## Body Weights
| DEPOSITOR\_STUDY\_NUMBER | study\_id | CHEMICAL | ENDPOINT | ENDPOINT\_UNIT | SEX | table\_id | OUTPUT\_TYPE | PHASE\_TYPE | PHASE\_START | id | GROUP\_NAME | Converted\_Dose\_Units | STE | MULT\_COMP\_SIGNIF | NUM\_DECIMAL\_DIGIT | DEATH\_PHASE\_TYPE | DEATH\_PHASE\_TIME\_UNIT | LEGEND\_ID | SORT\_ORDER | TABLE\_HEADER | DEATH\_PHASE\_TIME | DOSE\_UNIT | original\_doses | dataset\_name | xlabel | ylabel | dataset\_index | doses\_dropped | model\_name | model\_index | model\_version | has\_output | execution\_halted | BMD | BMDL | BMDU | CSF | AIC | pvalue1 | pvalue2 | pvalue3 | pvalue4 | Chi2 | df | residual\_of\_interest | warnings | logic\_bin | logic\_cautions | logic\_warnings | logic\_failures | recommended | recommended\_variable | dfile | outfile | stdout | stderr |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Body Weight | g | Male | I04 | Body Weights | SD | 4 | X-C10866B|Male|Body Weights|I04|4 | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 1 | Mean Body Weight Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Body Weight SD4 | Dose (mg/kg) | X-C10866B|Male|Body Weights|I04|4 | 0 | 0 | Linear | 0 | 2.21 | True | False | 278.244 | 187.298 | 536.529 | -999 | 140.071643 | 0.0729 | 0.8914 | 0.8914 | 0.6931 | 1.453160 | 3 | -0.24300 | NaN | valid | NaN | NaN | NaN | True | AIC | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-h8cp7464.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-h8cp7464.plt\n \t\t\t\t\t\t\tTue Jul 06 12:34:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 92.5624\n rho = 0 Specified\n beta\_0 = 250.124\n beta\_1 = -0.0318389\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -5.6e-011 -3e-010\n\n beta\_0 -5.6e-011 1 -0.73\n\n beta\_1 -3e-010 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 78.4817 22.198 34.9745 121.989\n beta\_0 250.124 2.58491 245.058 255.19\n beta\_1 -0.0318389 0.00820465 -0.0479197 -0.0157581\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 247 250 8.48 8.86 -0.748\n 77 5 251 248 7.73 8.86 0.88\n 153 5 246 245 11.9 8.86 0.133\n 306 5 239 240 9.32 8.86 -0.243\n 611 5 231 231 10.1 8.86 -0.0228\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -66.309243 6 144.618487\n A2 -65.750363 10 151.500726\n A3 -66.309243 6 144.618487\n fitted -67.035821 3 140.071643\n R -72.929294 2 149.858588\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.3579 8 0.0729\n Test 2 1.11776 4 0.8914\n Test 3 1.11776 4 0.8914\n Test 4 1.45316 3 0.6931\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 278.244\n\n\n BMDL = 187.298\n\n\n BMDU = 536.529\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Body Weight | g | Male | I04 | Body Weights | SD | 4 | X-C10866B|Male|Body Weights|I04|4 | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 1 | Mean Body Weight Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Body Weight SD4 | Dose (mg/kg) | X-C10866B|Male|Body Weights|I04|4 | 0 | 0 | Polynomial-2 | 1 | 2.21 | True | False | 319.027 | 188.177 | 575.952 | -999 | 141.995175 | 0.0729 | 0.8914 | 0.8914 | 0.5024 | 1.376690 | 2 | -0.42300 | NaN | valid | NaN | NaN | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-wpof4ujg.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-wpof4ujg.plt\n \t\t\t\t\t\t\tTue Jul 06 12:34:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 92.5624\n rho = 0 Specified\n beta\_0 = 249.525\n beta\_1 = -0.0235097\n beta\_2 = -1.32174e-005\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1 beta\_2\n\n alpha 1 -2.7e-012 -1.4e-013 -8.7e-014\n\n beta\_0 -2.7e-012 1 -0.77 0.64\n\n beta\_1 -1.4e-013 -0.77 1 -0.96\n\n beta\_2 -8.7e-014 0.64 -0.96 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 78.242 22.1302 34.8677 121.616\n beta\_0 249.525 3.36794 242.924 256.126\n beta\_1 -0.0235097 0.0311928 -0.0846463 0.037627\n beta\_2 -1.32174e-005 4.77611e-005 -0.000106827 8.03926e-005\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 247 250 8.48 8.85 -0.598\n 77 5 251 248 7.73 8.85 0.891\n 153 5 246 246 11.9 8.85 0.0408\n 306 5 239 241 9.32 8.85 -0.423\n 611 5 231 230 10.1 8.85 0.0894\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -66.309243 6 144.618487\n A2 -65.750363 10 151.500726\n A3 -66.309243 6 144.618487\n fitted -66.997587 4 141.995175\n R -72.929294 2 149.858588\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.3579 8 0.0729\n Test 2 1.11776 4 0.8914\n Test 3 1.11776 4 0.8914\n Test 4 1.37669 2 0.5024\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 319.027\n\n\n BMDL = 188.177\n\n\n BMDU = 575.952\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Body Weight | g | Male | I04 | Body Weights | SD | 4 | X-C10866B|Male|Body Weights|I04|4 | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 1 | Mean Body Weight Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Body Weight SD4 | Dose (mg/kg) | X-C10866B|Male|Body Weights|I04|4 | 0 | 0 | Polynomial-3 | 2 | 2.21 | True | False | 319.027 | 188.177 | 575.952 | -999 | 141.995175 | 0.0729 | 0.8914 | 0.8914 | 0.5024 | 1.376690 | 2 | -0.42300 | NaN | valid | NaN | NaN | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-i3vkk1go.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-i3vkk1go.plt\n \t\t\t\t\t\t\tTue Jul 06 12:34:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 92.5624\n rho = 0 Specified\n beta\_0 = 247.798\n beta\_1 = 0\n beta\_2 = -0.000353656\n beta\_3 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1 beta\_2\n\n alpha 1 -5e-009 -3.9e-008 4.7e-008\n\n beta\_0 -5e-009 1 -0.77 0.64\n\n beta\_1 -3.9e-008 -0.77 1 -0.96\n\n beta\_2 4.7e-008 0.64 -0.96 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 78.242 22.1302 34.8677 121.616\n beta\_0 249.525 3.36794 242.924 256.126\n beta\_1 -0.0235097 0.0311928 -0.0846464 0.037627\n beta\_2 -1.32174e-005 4.77611e-005 -0.000106827 8.03926e-005\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 247 250 8.48 8.85 -0.598\n 77 5 251 248 7.73 8.85 0.891\n 153 5 246 246 11.9 8.85 0.0408\n 306 5 239 241 9.32 8.85 -0.423\n 611 5 231 230 10.1 8.85 0.0894\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -66.309243 6 144.618487\n A2 -65.750363 10 151.500726\n A3 -66.309243 6 144.618487\n fitted -66.997587 4 141.995175\n R -72.929294 2 149.858588\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.3579 8 0.0729\n Test 2 1.11776 4 0.8914\n Test 3 1.11776 4 0.8914\n Test 4 1.37669 2 0.5024\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 319.027\n\n\n BMDL = 188.177\n\n\n BMDU = 575.952\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Body Weight | g | Male | I04 | Body Weights | SD | 4 | X-C10866B|Male|Body Weights|I04|4 | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 1 | Mean Body Weight Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Body Weight SD4 | Dose (mg/kg) | X-C10866B|Male|Body Weights|I04|4 | 0 | 0 | Polynomial-4 | 3 | 2.21 | True | False | 319.027 | 188.177 | 575.952 | -999 | 141.995175 | 0.0729 | 0.8914 | 0.8914 | 0.5024 | 1.376690 | 2 | -0.42300 | NaN | valid | NaN | NaN | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-9n9i99fr.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-9n9i99fr.plt\n \t\t\t\t\t\t\tTue Jul 06 12:34:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 92.5624\n rho = 0 Specified\n beta\_0 = 247.16\n beta\_1 = 0\n beta\_2 = -0.00193489\n beta\_3 = 0\n beta\_4 = -5.28001e-009\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1 beta\_2\n\n alpha 1 8e-008 -2e-007 1.5e-007\n\n beta\_0 8e-008 1 -0.77 0.64\n\n beta\_1 -2e-007 -0.77 1 -0.96\n\n beta\_2 1.5e-007 0.64 -0.96 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 78.242 22.1302 34.8677 121.616\n beta\_0 249.525 3.36794 242.924 256.126\n beta\_1 -0.0235097 0.0311928 -0.0846464 0.037627\n beta\_2 -1.32173e-005 4.77611e-005 -0.000106827 8.03926e-005\n beta\_3 0 NA\n beta\_4 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 247 250 8.48 8.85 -0.598\n 77 5 251 248 7.73 8.85 0.891\n 153 5 246 246 11.9 8.85 0.0408\n 306 5 239 241 9.32 8.85 -0.423\n 611 5 231 230 10.1 8.85 0.0894\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -66.309243 6 144.618487\n A2 -65.750363 10 151.500726\n A3 -66.309243 6 144.618487\n fitted -66.997587 4 141.995175\n R -72.929294 2 149.858588\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.3579 8 0.0729\n Test 2 1.11776 4 0.8914\n Test 3 1.11776 4 0.8914\n Test 4 1.37669 2 0.5024\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 319.027\n\n\n BMDL = 188.177\n\n\n BMDU = 575.952\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Body Weight | g | Male | I04 | Body Weights | SD | 4 | X-C10866B|Male|Body Weights|I04|4 | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 1 | Mean Body Weight Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Body Weight SD4 | Dose (mg/kg) | X-C10866B|Male|Body Weights|I04|4 | 0 | 0 | Power | 4 | 2.19 | True | False | 329.161 | 189.734 | 569.321 | -999 | 141.864123 | 0.0729 | 0.8914 | 0.8914 | 0.5364 | 1.245640 | 2 | -0.44300 | NaN | valid | NaN | NaN | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-bbb070uw.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-bbb070uw.plt\n \t\t\t\t\t\t\tTue Jul 06 12:34:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The power is restricted to be greater than or equal to 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 92.5624\n rho = 0 Specified\n control = 230.58\n slope = 306.481\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha control slope power\n\n alpha 1 -1.1e-007 4.7e-008 4.2e-008\n\n control -1.1e-007 1 -0.67 -0.64\n\n slope 4.7e-008 -0.67 1 1\n\n power 4.2e-008 -0.64 1 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 77.833 22.0145 34.6854 120.981\n control 249.22 3.13105 243.083 255.357\n slope -0.00623623 0.0257157 -0.0566382 0.0441657\n power 1.25155 0.633463 0.00998492 2.49311\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 247 249 8.48 8.82 -0.522\n 77 5 251 248 7.73 8.82 0.855\n 153 5 246 246 11.9 8.82 -0.0147\n 306 5 239 241 9.32 8.82 -0.443\n 611 5 231 230 10.1 8.82 0.125\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -66.309243 6 144.618487\n A2 -65.750363 10 151.500726\n A3 -66.309243 6 144.618487\n fitted -66.932061 4 141.864123\n R -72.929294 2 149.858588\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.3579 8 0.0729\n Test 2 1.11776 4 0.8914\n Test 3 1.11776 4 0.8914\n Test 4 1.24564 2 0.5364\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 329.161 \n\n\n BMDL = 189.734 \n\n\n BMDU = 569.321 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Body Weight | g | Male | I04 | Body Weights | SD | 4 | X-C10866B|Male|Body Weights|I04|4 | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 1 | Mean Body Weight Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Body Weight SD4 | Dose (mg/kg) | X-C10866B|Male|Body Weights|I04|4 | 0 | 0 | Hill | 5 | 2.18 | True | False | 285.940 | 141.473 | 541.085 | -999 | 143.329005 | 0.0729 | 0.8914 | 0.8914 | 0.3993 | 0.710518 | 1 | 0.05380 | NaN | valid | NaN | NaN | NaN | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-2ikrppth.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-2ikrppth.plt\n \t\t\t\t\t\t\tTue Jul 06 12:34:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n Power parameter restricted to be greater than 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 92.5624\n rho = 0 Specified\n intercept = 247.16\n v = -16.58\n n = 2.69674\n k = 324.976\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha intercept v n k\n\n alpha 1 -5.7e-008 1.4e-009 1.2e-009 2.9e-008\n\n intercept -5.7e-008 1 -0.46 -0.45 -0.0055\n\n v 1.4e-009 -0.46 1 0.85 -0.82\n\n n 1.2e-009 -0.45 0.85 1 -0.67\n\n k 2.9e-008 -0.0055 -0.82 -0.67 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 76.1847 21.5483 33.9508 118.419\n intercept 248.949 2.93903 243.188 254.709\n v -21.398 12.954 -46.7874 3.99145\n n 2.84108 2.9751 -2.99001 8.67217\n k 326.014 185.424 -37.4102 689.438\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 247 249 8.48 8.73 -0.458\n 77 5 251 249 7.73 8.73 0.656\n 153 5 246 247 11.9 8.73 -0.239\n 306 5 239 239 9.32 8.73 0.0538\n 611 5 231 231 10.1 8.73 -0.0119\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -66.309243 6 144.618487\n A2 -65.750363 10 151.500726\n A3 -66.309243 6 144.618487\n fitted -66.664503 5 143.329005\n R -72.929294 2 149.858588\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.3579 8 0.0729\n Test 2 1.11776 4 0.8914\n Test 3 1.11776 4 0.8914\n Test 4 0.710518 1 0.3993\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 285.94\n\n BMDL = 141.473\n\n BMDU = 541.085\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Body Weight | g | Male | I04 | Body Weights | SD | 4 | X-C10866B|Male|Body Weights|I04|4 | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 1 | Mean Body Weight Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Body Weight SD4 | Dose (mg/kg) | X-C10866B|Male|Body Weights|I04|4 | 0 | 0 | Exponential-M2 | 6 | 1.11 | True | False | 272.458 | 180.450 | 536.451 | -999 | 140.098400 | 0.0729 | 0.8914 | 0.8914 | 0.6869 | 1.480000 | 3 | -0.21520 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-gde\_sx3y.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:34:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha 4.30474 \n rho 0 Specified\n a 235.432 \n b 0.000132749 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha 4.36394 22.2218\n a 250.206 2.62349\n b 0.000132382 3.46417e-005\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 247.2 8.483\n 77 5 251.2 7.732\n 153 5 245.8 11.89\n 306 5 239.4 9.316\n 611 5 230.6 10.15\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 250.2 8.864 -0.7684\n 77 247.7 8.864 0.8808\n 153 245.2 8.864 0.1491\n 306 240.3 8.864 -0.2152\n 611 230.8 8.864 -0.04661\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -66.30924 6 144.6185\n A2 -65.75036 10 151.5007\n A3 -66.30924 6 144.6185\n R -72.92929 2 149.8586\n 2 -67.04921 3 140.0984\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 14.36 8 0.0729\n Test 2 1.118 4 0.8914\n Test 3 1.118 4 0.8914\n Test 4 1.48 3 0.6869\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is greater than .1. Model 2 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 272.458\n\n BMDL = 180.45\n\n BMDU = 536.451\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Body Weight | g | Male | I04 | Body Weights | SD | 4 | X-C10866B|Male|Body Weights|I04|4 | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 1 | Mean Body Weight Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Body Weight SD4 | Dose (mg/kg) | X-C10866B|Male|Body Weights|I04|4 | 0 | 0 | Exponential-M3 | 7 | 1.11 | True | False | 327.538 | 183.472 | 568.124 | -999 | 141.844400 | 0.0729 | 0.8914 | 0.8914 | 0.5417 | 1.226000 | 2 | -0.43270 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-r6uu0ih9.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:34:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha 4.30474 \n rho 0 Specified\n a 235.432 \n b 0.000132749 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha 4.35378 21.9997\n a 249.223 3.47559\n b 0.000226486 0.000398465\n d 1.27767 0.987046\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 247.2 8.483\n 77 5 251.2 7.732\n 153 5 245.8 11.89\n 306 5 239.4 9.316\n 611 5 230.6 10.15\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 249.2 8.819 -0.5232\n 77 247.8 8.819 0.8481\n 153 245.9 8.819 -0.01805\n 306 241.1 8.819 -0.4327\n 611 230.1 8.819 0.1259\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -66.30924 6 144.6185\n A2 -65.75036 10 151.5007\n A3 -66.30924 6 144.6185\n R -72.92929 2 149.8586\n 3 -66.9222 4 141.8444\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 14.36 8 0.0729\n Test 2 1.118 4 0.8914\n Test 3 1.118 4 0.8914\n Test 5a 1.226 2 0.5417\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is greater than .1. Model 3 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 327.538\n\n BMDL = 183.472\n\n BMDU = 568.124\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Body Weight | g | Male | I04 | Body Weights | SD | 4 | X-C10866B|Male|Body Weights|I04|4 | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 1 | Mean Body Weight Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Body Weight SD4 | Dose (mg/kg) | X-C10866B|Male|Body Weights|I04|4 | 0 | 0 | Exponential-M4 | 8 | 1.11 | True | False | 272.458 | 125.108 | 536.451 | -999 | 140.098400 | 0.0729 | 0.8914 | 0.8914 | 0.6869 | 1.480000 | 3 | -0.21520 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-kr377k2v.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:34:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha 4.30474 \n rho 0 Specified\n a 263.718 \n b 0.00241846 \n c 0.832708 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha 4.36394 22.2218\n a 250.206 2.62075\n b 0.000132382 3.45716e-005\n c 0 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 247.2 8.483\n 77 5 251.2 7.732\n 153 5 245.8 11.89\n 306 5 239.4 9.316\n 611 5 230.6 10.15\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 250.2 8.864 -0.7684\n 77 247.7 8.864 0.8808\n 153 245.2 8.864 0.1491\n 306 240.3 8.864 -0.2152\n 611 230.8 8.864 -0.04661\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -66.30924 6 144.6185\n A2 -65.75036 10 151.5007\n A3 -66.30924 6 144.6185\n R -72.92929 2 149.8586\n 4 -67.04921 3 140.0984\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 14.36 8 0.0729\n Test 2 1.118 4 0.8914\n Test 3 1.118 4 0.8914\n Test 6a 1.48 3 0.6869\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is greater than .1. Model 4 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 272.458\n\n BMDL = 125.108\n\n BMDU = 536.451\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Body Weight | g | Male | I04 | Body Weights | SD | 4 | X-C10866B|Male|Body Weights|I04|4 | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 1 | Mean Body Weight Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Body Weight SD4 | Dose (mg/kg) | X-C10866B|Male|Body Weights|I04|4 | 0 | 0 | Exponential-M5 | 9 | 1.11 | True | False | 289.255 | 142.229 | 542.372 | -999 | 143.350100 | 0.0729 | 0.8914 | 0.8914 | 0.3924 | 0.731600 | 1 | 0.04042 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-a1xzwrkq.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:34:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha 4.30474 \n rho 0 Specified\n a 263.718 \n b 0.00241846 \n c 0.832708 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha 4.334 21.5665\n a 248.923 2.96199\n b 0.00290078 0.00103994\n c 0.925459 0.0240859\n d 2.579 2.64713\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 247.2 8.483\n 77 5 251.2 7.732\n 153 5 245.8 11.89\n 306 5 239.4 9.316\n 611 5 230.6 10.15\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 248.9 8.732 -0.4515\n 77 248.5 8.732 0.6713\n 153 246.8 8.732 -0.2547\n 306 239.3 8.732 0.04042\n 611 230.6 8.732 -0.005541\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -66.30924 6 144.6185\n A2 -65.75036 10 151.5007\n A3 -66.30924 6 144.6185\n R -72.92929 2 149.8586\n 5 -66.67505 5 143.3501\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 14.36 8 0.0729\n Test 2 1.118 4 0.8914\n Test 3 1.118 4 0.8914\n Test 7a 0.7316 1 0.3924\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is greater than .1. Model 5 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 289.255\n\n BMDL = 142.229\n\n BMDU = 542.372\n | NaN | NaN |

## Organ Weights
| DEPOSITOR\_STUDY\_NUMBER | study\_id | CHEMICAL | ENDPOINT | ENDPOINT\_UNIT | SEX | table\_id | OUTPUT\_TYPE | id | GROUP\_NAME | Converted\_Dose\_Units | STE | MULT\_COMP\_SIGNIF | NUM\_DECIMAL\_DIGIT | DEATH\_PHASE\_TYPE | DEATH\_PHASE\_TIME\_UNIT | LEGEND\_ID | SORT\_ORDER | TABLE\_HEADER | DEATH\_PHASE\_TIME | DOSE\_UNIT | original\_doses | dataset\_name | xlabel | ylabel | dataset\_index | doses\_dropped | model\_name | model\_index | model\_version | has\_output | execution\_halted | BMD | BMDL | BMDU | CSF | AIC | pvalue1 | pvalue2 | pvalue3 | pvalue4 | Chi2 | df | residual\_of\_interest | warnings | logic\_bin | logic\_cautions | logic\_warnings | logic\_failures | recommended | recommended\_variable | dfile | outfile | stdout | stderr |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 0 | Linear | 0 | 2.21 | True | False | 242.4780 | 130.156000 | 590.215 | -999 | -5.724846 | 0.00025 | <0.0001 | 0.1530 | 0.02142 | 11.506800 | 4 | 0.06420 | THE MODEL HAS PROBABLY NOT CONVERGED!!!\nTHIS USUALLY MEANS THE MODEL HAS NOT CONVERGED! | warning | Warning(s): THE MODEL HAS PROBABLY NOT CONVERGED!!!; THIS USUALLY MEANS THE MODEL HAS NOT CONVERGED! | Goodness of fit p-value is less than threshold (0.0214 < 0.1) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741\n611.000000 5 6.947316 1.370320 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-20rhbjjy.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-20rhbjjy.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:38 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = -0.772623\n rho = 0\n beta\_0 = 6.91674\n beta\_1 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha beta\_0 beta\_1\n\n lalpha 1 0.71 NA \n\n beta\_0 0.71 1 NA \n\n beta\_1 NA NA NA \n\n\nNA - This parameter's variance has been estimated as zero or less.\nTHE MODEL HAS PROBABLY NOT CONVERGED!!!\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -36.6669 NA NA NA\n rho 18 NA\n beta\_0 6.76604 NA NA NA\n beta\_1 0.00133726 NA NA NA\n\nAt least some variance estimates are negative.\nTHIS USUALLY MEANS THE MODEL HAS NOT CONVERGED!\nTry again from another starting point.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 6.82 6.77 0.502 0.324 0.399\n 77 5 6.91 6.87 0.157 0.371 0.272\n 153 5 6.96 6.97 0.292 0.424 -0.0619\n 306 5 7.19 7.18 0.264 0.55 0.0642\n 611 5 6.95 7.58 1.37 0.905 -1.57\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -0.052913 6 12.105825\n A2 14.250977 10 -8.501954\n A3 11.615840 7 -9.231679\n fitted 5.862423 3 -5.724846\n R -0.543375 2 5.086750\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 29.5887 8 0.0002498\n Test 2 28.6078 4 <.0001\n Test 3 5.27027 3 0.153\n Test 4 11.5068 4 0.02142\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 242.478\n\n\n BMDL = 130.156\n\n\n BMDU = 590.215\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 0 | Polynomial-2 | 1 | 2.21 | True | False | 323.1920 | 200.900000 | 497.747 | -999 | -9.364816 | 0.00025 | <0.0001 | 0.1530 | 0.09658 | 7.866860 | 4 | 0.31200 | THE MODEL HAS PROBABLY NOT CONVERGED!!!\nTHIS USUALLY MEANS THE MODEL HAS NOT CONVERGED! | warning | Warning(s): THE MODEL HAS PROBABLY NOT CONVERGED!!!; THIS USUALLY MEANS THE MODEL HAS NOT CONVERGED! | Goodness of fit p-value is less than threshold (0.0966 < 0.1) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741\n611.000000 5 6.947316 1.370320 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-04ftbw9r.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-04ftbw9r.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:38 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = -0.772623\n rho = 0\n beta\_0 = 6.79035\n beta\_1 = 0\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_1 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha beta\_0 beta\_2\n\n lalpha 1 0.18 NA \n\n beta\_0 0.18 1 NA \n\n beta\_2 NA NA NA \n\n\nNA - This parameter's variance has been estimated as zero or less.\nTHE MODEL HAS PROBABLY NOT CONVERGED!!!\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -36.983 NA NA NA\n rho 18 NA\n beta\_0 6.85142 NA NA NA\n beta\_1 0 NA\n beta\_2 2.96725e-006 NA NA NA\n\nAt least some variance estimates are negative.\nTHIS USUALLY MEANS THE MODEL HAS NOT CONVERGED!\nTry again from another starting point.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 6.82 6.85 0.502 0.31 -0.199\n 77 5 6.91 6.87 0.157 0.317 0.319\n 153 5 6.96 6.92 0.292 0.339 0.251\n 306 5 7.19 7.13 0.264 0.443 0.312\n 611 5 6.95 7.96 1.37 1.19 -1.89\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -0.052913 6 12.105825\n A2 14.250977 10 -8.501954\n A3 11.615840 7 -9.231679\n fitted 7.682408 3 -9.364816\n R -0.543375 2 5.086750\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 29.5887 8 0.0002498\n Test 2 28.6078 4 <.0001\n Test 3 5.27027 3 0.153\n Test 4 7.86686 4 0.09658\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 323.192\n\n\n BMDL = 200.9\n\n\n BMDU = 497.747\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 0 | Polynomial-3 | 2 | 2.21 | True | False | 375.4550 | 210.933000 | 523.609 | -999 | -7.822164 | 0.00025 | <0.0001 | 0.1530 | 0.05993 | 7.409520 | 3 | 0.70200 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0599 < 0.1) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741\n611.000000 5 6.947316 1.370320 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-ybfiuth4.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-ybfiuth4.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:39 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = -0.772623\n rho = 0\n beta\_0 = 6.8323\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_1 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha beta\_0 beta\_2 beta\_3\n\n lalpha 1 0.077 -0.064 -0.27\n\n beta\_0 0.077 1 -0.68 0.76\n\n beta\_2 -0.064 -0.68 1 -1.1\n\n beta\_3 -0.27 0.76 -1.1 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -37.0665 0.216849 -37.4915 -36.6414\n rho 18 NA\n beta\_0 6.8889 0.10002 6.69287 7.08494\n beta\_1 0 NA\n beta\_2 5.53445e-007 3.8429e-006 -6.9785e-006 8.08539e-006\n beta\_3 4.42521e-009 4.68072e-009 -4.74883e-009 1.35993e-008\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 6.82 6.89 0.502 0.312 -0.466\n 77 5 6.91 6.89 0.157 0.314 0.143\n 153 5 6.96 6.92 0.292 0.324 0.284\n 306 5 7.19 7.07 0.264 0.393 0.702\n 611 5 6.95 8.1 1.37 1.35 -1.92\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -0.052913 6 12.105825\n A2 14.250977 10 -8.501954\n A3 11.615840 7 -9.231679\n fitted 7.911082 4 -7.822164\n R -0.543375 2 5.086750\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 29.5887 8 0.0002498\n Test 2 28.6078 4 <.0001\n Test 3 5.27027 3 0.153\n Test 4 7.40952 3 0.05993\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 375.455\n\n\n BMDL = 210.933\n\n\n BMDU = 523.609\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 0 | Polynomial-4 | 3 | 2.21 | True | False | 375.4550 | 207.529000 | 539.872 | -999 | -7.822164 | 0.00025 | <0.0001 | 0.1530 | 0.05993 | 7.409520 | 3 | 0.70200 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0599 < 0.1) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741\n611.000000 5 6.947316 1.370320 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-nefz8aew.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-nefz8aew.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:38 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = -0.772623\n rho = 0\n beta\_0 = 6.82383\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = 0\n beta\_4 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_1 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha beta\_0 beta\_2 beta\_3\n\n lalpha 1 0.077 -0.064 -0.27\n\n beta\_0 0.077 1 -0.68 0.76\n\n beta\_2 -0.064 -0.68 1 -1.1\n\n beta\_3 -0.27 0.76 -1.1 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -37.0665 0.216849 -37.4915 -36.6414\n rho 18 NA\n beta\_0 6.8889 0.10002 6.69287 7.08494\n beta\_1 0 NA\n beta\_2 5.53442e-007 3.8429e-006 -6.9785e-006 8.08538e-006\n beta\_3 4.42522e-009 4.68072e-009 -4.74882e-009 1.35993e-008\n beta\_4 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 6.82 6.89 0.502 0.312 -0.466\n 77 5 6.91 6.89 0.157 0.314 0.143\n 153 5 6.96 6.92 0.292 0.324 0.284\n 306 5 7.19 7.07 0.264 0.393 0.702\n 611 5 6.95 8.1 1.37 1.35 -1.92\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -0.052913 6 12.105825\n A2 14.250977 10 -8.501954\n A3 11.615840 7 -9.231679\n fitted 7.911082 4 -7.822164\n R -0.543375 2 5.086750\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 29.5887 8 0.0002498\n Test 2 28.6078 4 <.0001\n Test 3 5.27027 3 0.153\n Test 4 7.40952 3 0.05993\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 375.455\n\n\n BMDL = 207.529\n\n\n BMDU = 539.872\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 0 | Power | 4 | 2.19 | True | False | 372.1510 | 215.717000 | 591.195 | -999 | -7.835765 | 0.00025 | <0.0001 | 0.1530 | 0.06029 | 7.395910 | 3 | 0.67700 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0603 < 0.1) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741\n611.000000 5 6.947316 1.370320 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-\_rikbbqq.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-\_rikbbqq.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:39 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n The power is restricted to be greater than or equal to 1\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = -0.772623\n rho = 0\n control = 6.82383\n slope = 0.0340499\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha control slope power\n\n lalpha 1 -0.45 0.16 -0.18\n\n control -0.45 1 -0.57 0.57\n\n slope 0.16 -0.57 1 -1\n\n power -0.18 0.57 -1 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -37.0654 0.401496 -37.8523 -36.2785\n rho 18 NA\n control 6.88857 0.0892598 6.71363 7.06352\n slope 2.8863e-008 2.31017e-007 -4.23922e-007 4.81648e-007\n power 2.73626 1.25971 0.267283 5.20524\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 6.82 6.89 0.502 0.312 -0.464\n 77 5 6.91 6.89 0.157 0.314 0.153\n 153 5 6.96 6.92 0.292 0.324 0.296\n 306 5 7.19 7.07 0.264 0.395 0.677\n 611 5 6.95 8.1 1.37 1.34 -1.92\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -0.052913 6 12.105825\n A2 14.250977 10 -8.501954\n A3 11.615840 7 -9.231679\n fitted 7.917882 4 -7.835765\n R -0.543375 2 5.086750\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 29.5887 8 0.0002498\n Test 2 28.6078 4 <.0001\n Test 3 5.27027 3 0.153\n Test 4 7.39591 3 0.06029\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 372.151 \n\n\n BMDL = 215.717 \n\n\n BMDU = 591.195 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 0 | Hill | 5 | 2.18 | True | False | 357.1590 | -999.000000 | -999.000 | -999 | -5.857208 | 0.00025 | <0.0001 | 0.1530 | 0.02504 | 7.374470 | 2 | 0.63800 | BMDL computation failed. | failure | Warning(s): BMDL computation failed. | Goodness of fit p-value is less than threshold (0.025 < 0.1) | BMDL does not exist | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741\n611.000000 5 6.947316 1.370320 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-ba06ttmd.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-ba06ttmd.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:38 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n Power parameter restricted to be greater than 1\n The variance is to be modeled as Var(i) = exp(lalpha + rho \* ln(mean(i)))\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = -0.772623\n rho = 0\n intercept = 6.82383\n v = 0.367191\n n = 0.393541\n k = 427.017\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha intercept v n k\n\n lalpha 1 -0.43 -0.03 -0.024 0.00068\n\n intercept -0.43 1 -0.4 0.46 -0.4\n\n v -0.03 -0.4 1 -0.99 1\n\n n -0.024 0.46 -0.99 1 -0.99\n\n k 0.00068 -0.4 1 -0.99 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -37.0657 0.40153 -37.8527 -36.2787\n rho 18 NA\n intercept 6.89312 0.0927964 6.71124 7.07499\n v 1.97169 11.3233 -20.2215 24.1649\n n 3.93801 12.2325 -20.0372 27.9132\n k 544.904 1830.85 -3043.49 4133.3\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 6.82 6.89 0.502 0.314 -0.493\n 77 5 6.91 6.89 0.157 0.314 0.144\n 153 5 6.96 6.91 0.292 0.32 0.368\n 306 5 7.19 7.08 0.264 0.398 0.638\n 611 5 6.95 8.1 1.37 1.34 -1.92\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -0.052913 6 12.105825\n A2 14.250977 10 -8.501954\n A3 11.615840 7 -9.231679\n fitted 7.928604 5 -5.857208\n R -0.543375 2 5.086750\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 29.5887 8 0.0002498\n Test 2 28.6078 4 <.0001\n Test 3 5.27027 3 0.153\n Test 4 7.37447 2 0.02504\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 357.159\n\n\nBMDL computation failed.\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 0 | Exponential-M2 | 6 | 1.11 | True | False | 1.0000 | -999.000000 | -999.000 | -999 | 9.086750 | 0.00025 | <0.0001 | 0.1530 | <0.0001 | 24.320000 | 3 | -0.51670 | NaN | failure | Minimum dose/BMD ratio is greater than threshold (77.0 > 3.0) | NaN | BMDL does not exist | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741\n611.000000 5 6.947316 1.370320 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-d67rll7p.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:39 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha 34.1205 \n rho -18.566 \n a 6.91579 \n b 3.15429e-005 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha 34.9122 NA\n rho -18.4776 NA\n a 6.96706 NA\n b 0 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 6.824 0.502\n 77 5 6.914 0.1567\n 153 5 6.959 0.2917\n 306 5 7.191 0.2637\n 611 5 6.947 1.37\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 6.967 0.6199 -0.5167\n 77 6.967 0.6199 -0.1905\n 153 6.967 0.6199 -0.02943\n 306 6.967 0.6199 0.8079\n 611 6.967 0.6199 -0.07124\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -0.05291253 6 12.10583\n A2 14.25098 10 -8.501954\n A3 11.61584 7 -9.231679\n R -0.5433752 2 5.08675\n 2 -0.5433752 4 9.08675\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 29.59 8 0.0002498\n Test 2 28.61 4 < 0.0001\n Test 3 5.27 3 0.153\n Test 4 24.32 3 < 0.0001\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 1.#INF\n\n BMDL = Bad\_Completion\n\n BMDU = Bad\_Completion\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 0 | Exponential-M3 | 7 | 1.11 | True | False | 373.8740 | 214.745000 | 591.964 | -999 | -5.830699 | 0.00025 | <0.0001 | 0.1530 | 0.02471 | 7.401000 | 2 | 0.68340 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0247 < 0.1) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741\n611.000000 5 6.947316 1.370320 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-hxhnvhq4.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:39 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha 34.1205 \n rho -18.566 \n a 6.91579 \n b 3.15429e-005 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha -37.0652 0.402119\n rho 18 NA\n a 6.88817 0.000314695\n b 0.000822108 1.3022\n d 2.64163 0\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 6.824 0.502\n 77 5 6.914 0.1567\n 153 5 6.959 0.2917\n 306 5 7.191 0.2637\n 611 5 6.947 1.37\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 6.888 0.3121 -0.4609\n 77 6.893 0.3141 0.1522\n 153 6.917 0.3241 0.2888\n 306 7.07 0.3948 0.6834\n 611 8.101 1.344 -1.92\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -0.05291253 6 12.10583\n A2 14.25098 10 -8.501954\n A3 11.61584 7 -9.231679\n R -0.5433752 2 5.08675\n 3 7.91535 5 -5.830699\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 29.59 8 0.0002498\n Test 2 28.61 4 < 0.0001\n Test 3 5.27 3 0.153\n Test 5a 7.401 2 0.02471\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 373.874\n\n BMDL = 214.745\n\n BMDU = 591.964\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 0 | Exponential-M4 | 8 | 1.11 | True | False | -999.0000 | 0.000000 | 0.000 | -999 | 11.086750 | 0.00025 | <0.0001 | 0.1530 | <0.0001 | 24.320000 | 2 | -999.00000 | NaN | failure | NaN | Residual of Interest does not exist | BMD does not exist | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741\n611.000000 5 6.947316 1.370320 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-uov86z6k.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:38 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha 34.1205 \n rho -18.566 \n a 6.48264 \n b 0.00163673 \n c 1.16474 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha 34.7042 632933\n rho -18.3705 326053\n a 6.96707 0.124936\n b 0.00112241 2.66058\n c 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 6.824 0.502\n 77 5 6.914 0.1567\n 153 5 6.959 0.2917\n 306 5 7.191 0.2637\n 611 5 6.947 1.37\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 6.967 0.6199 -0.5167\n 77 6.967 0.6199 -0.1905\n 153 6.967 0.6199 -0.02944\n 306 6.967 0.6199 0.8079\n 611 6.967 0.6199 -0.07125\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -0.05291253 6 12.10583\n A2 14.25098 10 -8.501954\n A3 11.61584 7 -9.231679\n R -0.5433752 2 5.08675\n 4 -0.5433752 5 11.08675\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 29.59 8 0.0002498\n Test 2 28.61 4 < 0.0001\n Test 3 5.27 3 0.153\n Test 6a 24.32 2 < 0.0001\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is less than .1. Model 4 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = Not\_Computed\n\n BMDL = 0\n\n BMDU = 0\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 0 | Exponential-M5 | 9 | 1.11 | True | False | 64226.7000 | 65.481200 | 6110000.000 | -999 | 13.086750 | 0.00025 | <0.0001 | 0.1530 | <0.0001 | 24.320000 | 1 | -0.07124 | NaN | warning | BMD/BMDL ratio is greater than threshold (9.81e+02 > 5.0) | BMD/BMDL ratio is greater than threshold (9.81e+02 > 20.0)\nBMD/high dose ratio is greater than threshold (1.05e+02 > 1.0) | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741\n611.000000 5 6.947316 1.370320 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-2tiy\_8sf.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:39 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha 34.1205 \n rho -18.566 \n a 6.48264 \n b 1.50857e-005 \n c 1.16474 \n d 8 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha 34.9708 NA\n rho -18.5078 NA\n a 6.96706 NA\n b 1.50857e-005 NA\n c 1.16474 NA\n d 8 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 6.824 0.502\n 77 5 6.914 0.1567\n 153 5 6.959 0.2917\n 306 5 7.191 0.2637\n 611 5 6.947 1.37\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 6.967 0.6199 -0.5167\n 77 6.967 0.6199 -0.1905\n 153 6.967 0.6199 -0.02943\n 306 6.967 0.6199 0.8079\n 611 6.967 0.6199 -0.07124\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -0.05291253 6 12.10583\n A2 14.25098 10 -8.501954\n A3 11.61584 7 -9.231679\n R -0.5433752 2 5.08675\n 5 -0.5433752 6 13.08675\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 29.59 8 0.0002498\n Test 2 28.61 4 < 0.0001\n Test 3 5.27 3 0.153\n Test 7a 24.32 1 < 0.0001\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is less than .1. Model 5 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 64226.7\n\n BMDL = 65.4812\n\n BMDU = 6.11e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 1 | Linear | 0 | 2.21 | True | False | 287.2430 | 153.671000 | 1122.710 | -999 | -22.644841 | 0.1093 | 0.08867 | 0.1386 | 0.625 | 0.939905 | 2 | 0.09340 | NaN | valid | NaN | NaN | NaN | True | AIC | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-snoahh3x.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-snoahh3x.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:42 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = -2.22742\n rho = 0\n beta\_0 = 6.81332\n beta\_1 = 0.00118416\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 -0.18 0.21\n\n rho -1 1 0.18 -0.21\n\n beta\_0 -0.18 0.18 1 -0.85\n\n beta\_1 0.21 -0.21 -0.85 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 34.1988 27.6451 -19.9847 88.3823\n rho -18.9184 14.2376 -46.8237 8.98687\n beta\_0 6.80638 0.116818 6.57742 7.03534\n beta\_1 0.00122803 0.000557847 0.000134668 0.00232139\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 6.82 6.81 0.502 0.353 0.111\n 77 5 6.91 6.9 0.157 0.31 0.0961\n 153 5 6.96 6.99 0.292 0.273 -0.29\n 306 5 7.19 7.18 0.264 0.212 0.0934\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 14.505680 5 -19.011359\n A2 17.768339 8 -19.536679\n A3 15.792373 6 -19.584746\n fitted 15.322421 4 -22.644841\n R 12.575874 2 -21.151749\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 10.3849 6 0.1093\n Test 2 6.52532 3 0.08867\n Test 3 3.95193 2 0.1386\n Test 4 0.939905 2 0.625\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 287.243\n\n\n BMDL = 153.671\n\n\n BMDU = 1122.71\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 1 | Polynomial-2 | 1 | 2.21 | True | False | 287.2430 | 153.671000 | 1122.710 | -999 | -22.644841 | 0.1093 | 0.08867 | 0.1386 | 0.625 | 0.939905 | 2 | 0.09340 | NaN | valid | NaN | NaN | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-95mgthu\_.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-95mgthu\_.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:42 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = -2.22742\n rho = 0\n beta\_0 = 6.8313\n beta\_1 = 0.000698455\n beta\_2 = 1.53241e-006\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 -0.18 0.21\n\n rho -1 1 0.18 -0.21\n\n beta\_0 -0.18 0.18 1 -0.85\n\n beta\_1 0.21 -0.21 -0.85 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 34.1988 27.6451 -19.9847 88.3822\n rho -18.9184 14.2376 -46.8236 8.98686\n beta\_0 6.80638 0.116818 6.57742 7.03534\n beta\_1 0.00122803 0.000557847 0.000134669 0.00232139\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 6.82 6.81 0.502 0.353 0.111\n 77 5 6.91 6.9 0.157 0.31 0.0961\n 153 5 6.96 6.99 0.292 0.273 -0.29\n 306 5 7.19 7.18 0.264 0.212 0.0934\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 14.505680 5 -19.011359\n A2 17.768339 8 -19.536679\n A3 15.792373 6 -19.584746\n fitted 15.322421 4 -22.644841\n R 12.575874 2 -21.151749\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 10.3849 6 0.1093\n Test 2 6.52532 3 0.08867\n Test 3 3.95193 2 0.1386\n Test 4 0.939905 2 0.625\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 287.243\n\n\n BMDL = 153.671\n\n\n BMDU = 1122.71\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 1 | Polynomial-3 | 2 | 2.21 | True | False | 287.2430 | 153.671000 | 1122.710 | -999 | -22.644841 | 0.1093 | 0.08867 | 0.1386 | 0.625 | 0.939905 | 2 | 0.09340 | NaN | valid | NaN | NaN | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-i8a\_epi9.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-i8a\_epi9.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:42 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = -2.22742\n rho = 0\n beta\_0 = 6.82383\n beta\_1 = 0.00177328\n beta\_2 = 0\n beta\_3 = 2.5793e-008\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 -0.18 0.21\n\n rho -1 1 0.18 -0.21\n\n beta\_0 -0.18 0.18 1 -0.85\n\n beta\_1 0.21 -0.21 -0.85 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 34.1988 27.6451 -19.9847 88.3823\n rho -18.9184 14.2376 -46.8236 8.98685\n beta\_0 6.80638 0.116818 6.57742 7.03534\n beta\_1 0.00122803 0.000557847 0.000134669 0.00232139\n beta\_2 0 NA\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 6.82 6.81 0.502 0.353 0.111\n 77 5 6.91 6.9 0.157 0.31 0.0961\n 153 5 6.96 6.99 0.292 0.273 -0.29\n 306 5 7.19 7.18 0.264 0.212 0.0934\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 14.505680 5 -19.011359\n A2 17.768339 8 -19.536679\n A3 15.792373 6 -19.584746\n fitted 15.322421 4 -22.644841\n R 12.575874 2 -21.151749\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 10.3849 6 0.1093\n Test 2 6.52532 3 0.08867\n Test 3 3.95193 2 0.1386\n Test 4 0.939905 2 0.625\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 287.243\n\n\n BMDL = 153.671\n\n\n BMDU = 1122.71\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 1 | Polynomial-4 | 3 | 2.21 | True | False | 287.2430 | 153.671000 | 1122.710 | -999 | -22.644841 | 0.1093 | 0.08867 | 0.1386 | 0.625 | 0.939905 | 2 | 0.09340 | NaN | valid | NaN | NaN | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-7zdhdi1r.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-7zdhdi1r.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:42 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = -2.22742\n rho = 0\n beta\_0 = -4.68234\n beta\_1 = 0.0104494\n beta\_2 = 5.40018e-005\n beta\_3 = 0\n beta\_4 = 4.4497e-010\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 -0.18 0.21\n\n rho -1 1 0.18 -0.21\n\n beta\_0 -0.18 0.18 1 -0.85\n\n beta\_1 0.21 -0.21 -0.85 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 34.1988 27.6451 -19.9847 88.3822\n rho -18.9184 14.2376 -46.8236 8.98687\n beta\_0 6.80638 0.116818 6.57742 7.03534\n beta\_1 0.00122803 0.000557847 0.000134669 0.00232139\n beta\_2 1.59928e-133 NA\n beta\_3 0 NA\n beta\_4 -0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 6.82 6.81 0.502 0.353 0.111\n 77 5 6.91 6.9 0.157 0.31 0.0961\n 153 5 6.96 6.99 0.292 0.273 -0.29\n 306 5 7.19 7.18 0.264 0.212 0.0934\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 14.505680 5 -19.011359\n A2 17.768339 8 -19.536679\n A3 15.792373 6 -19.584746\n fitted 15.322421 4 -22.644841\n R 12.575874 2 -21.151749\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 10.3849 6 0.1093\n Test 2 6.52532 3 0.08867\n Test 3 3.95193 2 0.1386\n Test 4 0.939905 2 0.625\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 287.243\n\n\n BMDL = 153.671\n\n\n BMDU = 1122.71\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 1 | Power | 4 | 2.19 | True | False | 287.2430 | 153.671000 | 1122.710 | -999 | -22.644841 | 0.1093 | 0.08867 | 0.1386 | 0.625 | 0.939905 | 2 | 0.09340 | NaN | valid | NaN | NaN | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-pel70dxb.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-pel70dxb.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:42 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n The power is restricted to be greater than or equal to 1\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = -2.22742\n rho = 0\n control = 6.82383\n slope = 0.00109243\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho control slope\n\n lalpha 1 -1 0.4 -0.46\n\n rho -1 1 -0.39 0.46\n\n control 0.4 -0.39 1 -0.84\n\n slope -0.46 0.46 -0.84 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 34.1988 30.552 -25.682 94.0795\n rho -18.9184 15.7182 -49.7255 11.8887\n control 6.80638 0.111408 6.58802 7.02474\n slope 0.00122803 0.000523136 0.000202701 0.00225336\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 6.82 6.81 0.502 0.353 0.111\n 77 5 6.91 6.9 0.157 0.31 0.0961\n 153 5 6.96 6.99 0.292 0.273 -0.29\n 306 5 7.19 7.18 0.264 0.212 0.0934\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 14.505680 5 -19.011359\n A2 17.768339 8 -19.536679\n A3 15.792373 6 -19.584746\n fitted 15.322421 4 -22.644841\n R 12.575874 2 -21.151749\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 10.3849 6 0.1093\n Test 2 6.52532 3 0.08867\n Test 3 3.95193 2 0.1386\n Test 4 0.939905 2 0.625\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 287.243 \n\n\n BMDL = 153.671 \n\n\n BMDU = 1122.71 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 1 | Hill | 5 | 2.18 | True | False | 283.3170 | -999.000000 | -999.000 | -999 | -20.818639 | 0.1093 | 0.08867 | 0.1386 | 0.3814 | 0.766107 | 1 | 0.32400 | BMDL computation failed. | failure | Warning(s): BMDL computation failed. | NaN | BMDL does not exist | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-uq1ii937.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-uq1ii937.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:42 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n Power parameter restricted to be greater than 1\n The variance is to be modeled as Var(i) = exp(lalpha + rho \* ln(mean(i)))\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = -2.22742\n rho = 0\n intercept = 6.82383\n v = 0.367191\n n = 0.590312\n k = 427.017\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -n \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho intercept v k\n\n lalpha 1 -1 0.23 -0.33 -0.21\n\n rho -1 1 -0.23 0.33 0.21\n\n intercept 0.23 -0.23 1 0.32 0.55\n\n v -0.33 0.33 0.32 1 0.96\n\n k -0.21 0.21 0.55 0.96 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 36.8817 30.0746 -22.0634 95.8268\n rho -20.3084 15.4741 -50.6371 10.0203\n intercept 6.76731 0.157841 6.45795 7.07667\n v 0.822422 1.38943 -1.90081 3.54565\n n 1 NA\n k 334.467 1073.21 -1768.98 2437.92\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 6.82 6.77 0.502 0.377 0.335\n 77 5 6.91 6.92 0.157 0.3 -0.0519\n 153 5 6.96 7.03 0.292 0.258 -0.577\n 306 5 7.19 7.16 0.264 0.213 0.324\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 14.505680 5 -19.011359\n A2 17.768339 8 -19.536679\n A3 15.792373 6 -19.584746\n fitted 15.409320 5 -20.818639\n R 12.575874 2 -21.151749\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 10.3849 6 0.1093\n Test 2 6.52532 3 0.08867\n Test 3 3.95193 2 0.1386\n Test 4 0.766107 1 0.3814\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 283.317\n\n\nBMDL computation failed.\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 1 | Exponential-M2 | 6 | 1.11 | True | False | 288.0920 | 156.917000 | 1106.190 | -999 | -22.631020 | 0.1093 | 0.08867 | 0.1386 | 0.6207 | 0.953700 | 2 | 0.08887 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-9bo4vic8.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:42 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha 22.5684 \n rho -12.9381 \n a 6.81474 \n b 0.000168857 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha 34.1274 30.6896\n rho -18.881 15.7889\n a 6.80826 0.110145\n b 0.000174913 7.4678e-005\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 6.824 0.502\n 77 5 6.914 0.1567\n 153 5 6.959 0.2917\n 306 5 7.191 0.2637\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 6.808 0.3519 0.09898\n 77 6.901 0.3099 0.09868\n 153 6.993 0.2733 -0.2783\n 306 7.183 0.2123 0.08887\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 14.50568 5 -19.01136\n A2 17.76834 8 -19.53668\n A3 15.79237 6 -19.58475\n R 12.57587 2 -21.15175\n 2 15.31551 4 -22.63102\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 10.38 6 0.1093\n Test 2 6.525 3 0.08867\n Test 3 3.952 2 0.1386\n Test 4 0.9537 2 0.6207\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is greater than .1. Model 2 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 288.092\n\n BMDL = 156.917\n\n BMDU = 1106.19\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 1 | Exponential-M3 | 7 | 1.11 | True | False | 288.0920 | 156.917000 | 1106.190 | -999 | -22.631020 | 0.1093 | 0.08867 | 0.1386 | 0.6207 | 0.953700 | 2 | 0.08887 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-gpkd\_qng.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:42 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha 22.5684 \n rho -12.9381 \n a 6.81474 \n b 0.000168857 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha 34.1274 30.6896\n rho -18.881 15.7889\n a 6.80826 0.110145\n b 0.000174913 7.4678e-005\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 6.824 0.502\n 77 5 6.914 0.1567\n 153 5 6.959 0.2917\n 306 5 7.191 0.2637\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 6.808 0.3519 0.09898\n 77 6.901 0.3099 0.09868\n 153 6.993 0.2733 -0.2783\n 306 7.183 0.2123 0.08887\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 14.50568 5 -19.01136\n A2 17.76834 8 -19.53668\n A3 15.79237 6 -19.58475\n R 12.57587 2 -21.15175\n 3 15.31551 4 -22.63102\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 10.38 6 0.1093\n Test 2 6.525 3 0.08867\n Test 3 3.952 2 0.1386\n Test 5a 0.9537 2 0.6207\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is greater than .1. Model 3 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 288.092\n\n BMDL = 156.917\n\n BMDU = 1106.19\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 1 | Exponential-M4 | 8 | 1.11 | True | False | 281.6060 | 2.417100 | 3060000.000 | -999 | -20.789270 | 0.1093 | 0.08867 | 0.1386 | 0.3725 | 0.795500 | 1 | 0.27730 | NaN | warning | BMD/BMDL ratio is greater than threshold (1.17e+02 > 5.0) | BMD/BMDL ratio is greater than threshold (1.17e+02 > 20.0) | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-d4vfzl7l.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:43 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha 22.5684 \n rho -12.9381 \n a 6.48264 \n b 0.00376778 \n c 1.16474 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha 36.3234 29.9865\n rho -20.0193 15.4281\n a 6.77462 0.14857\n b 0.00355814 0.00927107\n c 1.08679 0.126492\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 6.824 0.502\n 77 5 6.914 0.1567\n 153 5 6.959 0.2917\n 306 5 7.191 0.2637\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 6.775 0.3721 0.2957\n 77 6.916 0.3028 -0.00946\n 153 7.021 0.2601 -0.5378\n 306 7.165 0.2125 0.2773\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 14.50568 5 -19.01136\n A2 17.76834 8 -19.53668\n A3 15.79237 6 -19.58475\n R 12.57587 2 -21.15175\n 4 15.39464 5 -20.78927\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 10.38 6 0.1093\n Test 2 6.525 3 0.08867\n Test 3 3.952 2 0.1386\n Test 6a 0.7955 1 0.3725\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is greater than .1. Model 4 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 281.606\n\n BMDL = 2.4171\n\n BMDU = 3.06e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Brain Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22451232473798627,.070080166139002295,.13044420508190807,.11794844490488542,.61282572043293393 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 200 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Brain Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 0 | 1 | Exponential-M5 | 9 | 1.11 | True | False | 281.6060 | 1.873560 | 3060000.000 | -999 | -20.789270 | 0.1093 | 0.08867 | 0.1386 | 0.3725 | 0.795500 | 1 | 0.27730 | NaN | warning | BMD/BMDL ratio is greater than threshold (1.5e+02 > 5.0) | BMD/BMDL ratio is greater than threshold (1.5e+02 > 20.0) | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 6.823832 0.502025\n77.000000 5 6.914246 0.156704\n153.000000 5 6.958906 0.291682\n306.000000 5 7.191023 0.263741 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-y0261p16.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:42 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha 22.5684 \n rho -12.9381 \n a 6.48264 \n b 0.00376778 \n c 1.16474 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha 36.3236 29.9865\n rho -20.0194 15.4281\n a 6.77462 0.148569\n b 0.00355818 0.00927097\n c 1.08679 0.126488\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 6.824 0.502\n 77 5 6.914 0.1567\n 153 5 6.959 0.2917\n 306 5 7.191 0.2637\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 6.775 0.3721 0.2957\n 77 6.916 0.3028 -0.009461\n 153 7.021 0.2601 -0.5378\n 306 7.165 0.2125 0.2773\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 14.50568 5 -19.01136\n A2 17.76834 8 -19.53668\n A3 15.79237 6 -19.58475\n R 12.57587 2 -21.15175\n 5 15.39464 5 -20.78927\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 10.38 6 0.1093\n Test 2 6.525 3 0.08867\n Test 3 3.952 2 0.1386\n Test 7a 0.7955 1 0.3725\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is greater than .1. Model 5 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 281.606\n\n BMDL = 1.87356\n\n BMDU = 3.06e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Absolute | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22529092303064485,.27300183149568791,.37182522776164595,.42494705552574435,.46315943979008634 | 2,0,0,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Absolute | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 1 | 0 | Linear | 0 | 2.21 | True | False | 381.0800 | 228.554000 | 1137.450 | -999 | 18.109621 | 0.0671 | 0.622 | 0.6220 | 0.1188 | 5.857320 | 3 | 1.33000 | NaN | warning | NaN | Ratio of modeled to actual stdev. at control is greater than threshold (1.55 > 1.5) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 10.354000 0.503766\n77.000000 5 11.230000 0.610451\n153.000000 5 11.288000 0.831426\n306.000000 5 11.950000 0.950211\n611.000000 4 11.750000 0.926319 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-uvachm5w.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-uvachm5w.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:47 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.602979\n rho = 0 Specified\n beta\_0 = 10.8716\n beta\_1 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -4e-008 -3e-008\n\n beta\_0 -4e-008 1 -0.72\n\n beta\_1 -3e-008 -0.72 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.609307 0.175892 0.264566 0.954049\n beta\_0 10.8589 0.229724 10.4087 11.3092\n beta\_1 0.00204834 0.000775105 0.000529161 0.00356752\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 10.4 10.9 0.504 0.781 -1.45\n 77 5 11.2 11 0.61 0.781 0.611\n 153 5 11.3 11.2 0.831 0.781 0.331\n 306 5 11.9 11.5 0.95 0.781 1.33\n 611 4 11.8 12.1 0.926 0.781 -0.924\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -3.126150 6 18.252299\n A2 -1.812630 10 23.625259\n A3 -3.126150 6 18.252299\n fitted -6.054810 3 18.109621\n R -9.119681 2 22.239361\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.6141 8 0.0671\n Test 2 2.62704 4 0.622\n Test 3 2.62704 4 0.622\n Test 4 5.85732 3 0.1188\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 381.08\n\n\n BMDL = 228.554\n\n\n BMDU = 1137.45\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Absolute | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22529092303064485,.27300183149568791,.37182522776164595,.42494705552574435,.46315943979008634 | 2,0,0,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Absolute | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 1 | 0 | Polynomial-2 | 1 | 2.21 | True | False | 381.0800 | 228.554000 | 1137.450 | -999 | 18.109621 | 0.0671 | 0.622 | 0.6220 | 0.1188 | 5.857320 | 3 | 1.33000 | NaN | warning | NaN | Ratio of modeled to actual stdev. at control is greater than threshold (1.55 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 10.354000 0.503766\n77.000000 5 11.230000 0.610451\n153.000000 5 11.288000 0.831426\n306.000000 5 11.950000 0.950211\n611.000000 4 11.750000 0.926319 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-klsoy6ia.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-klsoy6ia.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:47 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.602979\n rho = 0 Specified\n beta\_0 = 10.458\n beta\_1 = 0\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -4.1e-008 2.5e-008\n\n beta\_0 -4.1e-008 1 -0.72\n\n beta\_1 2.5e-008 -0.72 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.609307 0.175892 0.264566 0.954049\n beta\_0 10.8589 0.229724 10.4087 11.3092\n beta\_1 0.00204834 0.000775105 0.000529161 0.00356752\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 10.4 10.9 0.504 0.781 -1.45\n 77 5 11.2 11 0.61 0.781 0.611\n 153 5 11.3 11.2 0.831 0.781 0.331\n 306 5 11.9 11.5 0.95 0.781 1.33\n 611 4 11.8 12.1 0.926 0.781 -0.924\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -3.126150 6 18.252299\n A2 -1.812630 10 23.625259\n A3 -3.126150 6 18.252299\n fitted -6.054810 3 18.109621\n R -9.119681 2 22.239361\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.6141 8 0.0671\n Test 2 2.62704 4 0.622\n Test 3 2.62704 4 0.622\n Test 4 5.85732 3 0.1188\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 381.08\n\n\n BMDL = 228.554\n\n\n BMDU = 1137.45\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Absolute | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22529092303064485,.27300183149568791,.37182522776164595,.42494705552574435,.46315943979008634 | 2,0,0,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Absolute | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 1 | 0 | Polynomial-3 | 2 | 2.21 | True | False | 381.0800 | 228.554000 | 1137.450 | -999 | 18.109621 | 0.0671 | 0.622 | 0.6220 | 0.1188 | 5.857320 | 3 | 1.33000 | NaN | warning | NaN | Ratio of modeled to actual stdev. at control is greater than threshold (1.55 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 10.354000 0.503766\n77.000000 5 11.230000 0.610451\n153.000000 5 11.288000 0.831426\n306.000000 5 11.950000 0.950211\n611.000000 4 11.750000 0.926319 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-dzannlj7.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-dzannlj7.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:46 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.602979\n rho = 0 Specified\n beta\_0 = 10.4187\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -3.8e-008 1e-007\n\n beta\_0 -3.8e-008 1 -0.72\n\n beta\_1 1e-007 -0.72 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.609307 0.175892 0.264566 0.954049\n beta\_0 10.8589 0.229724 10.4087 11.3092\n beta\_1 0.00204834 0.000775105 0.000529161 0.00356752\n beta\_2 0 NA\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 10.4 10.9 0.504 0.781 -1.45\n 77 5 11.2 11 0.61 0.781 0.611\n 153 5 11.3 11.2 0.831 0.781 0.331\n 306 5 11.9 11.5 0.95 0.781 1.33\n 611 4 11.8 12.1 0.926 0.781 -0.924\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -3.126150 6 18.252299\n A2 -1.812630 10 23.625259\n A3 -3.126150 6 18.252299\n fitted -6.054810 3 18.109621\n R -9.119681 2 22.239361\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.6141 8 0.0671\n Test 2 2.62704 4 0.622\n Test 3 2.62704 4 0.622\n Test 4 5.85732 3 0.1188\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 381.08\n\n\n BMDL = 228.554\n\n\n BMDU = 1137.45\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Absolute | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22529092303064485,.27300183149568791,.37182522776164595,.42494705552574435,.46315943979008634 | 2,0,0,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Absolute | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 1 | 0 | Polynomial-4 | 3 | 2.21 | True | False | 381.0800 | 228.554000 | 1137.450 | -999 | 18.109621 | 0.0671 | 0.622 | 0.6220 | 0.1188 | 5.857320 | 3 | 1.33000 | NaN | warning | NaN | Ratio of modeled to actual stdev. at control is greater than threshold (1.55 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 10.354000 0.503766\n77.000000 5 11.230000 0.610451\n153.000000 5 11.288000 0.831426\n306.000000 5 11.950000 0.950211\n611.000000 4 11.750000 0.926319 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-du\_an1gu.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-du\_an1gu.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:46 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.602979\n rho = 0 Specified\n beta\_0 = 10.354\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = 0\n beta\_4 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 1.7e-008 -2e-008\n\n beta\_0 1.7e-008 1 -0.72\n\n beta\_1 -2e-008 -0.72 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.609307 0.175892 0.264566 0.954049\n beta\_0 10.8589 0.229724 10.4087 11.3092\n beta\_1 0.00204834 0.000775105 0.000529161 0.00356752\n beta\_2 0 NA\n beta\_3 0 NA\n beta\_4 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 10.4 10.9 0.504 0.781 -1.45\n 77 5 11.2 11 0.61 0.781 0.611\n 153 5 11.3 11.2 0.831 0.781 0.331\n 306 5 11.9 11.5 0.95 0.781 1.33\n 611 4 11.8 12.1 0.926 0.781 -0.924\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -3.126150 6 18.252299\n A2 -1.812630 10 23.625259\n A3 -3.126150 6 18.252299\n fitted -6.054810 3 18.109621\n R -9.119681 2 22.239361\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.6141 8 0.0671\n Test 2 2.62704 4 0.622\n Test 3 2.62704 4 0.622\n Test 4 5.85732 3 0.1188\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 381.08\n\n\n BMDL = 228.554\n\n\n BMDU = 1137.45\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Absolute | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22529092303064485,.27300183149568791,.37182522776164595,.42494705552574435,.46315943979008634 | 2,0,0,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Absolute | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 1 | 0 | Power | 4 | 2.19 | True | False | 381.0800 | 228.554000 | 1137.450 | -999 | 18.109621 | 0.0671 | 0.622 | 0.6220 | 0.1188 | 5.857320 | 3 | 1.33000 | NaN | warning | NaN | Ratio of modeled to actual stdev. at control is greater than threshold (1.55 > 1.5) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 10.354000 0.503766\n77.000000 5 11.230000 0.610451\n153.000000 5 11.288000 0.831426\n306.000000 5 11.950000 0.950211\n611.000000 4 11.750000 0.926319 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-8euqyazp.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-8euqyazp.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:47 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The power is restricted to be greater than or equal to 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.602979\n rho = 0 Specified\n control = 10.354\n slope = 0.257652\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha control slope\n\n alpha 1 -2.4e-009 2.2e-009\n\n control -2.4e-009 1 -0.72\n\n slope 2.2e-009 -0.72 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.609307 0.175892 0.264566 0.954049\n control 10.8589 0.229724 10.4087 11.3092\n slope 0.00204834 0.000775105 0.000529161 0.00356752\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 10.4 10.9 0.504 0.781 -1.45\n 77 5 11.2 11 0.61 0.781 0.611\n 153 5 11.3 11.2 0.831 0.781 0.331\n 306 5 11.9 11.5 0.95 0.781 1.33\n 611 4 11.8 12.1 0.926 0.781 -0.924\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -3.126150 6 18.252299\n A2 -1.812630 10 23.625259\n A3 -3.126150 6 18.252299\n fitted -6.054810 3 18.109621\n R -9.119681 2 22.239361\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.6141 8 0.0671\n Test 2 2.62704 4 0.622\n Test 3 2.62704 4 0.622\n Test 4 5.85732 3 0.1188\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 381.08 \n\n\n BMDL = 228.554 \n\n\n BMDU = 1137.45 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Absolute | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22529092303064485,.27300183149568791,.37182522776164595,.42494705552574435,.46315943979008634 | 2,0,0,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Absolute | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 1 | 0 | Hill | 5 | 2.18 | True | False | 63.0792 | 0.000119 | 372.013 | -999 | 17.319110 | 0.0671 | 0.622 | 0.6220 | 0.3017 | 1.066810 | 1 | 0.21900 | NaN | warning | BMD/BMDL ratio is greater than threshold (5.31e+05 > 5.0) | BMD/BMDL ratio is greater than threshold (5.31e+05 > 20.0) | NaN | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 10.354000 0.503766\n77.000000 5 11.230000 0.610451\n153.000000 5 11.288000 0.831426\n306.000000 5 11.950000 0.950211\n611.000000 4 11.750000 0.926319 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-mytseqm4.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-mytseqm4.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:47 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n Power parameter restricted to be greater than 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.602979\n rho = 0 Specified\n intercept = 10.354\n v = 1.596\n n = 0.516929\n k = 83.8562\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha intercept v n k\n\n alpha 1 4e-007 5.3e-007 -3.3e-007 6.5e-008\n\n intercept 4e-007 1 -0.41 0.13 0.31\n\n v 5.3e-007 -0.41 1 -0.82 0.54\n\n n -3.3e-007 0.13 -0.82 1 -0.38\n\n k 6.5e-008 0.31 0.54 -0.38 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.499057 0.144066 0.216694 0.78142\n intercept 10.3585 0.31766 9.73591 10.9811\n v 1.65464 0.867816 -0.0462493 3.35553\n n 1.17249 1.72816 -2.21464 4.55962\n k 81.0784 78.9626 -73.6854 235.842\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 10.4 10.4 0.504 0.706 -0.0143\n 77 5 11.2 11.2 0.61 0.706 0.219\n 153 5 11.3 11.5 0.831 0.706 -0.609\n 306 5 11.9 11.7 0.95 0.706 0.712\n 611 4 11.8 11.9 0.926 0.706 -0.344\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -3.126150 6 18.252299\n A2 -1.812630 10 23.625259\n A3 -3.126150 6 18.252299\n fitted -3.659555 5 17.319110\n R -9.119681 2 22.239361\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.6141 8 0.0671\n Test 2 2.62704 4 0.622\n Test 3 2.62704 4 0.622\n Test 4 1.06681 1 0.3017\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 63.0792\n\n BMDL = 0.000118776\n\n BMDU = 372.013\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Absolute | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22529092303064485,.27300183149568791,.37182522776164595,.42494705552574435,.46315943979008634 | 2,0,0,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Absolute | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 1 | 0 | Exponential-M2 | 6 | 1.11 | True | False | 399.9840 | 246.025000 | 1184.990 | -999 | 18.285940 | 0.0671 | 0.622 | 0.6220 | 0.11 | 6.034000 | 3 | 1.36400 | NaN | valid | NaN | NaN | NaN | True | AIC | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 10.354000 0.503766\n77.000000 5 11.230000 0.610451\n153.000000 5 11.288000 0.831426\n306.000000 5 11.950000 0.950211\n611.000000 4 11.750000 0.926319 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-sy3yg\_g3.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:47 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha -0.739488 \n rho 0 Specified\n a 10.8494 \n b 0.000183253 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha -0.488086 0.177189\n a 10.8777 0.224787\n b 0.000173877 6.58692e-005\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 10.35 0.5038\n 77 5 11.23 0.6105\n 153 5 11.29 0.8314\n 306 5 11.95 0.9502\n 611 4 11.75 0.9263\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 10.88 0.7835 -1.495\n 77 11.02 0.7835 0.5869\n 153 11.17 0.7835 0.3339\n 306 11.47 0.7835 1.364\n 611 12.1 0.7835 -0.8858\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -3.12615 6 18.2523\n A2 -1.81263 10 23.62526\n A3 -3.12615 6 18.2523\n R -9.119681 2 22.23936\n 2 -6.142969 3 18.28594\n\n\n Additive constant for all log-likelihoods = -22.05. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 14.61 8 0.0671\n Test 2 2.627 4 0.622\n Test 3 2.627 4 0.622\n Test 4 6.034 3 0.11\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is greater than .1. Model 2 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 399.984\n\n BMDL = 246.025\n\n BMDU = 1184.99\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Absolute | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22529092303064485,.27300183149568791,.37182522776164595,.42494705552574435,.46315943979008634 | 2,0,0,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Absolute | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 1 | 0 | Exponential-M3 | 7 | 1.11 | True | False | 399.9840 | 246.025000 | 1184.990 | -999 | 18.285940 | 0.0671 | 0.622 | 0.6220 | 0.11 | 6.034000 | 3 | 1.36400 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 10.354000 0.503766\n77.000000 5 11.230000 0.610451\n153.000000 5 11.288000 0.831426\n306.000000 5 11.950000 0.950211\n611.000000 4 11.750000 0.926319 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-1tm\_r6ef.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:47 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha -0.739488 \n rho 0 Specified\n a 10.8494 \n b 0.000183253 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha -0.488086 0.177189\n a 10.8777 0.224787\n b 0.000173877 6.58692e-005\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 10.35 0.5038\n 77 5 11.23 0.6105\n 153 5 11.29 0.8314\n 306 5 11.95 0.9502\n 611 4 11.75 0.9263\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 10.88 0.7835 -1.495\n 77 11.02 0.7835 0.5869\n 153 11.17 0.7835 0.3339\n 306 11.47 0.7835 1.364\n 611 12.1 0.7835 -0.8858\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -3.12615 6 18.2523\n A2 -1.81263 10 23.62526\n A3 -3.12615 6 18.2523\n R -9.119681 2 22.23936\n 3 -6.142969 3 18.28594\n\n\n Additive constant for all log-likelihoods = -22.05. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 14.61 8 0.0671\n Test 2 2.627 4 0.622\n Test 3 2.627 4 0.622\n Test 5a 6.034 3 0.11\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is greater than .1. Model 3 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 399.984\n\n BMDL = 246.025\n\n BMDU = 1184.99\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Absolute | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22529092303064485,.27300183149568791,.37182522776164595,.42494705552574435,.46315943979008634 | 2,0,0,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Absolute | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 1 | 0 | Exponential-M4 | 8 | 1.11 | True | False | 70.7856 | 0.342576 | 335.343 | -999 | 15.224390 | 0.0671 | 0.622 | 0.6220 | 0.6151 | 0.972100 | 2 | 0.35260 | NaN | warning | BMD/BMDL ratio is greater than threshold (2.07e+02 > 5.0) | BMD/BMDL ratio is greater than threshold (2.07e+02 > 20.0) | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 10.354000 0.503766\n77.000000 5 11.230000 0.610451\n153.000000 5 11.288000 0.831426\n306.000000 5 11.950000 0.950211\n611.000000 4 11.750000 0.926319 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-drdo76th.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:47 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha -0.739488 \n rho 0 Specified\n a 9.8363 \n b 0.00278729 \n c 1.27563 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha -0.698984 0.143497\n a 10.3709 0.308805\n b 0.00909004 0.0058484\n c 1.14327 0.0424934\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 10.35 0.5038\n 77 5 11.23 0.6105\n 153 5 11.29 0.8314\n 306 5 11.95 0.9502\n 611 4 11.75 0.9263\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 10.37 0.705 -0.05354\n 77 11.12 0.705 0.3526\n 153 11.49 0.705 -0.6308\n 306 11.76 0.705 0.5878\n 611 11.85 0.705 -0.2863\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -3.12615 6 18.2523\n A2 -1.81263 10 23.62526\n A3 -3.12615 6 18.2523\n R -9.119681 2 22.23936\n 4 -3.612194 4 15.22439\n\n\n Additive constant for all log-likelihoods = -22.05. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 14.61 8 0.0671\n Test 2 2.627 4 0.622\n Test 3 2.627 4 0.622\n Test 6a 0.9721 2 0.6151\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is greater than .1. Model 4 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 70.7856\n\n BMDL = 0.342576\n\n BMDU = 335.343\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Absolute | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .22529092303064485,.27300183149568791,.37182522776164595,.42494705552574435,.46315943979008634 | 2,0,0,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Absolute | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 1 | 0 | Exponential-M5 | 9 | 1.11 | True | False | 70.7857 | 0.293964 | 335.343 | -999 | 15.224390 | 0.0671 | 0.622 | 0.6220 | 0.6151 | 0.972100 | 2 | 0.35260 | NaN | warning | BMD/BMDL ratio is greater than threshold (2.41e+02 > 5.0) | BMD/BMDL ratio is greater than threshold (2.41e+02 > 20.0) | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 10.354000 0.503766\n77.000000 5 11.230000 0.610451\n153.000000 5 11.288000 0.831426\n306.000000 5 11.950000 0.950211\n611.000000 4 11.750000 0.926319 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-7l2yy\_ru.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:47 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha -0.739488 \n rho 0 Specified\n a 9.8363 \n b 0.00278729 \n c 1.27563 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha -0.698984 0.143498\n a 10.3709 0.308805\n b 0.00909004 0.00584841\n c 1.14327 0.0424934\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 10.35 0.5038\n 77 5 11.23 0.6105\n 153 5 11.29 0.8314\n 306 5 11.95 0.9502\n 611 4 11.75 0.9263\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 10.37 0.705 -0.05355\n 77 11.12 0.705 0.3526\n 153 11.49 0.705 -0.6308\n 306 11.76 0.705 0.5878\n 611 11.85 0.705 -0.2863\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -3.12615 6 18.2523\n A2 -1.81263 10 23.62526\n A3 -3.12615 6 18.2523\n R -9.119681 2 22.23936\n 5 -3.612194 4 15.22439\n\n\n Additive constant for all log-likelihoods = -22.05. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 14.61 8 0.0671\n Test 2 2.627 4 0.622\n Test 3 2.627 4 0.622\n Test 7a 0.9721 2 0.6151\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is greater than .1. Model 5 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 70.7857\n\n BMDL = 0.293964\n\n BMDU = 335.343\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .76656518330133239,.71738015062344429,.95149604071998772,1.1689047416798897,1.5939810554911218 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 2 | 0 | Linear | 0 | 2.21 | True | False | 154.2420 | 114.214000 | 234.285 | -999 | 71.179863 | <0.0001 | 0.5877 | 0.5877 | 0.0596 | 7.421750 | 3 | 0.27700 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0596 < 0.1) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 41.900622 1.714092\n77.000000 5 44.700437 1.604111\n153.000000 5 45.914457 2.127610\n306.000000 5 49.870111 2.613750\n611.000000 4 51.300099 3.187962 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-vi8pqvsl.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-vi8pqvsl.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:50 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 5.15622\n rho = 0 Specified\n beta\_0 = 43.3292\n beta\_1 = 0.0148557\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -4.9e-007 7e-007\n\n beta\_0 -4.9e-007 1 -0.72\n\n beta\_1 7e-007 -0.72 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 5.56128 1.6054 2.41475 8.70781\n beta\_0 43.2828 0.694025 41.9225 44.643\n beta\_1 0.0152892 0.00234169 0.0106996 0.0198788\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 41.9 43.3 1.71 2.36 -1.31\n 77 5 44.7 44.5 1.6 2.36 0.228\n 153 5 45.9 45.6 2.13 2.36 0.277\n 306 5 49.9 48 2.61 2.36 1.81\n 611 4 51.3 52.6 3.19 2.36 -1.12\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -28.879056 6 69.758112\n A2 -27.466920 10 74.933840\n A3 -28.879056 6 69.758112\n fitted -32.589931 3 71.179863\n R -44.843049 2 93.686099\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 34.7523 8 <.0001\n Test 2 2.82427 4 0.5877\n Test 3 2.82427 4 0.5877\n Test 4 7.42175 3 0.0596\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 154.242\n\n\n BMDL = 114.214\n\n\n BMDU = 234.285\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .76656518330133239,.71738015062344429,.95149604071998772,1.1689047416798897,1.5939810554911218 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 2 | 0 | Polynomial-2 | 1 | 2.21 | True | False | 154.2420 | 114.214000 | 236.078 | -999 | 71.179863 | <0.0001 | 0.5877 | 0.5877 | 0.0596 | 7.421750 | 3 | 0.27700 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0596 < 0.1) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 41.900622 1.714092\n77.000000 5 44.700437 1.604111\n153.000000 5 45.914457 2.127610\n306.000000 5 49.870111 2.613750\n611.000000 4 51.300099 3.187962 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-lrih5wwt.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-lrih5wwt.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:50 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 5.15622\n rho = 0 Specified\n beta\_0 = 41.8934\n beta\_1 = 0.0348289\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 1.9e-007 -5.4e-008\n\n beta\_0 1.9e-007 1 -0.72\n\n beta\_1 -5.4e-008 -0.72 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 5.56128 1.6054 2.41475 8.70781\n beta\_0 43.2828 0.694025 41.9225 44.643\n beta\_1 0.0152892 0.00234169 0.0106996 0.0198788\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 41.9 43.3 1.71 2.36 -1.31\n 77 5 44.7 44.5 1.6 2.36 0.228\n 153 5 45.9 45.6 2.13 2.36 0.277\n 306 5 49.9 48 2.61 2.36 1.81\n 611 4 51.3 52.6 3.19 2.36 -1.12\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -28.879056 6 69.758112\n A2 -27.466920 10 74.933840\n A3 -28.879056 6 69.758112\n fitted -32.589931 3 71.179863\n R -44.843049 2 93.686099\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 34.7523 8 <.0001\n Test 2 2.82427 4 0.5877\n Test 3 2.82427 4 0.5877\n Test 4 7.42175 3 0.0596\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 154.242\n\n\n BMDL = 114.214\n\n\n BMDU = 236.078\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .76656518330133239,.71738015062344429,.95149604071998772,1.1689047416798897,1.5939810554911218 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 2 | 0 | Polynomial-3 | 2 | 2.21 | True | False | 154.2420 | 114.214000 | 236.078 | -999 | 71.179863 | <0.0001 | 0.5877 | 0.5877 | 0.0596 | 7.421750 | 3 | 0.27700 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0596 < 0.1) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 41.900622 1.714092\n77.000000 5 44.700437 1.604111\n153.000000 5 45.914457 2.127610\n306.000000 5 49.870111 2.613750\n611.000000 4 51.300099 3.187962 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-w4fbwdza.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-w4fbwdza.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:50 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 5.15622\n rho = 0 Specified\n beta\_0 = 42.0476\n beta\_1 = 0.0288796\n beta\_2 = 0\n beta\_3 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -3.8e-007 8.5e-007\n\n beta\_0 -3.8e-007 1 -0.72\n\n beta\_1 8.5e-007 -0.72 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 5.56128 1.6054 2.41475 8.70781\n beta\_0 43.2828 0.694025 41.9225 44.643\n beta\_1 0.0152892 0.00234169 0.0106996 0.0198788\n beta\_2 0 NA\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 41.9 43.3 1.71 2.36 -1.31\n 77 5 44.7 44.5 1.6 2.36 0.228\n 153 5 45.9 45.6 2.13 2.36 0.277\n 306 5 49.9 48 2.61 2.36 1.81\n 611 4 51.3 52.6 3.19 2.36 -1.12\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -28.879056 6 69.758112\n A2 -27.466920 10 74.933840\n A3 -28.879056 6 69.758112\n fitted -32.589931 3 71.179863\n R -44.843049 2 93.686099\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 34.7523 8 <.0001\n Test 2 2.82427 4 0.5877\n Test 3 2.82427 4 0.5877\n Test 4 7.42175 3 0.0596\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 154.242\n\n\n BMDL = 114.214\n\n\n BMDU = 236.078\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .76656518330133239,.71738015062344429,.95149604071998772,1.1689047416798897,1.5939810554911218 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 2 | 0 | Polynomial-4 | 3 | 2.21 | True | False | 154.2420 | 114.214000 | 236.078 | -999 | 71.179863 | <0.0001 | 0.5877 | 0.5877 | 0.0596 | 7.421750 | 3 | 0.27700 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0596 < 0.1) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 41.900622 1.714092\n77.000000 5 44.700437 1.604111\n153.000000 5 45.914457 2.127610\n306.000000 5 49.870111 2.613750\n611.000000 4 51.300099 3.187962 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-scfnjvqw.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-scfnjvqw.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:50 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 5.15622\n rho = 0 Specified\n beta\_0 = 41.9006\n beta\_1 = 0.0578011\n beta\_2 = 0\n beta\_3 = 1.22894e-006\n beta\_4 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -8.7e-007 9.7e-007\n\n beta\_0 -8.7e-007 1 -0.72\n\n beta\_1 9.7e-007 -0.72 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 5.56128 1.6054 2.41475 8.70781\n beta\_0 43.2828 0.694025 41.9225 44.643\n beta\_1 0.0152892 0.00234169 0.0106996 0.0198788\n beta\_2 0 NA\n beta\_3 0 NA\n beta\_4 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 41.9 43.3 1.71 2.36 -1.31\n 77 5 44.7 44.5 1.6 2.36 0.228\n 153 5 45.9 45.6 2.13 2.36 0.277\n 306 5 49.9 48 2.61 2.36 1.81\n 611 4 51.3 52.6 3.19 2.36 -1.12\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -28.879056 6 69.758112\n A2 -27.466920 10 74.933840\n A3 -28.879056 6 69.758112\n fitted -32.589931 3 71.179863\n R -44.843049 2 93.686099\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 34.7523 8 <.0001\n Test 2 2.82427 4 0.5877\n Test 3 2.82427 4 0.5877\n Test 4 7.42175 3 0.0596\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 154.242\n\n\n BMDL = 114.214\n\n\n BMDU = 236.078\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .76656518330133239,.71738015062344429,.95149604071998772,1.1689047416798897,1.5939810554911218 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 2 | 0 | Power | 4 | 2.19 | True | False | 154.2420 | 114.214000 | 237.776 | -999 | 71.179863 | <0.0001 | 0.5877 | 0.5877 | 0.0596 | 7.421750 | 3 | 0.27700 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0596 < 0.1) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 41.900622 1.714092\n77.000000 5 44.700437 1.604111\n153.000000 5 45.914457 2.127610\n306.000000 5 49.870111 2.613750\n611.000000 4 51.300099 3.187962 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-i4aprkg1.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-i4aprkg1.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:50 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The power is restricted to be greater than or equal to 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 5.15622\n rho = 0 Specified\n control = 41.9006\n slope = 0.170133\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha control slope\n\n alpha 1 4.3e-013 8.8e-013\n\n control 4.3e-013 1 -0.72\n\n slope 8.8e-013 -0.72 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 5.56128 1.6054 2.41475 8.70781\n control 43.2828 0.694025 41.9225 44.643\n slope 0.0152892 0.00234169 0.0106996 0.0198788\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 41.9 43.3 1.71 2.36 -1.31\n 77 5 44.7 44.5 1.6 2.36 0.228\n 153 5 45.9 45.6 2.13 2.36 0.277\n 306 5 49.9 48 2.61 2.36 1.81\n 611 4 51.3 52.6 3.19 2.36 -1.12\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -28.879056 6 69.758112\n A2 -27.466920 10 74.933840\n A3 -28.879056 6 69.758112\n fitted -32.589931 3 71.179863\n R -44.843049 2 93.686099\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 34.7523 8 <.0001\n Test 2 2.82427 4 0.5877\n Test 3 2.82427 4 0.5877\n Test 4 7.42175 3 0.0596\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 154.242 \n\n\n BMDL = 114.214 \n\n\n BMDU = 237.776 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .76656518330133239,.71738015062344429,.95149604071998772,1.1689047416798897,1.5939810554911218 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 2 | 0 | Hill | 5 | 2.18 | True | False | 70.5848 | 29.566400 | 154.999 | -999 | 68.852731 | <0.0001 | 0.5877 | 0.5877 | 0.2955 | 1.094620 | 1 | 0.45600 | NaN | valid | NaN | NaN | NaN | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 41.900622 1.714092\n77.000000 5 44.700437 1.604111\n153.000000 5 45.914457 2.127610\n306.000000 5 49.870111 2.613750\n611.000000 4 51.300099 3.187962 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-ypiwyx46.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-ypiwyx46.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:50 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n Power parameter restricted to be greater than 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 5.15622\n rho = 0 Specified\n intercept = 41.9006\n v = 9.39948\n n = 0.259937\n k = 432.47\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha intercept v n k\n\n alpha 1 -4.2e-007 7.2e-008 -1.4e-008 -1.7e-007\n\n intercept -4.2e-007 1 -0.45 0.42 0.00049\n\n v 7.2e-008 -0.45 1 -0.9 0.87\n\n n -1.4e-008 0.42 -0.9 1 -0.78\n\n k -1.7e-007 0.00049 0.87 -0.78 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 4.27249 1.23336 1.85515 6.68983\n intercept 41.9921 0.951131 40.1279 43.8563\n v 11.5135 4.26845 3.14749 19.8795\n n 1.42973 0.815192 -0.168016 3.02748\n k 204.309 117.906 -26.7829 435.401\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 41.9 42 1.71 2.07 -0.0989\n 77 5 44.7 44.3 1.6 2.07 0.456\n 153 5 45.9 46.6 2.13 2.07 -0.715\n 306 5 49.9 49.4 2.61 2.07 0.545\n 611 4 51.3 51.5 3.19 2.07 -0.209\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -28.879056 6 69.758112\n A2 -27.466920 10 74.933840\n A3 -28.879056 6 69.758112\n fitted -29.426365 5 68.852731\n R -44.843049 2 93.686099\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 34.7523 8 <.0001\n Test 2 2.82427 4 0.5877\n Test 3 2.82427 4 0.5877\n Test 4 1.09462 1 0.2955\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 70.5848\n\n BMDL = 29.5664\n\n BMDU = 154.999\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .76656518330133239,.71738015062344429,.95149604071998772,1.1689047416798897,1.5939810554911218 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 2 | 0 | Exponential-M2 | 6 | 1.11 | True | False | 172.4860 | 129.612000 | 257.362 | -999 | 72.086310 | <0.0001 | 0.5877 | 0.5877 | 0.03969 | 8.328000 | 3 | 0.30840 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0397 < 0.1) | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 41.900622 1.714092\n77.000000 5 44.700437 1.604111\n153.000000 5 45.914457 2.127610\n306.000000 5 49.870111 2.613750\n611.000000 4 51.300099 3.187962 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-61vj7nyg.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:50 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha 1.40659 \n rho 0 Specified\n a 43.3048 \n b 0.000325895 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha 1.7536 1.6672\n a 43.4578 0.679678\n b 0.000312051 4.79598e-005\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 41.9 1.714\n 77 5 44.7 1.604\n 153 5 45.91 2.128\n 306 5 49.87 2.614\n 611 4 51.3 3.188\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 43.46 2.403 -1.449\n 77 44.51 2.403 0.1729\n 153 45.58 2.403 0.3084\n 306 47.81 2.403 1.915\n 611 52.59 2.403 -1.07\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -28.87906 6 69.75811\n A2 -27.46692 10 74.93384\n A3 -28.87906 6 69.75811\n R -44.84305 2 93.6861\n 2 -33.04316 3 72.08631\n\n\n Additive constant for all log-likelihoods = -22.05. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 34.75 8 < 0.0001\n Test 2 2.824 4 0.5877\n Test 3 2.824 4 0.5877\n Test 4 8.328 3 0.03969\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 172.486\n\n BMDL = 129.612\n\n BMDU = 257.362\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .76656518330133239,.71738015062344429,.95149604071998772,1.1689047416798897,1.5939810554911218 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 2 | 0 | Exponential-M3 | 7 | 1.11 | True | False | 172.4860 | 129.612000 | 260.416 | -999 | 72.086310 | <0.0001 | 0.5877 | 0.5877 | 0.03969 | 8.328000 | 3 | 0.30840 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0397 < 0.1) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 41.900622 1.714092\n77.000000 5 44.700437 1.604111\n153.000000 5 45.914457 2.127610\n306.000000 5 49.870111 2.613750\n611.000000 4 51.300099 3.187962 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-vj4hymcn.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:50 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha 1.40659 \n rho 0 Specified\n a 43.3048 \n b 0.000325895 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha 1.7536 1.6672\n a 43.4578 0.679678\n b 0.000312051 4.79598e-005\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 41.9 1.714\n 77 5 44.7 1.604\n 153 5 45.91 2.128\n 306 5 49.87 2.614\n 611 4 51.3 3.188\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 43.46 2.403 -1.449\n 77 44.51 2.403 0.1729\n 153 45.58 2.403 0.3084\n 306 47.81 2.403 1.915\n 611 52.59 2.403 -1.07\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -28.87906 6 69.75811\n A2 -27.46692 10 74.93384\n A3 -28.87906 6 69.75811\n R -44.84305 2 93.6861\n 3 -33.04316 3 72.08631\n\n\n Additive constant for all log-likelihoods = -22.05. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 34.75 8 < 0.0001\n Test 2 2.824 4 0.5877\n Test 3 2.824 4 0.5877\n Test 5a 8.328 3 0.03969\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 172.486\n\n BMDL = 129.612\n\n BMDU = 260.416\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .76656518330133239,.71738015062344429,.95149604071998772,1.1689047416798897,1.5939810554911218 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 2 | 0 | Exponential-M4 | 8 | 1.11 | True | False | 55.8399 | 33.683600 | 109.520 | -999 | 66.856540 | <0.0001 | 0.5877 | 0.5877 | 0.5774 | 1.098000 | 2 | 0.15530 | NaN | valid | NaN | NaN | NaN | True | AIC | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 41.900622 1.714092\n77.000000 5 44.700437 1.604111\n153.000000 5 45.914457 2.127610\n306.000000 5 49.870111 2.613750\n611.000000 4 51.300099 3.187962 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-hcmdpqtz.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:50 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha 1.40659 \n rho 0 Specified\n a 39.8056 \n b 0.00311249 \n c 1.3532 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha 1.45236 1.23356\n a 41.8144 0.848432\n b 0.00381167 0.00155013\n c 1.25786 0.0459667\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 41.9 1.714\n 77 5 44.7 1.604\n 153 5 45.91 2.128\n 306 5 49.87 2.614\n 611 4 51.3 3.188\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 41.81 2.067 0.09325\n 77 44.56 2.067 0.1553\n 153 46.58 2.067 -0.7188\n 306 49.24 2.067 0.6836\n 611 51.55 2.067 -0.2385\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -28.87906 6 69.75811\n A2 -27.46692 10 74.93384\n A3 -28.87906 6 69.75811\n R -44.84305 2 93.6861\n 4 -29.42827 4 66.85654\n\n\n Additive constant for all log-likelihoods = -22.05. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 34.75 8 < 0.0001\n Test 2 2.824 4 0.5877\n Test 3 2.824 4 0.5877\n Test 6a 1.098 2 0.5774\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is greater than .1. Model 4 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 55.8399\n\n BMDL = 33.6836\n\n BMDU = 109.52\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Liver Weight Relative | mg/g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | .76656518330133239,.71738015062344429,.95149604071998772,1.1689047416798897,1.5939810554911218 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 1250 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Liver Weight Relative | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 2 | 0 | Exponential-M5 | 9 | 1.11 | True | False | 72.0325 | 34.438400 | 157.068 | -999 | 68.600210 | <0.0001 | 0.5877 | 0.5877 | 0.3588 | 0.842100 | 1 | 0.50790 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 41.900622 1.714092\n77.000000 5 44.700437 1.604111\n153.000000 5 45.914457 2.127610\n306.000000 5 49.870111 2.613750\n611.000000 4 51.300099 3.187962 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-ovenlew5.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:50 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha 1.40659 \n rho 0 Specified\n a 39.8056 \n b 0.00311249 \n c 1.3532 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha 1.44168 1.22045\n a 42.0178 0.944032\n b 0.00450879 0.00143835\n c 1.22993 0.0504894\n d 1.27157 0.554968\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 41.9 1.714\n 77 5 44.7 1.604\n 153 5 45.91 2.128\n 306 5 49.87 2.614\n 611 4 51.3 3.188\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 42.02 2.056 -0.1275\n 77 44.23 2.056 0.5079\n 153 46.5 2.056 -0.6378\n 306 49.54 2.056 0.3637\n 611 51.42 2.056 -0.1189\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -28.87906 6 69.75811\n A2 -27.46692 10 74.93384\n A3 -28.87906 6 69.75811\n R -44.84305 2 93.6861\n 5 -29.30011 5 68.60021\n\n\n Additive constant for all log-likelihoods = -22.05. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 34.75 8 < 0.0001\n Test 2 2.824 4 0.5877\n Test 3 2.824 4 0.5877\n Test 7a 0.8421 1 0.3588\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is greater than .1. Model 5 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 72.0325\n\n BMDL = 34.4384\n\n BMDU = 157.068\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Terminal Body Weight | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 0 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Terminal Body Weight | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 3 | 0 | Linear | 0 | 2.21 | True | False | 278.2440 | 187.298000 | 536.529 | -999 | 140.071643 | 0.0729 | 0.8914 | 0.8914 | 0.6931 | 1.453160 | 3 | -0.24300 | NaN | valid | NaN | NaN | NaN | True | AIC | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-7ln\_0m\_u.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-7ln\_0m\_u.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 92.5624\n rho = 0 Specified\n beta\_0 = 250.124\n beta\_1 = -0.0318389\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -5.6e-011 -3e-010\n\n beta\_0 -5.6e-011 1 -0.73\n\n beta\_1 -3e-010 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 78.4817 22.198 34.9745 121.989\n beta\_0 250.124 2.58491 245.058 255.19\n beta\_1 -0.0318389 0.00820465 -0.0479197 -0.0157581\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 247 250 8.48 8.86 -0.748\n 77 5 251 248 7.73 8.86 0.88\n 153 5 246 245 11.9 8.86 0.133\n 306 5 239 240 9.32 8.86 -0.243\n 611 5 231 231 10.1 8.86 -0.0228\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -66.309243 6 144.618487\n A2 -65.750363 10 151.500726\n A3 -66.309243 6 144.618487\n fitted -67.035821 3 140.071643\n R -72.929294 2 149.858588\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.3579 8 0.0729\n Test 2 1.11776 4 0.8914\n Test 3 1.11776 4 0.8914\n Test 4 1.45316 3 0.6931\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 278.244\n\n\n BMDL = 187.298\n\n\n BMDU = 536.529\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Terminal Body Weight | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 0 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Terminal Body Weight | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 3 | 0 | Polynomial-2 | 1 | 2.21 | True | False | 319.0270 | 188.177000 | 575.952 | -999 | 141.995175 | 0.0729 | 0.8914 | 0.8914 | 0.5024 | 1.376690 | 2 | -0.42300 | NaN | valid | NaN | NaN | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-1l7\_q3ay.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-1l7\_q3ay.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:53 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 92.5624\n rho = 0 Specified\n beta\_0 = 249.525\n beta\_1 = -0.0235097\n beta\_2 = -1.32174e-005\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1 beta\_2\n\n alpha 1 -2.7e-012 -1.4e-013 -8.7e-014\n\n beta\_0 -2.7e-012 1 -0.77 0.64\n\n beta\_1 -1.4e-013 -0.77 1 -0.96\n\n beta\_2 -8.7e-014 0.64 -0.96 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 78.242 22.1302 34.8677 121.616\n beta\_0 249.525 3.36794 242.924 256.126\n beta\_1 -0.0235097 0.0311928 -0.0846463 0.037627\n beta\_2 -1.32174e-005 4.77611e-005 -0.000106827 8.03926e-005\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 247 250 8.48 8.85 -0.598\n 77 5 251 248 7.73 8.85 0.891\n 153 5 246 246 11.9 8.85 0.0408\n 306 5 239 241 9.32 8.85 -0.423\n 611 5 231 230 10.1 8.85 0.0894\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -66.309243 6 144.618487\n A2 -65.750363 10 151.500726\n A3 -66.309243 6 144.618487\n fitted -66.997587 4 141.995175\n R -72.929294 2 149.858588\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.3579 8 0.0729\n Test 2 1.11776 4 0.8914\n Test 3 1.11776 4 0.8914\n Test 4 1.37669 2 0.5024\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 319.027\n\n\n BMDL = 188.177\n\n\n BMDU = 575.952\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Terminal Body Weight | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 0 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Terminal Body Weight | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 3 | 0 | Polynomial-3 | 2 | 2.21 | True | False | 319.0270 | 188.177000 | 575.952 | -999 | 141.995175 | 0.0729 | 0.8914 | 0.8914 | 0.5024 | 1.376690 | 2 | -0.42300 | NaN | valid | NaN | NaN | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-45vr78bk.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-45vr78bk.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:53 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 92.5624\n rho = 0 Specified\n beta\_0 = 247.798\n beta\_1 = 0\n beta\_2 = -0.000353656\n beta\_3 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1 beta\_2\n\n alpha 1 -5e-009 -3.9e-008 4.7e-008\n\n beta\_0 -5e-009 1 -0.77 0.64\n\n beta\_1 -3.9e-008 -0.77 1 -0.96\n\n beta\_2 4.7e-008 0.64 -0.96 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 78.242 22.1302 34.8677 121.616\n beta\_0 249.525 3.36794 242.924 256.126\n beta\_1 -0.0235097 0.0311928 -0.0846464 0.037627\n beta\_2 -1.32174e-005 4.77611e-005 -0.000106827 8.03926e-005\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 247 250 8.48 8.85 -0.598\n 77 5 251 248 7.73 8.85 0.891\n 153 5 246 246 11.9 8.85 0.0408\n 306 5 239 241 9.32 8.85 -0.423\n 611 5 231 230 10.1 8.85 0.0894\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -66.309243 6 144.618487\n A2 -65.750363 10 151.500726\n A3 -66.309243 6 144.618487\n fitted -66.997587 4 141.995175\n R -72.929294 2 149.858588\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.3579 8 0.0729\n Test 2 1.11776 4 0.8914\n Test 3 1.11776 4 0.8914\n Test 4 1.37669 2 0.5024\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 319.027\n\n\n BMDL = 188.177\n\n\n BMDU = 575.952\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Terminal Body Weight | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 0 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Terminal Body Weight | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 3 | 0 | Polynomial-4 | 3 | 2.21 | True | False | 319.0270 | 188.177000 | 575.952 | -999 | 141.995175 | 0.0729 | 0.8914 | 0.8914 | 0.5024 | 1.376690 | 2 | -0.42300 | NaN | valid | NaN | NaN | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-1w7okw4z.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-1w7okw4z.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:53 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 92.5624\n rho = 0 Specified\n beta\_0 = 247.16\n beta\_1 = 0\n beta\_2 = -0.00193489\n beta\_3 = 0\n beta\_4 = -5.28001e-009\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1 beta\_2\n\n alpha 1 8e-008 -2e-007 1.5e-007\n\n beta\_0 8e-008 1 -0.77 0.64\n\n beta\_1 -2e-007 -0.77 1 -0.96\n\n beta\_2 1.5e-007 0.64 -0.96 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 78.242 22.1302 34.8677 121.616\n beta\_0 249.525 3.36794 242.924 256.126\n beta\_1 -0.0235097 0.0311928 -0.0846464 0.037627\n beta\_2 -1.32173e-005 4.77611e-005 -0.000106827 8.03926e-005\n beta\_3 0 NA\n beta\_4 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 247 250 8.48 8.85 -0.598\n 77 5 251 248 7.73 8.85 0.891\n 153 5 246 246 11.9 8.85 0.0408\n 306 5 239 241 9.32 8.85 -0.423\n 611 5 231 230 10.1 8.85 0.0894\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -66.309243 6 144.618487\n A2 -65.750363 10 151.500726\n A3 -66.309243 6 144.618487\n fitted -66.997587 4 141.995175\n R -72.929294 2 149.858588\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.3579 8 0.0729\n Test 2 1.11776 4 0.8914\n Test 3 1.11776 4 0.8914\n Test 4 1.37669 2 0.5024\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 319.027\n\n\n BMDL = 188.177\n\n\n BMDU = 575.952\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Terminal Body Weight | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 0 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Terminal Body Weight | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 3 | 0 | Power | 4 | 2.19 | True | False | 329.1610 | 189.734000 | 569.321 | -999 | 141.864123 | 0.0729 | 0.8914 | 0.8914 | 0.5364 | 1.245640 | 2 | -0.44300 | NaN | valid | NaN | NaN | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-0nmbox8t.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-0nmbox8t.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:53 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The power is restricted to be greater than or equal to 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 92.5624\n rho = 0 Specified\n control = 230.58\n slope = 306.481\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha control slope power\n\n alpha 1 -1.1e-007 4.7e-008 4.2e-008\n\n control -1.1e-007 1 -0.67 -0.64\n\n slope 4.7e-008 -0.67 1 1\n\n power 4.2e-008 -0.64 1 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 77.833 22.0145 34.6854 120.981\n control 249.22 3.13105 243.083 255.357\n slope -0.00623623 0.0257157 -0.0566382 0.0441657\n power 1.25155 0.633463 0.00998492 2.49311\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 247 249 8.48 8.82 -0.522\n 77 5 251 248 7.73 8.82 0.855\n 153 5 246 246 11.9 8.82 -0.0147\n 306 5 239 241 9.32 8.82 -0.443\n 611 5 231 230 10.1 8.82 0.125\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -66.309243 6 144.618487\n A2 -65.750363 10 151.500726\n A3 -66.309243 6 144.618487\n fitted -66.932061 4 141.864123\n R -72.929294 2 149.858588\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.3579 8 0.0729\n Test 2 1.11776 4 0.8914\n Test 3 1.11776 4 0.8914\n Test 4 1.24564 2 0.5364\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 329.161 \n\n\n BMDL = 189.734 \n\n\n BMDU = 569.321 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Terminal Body Weight | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 0 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Terminal Body Weight | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 3 | 0 | Hill | 5 | 2.18 | True | False | 285.9400 | 141.473000 | 541.085 | -999 | 143.329005 | 0.0729 | 0.8914 | 0.8914 | 0.3993 | 0.710518 | 1 | 0.05380 | NaN | valid | NaN | NaN | NaN | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-urfqdlmx.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-urfqdlmx.plt\n \t\t\t\t\t\t\tTue Jul 06 12:38:53 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n Power parameter restricted to be greater than 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 92.5624\n rho = 0 Specified\n intercept = 247.16\n v = -16.58\n n = 2.69674\n k = 324.976\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha intercept v n k\n\n alpha 1 -5.7e-008 1.4e-009 1.2e-009 2.9e-008\n\n intercept -5.7e-008 1 -0.46 -0.45 -0.0055\n\n v 1.4e-009 -0.46 1 0.85 -0.82\n\n n 1.2e-009 -0.45 0.85 1 -0.67\n\n k 2.9e-008 -0.0055 -0.82 -0.67 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 76.1847 21.5483 33.9508 118.419\n intercept 248.949 2.93903 243.188 254.709\n v -21.398 12.954 -46.7874 3.99145\n n 2.84108 2.9751 -2.99001 8.67217\n k 326.014 185.424 -37.4102 689.438\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 247 249 8.48 8.73 -0.458\n 77 5 251 249 7.73 8.73 0.656\n 153 5 246 247 11.9 8.73 -0.239\n 306 5 239 239 9.32 8.73 0.0538\n 611 5 231 231 10.1 8.73 -0.0119\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -66.309243 6 144.618487\n A2 -65.750363 10 151.500726\n A3 -66.309243 6 144.618487\n fitted -66.664503 5 143.329005\n R -72.929294 2 149.858588\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.3579 8 0.0729\n Test 2 1.11776 4 0.8914\n Test 3 1.11776 4 0.8914\n Test 4 0.710518 1 0.3993\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 285.94\n\n BMDL = 141.473\n\n BMDU = 541.085\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Terminal Body Weight | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 0 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Terminal Body Weight | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 3 | 0 | Exponential-M2 | 6 | 1.11 | True | False | 272.4580 | 180.450000 | 536.451 | -999 | 140.098400 | 0.0729 | 0.8914 | 0.8914 | 0.6869 | 1.480000 | 3 | -0.21520 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-isl1tdlv.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:53 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha 4.30474 \n rho 0 Specified\n a 235.432 \n b 0.000132749 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha 4.36394 22.2218\n a 250.206 2.62349\n b 0.000132382 3.46417e-005\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 247.2 8.483\n 77 5 251.2 7.732\n 153 5 245.8 11.89\n 306 5 239.4 9.316\n 611 5 230.6 10.15\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 250.2 8.864 -0.7684\n 77 247.7 8.864 0.8808\n 153 245.2 8.864 0.1491\n 306 240.3 8.864 -0.2152\n 611 230.8 8.864 -0.04661\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -66.30924 6 144.6185\n A2 -65.75036 10 151.5007\n A3 -66.30924 6 144.6185\n R -72.92929 2 149.8586\n 2 -67.04921 3 140.0984\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 14.36 8 0.0729\n Test 2 1.118 4 0.8914\n Test 3 1.118 4 0.8914\n Test 4 1.48 3 0.6869\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is greater than .1. Model 2 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 272.458\n\n BMDL = 180.45\n\n BMDU = 536.451\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Terminal Body Weight | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 0 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Terminal Body Weight | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 3 | 0 | Exponential-M3 | 7 | 1.11 | True | False | 327.5380 | 183.472000 | 568.124 | -999 | 141.844400 | 0.0729 | 0.8914 | 0.8914 | 0.5417 | 1.226000 | 2 | -0.43270 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-vmc4i1h4.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:53 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha 4.30474 \n rho 0 Specified\n a 235.432 \n b 0.000132749 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha 4.35378 21.9997\n a 249.223 3.47559\n b 0.000226486 0.000398465\n d 1.27767 0.987046\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 247.2 8.483\n 77 5 251.2 7.732\n 153 5 245.8 11.89\n 306 5 239.4 9.316\n 611 5 230.6 10.15\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 249.2 8.819 -0.5232\n 77 247.8 8.819 0.8481\n 153 245.9 8.819 -0.01805\n 306 241.1 8.819 -0.4327\n 611 230.1 8.819 0.1259\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -66.30924 6 144.6185\n A2 -65.75036 10 151.5007\n A3 -66.30924 6 144.6185\n R -72.92929 2 149.8586\n 3 -66.9222 4 141.8444\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 14.36 8 0.0729\n Test 2 1.118 4 0.8914\n Test 3 1.118 4 0.8914\n Test 5a 1.226 2 0.5417\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is greater than .1. Model 3 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 327.538\n\n BMDL = 183.472\n\n BMDU = 568.124\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Terminal Body Weight | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 0 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Terminal Body Weight | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 3 | 0 | Exponential-M4 | 8 | 1.11 | True | False | 272.4580 | 125.108000 | 536.451 | -999 | 140.098400 | 0.0729 | 0.8914 | 0.8914 | 0.6869 | 1.480000 | 3 | -0.21520 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-t9vom9de.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:53 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha 4.30474 \n rho 0 Specified\n a 263.718 \n b 0.00241846 \n c 0.832708 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha 4.36394 22.2218\n a 250.206 2.62075\n b 0.000132382 3.45716e-005\n c 0 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 247.2 8.483\n 77 5 251.2 7.732\n 153 5 245.8 11.89\n 306 5 239.4 9.316\n 611 5 230.6 10.15\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 250.2 8.864 -0.7684\n 77 247.7 8.864 0.8808\n 153 245.2 8.864 0.1491\n 306 240.3 8.864 -0.2152\n 611 230.8 8.864 -0.04661\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -66.30924 6 144.6185\n A2 -65.75036 10 151.5007\n A3 -66.30924 6 144.6185\n R -72.92929 2 149.8586\n 4 -67.04921 3 140.0984\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 14.36 8 0.0729\n Test 2 1.118 4 0.8914\n Test 3 1.118 4 0.8914\n Test 6a 1.48 3 0.6869\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is greater than .1. Model 4 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 272.458\n\n BMDL = 125.108\n\n BMDU = 536.451\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Terminal Body Weight | g | Male | PA06 | Organ Weights | X-C10866B|Male|Organ Weights|PA06| | 1, 2, 3, 4, 5 | mg/kg | 3.793758031292978,3.4578316905251425,5.3152046056572413,4.166341320631326,4.5390968264622904 | 2,0,0,0,1 | 1,1,1,1,1 | SD | day | NaN | 0 | Organ Weights Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Terminal Body Weight | Dose (mg/kg) | X-C10866B|Male|Organ Weights|PA06| | 3 | 0 | Exponential-M5 | 9 | 1.11 | True | False | 289.2550 | 142.229000 | 542.372 | -999 | 143.350100 | 0.0729 | 0.8914 | 0.8914 | 0.3924 | 0.731600 | 1 | 0.04042 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 247.160000 8.483101\n77.000000 5 251.160000 7.731947\n153.000000 5 245.780000 11.885159\n306.000000 5 239.420000 9.316222\n611.000000 5 230.580000 10.149729 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-2hz75210.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:38:53 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha 4.30474 \n rho 0 Specified\n a 263.718 \n b 0.00241846 \n c 0.832708 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha 4.334 21.5665\n a 248.923 2.96199\n b 0.00290078 0.00103994\n c 0.925459 0.0240859\n d 2.579 2.64713\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 247.2 8.483\n 77 5 251.2 7.732\n 153 5 245.8 11.89\n 306 5 239.4 9.316\n 611 5 230.6 10.15\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 248.9 8.732 -0.4515\n 77 248.5 8.732 0.6713\n 153 246.8 8.732 -0.2547\n 306 239.3 8.732 0.04042\n 611 230.6 8.732 -0.005541\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -66.30924 6 144.6185\n A2 -65.75036 10 151.5007\n A3 -66.30924 6 144.6185\n R -72.92929 2 149.8586\n 5 -66.67505 5 143.3501\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 14.36 8 0.0729\n Test 2 1.118 4 0.8914\n Test 3 1.118 4 0.8914\n Test 7a 0.7316 1 0.3924\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is greater than .1. Model 5 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 289.255\n\n BMDL = 142.229\n\n BMDU = 542.372\n | NaN | NaN |

## Clinical Chemistry
| DEPOSITOR\_STUDY\_NUMBER | study\_id | CHEMICAL | ENDPOINT | ENDPOINT\_UNIT | SEX | table\_id | OUTPUT\_TYPE | PHASE\_TYPE | PHASE\_START | id | GROUP\_NAME | Converted\_Dose\_Units | STE | MULT\_COMP\_SIGNIF | NUM\_DECIMAL\_DIGIT | DEATH\_PHASE\_TYPE | DEATH\_PHASE\_TIME\_UNIT | LEGEND\_ID | SORT\_ORDER | TABLE\_HEADER | DEATH\_PHASE\_TIME | DOSE\_UNIT | original\_doses | dataset\_name | xlabel | ylabel | dataset\_index | doses\_dropped | model\_name | model\_index | model\_version | has\_output | execution\_halted | BMD | BMDL | BMDU | CSF | AIC | pvalue1 | pvalue2 | pvalue3 | pvalue4 | Chi2 | df | residual\_of\_interest | warnings | logic\_bin | logic\_cautions | logic\_warnings | logic\_failures | recommended | recommended\_variable | dfile | outfile | stdout | stderr |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | A/G Ratio | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .014983919135108163,.03280013628629011,.020680692078115459,.029342751593028519,.034099546643330002 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 110 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: A/G Ratio | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 0 | 0 | Linear | 0 | 2.21 | True | False | 2.474410e+02 | 1.711930e+02 | 4.422000e+02 | -999 | -105.805864 | 0.000786 | 0.384200 | 0.3842 | 0.03824 | 8.410660 | 3 | -1.560000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0382 < 0.1)\nRatio of modeled to actual stdev. at control is greater than threshold (1.93 > 1.5) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 1.347926 0.033505\n77.000000 5 1.277884 0.073343\n153.000000 5 1.232263 0.046243\n306.000000 5 1.175592 0.065612\n611.000000 5 1.171317 0.076249 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-j5f1timy.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-j5f1timy.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:16 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.00375181\n rho = 0 Specified\n beta\_0 = 1.30109\n beta\_1 = -0.000261967\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 3e-009 -3.1e-009\n\n beta\_0 3e-009 1 -0.73\n\n beta\_1 -3.1e-009 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.00420183 0.00118846 0.0018725 0.00653117\n beta\_0 1.30109 0.0189139 1.26402 1.33816\n beta\_1 -0.000261967 6.00337e-005 -0.000379631 -0.000144303\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 1.35 1.3 0.0335 0.0648 1.62\n 77 5 1.28 1.28 0.0733 0.0648 -0.105\n 153 5 1.23 1.26 0.0462 0.0648 -0.992\n 306 5 1.18 1.22 0.0656 0.0648 -1.56\n 611 5 1.17 1.14 0.0762 0.0648 1.04\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 60.108262 6 -108.216524\n A2 62.190603 10 -104.381205\n A3 60.108262 6 -108.216524\n fitted 55.902932 3 -105.805864\n R 48.824694 2 -93.649388\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 26.7318 8 0.0007864\n Test 2 4.16468 4 0.3842\n Test 3 4.16468 4 0.3842\n Test 4 8.41066 3 0.03824\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 247.441\n\n\n BMDL = 171.193\n\n\n BMDU = 442.2\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | A/G Ratio | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .014983919135108163,.03280013628629011,.020680692078115459,.029342751593028519,.034099546643330002 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 110 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: A/G Ratio | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 0 | 0 | Polynomial-2 | 1 | 2.21 | True | False | 2.474410e+02 | 1.711930e+02 | 4.422000e+02 | -999 | -105.805864 | 0.000786 | 0.384200 | 0.3842 | 0.03824 | 8.410660 | 3 | -1.560000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0382 < 0.1)\nRatio of modeled to actual stdev. at control is greater than threshold (1.93 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 1.347926 0.033505\n77.000000 5 1.277884 0.073343\n153.000000 5 1.232263 0.046243\n306.000000 5 1.175592 0.065612\n611.000000 5 1.171317 0.076249 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-fippv6u9.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-fippv6u9.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:16 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.00375181\n rho = 0 Specified\n beta\_0 = 1.34316\n beta\_1 = -0.000847194\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -7e-008 -1.9e-008\n\n beta\_0 -7e-008 1 -0.73\n\n beta\_1 -1.9e-008 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.00420183 0.00118846 0.0018725 0.00653117\n beta\_0 1.30109 0.0189139 1.26402 1.33816\n beta\_1 -0.000261967 6.00337e-005 -0.000379631 -0.000144303\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 1.35 1.3 0.0335 0.0648 1.62\n 77 5 1.28 1.28 0.0733 0.0648 -0.105\n 153 5 1.23 1.26 0.0462 0.0648 -0.992\n 306 5 1.18 1.22 0.0656 0.0648 -1.56\n 611 5 1.17 1.14 0.0762 0.0648 1.04\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 60.108262 6 -108.216524\n A2 62.190603 10 -104.381205\n A3 60.108262 6 -108.216524\n fitted 55.902932 3 -105.805864\n R 48.824694 2 -93.649388\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 26.7318 8 0.0007864\n Test 2 4.16468 4 0.3842\n Test 3 4.16468 4 0.3842\n Test 4 8.41066 3 0.03824\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 247.441\n\n\n BMDL = 171.193\n\n\n BMDU = 442.2\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | A/G Ratio | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .014983919135108163,.03280013628629011,.020680692078115459,.029342751593028519,.034099546643330002 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 110 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: A/G Ratio | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 0 | 0 | Polynomial-3 | 2 | 2.21 | True | False | 2.474410e+02 | 1.711930e+02 | 4.422000e+02 | -999 | -105.805864 | 0.000786 | 0.384200 | 0.3842 | 0.03824 | 8.410660 | 3 | -1.560000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0382 < 0.1)\nRatio of modeled to actual stdev. at control is greater than threshold (1.93 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 1.347926 0.033505\n77.000000 5 1.277884 0.073343\n153.000000 5 1.232263 0.046243\n306.000000 5 1.175592 0.065612\n611.000000 5 1.171317 0.076249 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-2msp7v1x.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-2msp7v1x.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:16 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.00375181\n rho = 0 Specified\n beta\_0 = 1.34735\n beta\_1 = -0.00100872\n beta\_2 = 0\n beta\_3 = -9.40808e-010\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -2.7e-011 -3.2e-012\n\n beta\_0 -2.7e-011 1 -0.73\n\n beta\_1 -3.2e-012 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.00420183 0.00118846 0.0018725 0.00653117\n beta\_0 1.30109 0.0189139 1.26402 1.33816\n beta\_1 -0.000261967 6.00337e-005 -0.000379631 -0.000144303\n beta\_2 -0 NA\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 1.35 1.3 0.0335 0.0648 1.62\n 77 5 1.28 1.28 0.0733 0.0648 -0.105\n 153 5 1.23 1.26 0.0462 0.0648 -0.992\n 306 5 1.18 1.22 0.0656 0.0648 -1.56\n 611 5 1.17 1.14 0.0762 0.0648 1.04\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 60.108262 6 -108.216524\n A2 62.190603 10 -104.381205\n A3 60.108262 6 -108.216524\n fitted 55.902932 3 -105.805864\n R 48.824694 2 -93.649388\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 26.7318 8 0.0007864\n Test 2 4.16468 4 0.3842\n Test 3 4.16468 4 0.3842\n Test 4 8.41066 3 0.03824\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 247.441\n\n\n BMDL = 171.193\n\n\n BMDU = 442.2\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | A/G Ratio | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .014983919135108163,.03280013628629011,.020680692078115459,.029342751593028519,.034099546643330002 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 110 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: A/G Ratio | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 0 | 0 | Polynomial-4 | 3 | 2.21 | True | False | 2.474410e+02 | 1.711930e+02 | 4.422000e+02 | -999 | -105.805864 | 0.000786 | 0.384200 | 0.3842 | 0.03824 | 8.410660 | 3 | -1.560000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0382 < 0.1)\nRatio of modeled to actual stdev. at control is greater than threshold (1.93 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 1.347926 0.033505\n77.000000 5 1.277884 0.073343\n153.000000 5 1.232263 0.046243\n306.000000 5 1.175592 0.065612\n611.000000 5 1.171317 0.076249 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-w27j3v4l.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-w27j3v4l.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:16 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.00375181\n rho = 0 Specified\n beta\_0 = 1.34793\n beta\_1 = -0.00112166\n beta\_2 = 0\n beta\_3 = -5.87523e-009\n beta\_4 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -4.6e-008 2.9e-008\n\n beta\_0 -4.6e-008 1 -0.73\n\n beta\_1 2.9e-008 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.00420183 0.00118846 0.0018725 0.00653116\n beta\_0 1.30109 0.0189138 1.26402 1.33816\n beta\_1 -0.000261967 6.00337e-005 -0.000379631 -0.000144303\n beta\_2 0 NA\n beta\_3 -4.53552e-138 NA\n beta\_4 -2.47106e-140 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 1.35 1.3 0.0335 0.0648 1.62\n 77 5 1.28 1.28 0.0733 0.0648 -0.105\n 153 5 1.23 1.26 0.0462 0.0648 -0.992\n 306 5 1.18 1.22 0.0656 0.0648 -1.56\n 611 5 1.17 1.14 0.0762 0.0648 1.04\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 60.108262 6 -108.216524\n A2 62.190603 10 -104.381205\n A3 60.108262 6 -108.216524\n fitted 55.902932 3 -105.805864\n R 48.824694 2 -93.649388\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 26.7318 8 0.0007864\n Test 2 4.16468 4 0.3842\n Test 3 4.16468 4 0.3842\n Test 4 8.41066 3 0.03824\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 247.441\n\n\n BMDL = 171.193\n\n\n BMDU = 442.2\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | A/G Ratio | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .014983919135108163,.03280013628629011,.020680692078115459,.029342751593028519,.034099546643330002 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 110 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: A/G Ratio | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 0 | 0 | Power | 4 | 2.19 | True | False | 2.474410e+02 | 1.711930e+02 | 4.422000e+02 | -999 | -105.805864 | 0.000786 | 0.384200 | 0.3842 | 0.03824 | 8.410660 | 3 | -1.560000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0382 < 0.1)\nRatio of modeled to actual stdev. at control is greater than threshold (1.93 > 1.5) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 1.347926 0.033505\n77.000000 5 1.277884 0.073343\n153.000000 5 1.232263 0.046243\n306.000000 5 1.175592 0.065612\n611.000000 5 1.171317 0.076249 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-t6dowh6i.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-t6dowh6i.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:16 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The power is restricted to be greater than or equal to 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.00375181\n rho = 0 Specified\n control = 1.34793\n slope = -558903\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha control slope\n\n alpha 1 2.4e-011 9.4e-012\n\n control 2.4e-011 1 -0.73\n\n slope 9.4e-012 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.00420183 0.00118846 0.0018725 0.00653117\n control 1.30109 0.0189139 1.26402 1.33816\n slope -0.000261967 6.00337e-005 -0.000379631 -0.000144303\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 1.35 1.3 0.0335 0.0648 1.62\n 77 5 1.28 1.28 0.0733 0.0648 -0.105\n 153 5 1.23 1.26 0.0462 0.0648 -0.992\n 306 5 1.18 1.22 0.0656 0.0648 -1.56\n 611 5 1.17 1.14 0.0762 0.0648 1.04\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 60.108262 6 -108.216524\n A2 62.190603 10 -104.381205\n A3 60.108262 6 -108.216524\n fitted 55.902932 3 -105.805864\n R 48.824694 2 -93.649388\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 26.7318 8 0.0007864\n Test 2 4.16468 4 0.3842\n Test 3 4.16468 4 0.3842\n Test 4 8.41066 3 0.03824\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 247.441 \n\n\n BMDL = 171.193 \n\n\n BMDU = 442.2 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | A/G Ratio | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .014983919135108163,.03280013628629011,.020680692078115459,.029342751593028519,.034099546643330002 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 110 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: A/G Ratio | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 0 | 0 | Hill | 5 | 2.18 | True | False | 6.580620e+01 | 2.065610e+01 | 1.419750e+02 | -999 | -109.954309 | 0.000786 | 0.384200 | 0.3842 | 0.6086 | 0.262215 | 1 | -1.230000e-01 | NaN | warning | NaN | Ratio of modeled to actual stdev. at control is greater than threshold (1.64 > 1.5) | NaN | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 1.347926 0.033505\n77.000000 5 1.277884 0.073343\n153.000000 5 1.232263 0.046243\n306.000000 5 1.175592 0.065612\n611.000000 5 1.171317 0.076249 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-k8w3yayp.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-k8w3yayp.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:16 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n Power parameter restricted to be greater than 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.00375181\n rho = 0 Specified\n intercept = 1.34793\n v = -0.176609\n n = 2.20112\n k = 107.423\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha intercept v n k\n\n alpha 1 2.9e-009 -3.5e-008 -4.2e-008 -1.4e-008\n\n intercept 2.9e-009 1 -0.59 -0.22 -0.39\n\n v -3.5e-008 -0.59 1 0.74 -0.34\n\n n -4.2e-008 -0.22 0.74 1 -0.34\n\n k -1.4e-008 -0.39 -0.34 -0.34 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.00303309 0.000857888 0.00135166 0.00471452\n intercept 1.34735 0.0247725 1.2988 1.39591\n v -0.189368 0.0472991 -0.282073 -0.0966639\n n 1.75878 1.18815 -0.569954 4.08751\n k 109.238 41.7014 27.5043 190.971\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 1.35 1.35 0.0335 0.0551 0.0232\n 77 5 1.28 1.28 0.0733 0.0551 -0.123\n 153 5 1.23 1.23 0.0462 0.0551 0.278\n 306 5 1.18 1.18 0.0656 0.0551 -0.365\n 611 5 1.17 1.17 0.0762 0.0551 0.186\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 60.108262 6 -108.216524\n A2 62.190603 10 -104.381205\n A3 60.108262 6 -108.216524\n fitted 59.977155 5 -109.954309\n R 48.824694 2 -93.649388\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 26.7318 8 0.0007864\n Test 2 4.16468 4 0.3842\n Test 3 4.16468 4 0.3842\n Test 4 0.262215 1 0.6086\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 65.8062\n\n BMDL = 20.6561\n\n BMDU = 141.975\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | A/G Ratio | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .014983919135108163,.03280013628629011,.020680692078115459,.029342751593028519,.034099546643330002 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 110 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: A/G Ratio | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 0 | 0 | Exponential-M2 | 6 | 1.11 | True | False | 2.296500e+02 | 1.560350e+02 | 4.175690e+02 | -999 | -106.242200 | 0.000786 | 0.384200 | 0.3842 | 0.04655 | 7.974000 | 3 | -1.506000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0466 < 0.1) | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 1.347926 0.033505\n77.000000 5 1.277884 0.073343\n153.000000 5 1.232263 0.046243\n306.000000 5 1.175592 0.065612\n611.000000 5 1.171317 0.076249 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-899ob\_t3.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:16 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha -5.80866 \n rho 0 Specified\n a 1.18083 \n b 0.000210501 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha -5.48969 0.00116789\n a 1.30377 0.0190718\n b 0.000220085 4.93277e-005\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 1.348 0.03351\n 77 5 1.278 0.07334\n 153 5 1.232 0.04624\n 306 5 1.176 0.06561\n 611 5 1.171 0.07625\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 1.304 0.06426 1.536\n 77 1.282 0.06426 -0.1385\n 153 1.261 0.06426 -0.9862\n 306 1.219 0.06426 -1.506\n 611 1.14 0.06426 1.099\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 60.10826 6 -108.2165\n A2 62.1906 10 -104.3812\n A3 60.10826 6 -108.2165\n R 48.82469 2 -93.64939\n 2 56.12112 3 -106.2422\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 26.73 8 0.0007864\n Test 2 4.165 4 0.3842\n Test 3 4.165 4 0.3842\n Test 4 7.974 3 0.04655\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 229.65\n\n BMDL = 156.035\n\n BMDU = 417.569\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | A/G Ratio | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .014983919135108163,.03280013628629011,.020680692078115459,.029342751593028519,.034099546643330002 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 110 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: A/G Ratio | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 0 | 0 | Exponential-M3 | 7 | 1.11 | True | False | 2.296500e+02 | 1.560350e+02 | 4.175690e+02 | -999 | -106.242200 | 0.000786 | 0.384200 | 0.3842 | 0.04655 | 7.974000 | 3 | -1.506000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0466 < 0.1) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 1.347926 0.033505\n77.000000 5 1.277884 0.073343\n153.000000 5 1.232263 0.046243\n306.000000 5 1.175592 0.065612\n611.000000 5 1.171317 0.076249 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-7s45lddl.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:16 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha -5.80866 \n rho 0 Specified\n a 1.18083 \n b 0.000210501 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha -5.48969 0.00116789\n a 1.30377 0.019295\n b 0.000220085 5.04764e-005\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 1.348 0.03351\n 77 5 1.278 0.07334\n 153 5 1.232 0.04624\n 306 5 1.176 0.06561\n 611 5 1.171 0.07625\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 1.304 0.06426 1.536\n 77 1.282 0.06426 -0.1385\n 153 1.261 0.06426 -0.9862\n 306 1.219 0.06426 -1.506\n 611 1.14 0.06426 1.099\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 60.10826 6 -108.2165\n A2 62.1906 10 -104.3812\n A3 60.10826 6 -108.2165\n R 48.82469 2 -93.64939\n 3 56.12112 3 -106.2422\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 26.73 8 0.0007864\n Test 2 4.165 4 0.3842\n Test 3 4.165 4 0.3842\n Test 5a 7.974 3 0.04655\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 229.65\n\n BMDL = 156.035\n\n BMDU = 417.569\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | A/G Ratio | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .014983919135108163,.03280013628629011,.020680692078115459,.029342751593028519,.034099546643330002 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 110 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: A/G Ratio | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 0 | 0 | Exponential-M4 | 8 | 1.11 | True | False | 5.133690e+01 | 2.698320e+01 | 1.214850e+02 | -999 | -111.925400 | 0.000786 | 0.384200 | 0.3842 | 0.8645 | 0.291100 | 2 | 1.612000e-01 | NaN | valid | NaN | NaN | NaN | True | AIC | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 1.347926 0.033505\n77.000000 5 1.277884 0.073343\n153.000000 5 1.232263 0.046243\n306.000000 5 1.175592 0.065612\n611.000000 5 1.171317 0.076249 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-v6s\_7qot.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:15 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha -5.80866 \n rho 0 Specified\n a 1.41532 \n b 0.00344767 \n c 0.788188 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha -5.79702 0.00085888\n a 1.35016 0.0235655\n b 0.00677691 0.00273569\n c 0.861099 0.0226097\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 1.348 0.03351\n 77 5 1.278 0.07334\n 153 5 1.232 0.04624\n 306 5 1.176 0.06561\n 611 5 1.171 0.07625\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 1.35 0.05511 -0.09056\n 77 1.274 0.05511 0.1612\n 153 1.229 0.05511 0.1278\n 306 1.186 0.05511 -0.4303\n 611 1.166 0.05511 0.2319\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 60.10826 6 -108.2165\n A2 62.1906 10 -104.3812\n A3 60.10826 6 -108.2165\n R 48.82469 2 -93.64939\n 4 59.96271 4 -111.9254\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 26.73 8 0.0007864\n Test 2 4.165 4 0.3842\n Test 3 4.165 4 0.3842\n Test 6a 0.2911 2 0.8645\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is greater than .1. Model 4 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 51.3369\n\n BMDL = 26.9832\n\n BMDU = 121.485\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | A/G Ratio | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .014983919135108163,.03280013628629011,.020680692078115459,.029342751593028519,.034099546643330002 | 2,0,1,2,2 | 2,2,2,2,2 | SD | day | NaN | 110 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: A/G Ratio | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 0 | 0 | Exponential-M5 | 9 | 1.11 | True | False | 6.404880e+01 | 2.754190e+01 | 1.455700e+02 | -999 | -110.106100 | 0.000786 | 0.384200 | 0.3842 | 0.7396 | 0.110500 | 1 | -1.243000e-01 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 1.347926 0.033505\n77.000000 5 1.277884 0.073343\n153.000000 5 1.232263 0.046243\n306.000000 5 1.175592 0.065612\n611.000000 5 1.171317 0.076249 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-\_9\_e0hy0.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:16 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha -5.80866 \n rho 0 Specified\n a 1.41532 \n b 0.00344767 \n c 0.788188 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha -5.80424 0.000852697\n a 1.34728 0.0246396\n b 0.00709815 0.0023433\n c 0.867271 0.0239882\n d 1.27236 0.685039\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 1.348 0.03351\n 77 5 1.278 0.07334\n 153 5 1.232 0.04624\n 306 5 1.176 0.06561\n 611 5 1.171 0.07625\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 1.347 0.05491 0.02627\n 77 1.281 0.05491 -0.1243\n 153 1.227 0.05491 0.2001\n 306 1.181 0.05491 -0.2073\n 611 1.169 0.05491 0.1052\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 60.10826 6 -108.2165\n A2 62.1906 10 -104.3812\n A3 60.10826 6 -108.2165\n R 48.82469 2 -93.64939\n 5 60.05304 5 -110.1061\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 26.73 8 0.0007864\n Test 2 4.165 4 0.3842\n Test 3 4.165 4 0.3842\n Test 7a 0.1105 1 0.7396\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is greater than .1. Model 5 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 64.0488\n\n BMDL = 27.5419\n\n BMDU = 145.57\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Albumin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .05830951894845305,.05830951894845305,.063245553203367527,.050990195135927799,.073484692283495301 | 2,0,0,0,1 | 2,2,2,2,2 | SD | day | NaN | 120 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Albumin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1 | 0 | Linear | 0 | 2.21 | True | False | 3.096080e+02 | 2.026710e+02 | 6.505970e+02 | -999 | -71.887892 | 0.123300 | 0.947400 | 0.9474 | 0.5645 | 2.038140 | 3 | -7.070000e-01 | NaN | valid | NaN | NaN | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 3.420000 0.130384\n77.000000 5 3.420000 0.130384\n153.000000 5 3.300000 0.141421\n306.000000 5 3.240000 0.114018\n611.000000 5 3.180000 0.164317 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-jdrpfavx.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-jdrpfavx.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:19 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.0188\n rho = 0 Specified\n beta\_0 = 3.40665\n beta\_1 = -0.000412586\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 4.1e-010 -2.9e-010\n\n beta\_0 4.1e-010 1 -0.73\n\n beta\_1 -2.9e-010 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.0163175 0.00461529 0.00727172 0.0253633\n beta\_0 3.40665 0.0372724 3.33359 3.4797\n beta\_1 -0.000412586 0.000118305 -0.000644459 -0.000180713\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 3.42 3.41 0.13 0.128 0.234\n 77 5 3.42 3.37 0.13 0.128 0.79\n 153 5 3.3 3.34 0.141 0.128 -0.762\n 306 5 3.24 3.28 0.114 0.128 -0.707\n 611 5 3.18 3.15 0.164 0.128 0.445\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 39.963017 6 -67.926034\n A2 40.328862 10 -60.657723\n A3 39.963017 6 -67.926034\n fitted 38.943946 3 -71.887892\n R 33.988636 2 -63.977273\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 12.6805 8 0.1233\n Test 2 0.731689 4 0.9474\n Test 3 0.731689 4 0.9474\n Test 4 2.03814 3 0.5645\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 309.608\n\n\n BMDL = 202.671\n\n\n BMDU = 650.597\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Albumin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .05830951894845305,.05830951894845305,.063245553203367527,.050990195135927799,.073484692283495301 | 2,0,0,0,1 | 2,2,2,2,2 | SD | day | NaN | 120 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Albumin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1 | 0 | Polynomial-2 | 1 | 2.21 | True | False | 3.096080e+02 | 2.026710e+02 | 6.505970e+02 | -999 | -71.887892 | 0.123300 | 0.947400 | 0.9474 | 0.5645 | 2.038140 | 3 | -7.070000e-01 | NaN | valid | NaN | NaN | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 3.420000 0.130384\n77.000000 5 3.420000 0.130384\n153.000000 5 3.300000 0.141421\n306.000000 5 3.240000 0.114018\n611.000000 5 3.180000 0.164317 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-axr9qa76.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-axr9qa76.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:19 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.0188\n rho = 0 Specified\n beta\_0 = 3.43943\n beta\_1 = -0.000868643\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -1.1e-007 1.1e-007\n\n beta\_0 -1.1e-007 1 -0.73\n\n beta\_1 1.1e-007 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.0163175 0.00461529 0.00727172 0.0253633\n beta\_0 3.40665 0.0372724 3.33359 3.4797\n beta\_1 -0.000412586 0.000118305 -0.000644459 -0.000180713\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 3.42 3.41 0.13 0.128 0.234\n 77 5 3.42 3.37 0.13 0.128 0.79\n 153 5 3.3 3.34 0.141 0.128 -0.762\n 306 5 3.24 3.28 0.114 0.128 -0.707\n 611 5 3.18 3.15 0.164 0.128 0.445\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 39.963017 6 -67.926034\n A2 40.328862 10 -60.657723\n A3 39.963017 6 -67.926034\n fitted 38.943946 3 -71.887892\n R 33.988636 2 -63.977273\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 12.6805 8 0.1233\n Test 2 0.731689 4 0.9474\n Test 3 0.731689 4 0.9474\n Test 4 2.03814 3 0.5645\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 309.608\n\n\n BMDL = 202.671\n\n\n BMDU = 650.597\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Albumin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .05830951894845305,.05830951894845305,.063245553203367527,.050990195135927799,.073484692283495301 | 2,0,0,0,1 | 2,2,2,2,2 | SD | day | NaN | 120 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Albumin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1 | 0 | Polynomial-3 | 2 | 2.21 | True | False | 3.096080e+02 | 2.026710e+02 | 6.505970e+02 | -999 | -71.887892 | 0.123300 | 0.947400 | 0.9474 | 0.5645 | 2.038140 | 3 | -7.070000e-01 | NaN | valid | NaN | NaN | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 3.420000 0.130384\n77.000000 5 3.420000 0.130384\n153.000000 5 3.300000 0.141421\n306.000000 5 3.240000 0.114018\n611.000000 5 3.180000 0.164317 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-h8xj31lk.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-h8xj31lk.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:19 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.0188\n rho = 0 Specified\n beta\_0 = 3.43177\n beta\_1 = -0.000573299\n beta\_2 = -7.85652e-007\n beta\_3 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -3.1e-009 -6.4e-011\n\n beta\_0 -3.1e-009 1 -0.73\n\n beta\_1 -6.4e-011 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.0163175 0.00461529 0.00727172 0.0253633\n beta\_0 3.40665 0.0372724 3.33359 3.4797\n beta\_1 -0.000412586 0.000118305 -0.000644459 -0.000180713\n beta\_2 -1.38483e-031 NA\n beta\_3 -1.13325e-034 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 3.42 3.41 0.13 0.128 0.234\n 77 5 3.42 3.37 0.13 0.128 0.79\n 153 5 3.3 3.34 0.141 0.128 -0.762\n 306 5 3.24 3.28 0.114 0.128 -0.707\n 611 5 3.18 3.15 0.164 0.128 0.445\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 39.963017 6 -67.926034\n A2 40.328862 10 -60.657723\n A3 39.963017 6 -67.926034\n fitted 38.943946 3 -71.887892\n R 33.988636 2 -63.977273\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 12.6805 8 0.1233\n Test 2 0.731689 4 0.9474\n Test 3 0.731689 4 0.9474\n Test 4 2.03814 3 0.5645\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 309.608\n\n\n BMDL = 202.671\n\n\n BMDU = 650.597\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Albumin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .05830951894845305,.05830951894845305,.063245553203367527,.050990195135927799,.073484692283495301 | 2,0,0,0,1 | 2,2,2,2,2 | SD | day | NaN | 120 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Albumin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1 | 0 | Polynomial-4 | 3 | 2.21 | True | False | 3.096080e+02 | 2.026710e+02 | 6.505970e+02 | -999 | -71.887892 | 0.123300 | 0.947400 | 0.9474 | 0.5645 | 2.038140 | 3 | -7.070000e-01 | NaN | valid | NaN | NaN | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 3.420000 0.130384\n77.000000 5 3.420000 0.130384\n153.000000 5 3.300000 0.141421\n306.000000 5 3.240000 0.114018\n611.000000 5 3.180000 0.164317 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-vpcbrwp1.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-vpcbrwp1.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:19 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.0188\n rho = 0 Specified\n beta\_0 = 3.42\n beta\_1 = 0\n beta\_2 = -2.99821e-005\n beta\_3 = 0\n beta\_4 = -9.74917e-011\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 2.2e-009 -2e-010\n\n beta\_0 2.2e-009 1 -0.73\n\n beta\_1 -2e-010 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.0163175 0.00461529 0.00727172 0.0253633\n beta\_0 3.40665 0.0372724 3.33359 3.4797\n beta\_1 -0.000412586 0.000118305 -0.000644459 -0.000180713\n beta\_2 -6.92417e-032 NA\n beta\_3 0 NA\n beta\_4 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 3.42 3.41 0.13 0.128 0.234\n 77 5 3.42 3.37 0.13 0.128 0.79\n 153 5 3.3 3.34 0.141 0.128 -0.762\n 306 5 3.24 3.28 0.114 0.128 -0.707\n 611 5 3.18 3.15 0.164 0.128 0.445\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 39.963017 6 -67.926034\n A2 40.328862 10 -60.657723\n A3 39.963017 6 -67.926034\n fitted 38.943946 3 -71.887892\n R 33.988636 2 -63.977273\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 12.6805 8 0.1233\n Test 2 0.731689 4 0.9474\n Test 3 0.731689 4 0.9474\n Test 4 2.03814 3 0.5645\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 309.608\n\n\n BMDL = 202.671\n\n\n BMDU = 650.597\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Albumin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .05830951894845305,.05830951894845305,.063245553203367527,.050990195135927799,.073484692283495301 | 2,0,0,0,1 | 2,2,2,2,2 | SD | day | NaN | 120 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Albumin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1 | 0 | Power | 4 | 2.19 | True | False | 3.096080e+02 | 2.026710e+02 | 6.505970e+02 | -999 | -71.887892 | 0.123300 | 0.947400 | 0.9474 | 0.5645 | 2.038140 | 3 | -7.070000e-01 | NaN | valid | NaN | NaN | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 3.420000 0.130384\n77.000000 5 3.420000 0.130384\n153.000000 5 3.300000 0.141421\n306.000000 5 3.240000 0.114018\n611.000000 5 3.180000 0.164317 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-ny1qurxc.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-ny1qurxc.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:19 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The power is restricted to be greater than or equal to 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.0188\n rho = 0 Specified\n control = 3.42\n slope = -151.142\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha control slope\n\n alpha 1 1.2e-010 2e-011\n\n control 1.2e-010 1 -0.73\n\n slope 2e-011 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.0163175 0.00461529 0.00727172 0.0253633\n control 3.40665 0.0372724 3.33359 3.4797\n slope -0.000412586 0.000118305 -0.000644459 -0.000180713\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 3.42 3.41 0.13 0.128 0.234\n 77 5 3.42 3.37 0.13 0.128 0.79\n 153 5 3.3 3.34 0.141 0.128 -0.762\n 306 5 3.24 3.28 0.114 0.128 -0.707\n 611 5 3.18 3.15 0.164 0.128 0.445\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 39.963017 6 -67.926034\n A2 40.328862 10 -60.657723\n A3 39.963017 6 -67.926034\n fitted 38.943946 3 -71.887892\n R 33.988636 2 -63.977273\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 12.6805 8 0.1233\n Test 2 0.731689 4 0.9474\n Test 3 0.731689 4 0.9474\n Test 4 2.03814 3 0.5645\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 309.608 \n\n\n BMDL = 202.671 \n\n\n BMDU = 650.597 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Albumin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .05830951894845305,.05830951894845305,.063245553203367527,.050990195135927799,.073484692283495301 | 2,0,0,0,1 | 2,2,2,2,2 | SD | day | NaN | 120 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Albumin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1 | 0 | Hill | 5 | 2.18 | True | False | 1.617570e+02 | 6.618560e+01 | 3.733210e+09 | -999 | -69.532787 | 0.123300 | 0.947400 | 0.9474 | 0.5306 | 0.393247 | 1 | -2.870000e-01 | NaN | valid | NaN | NaN | NaN | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 3.420000 0.130384\n77.000000 5 3.420000 0.130384\n153.000000 5 3.300000 0.141421\n306.000000 5 3.240000 0.114018\n611.000000 5 3.180000 0.164317 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-25oge5dx.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-25oge5dx.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:19 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n Power parameter restricted to be greater than 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.0188\n rho = 0 Specified\n intercept = 3.42\n v = -0.24\n n = 0.792481\n k = 153\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha intercept v n k\n\n alpha 1 -5.1e-007 8.8e-007 2.6e-007 -4.3e-007\n\n intercept -5.1e-007 1 -0.55 -0.25 -0.23\n\n v 8.8e-007 -0.55 1 0.8 -0.57\n\n n 2.6e-007 -0.25 0.8 1 -0.66\n\n k -4.3e-007 -0.23 -0.57 -0.66 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.0152785 0.00432141 0.00680867 0.0237483\n intercept 3.43007 0.0486137 3.33479 3.52535\n v -0.244335 0.106379 -0.452835 -0.0358356\n n 2.77507 3.37451 -3.83885 9.38898\n k 160.39 90.2988 -16.5922 337.373\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 3.42 3.43 0.13 0.124 -0.182\n 77 5 3.42 3.4 0.13 0.124 0.328\n 153 5 3.3 3.32 0.141 0.124 -0.287\n 306 5 3.24 3.22 0.114 0.124 0.351\n 611 5 3.18 3.19 0.164 0.124 -0.209\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 39.963017 6 -67.926034\n A2 40.328862 10 -60.657723\n A3 39.963017 6 -67.926034\n fitted 39.766394 5 -69.532787\n R 33.988636 2 -63.977273\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 12.6805 8 0.1233\n Test 2 0.731689 4 0.9474\n Test 3 0.731689 4 0.9474\n Test 4 0.393247 1 0.5306\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 161.757\n\n BMDL = 66.1856\n\n BMDU = 3.73321e+009\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Albumin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .05830951894845305,.05830951894845305,.063245553203367527,.050990195135927799,.073484692283495301 | 2,0,0,0,1 | 2,2,2,2,2 | SD | day | NaN | 120 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Albumin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1 | 0 | Exponential-M2 | 6 | 1.11 | True | False | 3.008780e+02 | 1.938560e+02 | 6.429730e+02 | -999 | -71.966240 | 0.123300 | 0.947400 | 0.9474 | 0.5808 | 1.960000 | 3 | -6.798000e-01 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 3.420000 0.130384\n77.000000 5 3.420000 0.130384\n153.000000 5 3.300000 0.141421\n306.000000 5 3.240000 0.114018\n611.000000 5 3.180000 0.164317 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-riock62m.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:19 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha -4.19704 \n rho 0 Specified\n a 3.21693 \n b 0.000125133 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha -4.11865 0.00460085\n a 3.40844 0.0376455\n b 0.000126752 3.63537e-005\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 3.42 0.1304\n 77 5 3.42 0.1304\n 153 5 3.3 0.1414\n 306 5 3.24 0.114\n 611 5 3.18 0.1643\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 3.408 0.1275 0.2027\n 77 3.375 0.1275 0.783\n 153 3.343 0.1275 -0.7535\n 306 3.279 0.1275 -0.6798\n 611 3.154 0.1275 0.4482\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 39.96302 6 -67.92603\n A2 40.32886 10 -60.65772\n A3 39.96302 6 -67.92603\n R 33.98864 2 -63.97727\n 2 38.98312 3 -71.96624\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 12.68 8 0.1233\n Test 2 0.7317 4 0.9474\n Test 3 0.7317 4 0.9474\n Test 4 1.96 3 0.5808\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is greater than .1. Model 2 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 300.878\n\n BMDL = 193.856\n\n BMDU = 642.973\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Albumin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .05830951894845305,.05830951894845305,.063245553203367527,.050990195135927799,.073484692283495301 | 2,0,0,0,1 | 2,2,2,2,2 | SD | day | NaN | 120 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Albumin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1 | 0 | Exponential-M3 | 7 | 1.11 | True | False | 3.008780e+02 | 1.938560e+02 | 6.429730e+02 | -999 | -71.966240 | 0.123300 | 0.947400 | 0.9474 | 0.5808 | 1.960000 | 3 | -6.798000e-01 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 3.420000 0.130384\n77.000000 5 3.420000 0.130384\n153.000000 5 3.300000 0.141421\n306.000000 5 3.240000 0.114018\n611.000000 5 3.180000 0.164317 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-x0yo9ja5.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:19 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha -4.19704 \n rho 0 Specified\n a 3.21693 \n b 0.000125133 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha -4.11865 0.00460085\n a 3.40844 0.0377706\n b 0.000126752 3.65883e-005\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 3.42 0.1304\n 77 5 3.42 0.1304\n 153 5 3.3 0.1414\n 306 5 3.24 0.114\n 611 5 3.18 0.1643\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 3.408 0.1275 0.2027\n 77 3.375 0.1275 0.783\n 153 3.343 0.1275 -0.7535\n 306 3.279 0.1275 -0.6798\n 611 3.154 0.1275 0.4482\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 39.96302 6 -67.92603\n A2 40.32886 10 -60.65772\n A3 39.96302 6 -67.92603\n R 33.98864 2 -63.97727\n 3 38.98312 3 -71.96624\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 12.68 8 0.1233\n Test 2 0.7317 4 0.9474\n Test 3 0.7317 4 0.9474\n Test 5a 1.96 3 0.5808\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is greater than .1. Model 3 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 300.878\n\n BMDL = 193.856\n\n BMDU = 642.973\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Albumin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .05830951894845305,.05830951894845305,.063245553203367527,.050990195135927799,.073484692283495301 | 2,0,0,0,1 | 2,2,2,2,2 | SD | day | NaN | 120 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Albumin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1 | 0 | Exponential-M4 | 8 | 1.11 | True | False | 1.675910e+02 | 6.321530e+01 | 5.386320e+02 | -999 | -70.905680 | 0.123300 | 0.947400 | 0.9474 | 0.6004 | 1.020000 | 2 | -4.057000e-01 | NaN | valid | NaN | NaN | NaN | True | BMDL | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 3.420000 0.130384\n77.000000 5 3.420000 0.130384\n153.000000 5 3.300000 0.141421\n306.000000 5 3.240000 0.114018\n611.000000 5 3.180000 0.164317 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-3l\_twgvj.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:19 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha -4.19704 \n rho 0 Specified\n a 3.591 \n b 0.0024995 \n c 0.843378 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha -4.15623 0.00443117\n a 3.43933 0.0501098\n b 0.00303733 0.00305791\n c 0.908772 0.0407013\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 3.42 0.1304\n 77 5 3.42 0.1304\n 153 5 3.3 0.1414\n 306 5 3.24 0.114\n 611 5 3.18 0.1643\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 3.439 0.1252 -0.3454\n 77 3.374 0.1252 0.8236\n 153 3.323 0.1252 -0.4057\n 306 3.249 0.1252 -0.1686\n 611 3.175 0.1252 0.09613\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 39.96302 6 -67.92603\n A2 40.32886 10 -60.65772\n A3 39.96302 6 -67.92603\n R 33.98864 2 -63.97727\n 4 39.45284 4 -70.90568\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 12.68 8 0.1233\n Test 2 0.7317 4 0.9474\n Test 3 0.7317 4 0.9474\n Test 6a 1.02 2 0.6004\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is greater than .1. Model 4 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 167.591\n\n BMDL = 63.2153\n\n BMDU = 538.632\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Albumin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .05830951894845305,.05830951894845305,.063245553203367527,.050990195135927799,.073484692283495301 | 2,0,0,0,1 | 2,2,2,2,2 | SD | day | NaN | 120 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Albumin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1 | 0 | Exponential-M5 | 9 | 1.11 | True | False | 1.754820e+02 | 6.789370e+01 | 6.110000e+06 | -999 | -69.323140 | 0.123300 | 0.947400 | 0.9474 | 0.4375 | 0.602900 | 1 | -4.698000e-01 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 3.420000 0.130384\n77.000000 5 3.420000 0.130384\n153.000000 5 3.300000 0.141421\n306.000000 5 3.240000 0.114018\n611.000000 5 3.180000 0.164317 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-0v9yuko2.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:19 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha -4.19704 \n rho 0 Specified\n a 3.591 \n b 0.0024995 \n c 0.843378 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha -4.17293 0.00435779\n a 3.43113 0.0503279\n b 0.0046151 0.00248348\n c 0.928147 0.0232111\n d 1.69047 1.21396\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 3.42 0.1304\n 77 5 3.42 0.1304\n 153 5 3.3 0.1414\n 306 5 3.24 0.114\n 611 5 3.18 0.1643\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 3.431 0.1241 -0.2005\n 77 3.392 0.1241 0.5086\n 153 3.326 0.1241 -0.4698\n 306 3.226 0.1241 0.2583\n 611 3.185 0.1241 -0.0966\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 39.96302 6 -67.92603\n A2 40.32886 10 -60.65772\n A3 39.96302 6 -67.92603\n R 33.98864 2 -63.97727\n 5 39.66157 5 -69.32314\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 12.68 8 0.1233\n Test 2 0.7317 4 0.9474\n Test 3 0.7317 4 0.9474\n Test 7a 0.6029 1 0.4375\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is greater than .1. Model 5 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 175.482\n\n BMDL = 67.8937\n\n BMDU = 6.11e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 0 | Linear | 0 | 2.21 | True | False | 6.842230e+02 | 3.529920e+02 | 2.775170e+03 | -999 | 159.007298 | 0.017150 | 0.009598 | 0.1665 | 0.05625 | 7.551660 | 3 | 6.580000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0563 < 0.1)\nBMD/high dose ratio is greater than threshold (1.12 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (1.58 > 1.5) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581\n611.000000 5 18.880000 9.130005 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-1z9\_tk55.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-1z9\_tk55.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:24 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 5.29328\n rho = 0\n beta\_0 = 32.9286\n beta\_1 = -0.0242746\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.054 -0.072\n\n rho -1 1 -0.054 0.072\n\n beta\_0 0.054 -0.054 1 -0.82\n\n beta\_1 -0.072 0.072 -0.82 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -2.61297 4.73119 -11.8859 6.65999\n rho 2.32679 1.43582 -0.487373 5.14096\n beta\_0 32.5391 4.1068 24.4899 40.5883\n beta\_1 -0.0227472 0.00976903 -0.0418942 -0.0036003\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 34.9 32.5 9.85 15.6 0.345\n 77 5 33.5 30.8 24.8 14.6 0.409\n 153 5 23.2 29.1 4.99 13.6 -0.967\n 306 5 26.4 25.6 13.2 11.8 0.149\n 611 5 18.9 18.6 9.13 8.14 0.0658\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -75.876689 6 163.753378\n A2 -69.191141 10 158.382282\n A3 -71.727820 7 157.455641\n fitted -75.503649 4 159.007298\n R -78.491679 2 160.983358\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 18.6011 8 0.01715\n Test 2 13.3711 4 0.009598\n Test 3 5.07336 3 0.1665\n Test 4 7.55166 3 0.05625\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 684.223\n\n\n BMDL = 352.992\n\n\n BMDU = 2775.17\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 0 | Polynomial-2 | 1 | 2.21 | True | False | 6.842240e+02 | 3.529920e+02 | 2.775170e+03 | -999 | 159.007298 | 0.017150 | 0.009598 | 0.1665 | 0.05625 | 7.551660 | 3 | 6.580000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0563 < 0.1)\nBMD/high dose ratio is greater than threshold (1.12 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (1.58 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581\n611.000000 5 18.880000 9.130005 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-qd634yc0.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-qd634yc0.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:24 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 5.29328\n rho = 0\n beta\_0 = 34.5489\n beta\_1 = -0.0468132\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.054 -0.072\n\n rho -1 1 -0.054 0.072\n\n beta\_0 0.054 -0.054 1 -0.82\n\n beta\_1 -0.072 0.072 -0.82 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -2.613 4.7312 -11.886 6.65997\n rho 2.3268 1.43583 -0.487369 5.14097\n beta\_0 32.5391 4.1068 24.4899 40.5883\n beta\_1 -0.0227472 0.00976903 -0.0418942 -0.00360027\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 34.9 32.5 9.85 15.6 0.345\n 77 5 33.5 30.8 24.8 14.6 0.409\n 153 5 23.2 29.1 4.99 13.6 -0.967\n 306 5 26.4 25.6 13.2 11.8 0.149\n 611 5 18.9 18.6 9.13 8.14 0.0658\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -75.876689 6 163.753378\n A2 -69.191141 10 158.382282\n A3 -71.727820 7 157.455641\n fitted -75.503649 4 159.007298\n R -78.491679 2 160.983358\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 18.6011 8 0.01715\n Test 2 13.3711 4 0.009598\n Test 3 5.07336 3 0.1665\n Test 4 7.55166 3 0.05625\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 684.224\n\n\n BMDL = 352.992\n\n\n BMDU = 2775.17\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 0 | Polynomial-3 | 2 | 2.21 | True | False | 6.842240e+02 | 3.529920e+02 | 2.775170e+03 | -999 | 159.007298 | 0.017150 | 0.009598 | 0.1665 | 0.05625 | 7.551660 | 3 | 6.580000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0563 < 0.1)\nBMD/high dose ratio is greater than threshold (1.12 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (1.58 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581\n611.000000 5 18.880000 9.130005 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-1ixd50u2.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-1ixd50u2.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:24 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 5.29328\n rho = 0\n beta\_0 = 36.162\n beta\_1 = -0.109022\n beta\_2 = 0\n beta\_3 = -3.62331e-007\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.054 -0.072\n\n rho -1 1 -0.054 0.072\n\n beta\_0 0.054 -0.054 1 -0.82\n\n beta\_1 -0.072 0.072 -0.82 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -2.613 4.73119 -11.886 6.65997\n rho 2.3268 1.43583 -0.487369 5.14097\n beta\_0 32.5391 4.1068 24.4899 40.5883\n beta\_1 -0.0227472 0.00976903 -0.0418942 -0.00360027\n beta\_2 0 NA\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 34.9 32.5 9.85 15.6 0.345\n 77 5 33.5 30.8 24.8 14.6 0.409\n 153 5 23.2 29.1 4.99 13.6 -0.967\n 306 5 26.4 25.6 13.2 11.8 0.149\n 611 5 18.9 18.6 9.13 8.14 0.0658\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -75.876689 6 163.753378\n A2 -69.191141 10 158.382282\n A3 -71.727820 7 157.455641\n fitted -75.503649 4 159.007298\n R -78.491679 2 160.983358\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 18.6011 8 0.01715\n Test 2 13.3711 4 0.009598\n Test 3 5.07336 3 0.1665\n Test 4 7.55166 3 0.05625\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 684.224\n\n\n BMDL = 352.992\n\n\n BMDU = 2775.17\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 0 | Polynomial-4 | 3 | 2.21 | True | False | 6.842260e+02 | 3.529920e+02 | 2.775170e+03 | -999 | 159.007298 | 0.017150 | 0.009598 | 0.1665 | 0.05625 | 7.551660 | 3 | 6.580000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0563 < 0.1)\nBMD/high dose ratio is greater than threshold (1.12 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (1.58 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581\n611.000000 5 18.880000 9.130005 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-s9odfciq.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-s9odfciq.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:24 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 5.29328\n rho = 0\n beta\_0 = 34.94\n beta\_1 = 0\n beta\_2 = -0.00267628\n beta\_3 = 0\n beta\_4 = -1.01175e-008\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.054 -0.072\n\n rho -1 1 -0.054 0.072\n\n beta\_0 0.054 -0.054 1 -0.82\n\n beta\_1 -0.072 0.072 -0.82 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -2.61301 4.7312 -11.886 6.65998\n rho 2.3268 1.43583 -0.48737 5.14098\n beta\_0 32.5391 4.1068 24.4899 40.5883\n beta\_1 -0.0227472 0.00976903 -0.0418941 -0.00360022\n beta\_2 0 NA\n beta\_3 0 NA\n beta\_4 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 34.9 32.5 9.85 15.6 0.345\n 77 5 33.5 30.8 24.8 14.6 0.409\n 153 5 23.2 29.1 4.99 13.6 -0.967\n 306 5 26.4 25.6 13.2 11.8 0.149\n 611 5 18.9 18.6 9.13 8.14 0.0658\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -75.876689 6 163.753378\n A2 -69.191141 10 158.382282\n A3 -71.727820 7 157.455641\n fitted -75.503649 4 159.007298\n R -78.491679 2 160.983358\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 18.6011 8 0.01715\n Test 2 13.3711 4 0.009598\n Test 3 5.07336 3 0.1665\n Test 4 7.55166 3 0.05625\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 684.226\n\n\n BMDL = 352.992\n\n\n BMDU = 2775.17\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 0 | Power | 4 | 2.19 | True | False | 6.842240e+02 | 3.529920e+02 | 2.775170e+03 | -999 | 159.007298 | 0.017150 | 0.009598 | 0.1665 | 0.05625 | 7.551660 | 3 | 6.580000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0563 < 0.1)\nBMD/high dose ratio is greater than threshold (1.12 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (1.58 > 1.5) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581\n611.000000 5 18.880000 9.130005 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-0kam5fpz.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-0kam5fpz.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:24 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n The power is restricted to be greater than or equal to 1\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 5.29328\n rho = 0\n control = 18.88\n slope = 87.5924\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho control slope\n\n lalpha 1 -1 0.4 -0.6\n\n rho -1 1 -0.43 0.61\n\n control 0.4 -0.43 1 -0.82\n\n slope -0.6 0.61 -0.82 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -2.613 6.04841 -14.4677 9.24166\n rho 2.3268 1.83896 -1.27749 5.93109\n control 32.5391 4.12218 24.4598 40.6184\n slope -0.0227472 0.00980372 -0.0419622 -0.00353226\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 34.9 32.5 9.85 15.6 0.345\n 77 5 33.5 30.8 24.8 14.6 0.409\n 153 5 23.2 29.1 4.99 13.6 -0.967\n 306 5 26.4 25.6 13.2 11.8 0.149\n 611 5 18.9 18.6 9.13 8.14 0.0658\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -75.876689 6 163.753378\n A2 -69.191141 10 158.382282\n A3 -71.727820 7 157.455641\n fitted -75.503649 4 159.007298\n R -78.491679 2 160.983358\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 18.6011 8 0.01715\n Test 2 13.3711 4 0.009598\n Test 3 5.07336 3 0.1665\n Test 4 7.55166 3 0.05625\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 684.224 \n\n\n BMDL = 352.992 \n\n\n BMDU = 2775.17 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 0 | Hill | 5 | 2.18 | True | False | -9.990000e+02 | -9.990000e+02 | -9.990000e+02 | -999 | 158.112912 | 0.017150 | 0.009598 | 0.1665 | 0.09743 | 4.657270 | 2 | -9.990000e+02 | BMR value is not in the range of the mean function | failure | Warning(s): BMR value is not in the range of the mean function | Residual of Interest does not exist\nGoodness of fit p-value is less than threshold (0.0974 < 0.1)\nRatio of modeled to actual stdev. at control is greater than threshold (1.72 > 1.5) | BMD does not exist\nBMDL does not exist | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581\n611.000000 5 18.880000 9.130005 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-5bwbn6ay.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-5bwbn6ay.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:24 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n Power parameter restricted to be greater than 1\n The variance is to be modeled as Var(i) = exp(lalpha + rho \* ln(mean(i)))\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 5.29328\n rho = 0\n intercept = 34.94\n v = -16.06\n n = 3.30831\n k = 125.33\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -n \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho intercept v k\n\n lalpha 1 -1 0.55 -0.68 0.014\n\n rho -1 1 -0.58 0.69 -0.014\n\n intercept 0.55 -0.58 1 -0.91 -0.036\n\n v -0.68 0.69 -0.91 1 0.023\n\n k 0.014 -0.014 -0.036 0.023 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -4.95434 6.5234 -17.74 7.83128\n rho 3.00366 1.99106 -0.898744 6.90607\n intercept 34.2155 5.35631 23.7173 44.7136\n v -11.4223 5.86167 -22.911 0.0663189\n n 18 NA\n k 107.198 63.903 -18.0499 232.445\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 34.9 34.2 9.85 16.9 0.0958\n 77 5 33.5 34.2 24.8 16.9 -0.0961\n 153 5 23.2 22.8 4.99 9.2 0.0846\n 306 5 26.4 22.8 13.2 9.19 0.868\n 611 5 18.9 22.8 9.13 9.19 -0.952\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -75.876689 6 163.753378\n A2 -69.191141 10 158.382282\n A3 -71.727820 7 157.455641\n fitted -74.056456 5 158.112912\n R -78.491679 2 160.983358\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 18.6011 8 0.01715\n Test 2 13.3711 4 0.009598\n Test 3 5.07336 3 0.1665\n Test 4 4.65727 2 0.09743\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n\n\nBMD computation failed\nBMR value is not in the range of the mean function | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 0 | Exponential-M2 | 6 | 1.11 | True | False | 6.854330e+02 | 2.623300e+02 | 4.045290e+03 | -999 | 158.931100 | 0.017150 | 0.009598 | 0.1665 | 0.05819 | 7.475000 | 3 | 4.383000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0582 < 0.1)\nBMD/high dose ratio is greater than threshold (1.12 > 1.0) | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581\n611.000000 5 18.880000 9.130005 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-1oeprd14.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:24 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha -3.42231 \n rho 2.49164 \n a 21.5064 \n b 0.000936893 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha -2.36644 5.93586\n rho 2.25114 1.80365\n a 33.2788 4.57147\n b 0.000941823 0.000421942\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 34.94 9.852\n 77 5 33.46 24.83\n 153 5 23.16 4.993\n 306 5 26.36 13.15\n 611 5 18.88 9.13\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 33.28 15.83 0.2347\n 77 30.95 14.59 0.3846\n 153 28.81 13.46 -0.9392\n 306 24.95 11.44 0.2762\n 611 18.72 8.282 0.04383\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -75.87669 6 163.7534\n A2 -69.19114 10 158.3823\n A3 -71.72782 7 157.4556\n R -78.49168 2 160.9834\n 2 -75.46554 4 158.9311\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 18.6 8 0.01715\n Test 2 13.37 4 0.009598\n Test 3 5.073 3 0.1665\n Test 4 7.475 3 0.05819\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 685.433\n\n BMDL = 262.33\n\n BMDU = 4045.29\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 0 | Exponential-M3 | 7 | 1.11 | True | False | 6.878290e+02 | 2.624220e+02 | 4.039890e+03 | -999 | 160.928900 | 0.017150 | 0.009598 | 0.1665 | 0.02383 | 7.473000 | 2 | 5.065000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0238 < 0.1)\nBMD/high dose ratio is greater than threshold (1.13 > 1.0) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581\n611.000000 5 18.880000 9.130005 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-sdlp7gxb.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:23 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha -3.42231 \n rho 2.49164 \n a 21.5064 \n b 0.000936893 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha -2.41883 6.26714\n rho 2.26696 1.90313\n a 33.1149 7.71695\n b 0.00095349 0.00329745\n d 1.0345 2.22105\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 34.94 9.852\n 77 5 33.46 24.83\n 153 5 23.16 4.993\n 306 5 26.36 13.15\n 611 5 18.88 9.13\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 33.11 15.76 0.2589\n 77 30.97 14.61 0.3817\n 153 28.89 13.5 -0.9487\n 306 25.04 11.48 0.2576\n 611 18.69 8.245 0.05065\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -75.87669 6 163.7534\n A2 -69.19114 10 158.3823\n A3 -71.72782 7 157.4556\n R -78.49168 2 160.9834\n 3 -75.46445 5 160.9289\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 18.6 8 0.01715\n Test 2 13.37 4 0.009598\n Test 3 5.073 3 0.1665\n Test 5a 7.473 2 0.02383\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 687.829\n\n BMDL = 262.422\n\n BMDU = 4039.89\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 0 | Exponential-M4 | 8 | 1.11 | True | False | 6.915650e+02 | 1.114130e+02 | 6.110000e+06 | -999 | 160.922100 | 0.017150 | 0.009598 | 0.1665 | 0.02392 | 7.466000 | 2 | 1.671000e-02 | NaN | warning | BMD/BMDL ratio is greater than threshold (6.21 > 5.0) | Goodness of fit p-value is less than threshold (0.0239 < 0.1)\nBMD/high dose ratio is greater than threshold (1.13 > 1.0) | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581\n611.000000 5 18.880000 9.130005 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-fuxyoor5.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:24 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha -3.42231 \n rho 2.49164 \n a 36.687 \n b 0.00182981 \n c 0.257312 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha -2.28749 5.98511\n rho 2.22713 1.81839\n a 33.5973 5.78761\n b 0.00137769 0.00459294\n c 0.22694 1.60101\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 34.94 9.852\n 77 5 33.46 24.83\n 153 5 23.16 4.993\n 306 5 26.36 13.15\n 611 5 18.88 9.13\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 33.6 15.96 0.1882\n 77 30.98 14.58 0.3799\n 153 28.66 13.37 -0.9202\n 306 24.66 11.31 0.3355\n 611 18.82 8.367 0.01671\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -75.87669 6 163.7534\n A2 -69.19114 10 158.3823\n A3 -71.72782 7 157.4556\n R -78.49168 2 160.9834\n 4 -75.46104 5 160.9221\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 18.6 8 0.01715\n Test 2 13.37 4 0.009598\n Test 3 5.073 3 0.1665\n Test 6a 7.466 2 0.02392\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is less than .1. Model 4 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 691.565\n\n BMDL = 111.413\n\n BMDU = 6.11e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 0 | Exponential-M5 | 9 | 1.11 | True | False | 8.289480e+02 | 7.833380e+01 | 6.110000e+06 | -999 | 162.861000 | 0.017150 | 0.009598 | 0.1665 | 0.006503 | 7.405000 | 1 | -2.679000e-02 | NaN | warning | BMD/BMDL ratio is greater than threshold (10.6 > 5.0) | Goodness of fit p-value is less than threshold (0.0065 < 0.1)\nBMD/high dose ratio is greater than threshold (1.36 > 1.0) | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581\n611.000000 5 18.880000 9.130005 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-nx26p8x1.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:24 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha -3.42231 \n rho 2.49164 \n a 36.687 \n b 0.00182981 \n c 0.257312 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha -2.48345 6.04171\n rho 2.2857 1.83574\n a 33.2124 5.7321\n b 0.0026097 0.00430755\n c 0.491651 0.519982\n d 1.32008 1.32721\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 34.94 9.852\n 77 5 33.46 24.83\n 153 5 23.16 4.993\n 306 5 26.36 13.15\n 611 5 18.88 9.13\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 33.21 15.82 0.2441\n 77 31.3 14.79 0.3266\n 153 28.87 13.48 -0.9465\n 306 24.36 11.1 0.4029\n 611 18.98 8.349 -0.02679\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -75.87669 6 163.7534\n A2 -69.19114 10 158.3823\n A3 -71.72782 7 157.4556\n R -78.49168 2 160.9834\n 5 -75.43051 6 162.861\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 18.6 8 0.01715\n Test 2 13.37 4 0.009598\n Test 3 5.073 3 0.1665\n Test 7a 7.405 1 0.006503\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is less than .1. Model 5 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 828.948\n\n BMDL = 78.3338\n\n BMDU = 6.11e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 1 | Linear | 0 | 2.21 | True | False | 5.442750e+02 | 1.793790e+02 | -9.990000e+02 | -999 | 132.952034 | 0.027580 | 0.008355 | 0.3572 | 0.005219 | 10.510900 | 2 | 3.410000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00522 < 0.1)\nBMD/high dose ratio is greater than threshold (1.78 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (1.57 > 1.5) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 4 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-zorue9y\_.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-zorue9y\_.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:27 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 5.42893\n rho = 0\n beta\_0 = 33.7115\n beta\_1 = -0.0315781\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.19 -0.25\n\n rho -1 1 -0.19 0.25\n\n beta\_0 0.19 -0.19 1 -0.81\n\n beta\_1 -0.25 0.25 -0.81 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -0.913216 10.3291 -21.158 19.3315\n rho 1.82436 3.05711 -4.16747 7.81619\n beta\_0 33.2799 5.21092 23.0667 43.4931\n beta\_1 -0.0284698 0.0267535 -0.0809058 0.0239662\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 34.9 33.3 9.85 15.5 0.24\n 77 5 33.5 31.1 24.8 14.6 0.364\n 153 5 23.2 28.9 4.99 13.6 -0.945\n 306 5 26.4 24.6 13.2 11.7 0.341\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -62.057820 5 134.115641\n A2 -56.191169 8 128.382337\n A3 -57.220579 6 126.441159\n fitted -62.476017 4 132.952034\n R -63.286312 2 130.572625\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.1903 6 0.02758\n Test 2 11.7333 3 0.008355\n Test 3 2.05882 2 0.3572\n Test 4 10.5109 2 0.005219\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 544.275\n\n\n BMDL = 179.379\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 1 | Polynomial-2 | 1 | 2.21 | True | False | 5.442730e+02 | 1.793790e+02 | -9.990000e+02 | -999 | 132.952034 | 0.027580 | 0.008355 | 0.3572 | 0.005219 | 10.510900 | 2 | 3.410000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00522 < 0.1)\nBMD/high dose ratio is greater than threshold (1.78 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (1.57 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 4 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-4zzsx4tu.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-4zzsx4tu.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:27 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 5.42893\n rho = 0\n beta\_0 = 36.3052\n beta\_1 = -0.101672\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.19 -0.25\n\n rho -1 1 -0.19 0.25\n\n beta\_0 0.19 -0.19 1 -0.81\n\n beta\_1 -0.25 0.25 -0.81 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -0.91319 10.3291 -21.1579 19.3315\n rho 1.82435 3.0571 -4.16746 7.81617\n beta\_0 33.2799 5.21092 23.0667 43.4931\n beta\_1 -0.0284699 0.0267536 -0.0809059 0.0239661\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 34.9 33.3 9.85 15.5 0.24\n 77 5 33.5 31.1 24.8 14.6 0.364\n 153 5 23.2 28.9 4.99 13.6 -0.945\n 306 5 26.4 24.6 13.2 11.7 0.341\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -62.057820 5 134.115641\n A2 -56.191169 8 128.382337\n A3 -57.220579 6 126.441159\n fitted -62.476017 4 132.952034\n R -63.286312 2 130.572625\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.1903 6 0.02758\n Test 2 11.7333 3 0.008355\n Test 3 2.05882 2 0.3572\n Test 4 10.5109 2 0.005219\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 544.273\n\n\n BMDL = 179.379\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 1 | Polynomial-3 | 2 | 2.21 | True | False | 5.442750e+02 | 1.793790e+02 | -9.990000e+02 | -999 | 132.952034 | 0.027580 | 0.008355 | 0.3572 | 0.005219 | 10.510900 | 2 | 3.410000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00522 < 0.1)\nBMD/high dose ratio is greater than threshold (1.78 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (1.57 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 4 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-frw064l6.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-frw064l6.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:27 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 5.42893\n rho = 0\n beta\_0 = 34.94\n beta\_1 = 0\n beta\_2 = -0.00184501\n beta\_3 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.19 -0.25\n\n rho -1 1 -0.19 0.25\n\n beta\_0 0.19 -0.19 1 -0.81\n\n beta\_1 -0.25 0.25 -0.81 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -0.913237 10.3292 -21.158 19.3315\n rho 1.82437 3.05711 -4.16747 7.8162\n beta\_0 33.2799 5.21093 23.0667 43.4931\n beta\_1 -0.0284698 0.0267536 -0.0809059 0.0239662\n beta\_2 0 NA\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 34.9 33.3 9.85 15.5 0.24\n 77 5 33.5 31.1 24.8 14.6 0.364\n 153 5 23.2 28.9 4.99 13.6 -0.945\n 306 5 26.4 24.6 13.2 11.7 0.341\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -62.057820 5 134.115641\n A2 -56.191169 8 128.382337\n A3 -57.220579 6 126.441159\n fitted -62.476017 4 132.952034\n R -63.286312 2 130.572625\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.1903 6 0.02758\n Test 2 11.7333 3 0.008355\n Test 3 2.05882 2 0.3572\n Test 4 10.5109 2 0.005219\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 544.275\n\n\n BMDL = 179.379\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 1 | Polynomial-4 | 3 | 2.21 | True | False | 5.442750e+02 | 1.793790e+02 | -9.990000e+02 | -999 | 132.952034 | 0.027580 | 0.008355 | 0.3572 | 0.005219 | 10.510900 | 2 | 3.410000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00522 < 0.1)\nBMD/high dose ratio is greater than threshold (1.78 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (1.57 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 4 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-9oqlltku.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-9oqlltku.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:27 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 5.42893\n rho = 0\n beta\_0 = -7.06409\n beta\_1 = 0\n beta\_2 = -0.00141919\n beta\_3 = 0\n beta\_4 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.19 -0.25\n\n rho -1 1 -0.19 0.25\n\n beta\_0 0.19 -0.19 1 -0.81\n\n beta\_1 -0.25 0.25 -0.81 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -0.913222 10.3292 -21.158 19.3315\n rho 1.82436 3.05712 -4.16747 7.8162\n beta\_0 33.2799 5.21092 23.0667 43.4931\n beta\_1 -0.0284698 0.0267535 -0.0809058 0.0239662\n beta\_2 0 NA\n beta\_3 0 NA\n beta\_4 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 34.9 33.3 9.85 15.5 0.24\n 77 5 33.5 31.1 24.8 14.6 0.364\n 153 5 23.2 28.9 4.99 13.6 -0.945\n 306 5 26.4 24.6 13.2 11.7 0.341\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -62.057820 5 134.115641\n A2 -56.191169 8 128.382337\n A3 -57.220579 6 126.441159\n fitted -62.476017 4 132.952034\n R -63.286312 2 130.572625\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.1903 6 0.02758\n Test 2 11.7333 3 0.008355\n Test 3 2.05882 2 0.3572\n Test 4 10.5109 2 0.005219\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 544.275\n\n\n BMDL = 179.379\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 1 | Power | 4 | 2.19 | True | False | 5.442750e+02 | 1.793790e+02 | -9.990000e+02 | -999 | 132.952034 | 0.027580 | 0.008355 | 0.3572 | 0.005219 | 10.510900 | 2 | 3.410000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00522 < 0.1)\nBMD/high dose ratio is greater than threshold (1.78 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (1.57 > 1.5) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-zg3douzj.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-zg3douzj.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:27 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n The power is restricted to be greater than or equal to 1\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 5.42893\n rho = 0\n control = 23.16\n slope = 408.443\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho control slope\n\n lalpha 1 -1 0.45 -0.62\n\n rho -1 1 -0.46 0.62\n\n control 0.45 -0.46 1 -0.81\n\n slope -0.62 0.62 -0.81 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -0.913218 12.7589 -25.9203 24.0939\n rho 1.82436 3.77655 -5.57755 9.22627\n control 33.2799 5.19966 23.0888 43.4711\n slope -0.0284698 0.0265556 -0.0805179 0.0235783\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 34.9 33.3 9.85 15.5 0.24\n 77 5 33.5 31.1 24.8 14.6 0.364\n 153 5 23.2 28.9 4.99 13.6 -0.945\n 306 5 26.4 24.6 13.2 11.7 0.341\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -62.057820 5 134.115641\n A2 -56.191169 8 128.382337\n A3 -57.220579 6 126.441159\n fitted -62.476017 4 132.952034\n R -63.286312 2 130.572625\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.1903 6 0.02758\n Test 2 11.7333 3 0.008355\n Test 3 2.05882 2 0.3572\n Test 4 10.5109 2 0.005219\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 544.275 \n\n\n BMDL = 179.379 \n\nWarning: optimum may not have been found. Bad completion code in Optimization routine.\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 1 | Hill | 5 | 2.18 | True | False | -9.990000e+02 | -9.990000e+02 | -9.990000e+02 | -999 | 130.617808 | 0.027580 | 0.008355 | 0.3572 | 0.01294 | 6.176650 | 1 | -9.990000e+02 | BMR value is not in the range of the mean function | failure | Warning(s): BMR value is not in the range of the mean function | Residual of Interest does not exist\nGoodness of fit p-value is less than threshold (0.0129 < 0.1)\nRatio of modeled to actual stdev. at control is greater than threshold (1.72 > 1.5) | BMD does not exist\nBMDL does not exist | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-yurfql\_x.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-yurfql\_x.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:27 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n Power parameter restricted to be greater than 1\n The variance is to be modeled as Var(i) = exp(lalpha + rho \* ln(mean(i)))\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 5.42893\n rho = 0\n intercept = 34.94\n v = -11.78\n n = 3.23209\n k = 109.54\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -n \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho intercept v k\n\n lalpha 1 -1 0.59 -0.75 -0.00084\n\n rho -1 1 -0.62 0.76 0.00091\n\n intercept 0.59 -0.62 1 -0.88 -0.039\n\n v -0.75 0.76 -0.88 1 0.031\n\n k -0.00084 0.00091 -0.039 0.031 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -8.01483 10.198 -28.0025 11.9728\n rho 3.87031 3.04709 -2.10189 9.8425\n intercept 34.21 5.35845 23.7076 44.7124\n v -9.45451 6.0807 -21.3725 2.46345\n n 18 NA\n k 106.512 57.5322 -6.24885 219.273\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 34.9 34.2 9.85 16.9 0.0965\n 77 5 33.5 34.2 24.8 16.9 -0.0956\n 153 5 23.2 24.8 4.99 9.06 -0.397\n 306 5 26.4 24.8 13.2 9.05 0.397\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -62.057820 5 134.115641\n A2 -56.191169 8 128.382337\n A3 -57.220579 6 126.441159\n fitted -60.308904 5 130.617808\n R -63.286312 2 130.572625\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.1903 6 0.02758\n Test 2 11.7333 3 0.008355\n Test 3 2.05882 2 0.3572\n Test 4 6.17665 1 0.01294\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n\n\nBMD computation failed\nBMR value is not in the range of the mean function | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 1 | Exponential-M2 | 6 | 1.11 | True | False | 5.792450e+02 | 1.375960e+02 | 3.060000e+06 | -999 | 132.902300 | 0.027580 | 0.008355 | 0.3572 | 0.00535 | 10.460000 | 2 | 3.729000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00535 < 0.1)\nBMD/high dose ratio is greater than threshold (1.89 > 1.0) | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 -1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-s3jfya4s.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:27 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha -10.1964 \n rho 4.46308 \n a 25.244 \n b 0.00105206 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha -0.342806 11.8885\n rho 1.65496 3.51809\n a 33.7384 5.47071\n b 0.00106098 0.000954069\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 34.94 9.852\n 77 5 33.46 24.83\n 153 5 23.16 4.993\n 306 5 26.36 13.15\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 33.74 15.49 0.1735\n 77 31.09 14.48 0.3658\n 153 28.68 13.54 -0.9119\n 306 24.39 11.84 0.3729\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -62.05782 5 134.1156\n A2 -56.19117 8 128.3823\n A3 -57.22058 6 126.4412\n R -63.28631 2 130.5726\n 2 -62.45115 4 132.9023\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 14.19 6 0.02758\n Test 2 11.73 3 0.008355\n Test 3 2.059 2 0.3572\n Test 4 10.46 2 0.00535\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 579.245\n\n BMDL = 137.596\n\n BMDU = 3.06e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 1 | Exponential-M3 | 7 | 1.11 | True | False | 5.782900e+02 | 1.376090e+02 | -9.990000e+02 | -999 | 134.901800 | 0.027580 | 0.008355 | 0.3572 | 0.001219 | 10.460000 | 1 | 3.718000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00122 < 0.1)\nBMD/high dose ratio is greater than threshold (1.89 > 1.0) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 -1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-ckw72xjs.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:27 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha -10.1964 \n rho 4.46308 \n a 25.244 \n b 0.00105206 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha -0.491932 NA\n rho 1.69907 NA\n a 33.6429 NA\n b 0.00108121 NA\n d 1.0265 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 34.94 9.852\n 77 5 33.46 24.83\n 153 5 23.16 4.993\n 306 5 26.36 13.15\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 33.64 15.5 0.1871\n 77 31.12 14.51 0.3607\n 153 28.73 13.56 -0.9194\n 306 24.4 11.8 0.3718\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -62.05782 5 134.1156\n A2 -56.19117 8 128.3823\n A3 -57.22058 6 126.4412\n R -63.28631 2 130.5726\n 3 -62.45091 5 134.9018\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 14.19 6 0.02758\n Test 2 11.73 3 0.008355\n Test 3 2.059 2 0.3572\n Test 5a 10.46 1 0.001219\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 578.29\n\n BMDL = 137.609\n\n BMDU = Bad\_Completion\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 1 | Exponential-M4 | 8 | 1.11 | True | False | -9.990000e+02 | 0.000000e+00 | 0.000000e+00 | -999 | 134.808900 | 0.027580 | 0.008355 | 0.3572 | 0.001282 | 10.370000 | 1 | -9.990000e+02 | NaN | failure | NaN | Residual of Interest does not exist\nGoodness of fit p-value is less than threshold (0.00128 < 0.1) | BMD does not exist | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 -1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-a1mi0glb.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:27 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha -10.1964 \n rho 4.46308 \n a 36.687 \n b 0.00641759 \n c 0.601225 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha 0.976087 11.5974\n rho 1.26353 3.43269\n a 35.0358 6.99974\n b 0.00502274 0.0126595\n c 0.613719 0.419586\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 34.94 9.852\n 77 5 33.46 24.83\n 153 5 23.16 4.993\n 306 5 26.36 13.15\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 35.04 15.41 -0.01391\n 77 30.7 14.17 0.4363\n 153 27.78 13.31 -0.7761\n 306 24.41 12.26 0.3551\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -62.05782 5 134.1156\n A2 -56.19117 8 128.3823\n A3 -57.22058 6 126.4412\n R -63.28631 2 130.5726\n 4 -62.40447 5 134.8089\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 14.19 6 0.02758\n Test 2 11.73 3 0.008355\n Test 3 2.059 2 0.3572\n Test 6a 10.37 1 0.001282\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is less than .1. Model 4 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = Not\_Computed\n\n BMDL = 0\n\n BMDU = 0\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 1 | Exponential-M5 | 9 | 1.11 | True | False | -9.990000e+02 | 0.000000e+00 | 0.000000e+00 | -999 | 132.596800 | 0.027580 | 0.008355 | 0.3572 | -999 | 6.156000 | 0 | -9.990000e+02 | NaN | failure | NaN | Residual of Interest does not exist\nZero degrees of freedom; saturated model | BMD does not exist | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 -1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795\n306.000000 5 26.360000 13.154581 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-2g41q7h9.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:27 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha -10.1964 \n rho 4.46308 \n a 36.687 \n b 0.00641759 \n c 0.601225 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha -8.03936 10.1944\n rho 3.87727 3.04618\n a 34.2003 5.34811\n b 0.00753824 0.011487\n c 0.723969 0.140735\n d 18 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 34.94 9.852\n 77 5 33.46 24.83\n 153 5 23.16 4.993\n 306 5 26.36 13.15\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 34.2 16.91 0.0978\n 77 34.2 16.91 -0.09781\n 153 24.76 9.042 -0.3957\n 306 24.76 9.042 0.3957\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -62.05782 5 134.1156\n A2 -56.19117 8 128.3823\n A3 -57.22058 6 126.4412\n R -63.28631 2 130.5726\n 5 -60.2984 6 132.5968\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 14.19 6 0.02758\n Test 2 11.73 3 0.008355\n Test 3 2.059 2 0.3572\n Test 7a 6.156 0 N/A\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n Degrees of freedom for Test 7a are less than or equal to 0.\n The Chi-Square test for fit is not valid.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = Not\_Computed\n\n BMDL = 0\n\n BMDU = 0\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 2 | Linear | 0 | 2.21 | True | False | 2.094080e+02 | 9.480790e+01 | 3.045390e+03 | -999 | 101.185780 | 0.009188 | 0.003160 | 0.2587 | 0.002447 | 9.179900 | 1 | 7.240000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00245 < 0.1)\nBMD/high dose ratio is greater than threshold (1.37 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (2.44 > 1.5) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 3 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-qucz38fy.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-qucz38fy.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:30 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 5.50611\n rho = 0\n beta\_0 = 36.4131\n beta\_1 = -0.0768668\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.84 -0.9\n\n rho -1 1 -0.84 0.9\n\n beta\_0 0.84 -0.84 1 -0.97\n\n beta\_1 -0.9 0.9 -0.97 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -9.21611 25.0636 -58.3399 39.9077\n rho 4.20828 7.27175 -10.0441 18.4606\n beta\_0 40.4348 13.3305 14.3074 66.5622\n beta\_1 -0.114444 0.113159 -0.336231 0.107343\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 34.9 40.4 9.85 24 -0.513\n 77 5 33.5 31.6 24.8 14.3 0.288\n 153 5 23.2 22.9 4.99 7.26 0.0724\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -47.122241 4 102.244482\n A2 -41.365177 6 94.730355\n A3 -42.002938 5 94.005876\n fitted -46.592890 4 101.185780\n R -48.100824 2 100.201649\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 13.4713 4 0.009188\n Test 2 11.5141 2 0.00316\n Test 3 1.27552 1 0.2587\n Test 4 9.1799 1 0.002447\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 209.408\n\n\n BMDL = 94.8079\n\n\n BMDU = 3045.39\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 2 | Polynomial-2 | 1 | 2.21 | True | False | 1.900540e+02 | 1.328370e+02 | 4.059020e+02 | -999 | 97.136206 | 0.009188 | 0.003160 | 0.2587 | 0.02351 | 5.130330 | 1 | 5.530000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0235 < 0.1)\nBMD/high dose ratio is greater than threshold (1.24 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (2.14 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 3 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-nbnu8\_\_b.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-nbnu8\_\_b.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:30 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 5.50611\n rho = 0\n beta\_0 = 34.94\n beta\_1 = 0\n beta\_2 = -0.000760167\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_1 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_2\n\n lalpha 1 -1 0.32 -0.39\n\n rho -1 1 -0.32 0.38\n\n beta\_0 0.32 -0.32 1 -0.94\n\n beta\_2 -0.39 0.38 -0.94 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -15.9788 8.22289 -32.0954 0.137778\n rho 6.12757 2.40249 1.41878 10.8364\n beta\_0 36.6863 6.22936 24.477 48.8957\n beta\_1 0 NA\n beta\_2 -0.000583177 0.000278451 -0.00112893 -3.74232e-005\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 34.9 36.7 9.85 21.1 -0.185\n 77 5 33.5 33.2 24.8 15.6 0.0333\n 153 5 23.2 23 4.99 5.06 0.0553\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -47.122241 4 102.244482\n A2 -41.365177 6 94.730355\n A3 -42.002938 5 94.005876\n fitted -44.568103 4 97.136206\n R -48.100824 2 100.201649\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 13.4713 4 0.009188\n Test 2 11.5141 2 0.00316\n Test 3 1.27552 1 0.2587\n Test 4 5.13033 1 0.02351\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 190.054\n\n\n BMDL = 132.837\n\n\n BMDU = 405.902\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 2 | Polynomial-3 | 2 | 2.21 | True | False | -9.999000e+03 | 6.881940e+01 | -9.990000e+02 | -999 | 102.201649 | 0.009188 | 0.003160 | 0.2587 | 0.002248 | 12.195800 | 2 | -9.990000e+02 | THE MODEL HAS PROBABLY NOT CONVERGED!!!\nTHIS USUALLY MEANS THE MODEL HAS NOT CONVERGED!\nBMD = 100\*(maximum dose) | warning | Warning(s): THE MODEL HAS PROBABLY NOT CONVERGED!!!; THIS USUALLY MEANS THE MODEL HAS NOT CONVERGED!; BMD = 100\*(maximum dose) | Residual of Interest does not exist\nGoodness of fit p-value is less than threshold (0.00225 < 0.1)\nRatio of modeled to actual stdev. at control is greater than threshold (1.52 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 3 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-fjn1t9qp.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-fjn1t9qp.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:30 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 5.50611\n rho = 0\n beta\_0 = -4836.93\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = -0.000201225\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_1 -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0\n\n lalpha NA NA NA \n\n rho NA NA NA \n\n beta\_0 NA NA NA \n\n\nNA - This parameter's variance has been estimated as zero or less.\nTHE MODEL HAS PROBABLY NOT CONVERGED!!!\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 329.141 NA NA NA\n rho -94.702 NA NA NA\n beta\_0 30.52 NA NA NA\n beta\_1 0 NA\n beta\_2 0 NA\n beta\_3 0 NA\n\nAt least some variance estimates are negative.\nTHIS USUALLY MEANS THE MODEL HAS NOT CONVERGED!\nTry again from another starting point.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 34.9 30.5 9.85 15 0.66\n 77 5 33.5 30.5 24.8 15 0.439\n 153 5 23.2 30.5 4.99 15 -1.1\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -47.122241 4 102.244482\n A2 -41.365177 6 94.730355\n A3 -42.002938 5 94.005876\n fitted -48.100824 3 102.201649\n R -48.100824 2 100.201649\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 13.4713 4 0.009188\n Test 2 11.5141 2 0.00316\n Test 3 1.27552 1 0.2587\n Test 4 12.1958 2 0.002248\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n\nBMD computation failed for BMR = 15.5399\nSetting BMD = 100\*(maximum dose) \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = -9999\n\n\n BMDL = 68.8194\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 2 | Polynomial-4 | 3 | 2.21 | True | False | 1.705700e+02 | 1.437070e+02 | 2.747740e+02 | -999 | 95.058069 | 0.009188 | 0.003160 | 0.2587 | 0.08063 | 3.052190 | 1 | 1.250000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0806 < 0.1)\nBMD/high dose ratio is greater than threshold (1.11 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (1.81 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 3 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-2d57hf4\_.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-2d57hf4\_.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:31 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 5.50611\n rho = 0\n beta\_0 = 40.8658\n beta\_1 = 0\n beta\_2 = -0.0285215\n beta\_3 = 0\n beta\_4 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_1 -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_4\n\n lalpha 1 -1 0.072 -0.084\n\n rho -1 1 -0.071 0.084\n\n beta\_0 0.072 -0.071 1 -0.94\n\n beta\_4 -0.084 0.084 -0.94 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -18.1169 6.94854 -31.7358 -4.49805\n rho 6.73387 2.03843 2.73863 10.7291\n beta\_0 34.6686 5.45893 23.9693 45.3679\n beta\_1 -1.26809e-023 NA\n beta\_2 -1.4837e-024 NA\n beta\_3 -0 NA\n beta\_4 -2.10483e-008 1.05195e-008 -4.16661e-008 -4.30558e-010\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 34.9 34.7 9.85 17.8 0.0341\n 77 5 33.5 33.9 24.8 16.6 -0.0633\n 153 5 23.2 23.1 4.99 4.56 0.0125\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -47.122241 4 102.244482\n A2 -41.365177 6 94.730355\n A3 -42.002938 5 94.005876\n fitted -43.529034 4 95.058069\n R -48.100824 2 100.201649\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 13.4713 4 0.009188\n Test 2 11.5141 2 0.00316\n Test 3 1.27552 1 0.2587\n Test 4 3.05219 1 0.08063\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 170.57\n\n\n BMDL = 143.707\n\n\n BMDU = 274.774\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 2 | Power | 4 | 2.19 | True | False | 1.566680e+02 | 1.458930e+02 | 2.641480e+02 | -999 | 94.524402 | 0.009188 | 0.003160 | 0.2587 | 0.1125 | 2.518530 | 1 | 8.040000e-07 | NaN | warning | NaN | BMD/high dose ratio is greater than threshold (1.02 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (1.72 > 1.5) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-c96ezt\_h.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-c96ezt\_h.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:31 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n The power is restricted to be greater than or equal to 1\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 5.50611\n rho = 0\n control = 34.94\n slope = -0.0769935\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho control slope\n\n lalpha 1 -1 0.71 -0.82\n\n rho -1 1 -0.74 0.84\n\n control 0.71 -0.74 1 -0.94\n\n slope -0.82 0.84 -0.94 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -18.4767 12.1871 -42.3629 5.40955\n rho 6.83214 3.70745 -0.434332 14.0986\n control 34.2 5.34797 23.7182 44.6819\n slope -5.23027e-039 2.70453e-039 -1.05311e-038 7.05046e-041\n power 18 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 34.9 34.2 9.85 16.9 0.0978\n 77 5 33.5 34.2 24.8 16.9 -0.0978\n 153 5 23.2 23.2 4.99 4.47 8.04e-007\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -47.122241 4 102.244482\n A2 -41.365177 6 94.730355\n A3 -42.002938 5 94.005876\n fitted -43.262201 4 94.524402\n R -48.100824 2 100.201649\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 13.4713 4 0.009188\n Test 2 11.5141 2 0.00316\n Test 3 1.27552 1 0.2587\n Test 4 2.51853 1 0.1125\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 156.668 \n\n\n BMDL = 145.893 \n\n\n BMDU = 264.148 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 2 | Hill | 5 | 2.18 | True | False | -9.990000e+02 | -9.990000e+02 | -9.990000e+02 | -999 | 130.617808 | 0.027580 | 0.008355 | 0.3572 | 0.01294 | 6.176650 | 1 | -9.990000e+02 | BMR value is not in the range of the mean function | failure | Warning(s): BMR value is not in the range of the mean function | Residual of Interest does not exist\nGoodness of fit p-value is less than threshold (0.0129 < 0.1)\nRatio of modeled to actual stdev. at control is greater than threshold (1.72 > 1.5) | BMD does not exist\nBMDL does not exist | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-yurfql\_x.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-yurfql\_x.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:27 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n Power parameter restricted to be greater than 1\n The variance is to be modeled as Var(i) = exp(lalpha + rho \* ln(mean(i)))\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 5.42893\n rho = 0\n intercept = 34.94\n v = -11.78\n n = 3.23209\n k = 109.54\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -n \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho intercept v k\n\n lalpha 1 -1 0.59 -0.75 -0.00084\n\n rho -1 1 -0.62 0.76 0.00091\n\n intercept 0.59 -0.62 1 -0.88 -0.039\n\n v -0.75 0.76 -0.88 1 0.031\n\n k -0.00084 0.00091 -0.039 0.031 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -8.01483 10.198 -28.0025 11.9728\n rho 3.87031 3.04709 -2.10189 9.8425\n intercept 34.21 5.35845 23.7076 44.7124\n v -9.45451 6.0807 -21.3725 2.46345\n n 18 NA\n k 106.512 57.5322 -6.24885 219.273\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 34.9 34.2 9.85 16.9 0.0965\n 77 5 33.5 34.2 24.8 16.9 -0.0956\n 153 5 23.2 24.8 4.99 9.06 -0.397\n 306 5 26.4 24.8 13.2 9.05 0.397\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -62.057820 5 134.115641\n A2 -56.191169 8 128.382337\n A3 -57.220579 6 126.441159\n fitted -60.308904 5 130.617808\n R -63.286312 2 130.572625\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 14.1903 6 0.02758\n Test 2 11.7333 3 0.008355\n Test 3 2.05882 2 0.3572\n Test 4 6.17665 1 0.01294\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n\n\nBMD computation failed\nBMR value is not in the range of the mean function | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 2 | Exponential-M2 | 6 | 1.11 | True | False | 2.582320e+02 | 7.262000e+01 | 1.530000e+06 | -999 | 102.227800 | 0.009188 | 0.003160 | 0.2587 | 0.001388 | 10.220000 | 1 | -2.390000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00139 < 0.1)\nBMD/high dose ratio is greater than threshold (1.69 > 1.0) | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 -1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-39mtvsgq.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:30 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha -13.6899 \n rho 5.41672 \n a 24.4454 \n b 0.00268296 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha -5.13512 15.2844\n rho 3.05822 4.49164\n a 37.5496 12.8272\n b 0.00286227 0.00362327\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 34.94 9.852\n 77 5 33.46 24.83\n 153 5 23.16 4.993\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 37.55 19.62 -0.2974\n 77 30.12 14.01 0.5329\n 153 24.23 10.04 -0.239\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -47.12224 4 102.2445\n A2 -41.36518 6 94.73035\n A3 -42.00294 5 94.00588\n R -48.10082 2 100.2016\n 2 -47.11391 4 102.2278\n\n\n Additive constant for all log-likelihoods = -13.78. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 13.47 4 0.009188\n Test 2 11.51 2 0.00316\n Test 3 1.276 1 0.2587\n Test 4 10.22 1 0.001388\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 258.232\n\n BMDL = 72.62\n\n BMDU = 1.53e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 2 | Exponential-M3 | 7 | 1.11 | True | False | 1.578320e+02 | 1.444850e+02 | 3.125860e+02 | -999 | 96.524410 | 0.009188 | 0.003160 | 0.2587 | -999 | 2.519000 | 0 | 1.324000e-06 | NaN | warning | NaN | Zero degrees of freedom; saturated model\nBMD/high dose ratio is greater than threshold (1.03 > 1.0) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 -1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-2d668124.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:30 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha -13.6899 \n rho 5.41672 \n a 24.4454 \n b 0.00268296 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha -18.4767 12.1871\n rho 6.83215 3.70747\n a 34.2 5.34798\n b 0.00620265 0.000157863\n d 18 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 34.94 9.852\n 77 5 33.46 24.83\n 153 5 23.16 4.993\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 34.2 16.91 0.09784\n 77 34.2 16.91 -0.09784\n 153 23.16 4.466 1.324e-006\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -47.12224 4 102.2445\n A2 -41.36518 6 94.73035\n A3 -42.00294 5 94.00588\n R -48.10082 2 100.2016\n 3 -43.2622 5 96.52441\n\n\n Additive constant for all log-likelihoods = -13.78. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 13.47 4 0.009188\n Test 2 11.51 2 0.00316\n Test 3 1.276 1 0.2587\n Test 5a 2.519 0 N/A\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n Degrees of freedom for Test 5a are less than or equal to 0.\n The Chi-Square test for fit is not valid.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 157.832\n\n BMDL = 144.485\n\n BMDU = 312.586\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 2 | Exponential-M4 | 8 | 1.11 | True | False | 2.582330e+02 | 1.248040e+00 | 1.530000e+06 | -999 | 102.227800 | 0.009188 | 0.003160 | 0.2587 | 0.001388 | 10.220000 | 1 | -2.390000e-01 | NaN | warning | BMD/BMDL ratio is greater than threshold (2.07e+02 > 5.0) | Goodness of fit p-value is less than threshold (0.00139 < 0.1)\nBMD/BMDL ratio is greater than threshold (2.07e+02 > 20.0)\nBMD/high dose ratio is greater than threshold (1.69 > 1.0) | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 -1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-kln87rtr.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:30 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha -13.6899 \n rho 5.41672 \n a 36.687 \n b 0.00264265 \n c 0.000631286 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha -5.1351 15.1127\n rho 3.05821 4.43641\n a 37.5496 8.03752\n b 0.00286226 0.00201301\n c 0 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 34.94 9.852\n 77 5 33.46 24.83\n 153 5 23.16 4.993\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 37.55 19.62 -0.2974\n 77 30.12 14.01 0.5329\n 153 24.23 10.04 -0.239\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -47.12224 4 102.2445\n A2 -41.36518 6 94.73035\n A3 -42.00294 5 94.00588\n R -48.10082 2 100.2016\n 4 -47.11391 4 102.2278\n\n\n Additive constant for all log-likelihoods = -13.78. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 13.47 4 0.009188\n Test 2 11.51 2 0.00316\n Test 3 1.276 1 0.2587\n Test 6a 10.22 1 0.001388\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is less than .1. Model 4 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 258.233\n\n BMDL = 1.24804\n\n BMDU = 1.53e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Bile salts/acids | umol/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 4.405859734489967,11.104845789113867,2.2328457179124581,5.8829074444529548,4.0830625760573396 | 1,0,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 250 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Bile salts/acids | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 2 | 2 | Exponential-M5 | 9 | 1.11 | True | False | -9.990000e+02 | 0.000000e+00 | 0.000000e+00 | -999 | 132.596800 | 0.027580 | 0.008355 | 0.3572 | -999 | 6.156000 | 0 | -9.990000e+02 | NaN | failure | NaN | Residual of Interest does not exist\nZero degrees of freedom; saturated model | BMD does not exist | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 -1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 34.940000 9.851802\n77.000000 5 33.460000 24.831190\n153.000000 5 23.160000 4.992795 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-2g41q7h9.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:27 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha -10.1964 \n rho 4.46308 \n a 36.687 \n b 0.00641759 \n c 0.601225 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha -8.03936 10.1944\n rho 3.87727 3.04618\n a 34.2003 5.34811\n b 0.00753824 0.011487\n c 0.723969 0.140735\n d 18 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 34.94 9.852\n 77 5 33.46 24.83\n 153 5 23.16 4.993\n 306 5 26.36 13.15\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 34.2 16.91 0.0978\n 77 34.2 16.91 -0.09781\n 153 24.76 9.042 -0.3957\n 306 24.76 9.042 0.3957\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -62.05782 5 134.1156\n A2 -56.19117 8 128.3823\n A3 -57.22058 6 126.4412\n R -63.28631 2 130.5726\n 5 -60.2984 6 132.5968\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 14.19 6 0.02758\n Test 2 11.73 3 0.008355\n Test 3 2.059 2 0.3572\n Test 7a 6.156 0 N/A\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n Degrees of freedom for Test 7a are less than or equal to 0.\n The Chi-Square test for fit is not valid.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = Not\_Computed\n\n BMDL = 0\n\n BMDU = 0\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 0 | Linear | 0 | 2.21 | True | False | 3.248090e+02 | 2.097740e+02 | 7.140430e+02 | -999 | 161.039879 | 0.005198 | 0.652200 | 0.6522 | 0.01661 | 10.242800 | 3 | -4.740000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0166 < 0.1) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708\n611.000000 5 149.000000 8.660254 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-708gp\_rm.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-708gp\_rm.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:34 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 150.66\n rho = 0 Specified\n beta\_0 = 124.163\n beta\_1 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 3.4e-007 -1.8e-007\n\n beta\_0 3.4e-007 1 -0.73\n\n beta\_1 -1.8e-007 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 181.561 51.3533 80.9109 282.212\n beta\_0 124.163 3.93163 116.458 131.869\n beta\_1 0.0414843 0.0124792 0.0170255 0.0659432\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 113 124 11.3 13.5 -1.82\n 77 5 141 127 17 13.5 2.2\n 153 5 132 131 11.5 13.5 0.181\n 306 5 134 137 11.3 13.5 -0.474\n 611 5 149 150 8.66 13.5 -0.0847\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -72.398526 6 156.797051\n A2 -71.169721 10 162.339442\n A3 -72.398526 6 156.797051\n fitted -77.519939 3 161.039879\n R -82.095601 2 168.191202\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 21.8518 8 0.005198\n Test 2 2.45761 4 0.6522\n Test 3 2.45761 4 0.6522\n Test 4 10.2428 3 0.01661\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 324.809\n\n\n BMDL = 209.774\n\n\n BMDU = 714.043\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 0 | Polynomial-2 | 1 | 2.21 | True | False | 3.248090e+02 | 2.097740e+02 | 7.140430e+02 | -999 | 161.039879 | 0.005198 | 0.652200 | 0.6522 | 0.01661 | 10.242800 | 3 | -4.740000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0166 < 0.1) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708\n611.000000 5 149.000000 8.660254 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-avv0umyc.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-avv0umyc.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:34 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 150.66\n rho = 0 Specified\n beta\_0 = 121.825\n beta\_1 = 0\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -1.8e-008 -6.6e-008\n\n beta\_0 -1.8e-008 1 -0.73\n\n beta\_1 -6.6e-008 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 181.562 51.3534 80.9108 282.212\n beta\_0 124.163 3.93163 116.458 131.869\n beta\_1 0.0414844 0.0124792 0.0170255 0.0659432\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 113 124 11.3 13.5 -1.82\n 77 5 141 127 17 13.5 2.2\n 153 5 132 131 11.5 13.5 0.181\n 306 5 134 137 11.3 13.5 -0.474\n 611 5 149 150 8.66 13.5 -0.0847\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -72.398526 6 156.797051\n A2 -71.169721 10 162.339442\n A3 -72.398526 6 156.797051\n fitted -77.519939 3 161.039879\n R -82.095601 2 168.191202\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 21.8518 8 0.005198\n Test 2 2.45761 4 0.6522\n Test 3 2.45761 4 0.6522\n Test 4 10.2428 3 0.01661\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 324.809\n\n\n BMDL = 209.774\n\n\n BMDU = 714.043\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 0 | Polynomial-3 | 2 | 2.21 | True | False | 3.248090e+02 | 2.097740e+02 | 7.140430e+02 | -999 | 161.039879 | 0.005198 | 0.652200 | 0.6522 | 0.01661 | 10.242800 | 3 | -4.740000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0166 < 0.1) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708\n611.000000 5 149.000000 8.660254 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-a99dfmby.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-a99dfmby.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:34 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 150.66\n rho = 0 Specified\n beta\_0 = 115.77\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -3.5e-008 6e-008\n\n beta\_0 -3.5e-008 1 -0.73\n\n beta\_1 6e-008 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 181.562 51.3534 80.9109 282.212\n beta\_0 124.163 3.93163 116.458 131.869\n beta\_1 0.0414844 0.0124792 0.0170255 0.0659432\n beta\_2 0 NA\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 113 124 11.3 13.5 -1.82\n 77 5 141 127 17 13.5 2.2\n 153 5 132 131 11.5 13.5 0.181\n 306 5 134 137 11.3 13.5 -0.474\n 611 5 149 150 8.66 13.5 -0.0847\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -72.398526 6 156.797051\n A2 -71.169721 10 162.339442\n A3 -72.398526 6 156.797051\n fitted -77.519939 3 161.039879\n R -82.095601 2 168.191202\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 21.8518 8 0.005198\n Test 2 2.45761 4 0.6522\n Test 3 2.45761 4 0.6522\n Test 4 10.2428 3 0.01661\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 324.809\n\n\n BMDL = 209.774\n\n\n BMDU = 714.043\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 0 | Polynomial-4 | 3 | 2.21 | True | False | 3.248090e+02 | 2.097740e+02 | 7.140430e+02 | -999 | 161.039879 | 0.005198 | 0.652200 | 0.6522 | 0.01661 | 10.242800 | 3 | -4.740000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0166 < 0.1) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708\n611.000000 5 149.000000 8.660254 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-bsh8dswf.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-bsh8dswf.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:34 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 150.66\n rho = 0 Specified\n beta\_0 = 113.2\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = 0\n beta\_4 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 1.9e-009 -6.3e-009\n\n beta\_0 1.9e-009 1 -0.73\n\n beta\_1 -6.3e-009 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 181.562 51.3534 80.9108 282.212\n beta\_0 124.163 3.93163 116.458 131.869\n beta\_1 0.0414844 0.0124792 0.0170255 0.0659432\n beta\_2 0 NA\n beta\_3 0 NA\n beta\_4 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 113 124 11.3 13.5 -1.82\n 77 5 141 127 17 13.5 2.2\n 153 5 132 131 11.5 13.5 0.181\n 306 5 134 137 11.3 13.5 -0.474\n 611 5 149 150 8.66 13.5 -0.0847\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -72.398526 6 156.797051\n A2 -71.169721 10 162.339442\n A3 -72.398526 6 156.797051\n fitted -77.519939 3 161.039879\n R -82.095601 2 168.191202\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 21.8518 8 0.005198\n Test 2 2.45761 4 0.6522\n Test 3 2.45761 4 0.6522\n Test 4 10.2428 3 0.01661\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 324.809\n\n\n BMDL = 209.774\n\n\n BMDU = 714.043\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 0 | Power | 4 | 2.19 | True | False | 3.248090e+02 | 2.097740e+02 | 7.140430e+02 | -999 | 161.039879 | 0.005198 | 0.652200 | 0.6522 | 0.01661 | 10.242800 | 3 | -4.740000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0166 < 0.1) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708\n611.000000 5 149.000000 8.660254 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-\_dtmwvkq.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-\_dtmwvkq.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:34 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The power is restricted to be greater than or equal to 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 150.66\n rho = 0 Specified\n control = 113.2\n slope = 12.0149\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha control slope\n\n alpha 1 1.1e-009 -5.5e-011\n\n control 1.1e-009 1 -0.73\n\n slope -5.5e-011 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 181.562 51.3534 80.9108 282.212\n control 124.163 3.93163 116.458 131.869\n slope 0.0414844 0.0124792 0.0170255 0.0659432\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 113 124 11.3 13.5 -1.82\n 77 5 141 127 17 13.5 2.2\n 153 5 132 131 11.5 13.5 0.181\n 306 5 134 137 11.3 13.5 -0.474\n 611 5 149 150 8.66 13.5 -0.0847\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -72.398526 6 156.797051\n A2 -71.169721 10 162.339442\n A3 -72.398526 6 156.797051\n fitted -77.519939 3 161.039879\n R -82.095601 2 168.191202\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 21.8518 8 0.005198\n Test 2 2.45761 4 0.6522\n Test 3 2.45761 4 0.6522\n Test 4 10.2428 3 0.01661\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 324.809 \n\n\n BMDL = 209.774 \n\n\n BMDU = 714.043 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 0 | Hill | 5 | 2.18 | True | False | 1.669730e+01 | 9.303490e-05 | 1.923160e+02 | -999 | 159.067007 | 0.005198 | 0.652200 | 0.6522 | 0.0435 | 6.269960 | 2 | -2.110000e-02 | NaN | warning | BMD/BMDL ratio is greater than threshold (1.79e+05 > 5.0)\nMinimum dose/BMD ratio is greater than threshold (4.61 > 3.0) | Goodness of fit p-value is less than threshold (0.0435 < 0.1)\nBMD/BMDL ratio is greater than threshold (1.79e+05 > 20.0) | NaN | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708\n611.000000 5 149.000000 8.660254 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-i5hcflpw.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-i5hcflpw.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:34 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n Power parameter restricted to be greater than 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 150.66\n rho = 0 Specified\n intercept = 113.2\n v = 35.8\n n = 0.148587\n k = 103.697\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -n \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha intercept v k\n\n alpha 1 -1.7e-006 8.6e-007 1.4e-006\n\n intercept -1.7e-006 1 -0.6 0.2\n\n v 8.6e-007 -0.6 1 0.58\n\n k 1.4e-006 0.2 0.58 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 154.885 43.808 69.0225 240.747\n intercept 113.317 5.61008 102.322 124.313\n v 28.6401 8.43103 12.1156 45.1646\n n 1 NA\n k 21.7279 46.1643 -68.7524 112.208\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 113 113 11.3 12.4 -0.0211\n 77 5 141 136 17 12.4 0.889\n 153 5 132 138 11.5 12.4 -1.22\n 306 5 134 140 11.3 12.4 -1.09\n 611 5 149 141 8.66 12.4 1.44\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -72.398526 6 156.797051\n A2 -71.169721 10 162.339442\n A3 -72.398526 6 156.797051\n fitted -75.533503 4 159.067007\n R -82.095601 2 168.191202\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 21.8518 8 0.005198\n Test 2 2.45761 4 0.6522\n Test 3 2.45761 4 0.6522\n Test 4 6.26996 2 0.0435\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 16.6973\n\n BMDL = 9.30349e-005\n\n BMDU = 192.316\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 0 | Exponential-M2 | 6 | 1.11 | True | False | 3.440570e+02 | 2.310890e+02 | 7.244710e+02 | -999 | 161.162800 | 0.005198 | 0.652200 | 0.6522 | 0.0157 | 10.370000 | 3 | -4.127000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0157 < 0.1) | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708\n611.000000 5 149.000000 8.660254 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-bj6jnfqm.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:34 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha 4.79188 \n rho 0 Specified\n a 123.875 \n b 0.0003141 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha 5.20651 51.6065\n a 124.549 3.80637\n b 0.000299267 8.87801e-005\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 113.2 11.34\n 77 5 140.6 16.98\n 153 5 131.6 11.55\n 306 5 134 11.31\n 611 5 149 8.66\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 124.5 13.51 -1.879\n 77 127.5 13.51 2.176\n 153 130.4 13.51 0.2013\n 306 136.5 13.51 -0.4127\n 611 149.5 13.51 -0.08906\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -72.39853 6 156.7971\n A2 -71.16972 10 162.3394\n A3 -72.39853 6 156.7971\n R -82.0956 2 168.1912\n 2 -77.58141 3 161.1628\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 21.85 8 0.005198\n Test 2 2.458 4 0.6522\n Test 3 2.458 4 0.6522\n Test 4 10.37 3 0.0157\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 344.057\n\n BMDL = 231.089\n\n BMDU = 724.471\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 0 | Exponential-M3 | 7 | 1.11 | True | False | 3.440570e+02 | 2.310890e+02 | 7.244710e+02 | -999 | 161.162800 | 0.005198 | 0.652200 | 0.6522 | 0.0157 | 10.370000 | 3 | -4.127000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0157 < 0.1) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708\n611.000000 5 149.000000 8.660254 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-41rs8mfe.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:34 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha 4.79188 \n rho 0 Specified\n a 123.875 \n b 0.0003141 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha 5.20651 51.6065\n a 124.549 3.80637\n b 0.000299267 8.87801e-005\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 113.2 11.34\n 77 5 140.6 16.98\n 153 5 131.6 11.55\n 306 5 134 11.31\n 611 5 149 8.66\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 124.5 13.51 -1.879\n 77 127.5 13.51 2.176\n 153 130.4 13.51 0.2013\n 306 136.5 13.51 -0.4127\n 611 149.5 13.51 -0.08906\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -72.39853 6 156.7971\n A2 -71.16972 10 162.3394\n A3 -72.39853 6 156.7971\n R -82.0956 2 168.1912\n 3 -77.58141 3 161.1628\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 21.85 8 0.005198\n Test 2 2.458 4 0.6522\n Test 3 2.458 4 0.6522\n Test 5a 10.37 3 0.0157\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 344.057\n\n BMDL = 231.089\n\n BMDU = 724.471\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 0 | Exponential-M4 | 8 | 1.11 | True | False | 3.718190e+00 | 8.583410e-03 | 1.947930e+02 | -999 | 159.399800 | 0.005198 | 0.652200 | 0.6522 | 0.03683 | 6.603000 | 2 | -8.224000e-07 | NaN | warning | BMD/BMDL ratio is greater than threshold (4.33e+02 > 5.0)\nMinimum dose/BMD ratio is greater than threshold (20.7 > 3.0) | Goodness of fit p-value is less than threshold (0.0368 < 0.1)\nBMD/BMDL ratio is greater than threshold (4.33e+02 > 20.0) | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708\n611.000000 5 149.000000 8.660254 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-fljp0j0o.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:34 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha 4.79188 \n rho 0 Specified\n a 107.54 \n b 0.00318038 \n c 1.45481 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha 5.05599 44.395\n a 113.2 5.60286\n b 0.180773 11.2913\n c 1.22615 0.0655403\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 113.2 11.34\n 77 5 140.6 16.98\n 153 5 131.6 11.55\n 306 5 134 11.31\n 611 5 149 8.66\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 113.2 12.53 -8.224e-007\n 77 138.8 12.53 0.3213\n 153 138.8 12.53 -1.285\n 306 138.8 12.53 -0.8567\n 611 138.8 12.53 1.82\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -72.39853 6 156.7971\n A2 -71.16972 10 162.3394\n A3 -72.39853 6 156.7971\n R -82.0956 2 168.1912\n 4 -75.69989 4 159.3998\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 21.85 8 0.005198\n Test 2 2.458 4 0.6522\n Test 3 2.458 4 0.6522\n Test 6a 6.603 2 0.03683\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is less than .1. Model 4 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 3.71819\n\n BMDL = 0.00858341\n\n BMDU = 194.793\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 0 | Exponential-M5 | 9 | 1.11 | True | False | 1.198700e+01 | 2.804230e-02 | 7.691210e+01 | -999 | 161.399800 | 0.005198 | 0.652200 | 0.6522 | 0.01018 | 6.603000 | 1 | 2.286000e-07 | NaN | warning | BMD/BMDL ratio is greater than threshold (4.27e+02 > 5.0)\nMinimum dose/BMD ratio is greater than threshold (6.42 > 3.0) | Goodness of fit p-value is less than threshold (0.0102 < 0.1)\nBMD/BMDL ratio is greater than threshold (4.27e+02 > 20.0) | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708\n611.000000 5 149.000000 8.660254 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-t0qn\_41v.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:34 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha 4.79188 \n rho 0 Specified\n a 107.54 \n b 0.00318038 \n c 1.45481 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha 5.05599 44.395\n a 113.2 5.60286\n b 0.0689413 50669.6\n c 1.22615 0.0655403\n d 2.08353 924327\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 113.2 11.34\n 77 5 140.6 16.98\n 153 5 131.6 11.55\n 306 5 134 11.31\n 611 5 149 8.66\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 113.2 12.53 2.286e-007\n 77 138.8 12.53 0.3213\n 153 138.8 12.53 -1.285\n 306 138.8 12.53 -0.8567\n 611 138.8 12.53 1.821\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -72.39853 6 156.7971\n A2 -71.16972 10 162.3394\n A3 -72.39853 6 156.7971\n R -82.0956 2 168.1912\n 5 -75.69989 5 161.3998\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 21.85 8 0.005198\n Test 2 2.458 4 0.6522\n Test 3 2.458 4 0.6522\n Test 7a 6.603 1 0.01018\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is less than .1. Model 5 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 11.987\n\n BMDL = 0.0280423\n\n BMDU = 76.9121\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 1 | Linear | 0 | 2.21 | True | False | 3.145430e+02 | 1.529670e+02 | 9.363600e+08 | -999 | 133.092147 | 0.048850 | 0.720800 | 0.7208 | 0.01174 | 8.889110 | 2 | -5.850000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0117 < 0.1)\nBMD/high dose ratio is greater than threshold (1.03 > 1.0) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-fij2nzbt.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-fij2nzbt.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:37 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 169.575\n rho = 0 Specified\n beta\_0 = 123.653\n beta\_1 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 6.5e-007 -9.6e-007\n\n beta\_0 6.5e-007 1 -0.76\n\n beta\_1 -9.6e-007 -0.76 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 211.581 66.9079 80.4441 342.718\n beta\_0 123.653 5.04321 113.769 133.538\n beta\_1 0.0462443 0.0287628 -0.0101297 0.102618\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 113 124 11.3 14.5 -1.61\n 77 5 141 127 17 14.5 2.06\n 153 5 132 131 11.5 14.5 0.134\n 306 5 134 138 11.3 14.5 -0.585\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -59.101517 5 128.203034\n A2 -58.433860 8 132.867719\n A3 -59.101517 5 128.203034\n fitted -63.546073 3 133.092147\n R -64.761601 2 133.523203\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 12.6555 6 0.04885\n Test 2 1.33532 3 0.7208\n Test 3 1.33532 3 0.7208\n Test 4 8.88911 2 0.01174\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 314.543\n\n\n BMDL = 152.967\n\n\n BMDU = 9.3636e+008\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 1 | Polynomial-2 | 1 | 2.21 | True | False | 3.145430e+02 | 1.529670e+02 | -9.990000e+02 | -999 | 133.092147 | 0.048850 | 0.720800 | 0.7208 | 0.01174 | 8.889110 | 2 | -5.850000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0117 < 0.1)\nBMD/high dose ratio is greater than threshold (1.03 > 1.0) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-moy21077.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-moy21077.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:37 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 169.575\n rho = 0 Specified\n beta\_0 = 116.686\n beta\_1 = 0\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -3.8e-007 -2.4e-007\n\n beta\_0 -3.8e-007 1 -0.76\n\n beta\_1 -2.4e-007 -0.76 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 211.581 66.9078 80.4441 342.718\n beta\_0 123.653 5.04321 113.769 133.538\n beta\_1 0.0462444 0.0287627 -0.0101296 0.102618\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 113 124 11.3 14.5 -1.61\n 77 5 141 127 17 14.5 2.06\n 153 5 132 131 11.5 14.5 0.134\n 306 5 134 138 11.3 14.5 -0.585\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -59.101517 5 128.203034\n A2 -58.433860 8 132.867719\n A3 -59.101517 5 128.203034\n fitted -63.546073 3 133.092147\n R -64.761601 2 133.523203\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 12.6555 6 0.04885\n Test 2 1.33532 3 0.7208\n Test 3 1.33532 3 0.7208\n Test 4 8.88911 2 0.01174\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 314.543\n\n\n BMDL = 152.967\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 1 | Polynomial-3 | 2 | 2.21 | True | False | 3.145430e+02 | 1.529670e+02 | -9.990000e+02 | -999 | 133.092147 | 0.048850 | 0.720800 | 0.7208 | 0.01174 | 8.889110 | 2 | -5.850000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0117 < 0.1)\nBMD/high dose ratio is greater than threshold (1.03 > 1.0) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-jbf9170k.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-jbf9170k.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:37 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 169.575\n rho = 0 Specified\n beta\_0 = 113.2\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 4.7e-007 -3.1e-007\n\n beta\_0 4.7e-007 1 -0.76\n\n beta\_1 -3.1e-007 -0.76 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 211.581 66.9077 80.4441 342.718\n beta\_0 123.653 5.04321 113.769 133.538\n beta\_1 0.0462444 0.0287627 -0.0101296 0.102618\n beta\_2 -0 NA\n beta\_3 2.01399e-136 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 113 124 11.3 14.5 -1.61\n 77 5 141 127 17 14.5 2.06\n 153 5 132 131 11.5 14.5 0.134\n 306 5 134 138 11.3 14.5 -0.585\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -59.101517 5 128.203034\n A2 -58.433860 8 132.867719\n A3 -59.101517 5 128.203034\n fitted -63.546073 3 133.092147\n R -64.761601 2 133.523203\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 12.6555 6 0.04885\n Test 2 1.33532 3 0.7208\n Test 3 1.33532 3 0.7208\n Test 4 8.88911 2 0.01174\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 314.543\n\n\n BMDL = 152.967\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 1 | Polynomial-4 | 3 | 2.21 | True | False | 3.145430e+02 | 1.529670e+02 | -9.990000e+02 | -999 | 133.092147 | 0.048850 | 0.720800 | 0.7208 | 0.01174 | 8.889110 | 2 | -5.850000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0117 < 0.1)\nBMD/high dose ratio is greater than threshold (1.03 > 1.0) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-5y67r7s4.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-5y67r7s4.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:37 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 169.575\n rho = 0 Specified\n beta\_0 = -101.995\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = 0\n beta\_4 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 5.5e-007 -4e-007\n\n beta\_0 5.5e-007 1 -0.76\n\n beta\_1 -4e-007 -0.76 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 211.581 66.9078 80.4441 342.718\n beta\_0 123.653 5.04321 113.769 133.538\n beta\_1 0.0462443 0.0287628 -0.0101296 0.102618\n beta\_2 0 NA\n beta\_3 0 NA\n beta\_4 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 113 124 11.3 14.5 -1.61\n 77 5 141 127 17 14.5 2.06\n 153 5 132 131 11.5 14.5 0.134\n 306 5 134 138 11.3 14.5 -0.585\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -59.101517 5 128.203034\n A2 -58.433860 8 132.867719\n A3 -59.101517 5 128.203034\n fitted -63.546073 3 133.092147\n R -64.761601 2 133.523203\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 12.6555 6 0.04885\n Test 2 1.33532 3 0.7208\n Test 3 1.33532 3 0.7208\n Test 4 8.88911 2 0.01174\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 314.543\n\n\n BMDL = 152.967\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 1 | Power | 4 | 2.19 | True | False | 3.145420e+02 | 1.529670e+02 | 3.060000e+06 | -999 | 133.092147 | 0.048850 | 0.720800 | 0.7208 | 0.01174 | 8.889110 | 2 | -5.850000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0117 < 0.1)\nBMD/high dose ratio is greater than threshold (1.03 > 1.0) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-et3oopwa.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-et3oopwa.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:37 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The power is restricted to be greater than or equal to 1\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 169.575\n rho = 0 Specified\n control = 113.2\n slope = 59.6288\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha control slope\n\n alpha 1 -1e-010 -6.3e-011\n\n control -1e-010 1 -0.76\n\n slope -6.3e-011 -0.76 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 211.581 66.9077 80.4441 342.718\n control 123.653 5.04321 113.769 133.538\n slope 0.0462444 0.0287627 -0.0101296 0.102618\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 113 124 11.3 14.5 -1.61\n 77 5 141 127 17 14.5 2.06\n 153 5 132 131 11.5 14.5 0.134\n 306 5 134 138 11.3 14.5 -0.585\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -59.101517 5 128.203034\n A2 -58.433860 8 132.867719\n A3 -59.101517 5 128.203034\n fitted -63.546073 3 133.092147\n R -64.761601 2 133.523203\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 12.6555 6 0.04885\n Test 2 1.33532 3 0.7208\n Test 3 1.33532 3 0.7208\n Test 4 8.88911 2 0.01174\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 314.542 \n\n\n BMDL = 152.967 \n\n\n BMDU = 3.06e+006 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 1 | Hill | 5 | 2.18 | True | False | 3.668930e-13 | 3.668930e-13 | 3.668950e-13 | -999 | 127.743238 | 0.048850 | 0.720800 | 0.7208 | 0.2146 | 1.540200 | 1 | -1.590000e-08 | NaN | valid | Minimum dose/BMD ratio is greater than threshold (2.1e+14 > 3.0) | NaN | NaN | True | AIC | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-012wqt80.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-012wqt80.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:37 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n Power parameter restricted to be greater than 1\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 169.575\n rho = 0 Specified\n intercept = 113.2\n v = 27.4\n n = 1.86078\n k = 115.5\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -k \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha intercept v n\n\n alpha 1 5e-009 -2e-008 -5.4e-006\n\n intercept 5e-009 1 -0.87 -4.1e-006\n\n v -2e-008 -0.87 1 -1.2e-005\n\n n -5.4e-006 -4.1e-006 -1.2e-005 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 146.52 46.3338 55.7076 237.333\n intercept 113.2 5.41332 102.59 123.81\n v 22.2 6.25076 9.94873 34.4513\n n 1.00006 2660.6 -5213.69 5215.69\n k 3.06e-013 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 113 113 11.3 12.1 -1.59e-008\n 77 5 141 135 17 12.1 0.961\n 153 5 132 135 11.5 12.1 -0.702\n 306 5 134 135 11.3 12.1 -0.259\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -59.101517 5 128.203034\n A2 -58.433860 8 132.867719\n A3 -59.101517 5 128.203034\n fitted -59.871619 4 127.743238\n R -64.761601 2 133.523203\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 12.6555 6 0.04885\n Test 2 1.33532 3 0.7208\n Test 3 1.33532 3 0.7208\n Test 4 1.5402 1 0.2146\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 3.66893e-013\n\n BMDL = 3.66893e-013\n\n BMDU = 3.66895e-013\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 1 | Exponential-M2 | 6 | 1.11 | True | False | 3.267160e+02 | 1.657720e+02 | 3.060000e+06 | -999 | 133.186900 | 0.048850 | 0.720800 | 0.7208 | 0.0112 | 8.984000 | 2 | -5.489000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0112 < 0.1)\nBMD/high dose ratio is greater than threshold (1.07 > 1.0) | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-9ofqvcpn.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:37 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha 4.91015 \n rho 0 Specified\n a 122.981 \n b 0.000381617 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha 5.35935 67.2256\n a 123.972 4.91195\n b 0.000340332 0.000214692\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 113.2 11.34\n 77 5 140.6 16.98\n 153 5 131.6 11.55\n 306 5 134 11.31\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 124 14.58 -1.652\n 77 127.3 14.58 2.045\n 153 130.6 14.58 0.1535\n 306 137.6 14.58 -0.5489\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -59.10152 5 128.203\n A2 -58.43386 8 132.8677\n A3 -59.10152 5 128.203\n R -64.7616 2 133.5232\n 2 -63.59347 3 133.1869\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 12.66 6 0.04885\n Test 2 1.335 3 0.7208\n Test 3 1.335 3 0.7208\n Test 4 8.984 2 0.0112\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 326.716\n\n BMDL = 165.772\n\n BMDU = 3.06e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 1 | Exponential-M3 | 7 | 1.11 | True | False | 3.267160e+02 | 1.657720e+02 | -9.990000e+02 | -999 | 133.186900 | 0.048850 | 0.720800 | 0.7208 | 0.0112 | 8.984000 | 2 | -5.489000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0112 < 0.1)\nBMD/high dose ratio is greater than threshold (1.07 > 1.0) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-37jvou3n.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:37 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha 4.91015 \n rho 0 Specified\n a 122.981 \n b 0.000381617 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha 5.35935 67.2257\n a 123.972 4.91195\n b 0.000340332 0.000214692\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 113.2 11.34\n 77 5 140.6 16.98\n 153 5 131.6 11.55\n 306 5 134 11.31\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 124 14.58 -1.652\n 77 127.3 14.58 2.045\n 153 130.6 14.58 0.1535\n 306 137.6 14.58 -0.5489\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -59.10152 5 128.203\n A2 -58.43386 8 132.8677\n A3 -59.10152 5 128.203\n R -64.7616 2 133.5232\n 3 -63.59347 3 133.1869\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 12.66 6 0.04885\n Test 2 1.335 3 0.7208\n Test 3 1.335 3 0.7208\n Test 5a 8.984 2 0.0112\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 326.716\n\n BMDL = 165.772\n\n BMDU = Bad\_Completion\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 1 | Exponential-M4 | 8 | 1.11 | True | False | 3.881050e+00 | 5.909220e-03 | 3.060000e+06 | -999 | 127.743200 | 0.048850 | 0.720800 | 0.7208 | 0.2146 | 1.540000 | 1 | -2.738000e-07 | NaN | warning | BMD/BMDL ratio is greater than threshold (6.57e+02 > 5.0)\nMinimum dose/BMD ratio is greater than threshold (19.8 > 3.0) | BMD/BMDL ratio is greater than threshold (6.57e+02 > 20.0) | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-\_5njqyzm.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:37 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha 4.91015 \n rho 0 Specified\n a 107.54 \n b 0.00491512 \n c 1.37279 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha 4.98716 46.3337\n a 113.2 5.41332\n b 0.203039 16.2436\n c 1.19611 0.0635139\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 113.2 11.34\n 77 5 140.6 16.98\n 153 5 131.6 11.55\n 306 5 134 11.31\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 113.2 12.1 -2.738e-007\n 77 135.4 12.1 0.9606\n 153 135.4 12.1 -0.702\n 306 135.4 12.1 -0.2586\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -59.10152 5 128.203\n A2 -58.43386 8 132.8677\n A3 -59.10152 5 128.203\n R -64.7616 2 133.5232\n 4 -59.87162 4 127.7432\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 12.66 6 0.04885\n Test 2 1.335 3 0.7208\n Test 3 1.335 3 0.7208\n Test 6a 1.54 1 0.2146\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is greater than .1. Model 4 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 3.88105\n\n BMDL = 0.00590922\n\n BMDU = 3.06e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 5.0734603575863284,7.5934182026278521,5.163332257370234,5.0596442562694071,3.872983346207417 | 2,1,1,1,2 | 1,1,1,1,1 | SD | day | NaN | 150 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 3 | 1 | Exponential-M5 | 9 | 1.11 | True | False | 2.017480e+01 | 3.680120e-02 | 3.060000e+06 | -999 | 129.743200 | 0.048850 | 0.720800 | 0.7208 | -999 | 1.540000 | 0 | -1.214000e-06 | NaN | warning | BMD/BMDL ratio is greater than threshold (5.48e+02 > 5.0)\nMinimum dose/BMD ratio is greater than threshold (3.82 > 3.0) | BMD/BMDL ratio is greater than threshold (5.48e+02 > 20.0)\nZero degrees of freedom; saturated model | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 113.200000 11.344602\n77.000000 5 140.600000 16.979399\n153.000000 5 131.600000 11.545562\n306.000000 5 134.000000 11.313708 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-6k5fhvxt.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:37 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha 4.91015 \n rho 0 Specified\n a 107.54 \n b 0.00491512 \n c 1.37279 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha 4.98716 46.3337\n a 113.2 5.41332\n b 0.0452035 506.222\n c 1.19611 0.0635139\n d 2.58549 23400.1\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 113.2 11.34\n 77 5 140.6 16.98\n 153 5 131.6 11.55\n 306 5 134 11.31\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 113.2 12.1 -1.214e-006\n 77 135.4 12.1 0.9606\n 153 135.4 12.1 -0.702\n 306 135.4 12.1 -0.2586\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -59.10152 5 128.203\n A2 -58.43386 8 132.8677\n A3 -59.10152 5 128.203\n R -64.7616 2 133.5232\n 5 -59.87162 5 129.7432\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 12.66 6 0.04885\n Test 2 1.335 3 0.7208\n Test 3 1.335 3 0.7208\n Test 7a 1.54 0 N/A\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n Degrees of freedom for Test 7a are less than or equal to 0.\n The Chi-Square test for fit is not valid.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 20.1748\n\n BMDL = 0.0368012\n\n BMDU = 3.06e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Creatinine | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .0074833147735478773,.003741657386773936,.010488088481701513,.0070710678118654779,.0037416573867739447 | 2,0,0,1,1 | 2,2,2,2,2 | SD | day | NaN | 20 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Creatinine | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 4 | 0 | Linear | 0 | 2.21 | True | False | 3.302410e+02 | 2.122600e+02 | 7.382310e+02 | -999 | -175.738438 | 0.002986 | 0.106800 | 0.1068 | 0.07859 | 6.798900 | 3 | -1.830000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0786 < 0.1) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 0.274000 0.016733\n77.000000 5 0.278000 0.008367\n153.000000 5 0.280000 0.023452\n306.000000 5 0.250000 0.015811\n611.000000 5 0.252000 0.008367 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-palmpdr7.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-palmpdr7.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:42 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.000243998\n rho = 0 Specified\n beta\_0 = 0.277919\n beta\_1 = -4.84687e-005\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -2.4e-009 2.4e-009\n\n beta\_0 -2.4e-009 1 -0.73\n\n beta\_1 2.4e-009 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.000256204 7.24654e-005 0.000114174 0.000398233\n beta\_0 0.277919 0.00467039 0.268765 0.287073\n beta\_1 -4.84687e-005 1.48241e-005 -7.75234e-005 -1.9414e-005\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 0.274 0.278 0.0167 0.016 -0.547\n 77 5 0.278 0.274 0.00837 0.016 0.533\n 153 5 0.28 0.271 0.0235 0.016 1.33\n 306 5 0.25 0.263 0.0158 0.016 -1.83\n 611 5 0.252 0.248 0.00837 0.016 0.516\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 94.268669 6 -176.537338\n A2 98.075000 10 -176.150000\n A3 94.268669 6 -176.537338\n fitted 90.869219 3 -175.738438\n R 86.419216 2 -168.838431\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 23.3116 8 0.002986\n Test 2 7.61266 4 0.1068\n Test 3 7.61266 4 0.1068\n Test 4 6.7989 3 0.07859\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 330.241\n\n\n BMDL = 212.26\n\n\n BMDU = 738.231\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Creatinine | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .0074833147735478773,.003741657386773936,.010488088481701513,.0070710678118654779,.0037416573867739447 | 2,0,0,1,1 | 2,2,2,2,2 | SD | day | NaN | 20 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Creatinine | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 4 | 0 | Polynomial-2 | 1 | 2.21 | True | False | 3.302410e+02 | 2.122600e+02 | 7.382310e+02 | -999 | -175.738438 | 0.002986 | 0.106800 | 0.1068 | 0.07859 | 6.798900 | 3 | -1.830000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0786 < 0.1) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 0.274000 0.016733\n77.000000 5 0.278000 0.008367\n153.000000 5 0.280000 0.023452\n306.000000 5 0.250000 0.015811\n611.000000 5 0.252000 0.008367 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-80q3eav7.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-80q3eav7.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:41 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.000243998\n rho = 0 Specified\n beta\_0 = 0.280555\n beta\_1 = -8.51354e-005\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -1.4e-008 -4.1e-009\n\n beta\_0 -1.4e-008 1 -0.73\n\n beta\_1 -4.1e-009 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.000256204 7.24654e-005 0.000114174 0.000398233\n beta\_0 0.277919 0.00467039 0.268765 0.287073\n beta\_1 -4.84687e-005 1.48241e-005 -7.75234e-005 -1.9414e-005\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 0.274 0.278 0.0167 0.016 -0.547\n 77 5 0.278 0.274 0.00837 0.016 0.533\n 153 5 0.28 0.271 0.0235 0.016 1.33\n 306 5 0.25 0.263 0.0158 0.016 -1.83\n 611 5 0.252 0.248 0.00837 0.016 0.516\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 94.268669 6 -176.537338\n A2 98.075000 10 -176.150000\n A3 94.268669 6 -176.537338\n fitted 90.869219 3 -175.738438\n R 86.419216 2 -168.838431\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 23.3116 8 0.002986\n Test 2 7.61266 4 0.1068\n Test 3 7.61266 4 0.1068\n Test 4 6.7989 3 0.07859\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 330.241\n\n\n BMDL = 212.26\n\n\n BMDU = 738.231\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Creatinine | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .0074833147735478773,.003741657386773936,.010488088481701513,.0070710678118654779,.0037416573867739447 | 2,0,0,1,1 | 2,2,2,2,2 | SD | day | NaN | 20 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Creatinine | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 4 | 0 | Polynomial-3 | 2 | 2.21 | True | False | 3.302410e+02 | 2.122600e+02 | 7.382310e+02 | -999 | -175.738438 | 0.002986 | 0.106800 | 0.1068 | 0.07859 | 6.798900 | 3 | -1.830000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0786 < 0.1) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 0.274000 0.016733\n77.000000 5 0.278000 0.008367\n153.000000 5 0.280000 0.023452\n306.000000 5 0.250000 0.015811\n611.000000 5 0.252000 0.008367 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-xntqrl0k.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-xntqrl0k.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:42 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.000243998\n rho = 0 Specified\n beta\_0 = 0.272958\n beta\_1 = 0\n beta\_2 = -1.43909e-006\n beta\_3 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 2.9e-008 5.7e-008\n\n beta\_0 2.9e-008 1 -0.73\n\n beta\_1 5.7e-008 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.000256204 7.24654e-005 0.000114174 0.000398233\n beta\_0 0.277919 0.00467039 0.268765 0.287073\n beta\_1 -4.84687e-005 1.48241e-005 -7.75234e-005 -1.9414e-005\n beta\_2 0 NA\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 0.274 0.278 0.0167 0.016 -0.547\n 77 5 0.278 0.274 0.00837 0.016 0.533\n 153 5 0.28 0.271 0.0235 0.016 1.33\n 306 5 0.25 0.263 0.0158 0.016 -1.83\n 611 5 0.252 0.248 0.00837 0.016 0.516\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 94.268669 6 -176.537338\n A2 98.075000 10 -176.150000\n A3 94.268669 6 -176.537338\n fitted 90.869219 3 -175.738438\n R 86.419216 2 -168.838431\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 23.3116 8 0.002986\n Test 2 7.61266 4 0.1068\n Test 3 7.61266 4 0.1068\n Test 4 6.7989 3 0.07859\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 330.241\n\n\n BMDL = 212.26\n\n\n BMDU = 738.231\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Creatinine | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .0074833147735478773,.003741657386773936,.010488088481701513,.0070710678118654779,.0037416573867739447 | 2,0,0,1,1 | 2,2,2,2,2 | SD | day | NaN | 20 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Creatinine | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 4 | 0 | Polynomial-4 | 3 | 2.21 | True | False | 3.302410e+02 | 2.122600e+02 | 7.382310e+02 | -999 | -175.738438 | 0.002986 | 0.106800 | 0.1068 | 0.07859 | 6.798900 | 3 | -1.830000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0786 < 0.1) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 0.274000 0.016733\n77.000000 5 0.278000 0.008367\n153.000000 5 0.280000 0.023452\n306.000000 5 0.250000 0.015811\n611.000000 5 0.252000 0.008367 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-\_iueuopf.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-\_iueuopf.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:42 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.000243998\n rho = 0 Specified\n beta\_0 = 0.274\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = -7.2523e-009\n beta\_4 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -3.1e-009 -5.2e-009\n\n beta\_0 -3.1e-009 1 -0.73\n\n beta\_1 -5.2e-009 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.000256204 7.24654e-005 0.000114174 0.000398233\n beta\_0 0.277919 0.00467039 0.268765 0.287073\n beta\_1 -4.84687e-005 1.48241e-005 -7.75234e-005 -1.9414e-005\n beta\_2 0 NA\n beta\_3 0 NA\n beta\_4 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 0.274 0.278 0.0167 0.016 -0.547\n 77 5 0.278 0.274 0.00837 0.016 0.533\n 153 5 0.28 0.271 0.0235 0.016 1.33\n 306 5 0.25 0.263 0.0158 0.016 -1.83\n 611 5 0.252 0.248 0.00837 0.016 0.516\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 94.268669 6 -176.537338\n A2 98.075000 10 -176.150000\n A3 94.268669 6 -176.537338\n fitted 90.869219 3 -175.738438\n R 86.419216 2 -168.838431\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 23.3116 8 0.002986\n Test 2 7.61266 4 0.1068\n Test 3 7.61266 4 0.1068\n Test 4 6.7989 3 0.07859\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 330.241\n\n\n BMDL = 212.26\n\n\n BMDU = 738.231\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Creatinine | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .0074833147735478773,.003741657386773936,.010488088481701513,.0070710678118654779,.0037416573867739447 | 2,0,0,1,1 | 2,2,2,2,2 | SD | day | NaN | 20 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Creatinine | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 4 | 0 | Power | 4 | 2.19 | True | False | 3.302410e+02 | 2.122600e+02 | 7.382310e+02 | -999 | -175.738438 | 0.002986 | 0.106800 | 0.1068 | 0.07859 | 6.798900 | 3 | -1.830000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0786 < 0.1) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 0.274000 0.016733\n77.000000 5 0.278000 0.008367\n153.000000 5 0.280000 0.023452\n306.000000 5 0.250000 0.015811\n611.000000 5 0.252000 0.008367 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-\_a8t8glj.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-\_a8t8glj.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:42 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The power is restricted to be greater than or equal to 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.000243998\n rho = 0 Specified\n control = 0.25\n slope = 16.3253\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha control slope\n\n alpha 1 4e-012 4.8e-013\n\n control 4e-012 1 -0.73\n\n slope 4.8e-013 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.000256204 7.24654e-005 0.000114174 0.000398233\n control 0.277919 0.00467039 0.268765 0.287073\n slope -4.84687e-005 1.48241e-005 -7.75234e-005 -1.9414e-005\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 0.274 0.278 0.0167 0.016 -0.547\n 77 5 0.278 0.274 0.00837 0.016 0.533\n 153 5 0.28 0.271 0.0235 0.016 1.33\n 306 5 0.25 0.263 0.0158 0.016 -1.83\n 611 5 0.252 0.248 0.00837 0.016 0.516\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 94.268669 6 -176.537338\n A2 98.075000 10 -176.150000\n A3 94.268669 6 -176.537338\n fitted 90.869219 3 -175.738438\n R 86.419216 2 -168.838431\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 23.3116 8 0.002986\n Test 2 7.61266 4 0.1068\n Test 3 7.61266 4 0.1068\n Test 4 6.7989 3 0.07859\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 330.241 \n\n\n BMDL = 212.26 \n\n\n BMDU = 738.231 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Creatinine | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .0074833147735478773,.003741657386773936,.010488088481701513,.0070710678118654779,.0037416573867739447 | 2,0,0,1,1 | 2,2,2,2,2 | SD | day | NaN | 20 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Creatinine | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 4 | 0 | Hill | 5 | 2.18 | True | False | 2.239130e+02 | 1.588660e+02 | 3.080840e+02 | -999 | -180.004962 | 0.002986 | 0.106800 | 0.1068 | 0.7663 | 0.532375 | 2 | 4.260000e-01 | NaN | valid | NaN | NaN | NaN | True | AIC | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 0.274000 0.016733\n77.000000 5 0.278000 0.008367\n153.000000 5 0.280000 0.023452\n306.000000 5 0.250000 0.015811\n611.000000 5 0.252000 0.008367 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-0asi5ygi.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-0asi5ygi.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:42 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n Power parameter restricted to be greater than 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.000243998\n rho = 0 Specified\n intercept = 0.274\n v = -0.024\n n = 2.62164\n k = 244.8\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -n \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha intercept v k\n\n alpha 1 -1e-006 4.1e-007 1.8e-006\n\n intercept -1e-006 1 -0.63 -0.044\n\n v 4.1e-007 -0.63 1 -0.079\n\n k 1.8e-006 -0.044 -0.079 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.0001994 5.63988e-005 8.88602e-005 0.00030994\n intercept 0.277342 0.00365103 0.270186 0.284498\n v -0.0263798 0.00579447 -0.0377368 -0.0150229\n n 18 NA\n k 222.161 186.148 -142.683 587.005\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 0.274 0.277 0.0167 0.0141 -0.529\n 77 5 0.278 0.277 0.00837 0.0141 0.104\n 153 5 0.28 0.277 0.0235 0.0141 0.426\n 306 5 0.25 0.251 0.0158 0.0141 -0.165\n 611 5 0.252 0.251 0.00837 0.0141 0.164\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 94.268669 6 -176.537338\n A2 98.075000 10 -176.150000\n A3 94.268669 6 -176.537338\n fitted 94.002481 4 -180.004962\n R 86.419216 2 -168.838431\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 23.3116 8 0.002986\n Test 2 7.61266 4 0.1068\n Test 3 7.61266 4 0.1068\n Test 4 0.532375 2 0.7663\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 223.913\n\n BMDL = 158.866\n\n BMDU = 308.084\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Creatinine | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .0074833147735478773,.003741657386773936,.010488088481701513,.0070710678118654779,.0037416573867739447 | 2,0,0,1,1 | 2,2,2,2,2 | SD | day | NaN | 20 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Creatinine | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 4 | 0 | Exponential-M2 | 6 | 1.11 | True | False | 3.186290e+02 | 1.995390e+02 | 7.329020e+02 | -999 | -175.804500 | 0.002986 | 0.106800 | 0.1068 | 0.08092 | 6.733000 | 3 | -1.793000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0809 < 0.1) | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 0.274000 0.016733\n77.000000 5 0.278000 0.008367\n153.000000 5 0.280000 0.023452\n306.000000 5 0.250000 0.015811\n611.000000 5 0.252000 0.008367 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-a6\_9a6rp.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:42 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha -8.54149 \n rho 0 Specified\n a 0.255482 \n b 0.000183661 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha -8.27218 7.22741e-005\n a 0.27819 0.00474787\n b 0.000185729 5.71949e-005\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 0.274 0.01673\n 77 5 0.278 0.008367\n 153 5 0.28 0.02345\n 306 5 0.25 0.01581\n 611 5 0.252 0.008367\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 0.2782 0.01599 -0.5861\n 77 0.2742 0.01599 0.5259\n 153 0.2704 0.01599 1.343\n 306 0.2628 0.01599 -1.793\n 611 0.2483 0.01599 0.5111\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 94.26867 6 -176.5373\n A2 98.075 10 -176.15\n A3 94.26867 6 -176.5373\n R 86.41922 2 -168.8384\n 2 90.90226 3 -175.8045\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 23.31 8 0.002986\n Test 2 7.613 4 0.1068\n Test 3 7.613 4 0.1068\n Test 4 6.733 3 0.08092\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 318.629\n\n BMDL = 199.539\n\n BMDU = 732.902\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Creatinine | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .0074833147735478773,.003741657386773936,.010488088481701513,.0070710678118654779,.0037416573867739447 | 2,0,0,1,1 | 2,2,2,2,2 | SD | day | NaN | 20 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Creatinine | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 4 | 0 | Exponential-M3 | 7 | 1.11 | True | False | 3.189390e+02 | 1.995390e+02 | 7.329000e+02 | -999 | -173.804500 | 0.002986 | 0.106800 | 0.1068 | 0.03451 | 6.733000 | 2 | -1.794000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0345 < 0.1) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 0.274000 0.016733\n77.000000 5 0.278000 0.008367\n153.000000 5 0.280000 0.023452\n306.000000 5 0.250000 0.015811\n611.000000 5 0.252000 0.008367 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-2jtle99m.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:42 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha -8.54149 \n rho 0 Specified\n a 0.255482 \n b 0.000183661 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha -8.27218 7.23422e-005\n a 0.278181 0.00682826\n b 0.000186241 0.000476824\n d 1.00131 0.952566\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 0.274 0.01673\n 77 5 0.278 0.008367\n 153 5 0.28 0.02345\n 306 5 0.25 0.01581\n 611 5 0.252 0.008367\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 0.2782 0.01599 -0.5849\n 77 0.2742 0.01599 0.5256\n 153 0.2704 0.01599 1.343\n 306 0.2628 0.01599 -1.794\n 611 0.2483 0.01599 0.5118\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 94.26867 6 -176.5373\n A2 98.075 10 -176.15\n A3 94.26867 6 -176.5373\n R 86.41922 2 -168.8384\n 3 90.90226 4 -173.8045\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 23.31 8 0.002986\n Test 2 7.613 4 0.1068\n Test 3 7.613 4 0.1068\n Test 5a 6.733 2 0.03451\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 318.939\n\n BMDL = 199.539\n\n BMDU = 732.9\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Creatinine | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .0074833147735478773,.003741657386773936,.010488088481701513,.0070710678118654779,.0037416573867739447 | 2,0,0,1,1 | 2,2,2,2,2 | SD | day | NaN | 20 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Creatinine | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 4 | 0 | Exponential-M4 | 8 | 1.11 | True | False | 2.556580e+02 | 1.012540e+02 | 9.595150e+02 | -999 | -174.018600 | 0.002986 | 0.106800 | 0.1068 | 0.03841 | 6.519000 | 2 | -1.580000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0384 < 0.1) | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 0.274000 0.016733\n77.000000 5 0.278000 0.008367\n153.000000 5 0.280000 0.023452\n306.000000 5 0.250000 0.015811\n611.000000 5 0.252000 0.008367 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-uakldp9m.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:42 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha -8.54149 \n rho 0 Specified\n a 0.294 \n b 0.00280783 \n c 0.809848 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha -8.28074 7.16578e-005\n a 0.279667 0.00581298\n b 0.0014313 0.00266193\n c 0.814277 0.222877\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 0.274 0.01673\n 77 5 0.278 0.008367\n 153 5 0.28 0.02345\n 306 5 0.25 0.01581\n 611 5 0.252 0.008367\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 0.2797 0.01592 -0.7961\n 77 0.2742 0.01592 0.5273\n 153 0.2695 0.01592 1.482\n 306 0.2612 0.01592 -1.58\n 611 0.2494 0.01592 0.3668\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 94.26867 6 -176.5373\n A2 98.075 10 -176.15\n A3 94.26867 6 -176.5373\n R 86.41922 2 -168.8384\n 4 91.00931 4 -174.0186\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 23.31 8 0.002986\n Test 2 7.613 4 0.1068\n Test 3 7.613 4 0.1068\n Test 6a 6.519 2 0.03841\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is less than .1. Model 4 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 255.658\n\n BMDL = 101.254\n\n BMDU = 959.515\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Creatinine | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .0074833147735478773,.003741657386773936,.010488088481701513,.0070710678118654779,.0037416573867739447 | 2,0,0,1,1 | 2,2,2,2,2 | SD | day | NaN | 20 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Creatinine | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 4 | 0 | Exponential-M5 | 9 | 1.11 | True | False | 2.632930e+02 | 1.576260e+02 | 3.078480e+02 | -999 | -178.013300 | 0.002986 | 0.106800 | 0.1068 | 0.4691 | 0.524000 | 1 | -1.584000e-01 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 0.274000 0.016733\n77.000000 5 0.278000 0.008367\n153.000000 5 0.280000 0.023452\n306.000000 5 0.250000 0.015811\n611.000000 5 0.252000 0.008367 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-seks3kgb.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:42 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha -8.54149 \n rho 0 Specified\n a 0.294 \n b 0.00280783 \n c 0.809848 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha -8.52053 5.63799e-005\n a 0.277334 0.00364547\n b 0.00374281 0.00697715\n c 0.905047 0.020018\n d 18 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 0.274 0.01673\n 77 5 0.278 0.008367\n 153 5 0.28 0.02345\n 306 5 0.25 0.01581\n 611 5 0.252 0.008367\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 0.2773 0.01412 -0.528\n 77 0.2773 0.01412 0.1055\n 153 0.2773 0.01412 0.4225\n 306 0.251 0.01412 -0.1584\n 611 0.251 0.01412 0.1584\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 94.26867 6 -176.5373\n A2 98.075 10 -176.15\n A3 94.26867 6 -176.5373\n R 86.41922 2 -168.8384\n 5 94.00666 5 -178.0133\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 23.31 8 0.002986\n Test 2 7.613 4 0.1068\n Test 3 7.613 4 0.1068\n Test 7a 0.524 1 0.4691\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is greater than .1. Model 5 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 263.293\n\n BMDL = 157.626\n\n BMDU = 307.848\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Globulin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .067823299831252584,.048989794855663599,.058309518948453119,.050990195135927972,.066332495807108066 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 100 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Globulin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 5 | 0 | Linear | 0 | 2.21 | True | False | 5.676480e+02 | 2.993790e+02 | -9.990000e+02 | -999 | -70.910238 | 0.326300 | 0.929700 | 0.9297 | 0.1755 | 4.950380 | 3 | -7.480000e-01 | NaN | valid | NaN | NaN | NaN | True | AIC | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 2.540000 0.151658\n77.000000 5 2.680000 0.109545\n153.000000 5 2.680000 0.130384\n306.000000 5 2.760000 0.114018\n611.000000 5 2.720000 0.148324 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-trty3tz9.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-trty3tz9.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.0174001\n rho = 0 Specified\n beta\_0 = 2.62336\n beta\_1 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -9.1e-008 1e-007\n\n beta\_0 -9.1e-008 1 -0.73\n\n beta\_1 1e-007 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.0169683 0.00479935 0.00756172 0.0263748\n beta\_0 2.62336 0.0380084 2.54886 2.69785\n beta\_1 0.000229478 0.000120641 -6.97431e-006 0.000465929\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 2.54 2.62 0.152 0.13 -1.43\n 77 5 2.68 2.64 0.11 0.13 0.669\n 153 5 2.68 2.66 0.13 0.13 0.37\n 306 5 2.76 2.69 0.114 0.13 1.14\n 611 5 2.72 2.76 0.148 0.13 -0.748\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 40.930307 6 -69.860613\n A2 41.362163 10 -62.724325\n A3 40.930307 6 -69.860613\n fitted 38.455119 3 -70.910238\n R 36.765537 2 -69.531073\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 9.19325 8 0.3263\n Test 2 0.863712 4 0.9297\n Test 3 0.863712 4 0.9297\n Test 4 4.95038 3 0.1755\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 567.648\n\n\n BMDL = 299.379\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Globulin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .067823299831252584,.048989794855663599,.058309518948453119,.050990195135927972,.066332495807108066 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 100 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Globulin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 5 | 0 | Polynomial-2 | 1 | 2.21 | True | False | 5.676480e+02 | 2.993790e+02 | 5.399210e+03 | -999 | -70.910238 | 0.326300 | 0.929700 | 0.9297 | 0.1755 | 4.950380 | 3 | -7.480000e-01 | NaN | valid | NaN | NaN | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 2.540000 0.151658\n77.000000 5 2.680000 0.109545\n153.000000 5 2.680000 0.130384\n306.000000 5 2.760000 0.114018\n611.000000 5 2.720000 0.148324 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-grpakrp6.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-grpakrp6.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.0174001\n rho = 0 Specified\n beta\_0 = 2.56187\n beta\_1 = 0\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -8e-010 -3.2e-010\n\n beta\_0 -8e-010 1 -0.73\n\n beta\_1 -3.2e-010 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.0169683 0.00479935 0.00756172 0.0263748\n beta\_0 2.62336 0.0380084 2.54886 2.69785\n beta\_1 0.000229477 0.000120641 -6.97435e-006 0.000465929\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 2.54 2.62 0.152 0.13 -1.43\n 77 5 2.68 2.64 0.11 0.13 0.669\n 153 5 2.68 2.66 0.13 0.13 0.37\n 306 5 2.76 2.69 0.114 0.13 1.14\n 611 5 2.72 2.76 0.148 0.13 -0.748\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 40.930307 6 -69.860613\n A2 41.362163 10 -62.724325\n A3 40.930307 6 -69.860613\n fitted 38.455119 3 -70.910238\n R 36.765537 2 -69.531073\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 9.19325 8 0.3263\n Test 2 0.863712 4 0.9297\n Test 3 0.863712 4 0.9297\n Test 4 4.95038 3 0.1755\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 567.648\n\n\n BMDL = 299.379\n\n\n BMDU = 5399.21\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Globulin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .067823299831252584,.048989794855663599,.058309518948453119,.050990195135927972,.066332495807108066 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 100 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Globulin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 5 | 0 | Polynomial-3 | 2 | 2.21 | True | False | 5.676480e+02 | 2.993790e+02 | 5.399210e+03 | -999 | -70.910238 | 0.326300 | 0.929700 | 0.9297 | 0.1755 | 4.950380 | 3 | -7.480000e-01 | NaN | valid | NaN | NaN | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 2.540000 0.151658\n77.000000 5 2.680000 0.109545\n153.000000 5 2.680000 0.130384\n306.000000 5 2.760000 0.114018\n611.000000 5 2.720000 0.148324 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-prvknkhw.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-prvknkhw.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.0174001\n rho = 0 Specified\n beta\_0 = 2.55053\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -4.6e-008 -1.8e-008\n\n beta\_0 -4.6e-008 1 -0.73\n\n beta\_1 -1.8e-008 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.0169683 0.00479935 0.00756172 0.0263748\n beta\_0 2.62336 0.0380084 2.54886 2.69785\n beta\_1 0.000229477 0.000120641 -6.97436e-006 0.000465929\n beta\_2 6.92417e-032 NA\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 2.54 2.62 0.152 0.13 -1.43\n 77 5 2.68 2.64 0.11 0.13 0.669\n 153 5 2.68 2.66 0.13 0.13 0.37\n 306 5 2.76 2.69 0.114 0.13 1.14\n 611 5 2.72 2.76 0.148 0.13 -0.748\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 40.930307 6 -69.860613\n A2 41.362163 10 -62.724325\n A3 40.930307 6 -69.860613\n fitted 38.455119 3 -70.910238\n R 36.765537 2 -69.531073\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 9.19325 8 0.3263\n Test 2 0.863712 4 0.9297\n Test 3 0.863712 4 0.9297\n Test 4 4.95038 3 0.1755\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 567.648\n\n\n BMDL = 299.379\n\n\n BMDU = 5399.21\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Globulin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .067823299831252584,.048989794855663599,.058309518948453119,.050990195135927972,.066332495807108066 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 100 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Globulin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 5 | 0 | Polynomial-4 | 3 | 2.21 | True | False | 5.676480e+02 | 2.993790e+02 | -9.990000e+02 | -999 | -70.910238 | 0.326300 | 0.929700 | 0.9297 | 0.1755 | 4.950380 | 3 | -7.480000e-01 | NaN | valid | NaN | NaN | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 2.540000 0.151658\n77.000000 5 2.680000 0.109545\n153.000000 5 2.680000 0.130384\n306.000000 5 2.760000 0.114018\n611.000000 5 2.720000 0.148324 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-pazmx1w2.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-pazmx1w2.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.0174001\n rho = 0 Specified\n beta\_0 = 2.54\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = 0\n beta\_4 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 1.1e-008 4.5e-009\n\n beta\_0 1.1e-008 1 -0.73\n\n beta\_1 4.5e-009 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.0169683 0.00479935 0.00756172 0.0263748\n beta\_0 2.62336 0.0380084 2.54886 2.69785\n beta\_1 0.000229477 0.000120641 -6.97435e-006 0.000465929\n beta\_2 -0 NA\n beta\_3 0 NA\n beta\_4 1.85475e-037 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 2.54 2.62 0.152 0.13 -1.43\n 77 5 2.68 2.64 0.11 0.13 0.669\n 153 5 2.68 2.66 0.13 0.13 0.37\n 306 5 2.76 2.69 0.114 0.13 1.14\n 611 5 2.72 2.76 0.148 0.13 -0.748\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 40.930307 6 -69.860613\n A2 41.362163 10 -62.724325\n A3 40.930307 6 -69.860613\n fitted 38.455119 3 -70.910238\n R 36.765537 2 -69.531073\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 9.19325 8 0.3263\n Test 2 0.863712 4 0.9297\n Test 3 0.863712 4 0.9297\n Test 4 4.95038 3 0.1755\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 567.648\n\n\n BMDL = 299.379\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Globulin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .067823299831252584,.048989794855663599,.058309518948453119,.050990195135927972,.066332495807108066 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 100 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Globulin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 5 | 0 | Power | 4 | 2.19 | True | False | 5.676480e+02 | 2.993790e+02 | 5.399210e+03 | -999 | -70.910238 | 0.326300 | 0.929700 | 0.9297 | 0.1755 | 4.950380 | 3 | -7.480000e-01 | NaN | valid | NaN | NaN | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 2.540000 0.151658\n77.000000 5 2.680000 0.109545\n153.000000 5 2.680000 0.130384\n306.000000 5 2.760000 0.114018\n611.000000 5 2.720000 0.148324 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-gcrd5bci.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-gcrd5bci.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The power is restricted to be greater than or equal to 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.0174001\n rho = 0 Specified\n control = 2.54\n slope = 0.0652351\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha control slope\n\n alpha 1 -9.2e-011 -9.3e-012\n\n control -9.2e-011 1 -0.73\n\n slope -9.3e-012 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.0169683 0.00479935 0.00756172 0.0263748\n control 2.62336 0.0380084 2.54886 2.69785\n slope 0.000229477 0.000120641 -6.97435e-006 0.000465929\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 2.54 2.62 0.152 0.13 -1.43\n 77 5 2.68 2.64 0.11 0.13 0.669\n 153 5 2.68 2.66 0.13 0.13 0.37\n 306 5 2.76 2.69 0.114 0.13 1.14\n 611 5 2.72 2.76 0.148 0.13 -0.748\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 40.930307 6 -69.860613\n A2 41.362163 10 -62.724325\n A3 40.930307 6 -69.860613\n fitted 38.455119 3 -70.910238\n R 36.765537 2 -69.531073\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 9.19325 8 0.3263\n Test 2 0.863712 4 0.9297\n Test 3 0.863712 4 0.9297\n Test 4 4.95038 3 0.1755\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 567.648 \n\n\n BMDL = 299.379 \n\n\n BMDU = 5399.21 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Globulin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .067823299831252584,.048989794855663599,.058309518948453119,.050990195135927972,.066332495807108066 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 100 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Globulin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 5 | 0 | Hill | 5 | 2.18 | True | False | 6.145590e+01 | 4.987880e-05 | 3.733210e+09 | -999 | -71.104300 | 0.326300 | 0.929700 | 0.9297 | 0.3845 | 0.756313 | 1 | 1.340000e-01 | NaN | warning | BMD/BMDL ratio is greater than threshold (1.23e+06 > 5.0) | BMD/BMDL ratio is greater than threshold (1.23e+06 > 20.0) | NaN | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 2.540000 0.151658\n77.000000 5 2.680000 0.109545\n153.000000 5 2.680000 0.130384\n306.000000 5 2.760000 0.114018\n611.000000 5 2.720000 0.148324 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-expvqeq2.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-expvqeq2.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n Power parameter restricted to be greater than 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 0.0174001\n rho = 0 Specified\n intercept = 2.54\n v = 0.22\n n = 0.645864\n k = 93.5\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha intercept v n k\n\n alpha 1 9.9e-008 -8.2e-009 1.3e-008 1.2e-007\n\n intercept 9.9e-008 1 -0.5 0.052 0.26\n\n v -8.2e-009 -0.5 1 -0.74 -0.13\n\n n 1.3e-008 0.052 -0.74 1 0.48\n\n k 1.2e-007 0.26 -0.13 0.48 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 0.0143476 0.00405812 0.00639385 0.0223014\n intercept 2.54022 0.0536562 2.43506 2.64539\n v 0.205679 0.111609 -0.0130716 0.424429\n n 1.16804 2.88586 -4.48813 6.82422\n k 46.2305 70.3826 -91.7168 184.178\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 2.54 2.54 0.152 0.12 -0.00413\n 77 5 2.68 2.67 0.11 0.12 0.134\n 153 5 2.68 2.71 0.13 0.12 -0.469\n 306 5 2.76 2.73 0.114 0.12 0.644\n 611 5 2.72 2.74 0.148 0.12 -0.304\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 40.930307 6 -69.860613\n A2 41.362163 10 -62.724325\n A3 40.930307 6 -69.860613\n fitted 40.552150 5 -71.104300\n R 36.765537 2 -69.531073\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 9.19325 8 0.3263\n Test 2 0.863712 4 0.9297\n Test 3 0.863712 4 0.9297\n Test 4 0.756313 1 0.3845\n\nThe p-value for Test 1 is greater than .05. There may not be a\ndiffence between responses and/or variances among the dose levels\nModelling the data with a dose/response curve may not be appropriate\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 61.4559\n\n BMDL = 4.98788e-005\n\n BMDU = 3.73321e+009\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Globulin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .067823299831252584,.048989794855663599,.058309518948453119,.050990195135927972,.066332495807108066 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 100 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Globulin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 5 | 0 | Exponential-M2 | 6 | 1.11 | True | False | 5.779270e+02 | 3.104060e+02 | 5.748950e+03 | -999 | -70.857430 | 0.326300 | 0.929700 | 0.9297 | 0.1716 | 5.003000 | 3 | -7.308000e-01 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 2.540000 0.151658\n77.000000 5 2.680000 0.109545\n153.000000 5 2.680000 0.130384\n306.000000 5 2.760000 0.114018\n611.000000 5 2.720000 0.148324 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-fwjy17t5.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha -4.27442 \n rho 0 Specified\n a 2.62228 \n b 8.6693e-005 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha -4.0743 0.0048095\n a 2.62456 0.0375674\n b 8.39027e-005 4.41775e-005\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 2.54 0.1517\n 77 5 2.68 0.1095\n 153 5 2.68 0.1304\n 306 5 2.76 0.114\n 611 5 2.72 0.1483\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 2.625 0.1304 -1.45\n 77 2.642 0.1304 0.659\n 153 2.658 0.1304 0.3692\n 306 2.693 0.1304 1.152\n 611 2.763 0.1304 -0.7308\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 40.93031 6 -69.86061\n A2 41.36216 10 -62.72433\n A3 40.93031 6 -69.86061\n R 36.76554 2 -69.53107\n 2 38.42871 3 -70.85743\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 9.193 8 0.3263\n Test 2 0.8637 4 0.9297\n Test 3 0.8637 4 0.9297\n Test 4 5.003 3 0.1716\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is greater than .1. Model 2 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 577.927\n\n BMDL = 310.406\n\n BMDU = 5748.95\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Globulin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .067823299831252584,.048989794855663599,.058309518948453119,.050990195135927972,.066332495807108066 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 100 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Globulin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 5 | 0 | Exponential-M3 | 7 | 1.11 | True | False | 5.779270e+02 | 3.104060e+02 | 5.748950e+03 | -999 | -70.857430 | 0.326300 | 0.929700 | 0.9297 | 0.1716 | 5.003000 | 3 | -7.308000e-01 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 2.540000 0.151658\n77.000000 5 2.680000 0.109545\n153.000000 5 2.680000 0.130384\n306.000000 5 2.760000 0.114018\n611.000000 5 2.720000 0.148324 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-fdd7pn8e.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha -4.27442 \n rho 0 Specified\n a 2.62228 \n b 8.6693e-005 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha -4.0743 0.0048095\n a 2.62456 0.0375674\n b 8.39027e-005 4.41775e-005\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 2.54 0.1517\n 77 5 2.68 0.1095\n 153 5 2.68 0.1304\n 306 5 2.76 0.114\n 611 5 2.72 0.1483\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 2.625 0.1304 -1.45\n 77 2.642 0.1304 0.659\n 153 2.658 0.1304 0.3692\n 306 2.693 0.1304 1.152\n 611 2.763 0.1304 -0.7308\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 40.93031 6 -69.86061\n A2 41.36216 10 -62.72433\n A3 40.93031 6 -69.86061\n R 36.76554 2 -69.53107\n 3 38.42871 3 -70.85743\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 9.193 8 0.3263\n Test 2 0.8637 4 0.9297\n Test 3 0.8637 4 0.9297\n Test 5a 5.003 3 0.1716\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is greater than .1. Model 3 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 577.927\n\n BMDL = 310.406\n\n BMDU = 5748.95\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Globulin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .067823299831252584,.048989794855663599,.058309518948453119,.050990195135927972,.066332495807108066 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 100 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Globulin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 5 | 0 | Exponential-M4 | 8 | 1.11 | True | False | 7.403930e+01 | 2.085250e-01 | 6.110000e+06 | -999 | -73.112380 | 0.326300 | 0.929700 | 0.9297 | 0.6879 | 0.748200 | 2 | 2.846000e-01 | NaN | warning | BMD/BMDL ratio is greater than threshold (3.55e+02 > 5.0) | BMD/BMDL ratio is greater than threshold (3.55e+02 > 20.0) | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 2.540000 0.151658\n77.000000 5 2.680000 0.109545\n153.000000 5 2.680000 0.130384\n306.000000 5 2.760000 0.114018\n611.000000 5 2.720000 0.148324 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-3kttye3y.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha -4.27442 \n rho 0 Specified\n a 2.413 \n b 0.00237958 \n c 1.20099 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha -4.24449 0.00405681\n a 2.54223 0.0534919\n b 0.0132429 0.0117082\n c 1.07539 0.0269476\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 2.54 0.1517\n 77 5 2.68 0.1095\n 153 5 2.68 0.1304\n 306 5 2.76 0.114\n 611 5 2.72 0.1483\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 2.542 0.1198 -0.04167\n 77 2.665 0.1198 0.2846\n 153 2.709 0.1198 -0.5344\n 306 2.731 0.1198 0.5497\n 611 2.734 0.1198 -0.2582\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 40.93031 6 -69.86061\n A2 41.36216 10 -62.72433\n A3 40.93031 6 -69.86061\n R 36.76554 2 -69.53107\n 4 40.55619 4 -73.11238\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 9.193 8 0.3263\n Test 2 0.8637 4 0.9297\n Test 3 0.8637 4 0.9297\n Test 6a 0.7482 2 0.6879\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is greater than .1. Model 4 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 74.0393\n\n BMDL = 0.208525\n\n BMDU = 6.11e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Globulin | g/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .067823299831252584,.048989794855663599,.058309518948453119,.050990195135927972,.066332495807108066 | 1,0,0,0,0 | 2,2,2,2,2 | SD | day | NaN | 100 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Globulin | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 5 | 0 | Exponential-M5 | 9 | 1.11 | True | False | 7.403930e+01 | 2.400450e-01 | -9.990000e+02 | -999 | -73.112380 | 0.326300 | 0.929700 | 0.9297 | 0.6879 | 0.748200 | 2 | 2.846000e-01 | NaN | warning | BMD/BMDL ratio is greater than threshold (3.08e+02 > 5.0) | BMD/BMDL ratio is greater than threshold (3.08e+02 > 20.0) | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 2.540000 0.151658\n77.000000 5 2.680000 0.109545\n153.000000 5 2.680000 0.130384\n306.000000 5 2.760000 0.114018\n611.000000 5 2.720000 0.148324 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-43gouvfu.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha -4.27442 \n rho 0 Specified\n a 2.413 \n b 0.00237958 \n c 1.20099 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha -4.2445 0.00405681\n a 2.54223 0.0534919\n b 0.0132429 0.0117081\n c 1.07539 0.0269476\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 2.54 0.1517\n 77 5 2.68 0.1095\n 153 5 2.68 0.1304\n 306 5 2.76 0.114\n 611 5 2.72 0.1483\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 2.542 0.1198 -0.04167\n 77 2.665 0.1198 0.2846\n 153 2.709 0.1198 -0.5344\n 306 2.731 0.1198 0.5497\n 611 2.734 0.1198 -0.2582\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 40.93031 6 -69.86061\n A2 41.36216 10 -62.72433\n A3 40.93031 6 -69.86061\n R 36.76554 2 -69.53107\n 5 40.55619 4 -73.11238\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 9.193 8 0.3263\n Test 2 0.8637 4 0.9297\n Test 3 0.8637 4 0.9297\n Test 7a 0.7482 2 0.6879\n\n\n The p-value for Test 1 is greater than .05. There may not be a\n diffence between responses and/or variances among the dose levels\n Modelling the data with a dose/response curve may not be appropriate.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is greater than .1. Model 5 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 74.0393\n\n BMDL = 0.240045\n\n BMDU = Bad\_Completion\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 0 | Linear | 0 | 2.21 | True | False | 2.696050e+02 | 1.828850e+02 | 5.084960e+02 | -999 | 124.475607 | 0.000141 | 0.399300 | 0.3993 | 0.002248 | 14.546300 | 3 | 3.990000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00225 < 0.1) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000\n611.000000 5 71.200000 5.674504 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-qnh4qmsi.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-qnh4qmsi.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 29.38\n rho = 0 Specified\n beta\_0 = 57.482\n beta\_1 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 1.9e-006 3.6e-007\n\n beta\_0 1.9e-006 1 -0.73\n\n beta\_1 3.6e-007 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 42.0569 11.8955 18.7422 65.3716\n beta\_0 57.482 1.89225 53.7732 61.1907\n beta\_1 0.0240542 0.00600613 0.0122824 0.035826\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 52 57.5 5 6.49 -1.89\n 77 5 66.8 59.3 7.56 6.49 2.57\n 153 5 59 61.2 4.85 6.49 -0.746\n 306 5 66 64.8 3 6.49 0.399\n 611 5 71.2 72.2 5.67 6.49 -0.338\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -51.964632 6 115.929265\n A2 -49.939758 10 119.879516\n A3 -51.964632 6 115.929265\n fitted -59.237804 3 124.475607\n R -65.433575 2 134.867151\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 30.9876 8 0.0001412\n Test 2 4.04975 4 0.3993\n Test 3 4.04975 4 0.3993\n Test 4 14.5463 3 0.002248\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 269.605\n\n\n BMDL = 182.885\n\n\n BMDU = 508.496\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 0 | Polynomial-2 | 1 | 2.21 | True | False | 2.696050e+02 | 1.828850e+02 | 5.086210e+02 | -999 | 124.475607 | 0.000141 | 0.399300 | 0.3993 | 0.002248 | 14.546300 | 3 | 3.990000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00225 < 0.1) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000\n611.000000 5 71.200000 5.674504 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-kx9dwhos.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-kx9dwhos.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 29.38\n rho = 0 Specified\n beta\_0 = 55.7419\n beta\_1 = 0\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -2.7e-007 5.7e-007\n\n beta\_0 -2.7e-007 1 -0.73\n\n beta\_1 5.7e-007 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 42.0569 11.8955 18.7422 65.3717\n beta\_0 57.482 1.89225 53.7732 61.1907\n beta\_1 0.0240542 0.00600613 0.0122824 0.035826\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 52 57.5 5 6.49 -1.89\n 77 5 66.8 59.3 7.56 6.49 2.57\n 153 5 59 61.2 4.85 6.49 -0.746\n 306 5 66 64.8 3 6.49 0.399\n 611 5 71.2 72.2 5.67 6.49 -0.338\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -51.964632 6 115.929265\n A2 -49.939758 10 119.879516\n A3 -51.964632 6 115.929265\n fitted -59.237804 3 124.475607\n R -65.433575 2 134.867151\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 30.9876 8 0.0001412\n Test 2 4.04975 4 0.3993\n Test 3 4.04975 4 0.3993\n Test 4 14.5463 3 0.002248\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 269.605\n\n\n BMDL = 182.885\n\n\n BMDU = 508.621\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 0 | Polynomial-3 | 2 | 2.21 | True | False | 2.696050e+02 | 1.828850e+02 | 5.138780e+02 | -999 | 124.475607 | 0.000141 | 0.399300 | 0.3993 | 0.002248 | 14.546300 | 3 | 3.990000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00225 < 0.1) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000\n611.000000 5 71.200000 5.674504 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-izsnyej7.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-izsnyej7.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 29.38\n rho = 0 Specified\n beta\_0 = 53.9265\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -1.5e-006 1.2e-007\n\n beta\_0 -1.5e-006 1 -0.73\n\n beta\_1 1.2e-007 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 42.0569 11.8955 18.7422 65.3717\n beta\_0 57.482 1.89225 53.7732 61.1907\n beta\_1 0.0240542 0.00600613 0.0122824 0.035826\n beta\_2 0 NA\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 52 57.5 5 6.49 -1.89\n 77 5 66.8 59.3 7.56 6.49 2.57\n 153 5 59 61.2 4.85 6.49 -0.746\n 306 5 66 64.8 3 6.49 0.399\n 611 5 71.2 72.2 5.67 6.49 -0.338\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -51.964632 6 115.929265\n A2 -49.939758 10 119.879516\n A3 -51.964632 6 115.929265\n fitted -59.237804 3 124.475607\n R -65.433575 2 134.867151\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 30.9876 8 0.0001412\n Test 2 4.04975 4 0.3993\n Test 3 4.04975 4 0.3993\n Test 4 14.5463 3 0.002248\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 269.605\n\n\n BMDL = 182.885\n\n\n BMDU = 513.878\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 0 | Polynomial-4 | 3 | 2.21 | True | False | 2.696050e+02 | 1.828850e+02 | 5.208290e+02 | -999 | 124.475607 | 0.000141 | 0.399300 | 0.3993 | 0.002248 | 14.546300 | 3 | 3.990000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00225 < 0.1) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000\n611.000000 5 71.200000 5.674504 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-8bhxs4uo.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-8bhxs4uo.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 29.38\n rho = 0 Specified\n beta\_0 = 52\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = 0\n beta\_4 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -2.4e-007 2.7e-007\n\n beta\_0 -2.4e-007 1 -0.73\n\n beta\_1 2.7e-007 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 42.0569 11.8955 18.7422 65.3716\n beta\_0 57.482 1.89225 53.7732 61.1907\n beta\_1 0.0240542 0.00600612 0.0122824 0.035826\n beta\_2 0 NA\n beta\_3 0 NA\n beta\_4 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 52 57.5 5 6.49 -1.89\n 77 5 66.8 59.3 7.56 6.49 2.57\n 153 5 59 61.2 4.85 6.49 -0.746\n 306 5 66 64.8 3 6.49 0.399\n 611 5 71.2 72.2 5.67 6.49 -0.338\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -51.964632 6 115.929265\n A2 -49.939758 10 119.879516\n A3 -51.964632 6 115.929265\n fitted -59.237804 3 124.475607\n R -65.433575 2 134.867151\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 30.9876 8 0.0001412\n Test 2 4.04975 4 0.3993\n Test 3 4.04975 4 0.3993\n Test 4 14.5463 3 0.002248\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 269.605\n\n\n BMDL = 182.885\n\n\n BMDU = 520.829\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 0 | Power | 4 | 2.19 | True | False | 2.696050e+02 | 1.828850e+02 | 5.084960e+02 | -999 | 124.475607 | 0.000141 | 0.399300 | 0.3993 | 0.002248 | 14.546300 | 3 | 3.990000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00225 < 0.1) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000\n611.000000 5 71.200000 5.674504 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-s92acyar.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-s92acyar.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The power is restricted to be greater than or equal to 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 29.38\n rho = 0 Specified\n control = 52\n slope = 4.08078\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha control slope\n\n alpha 1 3e-008 6.7e-009\n\n control 3e-008 1 -0.73\n\n slope 6.7e-009 -0.73 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 42.0569 11.8955 18.7422 65.3717\n control 57.482 1.89225 53.7732 61.1907\n slope 0.0240542 0.00600613 0.0122824 0.035826\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 52 57.5 5 6.49 -1.89\n 77 5 66.8 59.3 7.56 6.49 2.57\n 153 5 59 61.2 4.85 6.49 -0.746\n 306 5 66 64.8 3 6.49 0.399\n 611 5 71.2 72.2 5.67 6.49 -0.338\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -51.964632 6 115.929265\n A2 -49.939758 10 119.879516\n A3 -51.964632 6 115.929265\n fitted -59.237804 3 124.475607\n R -65.433575 2 134.867151\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 30.9876 8 0.0001412\n Test 2 4.04975 4 0.3993\n Test 3 4.04975 4 0.3993\n Test 4 14.5463 3 0.002248\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 269.605 \n\n\n BMDL = 182.885 \n\n\n BMDU = 508.496 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 0 | Hill | 5 | 2.18 | True | False | 3.138960e+01 | 7.978790e-05 | 2.337490e+02 | -999 | 123.059578 | 0.000141 | 0.399300 | 0.3993 | 0.003829 | 11.130300 | 2 | -1.420000e-01 | NaN | warning | BMD/BMDL ratio is greater than threshold (3.93e+05 > 5.0) | Goodness of fit p-value is less than threshold (0.00383 < 0.1)\nBMD/BMDL ratio is greater than threshold (3.93e+05 > 20.0) | NaN | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000\n611.000000 5 71.200000 5.674504 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-eyw3meca.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-eyw3meca.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:51 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n Power parameter restricted to be greater than 1\n A constant variance model is fit\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 29.38\n rho = 0 Specified\n intercept = 52\n v = 19.2\n n = 0.306054\n k = 104.054\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -n \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha intercept v k\n\n alpha 1 1.1e-006 -2e-006 -5.8e-007\n\n intercept 1.1e-006 1 -0.3 0.46\n\n v -2e-006 -0.3 1 0.65\n\n k -5.8e-007 0.46 0.65 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 36.6855 10.3762 16.3485 57.0225\n intercept 52.3854 2.88544 46.73 58.0407\n v 17.4826 4.88418 7.90974 27.0554\n n 1 NA\n k 59.2136 82.761 -102.995 221.422\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 52 52.4 5 6.06 -0.142\n 77 5 66.8 62.3 7.56 6.06 1.67\n 153 5 59 65 4.85 6.06 -2.21\n 306 5 66 67 3 6.06 -0.382\n 611 5 71.2 68.3 5.67 6.06 1.06\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -51.964632 6 115.929265\n A2 -49.939758 10 119.879516\n A3 -51.964632 6 115.929265\n fitted -57.529789 4 123.059578\n R -65.433575 2 134.867151\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 30.9876 8 0.0001412\n Test 2 4.04975 4 0.3993\n Test 3 4.04975 4 0.3993\n Test 4 11.1303 2 0.003829\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 31.3896\n\n BMDL = 7.97879e-005\n\n BMDU = 233.749\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 0 | Exponential-M2 | 6 | 1.11 | True | False | 2.939290e+02 | 2.069630e+02 | 5.315500e+02 | -999 | 124.756500 | 0.000141 | 0.399300 | 0.3993 | 0.00197 | 14.830000 | 3 | 4.866000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00197 < 0.1) | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000\n611.000000 5 71.200000 5.674504 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-tvy857a4.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:51 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha 3.15717 \n rho 0 Specified\n a 57.2958 \n b 0.000387527 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha 3.75026 12.0299\n a 57.776 1.82146\n b 0.000363863 8.9834e-005\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 52 5\n 77 5 66.8 7.563\n 153 5 59 4.848\n 306 5 66 3\n 611 5 71.2 5.675\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 57.78 6.522 -1.98\n 77 59.42 6.522 2.531\n 153 61.08 6.522 -0.7144\n 306 64.58 6.522 0.4866\n 611 72.16 6.522 -0.3293\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -51.96463 6 115.9293\n A2 -49.93976 10 119.8795\n A3 -51.96463 6 115.9293\n R -65.43358 2 134.8672\n 2 -59.37823 3 124.7565\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 30.99 8 0.0001412\n Test 2 4.05 4 0.3993\n Test 3 4.05 4 0.3993\n Test 4 14.83 3 0.00197\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 293.929\n\n BMDL = 206.963\n\n BMDU = 531.55\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 0 | Exponential-M3 | 7 | 1.11 | True | False | 2.939290e+02 | 2.069630e+02 | 5.315500e+02 | -999 | 124.756500 | 0.000141 | 0.399300 | 0.3993 | 0.00197 | 14.830000 | 3 | 4.866000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00197 < 0.1) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000\n611.000000 5 71.200000 5.674504 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-pyu1pi3x.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha 3.15717 \n rho 0 Specified\n a 57.2958 \n b 0.000387527 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha 3.75026 12.0299\n a 57.776 1.82146\n b 0.000363862 8.9834e-005\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 52 5\n 77 5 66.8 7.563\n 153 5 59 4.848\n 306 5 66 3\n 611 5 71.2 5.675\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 57.78 6.522 -1.98\n 77 59.42 6.522 2.531\n 153 61.08 6.522 -0.7144\n 306 64.58 6.522 0.4866\n 611 72.16 6.522 -0.3293\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -51.96463 6 115.9293\n A2 -49.93976 10 119.8795\n A3 -51.96463 6 115.9293\n R -65.43358 2 134.8672\n 3 -59.37823 3 124.7565\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 30.99 8 0.0001412\n Test 2 4.05 4 0.3993\n Test 3 4.05 4 0.3993\n Test 5a 14.83 3 0.00197\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 293.929\n\n BMDL = 206.963\n\n BMDU = 531.55\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 0 | Exponential-M4 | 8 | 1.11 | True | False | 8.905580e+01 | 4.026330e-01 | 3.608690e+02 | -999 | 124.551500 | 0.000141 | 0.399300 | 0.3993 | 0.001816 | 12.620000 | 2 | 2.467000e+00 | NaN | warning | BMD/BMDL ratio is greater than threshold (2.21e+02 > 5.0) | Goodness of fit p-value is less than threshold (0.00182 < 0.1)\nResidual of interest is greater than threshold (2.47 > 2.0)\nBMD/BMDL ratio is greater than threshold (2.21e+02 > 20.0) | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000\n611.000000 5 71.200000 5.674504 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-fi9p4xq9.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha 3.15717 \n rho 0 Specified\n a 49.4 \n b 0.00339903 \n c 1.51336 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha 3.66206 11.0143\n a 54.35 3.15921\n b 0.0055526 0.00575559\n c 1.29431 0.0859175\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 52 5\n 77 5 66.8 7.563\n 153 5 59 4.848\n 306 5 66 3\n 611 5 71.2 5.675\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 54.35 6.24 -0.8421\n 77 59.91 6.24 2.467\n 153 63.51 6.24 -1.615\n 306 67.42 6.24 -0.5092\n 611 69.81 6.24 0.4987\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -51.96463 6 115.9293\n A2 -49.93976 10 119.8795\n A3 -51.96463 6 115.9293\n R -65.43358 2 134.8672\n 4 -58.27574 4 124.5515\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 30.99 8 0.0001412\n Test 2 4.05 4 0.3993\n Test 3 4.05 4 0.3993\n Test 6a 12.62 2 0.001816\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is less than .1. Model 4 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 89.0558\n\n BMDL = 0.402633\n\n BMDU = 360.869\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 0 | Exponential-M5 | 9 | 1.11 | True | False | 8.905580e+01 | 3.515710e-01 | 3.608630e+02 | -999 | 124.551500 | 0.000141 | 0.399300 | 0.3993 | 0.001816 | 12.620000 | 2 | 2.467000e+00 | NaN | warning | BMD/BMDL ratio is greater than threshold (2.53e+02 > 5.0) | Goodness of fit p-value is less than threshold (0.00182 < 0.1)\nResidual of interest is greater than threshold (2.47 > 2.0)\nBMD/BMDL ratio is greater than threshold (2.53e+02 > 20.0) | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000\n611.000000 5 71.200000 5.674504 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-477acd5y.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:52 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha 3.15717 \n rho 0 Specified\n a 49.4 \n b 0.00339903 \n c 1.51336 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha 3.66206 11.0143\n a 54.35 3.15921\n b 0.0055526 0.00575559\n c 1.29431 0.0859175\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 52 5\n 77 5 66.8 7.563\n 153 5 59 4.848\n 306 5 66 3\n 611 5 71.2 5.675\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 54.35 6.24 -0.8421\n 77 59.91 6.24 2.467\n 153 63.51 6.24 -1.615\n 306 67.42 6.24 -0.5092\n 611 69.81 6.24 0.4987\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -51.96463 6 115.9293\n A2 -49.93976 10 119.8795\n A3 -51.96463 6 115.9293\n R -65.43358 2 134.8672\n 5 -58.27574 4 124.5515\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 30.99 8 0.0001412\n Test 2 4.05 4 0.3993\n Test 3 4.05 4 0.3993\n Test 7a 12.62 2 0.001816\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is less than .1. Model 5 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 89.0558\n\n BMDL = 0.351571\n\n BMDU = 360.863\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 1 | Linear | 0 | 2.21 | True | False | 2.016200e+02 | 1.181150e+02 | 6.809750e+02 | -999 | 102.028778 | 0.000843 | 0.259100 | 0.2591 | 0.001249 | 13.371100 | 2 | -8.620000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00125 < 0.1) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-c32090b5.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-c32090b5.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:57 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 28.675\n rho = 0 Specified\n beta\_0 = 56.5032\n beta\_1 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 3.9e-007 2.9e-007\n\n beta\_0 3.9e-007 1 -0.76\n\n beta\_1 2.9e-007 -0.76 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 44.7656 14.1561 17.0201 72.5111\n beta\_0 56.5032 2.31975 51.9566 61.0499\n beta\_1 0.0331848 0.0132301 0.00725418 0.0591153\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 52 56.5 5 6.69 -1.51\n 77 5 66.8 59.1 7.56 6.69 2.59\n 153 5 59 61.6 4.85 6.69 -0.862\n 306 5 66 66.7 3 6.69 -0.22\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -41.328821 5 92.657642\n A2 -39.317701 8 94.635403\n A3 -41.328821 5 92.657642\n fitted -48.014389 3 102.028778\n R -50.749493 2 105.498987\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 22.8636 6 0.0008435\n Test 2 4.02224 3 0.2591\n Test 3 4.02224 3 0.2591\n Test 4 13.3711 2 0.001249\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 201.62\n\n\n BMDL = 118.115\n\n\n BMDU = 680.975\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 1 | Polynomial-2 | 1 | 2.21 | True | False | 2.016200e+02 | 1.181150e+02 | 6.809750e+02 | -999 | 102.028778 | 0.000843 | 0.259100 | 0.2591 | 0.001249 | 13.371100 | 2 | -8.620000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00125 < 0.1) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-8aqakwp7.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-8aqakwp7.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:57 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 28.675\n rho = 0 Specified\n beta\_0 = 54.4356\n beta\_1 = 0\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -2e-007 1.6e-007\n\n beta\_0 -2e-007 1 -0.76\n\n beta\_1 1.6e-007 -0.76 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 44.7655 14.1561 17.0201 72.511\n beta\_0 56.5032 2.31975 51.9566 61.0499\n beta\_1 0.0331848 0.0132301 0.00725418 0.0591153\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 52 56.5 5 6.69 -1.51\n 77 5 66.8 59.1 7.56 6.69 2.59\n 153 5 59 61.6 4.85 6.69 -0.862\n 306 5 66 66.7 3 6.69 -0.22\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -41.328821 5 92.657642\n A2 -39.317701 8 94.635403\n A3 -41.328821 5 92.657642\n fitted -48.014389 3 102.028778\n R -50.749493 2 105.498987\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 22.8636 6 0.0008435\n Test 2 4.02224 3 0.2591\n Test 3 4.02224 3 0.2591\n Test 4 13.3711 2 0.001249\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 201.62\n\n\n BMDL = 118.115\n\n\n BMDU = 680.975\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 1 | Polynomial-3 | 2 | 2.21 | True | False | 2.016200e+02 | 1.181150e+02 | 6.809750e+02 | -999 | 102.028778 | 0.000843 | 0.259100 | 0.2591 | 0.001249 | 13.371100 | 2 | -8.620000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00125 < 0.1) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-g4ihsxio.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-g4ihsxio.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:57 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 28.675\n rho = 0 Specified\n beta\_0 = 52\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -1.3e-007 1.6e-007\n\n beta\_0 -1.3e-007 1 -0.76\n\n beta\_1 1.6e-007 -0.76 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 44.7656 14.1561 17.0201 72.511\n beta\_0 56.5032 2.31975 51.9566 61.0499\n beta\_1 0.0331848 0.0132301 0.00725417 0.0591153\n beta\_2 0 NA\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 52 56.5 5 6.69 -1.51\n 77 5 66.8 59.1 7.56 6.69 2.59\n 153 5 59 61.6 4.85 6.69 -0.862\n 306 5 66 66.7 3 6.69 -0.22\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -41.328821 5 92.657642\n A2 -39.317701 8 94.635403\n A3 -41.328821 5 92.657642\n fitted -48.014389 3 102.028778\n R -50.749493 2 105.498987\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 22.8636 6 0.0008435\n Test 2 4.02224 3 0.2591\n Test 3 4.02224 3 0.2591\n Test 4 13.3711 2 0.001249\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 201.62\n\n\n BMDL = 118.115\n\n\n BMDU = 680.975\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 1 | Polynomial-4 | 3 | 2.21 | True | False | 2.016200e+02 | 1.181150e+02 | 6.809750e+02 | -999 | 102.028778 | 0.000843 | 0.259100 | 0.2591 | 0.001249 | 13.371100 | 2 | -8.620000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00125 < 0.1) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-lrqjuiny.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-lrqjuiny.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:57 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 28.675\n rho = 0 Specified\n beta\_0 = -52.7739\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = 0\n beta\_4 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 3e-007 -4e-007\n\n beta\_0 3e-007 1 -0.76\n\n beta\_1 -4e-007 -0.76 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 44.7655 14.1561 17.0201 72.511\n beta\_0 56.5032 2.31975 51.9566 61.0499\n beta\_1 0.0331847 0.0132301 0.00725415 0.0591153\n beta\_2 0 NA\n beta\_3 0 NA\n beta\_4 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 52 56.5 5 6.69 -1.51\n 77 5 66.8 59.1 7.56 6.69 2.59\n 153 5 59 61.6 4.85 6.69 -0.862\n 306 5 66 66.7 3 6.69 -0.22\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -41.328821 5 92.657642\n A2 -39.317701 8 94.635403\n A3 -41.328821 5 92.657642\n fitted -48.014389 3 102.028778\n R -50.749493 2 105.498987\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 22.8636 6 0.0008435\n Test 2 4.02224 3 0.2591\n Test 3 4.02224 3 0.2591\n Test 4 13.3711 2 0.001249\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 201.62\n\n\n BMDL = 118.115\n\n\n BMDU = 680.975\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 1 | Power | 4 | 2.19 | True | False | 2.016200e+02 | 1.181150e+02 | 6.809750e+02 | -999 | 102.028778 | 0.000843 | 0.259100 | 0.2591 | 0.001249 | 13.371100 | 2 | -8.620000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00125 < 0.1) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-qeq0cwwh.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-qeq0cwwh.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:57 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The power is restricted to be greater than or equal to 1\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 28.675\n rho = 0 Specified\n control = 52\n slope = 13.7486\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha control slope\n\n alpha 1 1.5e-008 -1.8e-008\n\n control 1.5e-008 1 -0.76\n\n slope -1.8e-008 -0.76 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 44.7656 14.1561 17.0201 72.511\n control 56.5032 2.31975 51.9566 61.0499\n slope 0.0331847 0.0132301 0.00725417 0.0591153\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 52 56.5 5 6.69 -1.51\n 77 5 66.8 59.1 7.56 6.69 2.59\n 153 5 59 61.6 4.85 6.69 -0.862\n 306 5 66 66.7 3 6.69 -0.22\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -41.328821 5 92.657642\n A2 -39.317701 8 94.635403\n A3 -41.328821 5 92.657642\n fitted -48.014389 3 102.028778\n R -50.749493 2 105.498987\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 22.8636 6 0.0008435\n Test 2 4.02224 3 0.2591\n Test 3 4.02224 3 0.2591\n Test 4 13.3711 2 0.001249\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 201.62 \n\n\n BMDL = 118.115 \n\n\n BMDU = 680.975 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 1 | Hill | 5 | 2.18 | True | False | 2.770690e-13 | 2.770690e-13 | 2.770700e-13 | -999 | 97.406175 | 0.000843 | 0.259100 | 0.2591 | 0.009382 | 6.748530 | 1 | -3.420000e-07 | NaN | warning | Minimum dose/BMD ratio is greater than threshold (2.78e+14 > 3.0) | Goodness of fit p-value is less than threshold (0.00938 < 0.1) | NaN | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-siquiglq.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-siquiglq.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:57 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n Power parameter restricted to be greater than 1\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 28.675\n rho = 0 Specified\n intercept = 52\n v = 14.8\n n = 1.46883\n k = 115.5\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -k \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha intercept v n\n\n alpha 1 1.1e-007 -9.8e-008 -4.5e-006\n\n intercept 1.1e-007 1 -0.87 -3e-006\n\n v -9.8e-008 -0.87 1 -1.8e-005\n\n n -4.5e-006 -3e-006 -1.8e-005 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 32.1467 10.1657 12.2223 52.071\n intercept 52 2.53561 47.0303 56.9697\n v 11.9333 2.92787 6.19481 17.6719\n n 1.00274 3224.29 -6318.49 6320.49\n k 3.06e-013 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 52 52 5 5.67 -3.42e-007\n 77 5 66.8 63.9 7.56 5.67 1.13\n 153 5 59 63.9 4.85 5.67 -1.95\n 306 5 66 63.9 3 5.67 0.815\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -41.328821 5 92.657642\n A2 -39.317701 8 94.635403\n A3 -41.328821 5 92.657642\n fitted -44.703088 4 97.406175\n R -50.749493 2 105.498987\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 22.8636 6 0.0008435\n Test 2 4.02224 3 0.2591\n Test 3 4.02224 3 0.2591\n Test 4 6.74853 1 0.009382\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 2.77069e-013\n\n BMDL = 2.77069e-013\n\n BMDU = 2.7707e-013\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 1 | Exponential-M2 | 6 | 1.11 | True | False | 2.130840e+02 | 1.305120e+02 | 7.002960e+02 | -999 | 102.175900 | 0.000843 | 0.259100 | 0.2591 | 0.00116 | 13.520000 | 2 | -8.173000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00116 < 0.1) | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-sbpt61wi.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:56 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha 3.13288 \n rho 0 Specified\n a 56.189 \n b 0.000569503 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha 3.8088 14.2607\n a 56.7094 2.24895\n b 0.000525213 0.000210592\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 52 5\n 77 5 66.8 7.563\n 153 5 59 4.848\n 306 5 66 3\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 56.71 6.715 -1.568\n 77 59.05 6.715 2.581\n 153 61.45 6.715 -0.8173\n 306 66.6 6.715 -0.1987\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -41.32882 5 92.65764\n A2 -39.3177 8 94.6354\n A3 -41.32882 5 92.65764\n R -50.74949 2 105.499\n 2 -48.08797 3 102.1759\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 22.86 6 0.0008435\n Test 2 4.022 3 0.2591\n Test 3 4.022 3 0.2591\n Test 4 13.52 2 0.00116\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 213.084\n\n BMDL = 130.512\n\n BMDU = 700.296\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 1 | Exponential-M3 | 7 | 1.11 | True | False | 2.130840e+02 | 1.305120e+02 | 7.002960e+02 | -999 | 102.175900 | 0.000843 | 0.259100 | 0.2591 | 0.00116 | 13.520000 | 2 | -8.173000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00116 < 0.1) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-kl1mljtm.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:57 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha 3.13288 \n rho 0 Specified\n a 56.189 \n b 0.000569503 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha 3.8088 14.2607\n a 56.7094 2.24895\n b 0.000525214 0.000210592\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 52 5\n 77 5 66.8 7.563\n 153 5 59 4.848\n 306 5 66 3\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 56.71 6.715 -1.568\n 77 59.05 6.715 2.581\n 153 61.45 6.715 -0.8173\n 306 66.6 6.715 -0.1987\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -41.32882 5 92.65764\n A2 -39.3177 8 94.6354\n A3 -41.32882 5 92.65764\n R -50.74949 2 105.499\n 3 -48.08797 3 102.1759\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 22.86 6 0.0008435\n Test 2 4.022 3 0.2591\n Test 3 4.022 3 0.2591\n Test 5a 13.52 2 0.00116\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 213.084\n\n BMDL = 130.512\n\n BMDU = 700.296\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 1 | Exponential-M4 | 8 | 1.11 | True | False | 1.065570e+00 | 1.659230e-03 | 5.660530e+01 | -999 | 97.406180 | 0.000843 | 0.259100 | 0.2591 | 0.009382 | 6.749000 | 1 | 9.933000e-08 | NaN | warning | BMD/BMDL ratio is greater than threshold (6.42e+02 > 5.0)\nMinimum dose/BMD ratio is greater than threshold (72.3 > 3.0) | Goodness of fit p-value is less than threshold (0.00938 < 0.1)\nBMD/BMDL ratio is greater than threshold (6.42e+02 > 20.0) | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-w4ay9i5a.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:57 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha 3.13288 \n rho 0 Specified\n a 49.4 \n b 0.0059263 \n c 1.41984 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha 3.47031 10.1657\n a 52 2.53561\n b 0.604927 7.33008e+007\n c 1.22949 0.066233\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 52 5\n 77 5 66.8 7.563\n 153 5 59 4.848\n 306 5 66 3\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 52 5.67 9.933e-008\n 77 63.93 5.67 1.131\n 153 63.93 5.67 -1.946\n 306 63.93 5.67 0.8151\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -41.32882 5 92.65764\n A2 -39.3177 8 94.6354\n A3 -41.32882 5 92.65764\n R -50.74949 2 105.499\n 4 -44.70309 4 97.40618\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 22.86 6 0.0008435\n Test 2 4.022 3 0.2591\n Test 3 4.022 3 0.2591\n Test 6a 6.749 1 0.009382\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is less than .1. Model 4 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 1.06557\n\n BMDL = 0.00165923\n\n BMDU = 56.6053\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 1 | Exponential-M5 | 9 | 1.11 | True | False | 1.115610e+01 | 3.992100e-02 | 7.537020e+01 | -999 | 99.406180 | 0.000843 | 0.259100 | 0.2591 | -999 | 6.749000 | 0 | -3.169000e-10 | NaN | warning | BMD/BMDL ratio is greater than threshold (2.79e+02 > 5.0)\nMinimum dose/BMD ratio is greater than threshold (6.9 > 3.0) | BMD/BMDL ratio is greater than threshold (2.79e+02 > 20.0)\nZero degrees of freedom; saturated model | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680\n306.000000 5 66.000000 3.000000 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-0fvvr86\_.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:57 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha 3.13288 \n rho 0 Specified\n a 49.4 \n b 0.0059263 \n c 1.41984 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha 3.47031 10.1657\n a 52 2.53561\n b 0.0712123 1155.31\n c 1.22949 0.066233\n d 1.90841 18385.7\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 52 5\n 77 5 66.8 7.563\n 153 5 59 4.848\n 306 5 66 3\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 52 5.67 -3.169e-010\n 77 63.93 5.67 1.131\n 153 63.93 5.67 -1.946\n 306 63.93 5.67 0.8151\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -41.32882 5 92.65764\n A2 -39.3177 8 94.6354\n A3 -41.32882 5 92.65764\n R -50.74949 2 105.499\n 5 -44.70309 5 99.40618\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 22.86 6 0.0008435\n Test 2 4.022 3 0.2591\n Test 3 4.022 3 0.2591\n Test 7a 6.749 0 N/A\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n Degrees of freedom for Test 7a are less than or equal to 0.\n The Chi-Square test for fit is not valid.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 11.1561\n\n BMDL = 0.039921\n\n BMDU = 75.3702\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 2 | Linear | 0 | 2.21 | True | False | 1.630710e+02 | 7.585610e+01 | 2.340900e+08 | -999 | 81.499545 | 0.008003 | 0.517400 | 0.5174 | 0.001249 | 10.416800 | 1 | -1.130000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00125 < 0.1)\nBMD/high dose ratio is greater than threshold (1.07 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (1.5 > 1.5) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 3 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-2giga8ch.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-2giga8ch.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:59 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 35.2333\n rho = 0 Specified\n beta\_0 = 55.7344\n beta\_1 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 2.8e-007 -1.7e-006\n\n beta\_0 2.8e-007 1 -0.78\n\n beta\_1 -1.7e-006 -0.78 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 56.447 20.6115 16.0492 96.8449\n beta\_0 55.7344 3.07122 49.7149 61.7539\n beta\_1 0.0460726 0.0310568 -0.0147975 0.106943\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 52 55.7 5 7.51 -1.11\n 77 5 66.8 59.3 7.56 7.51 2.24\n 153 5 59 62.8 4.85 7.51 -1.13\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -32.541368 4 73.082736\n A2 -31.882499 6 75.764998\n A3 -32.541368 4 73.082736\n fitted -37.749773 3 81.499545\n R -38.776557 2 81.553114\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 13.7881 4 0.008003\n Test 2 1.31774 2 0.5174\n Test 3 1.31774 2 0.5174\n Test 4 10.4168 1 0.001249\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 163.071\n\n\n BMDL = 75.8561\n\n\n BMDU = 2.3409e+008\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 2 | Polynomial-2 | 1 | 2.21 | True | False | 1.630700e+02 | 7.585610e+01 | -9.990000e+02 | -999 | 81.499545 | 0.008003 | 0.517400 | 0.5174 | 0.001249 | 10.416800 | 1 | -1.130000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00125 < 0.1)\nBMD/high dose ratio is greater than threshold (1.07 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (1.5 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 3 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-j5bbsz10.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-j5bbsz10.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:59 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 35.2333\n rho = 0 Specified\n beta\_0 = 52\n beta\_1 = 0\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -1.2e-006 1.6e-006\n\n beta\_0 -1.2e-006 1 -0.78\n\n beta\_1 1.6e-006 -0.78 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 56.4469 20.6114 16.0492 96.8445\n beta\_0 55.7344 3.07121 49.7149 61.7539\n beta\_1 0.0460729 0.0310567 -0.0147971 0.106943\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 52 55.7 5 7.51 -1.11\n 77 5 66.8 59.3 7.56 7.51 2.24\n 153 5 59 62.8 4.85 7.51 -1.13\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -32.541368 4 73.082736\n A2 -31.882499 6 75.764998\n A3 -32.541368 4 73.082736\n fitted -37.749773 3 81.499545\n R -38.776557 2 81.553114\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 13.7881 4 0.008003\n Test 2 1.31774 2 0.5174\n Test 3 1.31774 2 0.5174\n Test 4 10.4168 1 0.001249\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 163.07\n\n\n BMDL = 75.8561\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 2 | Polynomial-3 | 2 | 2.21 | True | False | 1.630710e+02 | 7.585610e+01 | -9.990000e+02 | -999 | 81.499545 | 0.008003 | 0.517400 | 0.5174 | 0.001249 | 10.416800 | 1 | -1.130000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00125 < 0.1)\nBMD/high dose ratio is greater than threshold (1.07 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (1.5 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 3 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-l19zijoa.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-l19zijoa.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:59 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 35.2333\n rho = 0 Specified\n beta\_0 = -11983.5\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 2.7e-007 -4.8e-007\n\n beta\_0 2.7e-007 1 -0.78\n\n beta\_1 -4.8e-007 -0.78 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 56.4471 20.6116 16.0492 96.845\n beta\_0 55.7344 3.07122 49.7149 61.7539\n beta\_1 0.0460728 0.0310568 -0.0147974 0.106943\n beta\_2 0 NA\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 52 55.7 5 7.51 -1.11\n 77 5 66.8 59.3 7.56 7.51 2.24\n 153 5 59 62.8 4.85 7.51 -1.13\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -32.541368 4 73.082736\n A2 -31.882499 6 75.764998\n A3 -32.541368 4 73.082736\n fitted -37.749773 3 81.499545\n R -38.776557 2 81.553114\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 13.7881 4 0.008003\n Test 2 1.31774 2 0.5174\n Test 3 1.31774 2 0.5174\n Test 4 10.4168 1 0.001249\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 163.071\n\n\n BMDL = 75.8561\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 2 | Polynomial-4 | 3 | 2.21 | True | False | 1.630720e+02 | 7.585610e+01 | -9.990000e+02 | -999 | 81.499545 | 0.008003 | 0.517400 | 0.5174 | 0.001249 | 10.416800 | 1 | -1.130000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00125 < 0.1)\nBMD/high dose ratio is greater than threshold (1.07 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (1.5 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 3 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-6zamorwu.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-6zamorwu.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:59 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be positive\n A constant variance model is fit\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 35.2333\n rho = 0 Specified\n beta\_0 = 69.732\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = 0\n beta\_4 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 1.6e-006 -2e-006\n\n beta\_0 1.6e-006 1 -0.78\n\n beta\_1 -2e-006 -0.78 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 56.4472 20.6117 16.0491 96.8453\n beta\_0 55.7344 3.07122 49.7149 61.7539\n beta\_1 0.0460726 0.0310568 -0.0147976 0.106943\n beta\_2 0 NA\n beta\_3 0 NA\n beta\_4 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 52 55.7 5 7.51 -1.11\n 77 5 66.8 59.3 7.56 7.51 2.24\n 153 5 59 62.8 4.85 7.51 -1.13\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -32.541368 4 73.082736\n A2 -31.882499 6 75.764998\n A3 -32.541368 4 73.082736\n fitted -37.749773 3 81.499545\n R -38.776557 2 81.553114\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 13.7881 4 0.008003\n Test 2 1.31774 2 0.5174\n Test 3 1.31774 2 0.5174\n Test 4 10.4168 1 0.001249\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 163.072\n\n\n BMDL = 75.8561\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 2 | Power | 4 | 2.19 | True | False | 1.630710e+02 | 7.585610e+01 | 1.530000e+06 | -999 | 81.499545 | 0.008003 | 0.517400 | 0.5174 | 0.001249 | 10.416800 | 1 | -1.130000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00125 < 0.1)\nBMD/high dose ratio is greater than threshold (1.07 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (1.5 > 1.5) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-6gloxgp\_.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-6gloxgp\_.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:59 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The power is restricted to be greater than or equal to 1\n A constant variance model is fit\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 35.2333\n rho = 0 Specified\n control = 52\n slope = 1687.82\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha control slope\n\n alpha 1 -2.1e-009 -1.4e-009\n\n control -2.1e-009 1 -0.78\n\n slope -1.4e-009 -0.78 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 56.447 20.6115 16.0492 96.8449\n control 55.7344 3.07122 49.7149 61.7539\n slope 0.0460728 0.0310568 -0.0147973 0.106943\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 52 55.7 5 7.51 -1.11\n 77 5 66.8 59.3 7.56 7.51 2.24\n 153 5 59 62.8 4.85 7.51 -1.13\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -32.541368 4 73.082736\n A2 -31.882499 6 75.764998\n A3 -32.541368 4 73.082736\n fitted -37.749773 3 81.499545\n R -38.776557 2 81.553114\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 13.7881 4 0.008003\n Test 2 1.31774 2 0.5174\n Test 3 1.31774 2 0.5174\n Test 4 10.4168 1 0.001249\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 163.071 \n\n\n BMDL = 75.8561 \n\n\n BMDU = 1.53e+006 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 2 | Hill | 5 | 2.18 | True | False | 2.770690e-13 | 2.770690e-13 | 2.770700e-13 | -999 | 97.406175 | 0.000843 | 0.259100 | 0.2591 | 0.009382 | 6.748530 | 1 | -3.420000e-07 | NaN | warning | Minimum dose/BMD ratio is greater than threshold (2.78e+14 > 3.0) | Goodness of fit p-value is less than threshold (0.00938 < 0.1) | NaN | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-siquiglq.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-siquiglq.plt\n \t\t\t\t\t\t\tTue Jul 06 12:39:57 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n Power parameter restricted to be greater than 1\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 28.675\n rho = 0 Specified\n intercept = 52\n v = 14.8\n n = 1.46883\n k = 115.5\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -k \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha intercept v n\n\n alpha 1 1.1e-007 -9.8e-008 -4.5e-006\n\n intercept 1.1e-007 1 -0.87 -3e-006\n\n v -9.8e-008 -0.87 1 -1.8e-005\n\n n -4.5e-006 -3e-006 -1.8e-005 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 32.1467 10.1657 12.2223 52.071\n intercept 52 2.53561 47.0303 56.9697\n v 11.9333 2.92787 6.19481 17.6719\n n 1.00274 3224.29 -6318.49 6320.49\n k 3.06e-013 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 52 52 5 5.67 -3.42e-007\n 77 5 66.8 63.9 7.56 5.67 1.13\n 153 5 59 63.9 4.85 5.67 -1.95\n 306 5 66 63.9 3 5.67 0.815\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -41.328821 5 92.657642\n A2 -39.317701 8 94.635403\n A3 -41.328821 5 92.657642\n fitted -44.703088 4 97.406175\n R -50.749493 2 105.498987\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 22.8636 6 0.0008435\n Test 2 4.02224 3 0.2591\n Test 3 4.02224 3 0.2591\n Test 4 6.74853 1 0.009382\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 2.77069e-013\n\n BMDL = 2.77069e-013\n\n BMDU = 2.7707e-013\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 2 | Exponential-M2 | 6 | 1.11 | True | False | 1.729660e+02 | 8.397180e+01 | 1.530000e+06 | -999 | 81.630800 | 0.008003 | 0.517400 | 0.5174 | 0.001163 | 10.550000 | 1 | -1.069000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00116 < 0.1)\nBMD/high dose ratio is greater than threshold (1.13 > 1.0) | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-kk2jo54c.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:59 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha 3.33885 \n rho 0 Specified\n a 55.3201 \n b 0.000830772 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha 4.04205 20.7927\n a 55.9815 2.98984\n b 0.000731083 0.000511415\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 52 5\n 77 5 66.8 7.563\n 153 5 59 4.848\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 55.98 7.546 -1.18\n 77 59.22 7.546 2.245\n 153 62.61 7.546 -1.069\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -32.54137 4 73.08274\n A2 -31.8825 6 75.765\n A3 -32.54137 4 73.08274\n R -38.77656 2 81.55311\n 2 -37.8154 3 81.6308\n\n\n Additive constant for all log-likelihoods = -13.78. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 13.79 4 0.008003\n Test 2 1.318 2 0.5174\n Test 3 1.318 2 0.5174\n Test 4 10.55 1 0.001163\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 172.966\n\n BMDL = 83.9718\n\n BMDU = 1.53e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 2 | Exponential-M3 | 7 | 1.11 | True | False | 1.729660e+02 | 8.397180e+01 | -9.990000e+02 | -999 | 81.630800 | 0.008003 | 0.517400 | 0.5174 | 0.001163 | 10.550000 | 1 | -1.069000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00116 < 0.1)\nBMD/high dose ratio is greater than threshold (1.13 > 1.0) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-3emt8qz5.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:59 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha 3.33885 \n rho 0 Specified\n a 55.3201 \n b 0.000830772 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha 4.04205 20.7927\n a 55.9815 2.98983\n b 0.000731083 0.000511415\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 52 5\n 77 5 66.8 7.563\n 153 5 59 4.848\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 55.98 7.546 -1.18\n 77 59.22 7.546 2.245\n 153 62.61 7.546 -1.069\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -32.54137 4 73.08274\n A2 -31.8825 6 75.765\n A3 -32.54137 4 73.08274\n R -38.77656 2 81.55311\n 3 -37.8154 3 81.6308\n\n\n Additive constant for all log-likelihoods = -13.78. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 13.79 4 0.008003\n Test 2 1.318 2 0.5174\n Test 3 1.318 2 0.5174\n Test 5a 10.55 1 0.001163\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 172.966\n\n BMDL = 83.9718\n\n BMDU = Bad\_Completion\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 2 | Exponential-M4 | 8 | 1.11 | True | False | 3.478920e+00 | 7.479800e-03 | 1.530000e+06 | -999 | 77.692190 | 0.008003 | 0.517400 | 0.5174 | -999 | 4.609000 | 0 | -6.114000e-08 | NaN | warning | BMD/BMDL ratio is greater than threshold (4.65e+02 > 5.0)\nMinimum dose/BMD ratio is greater than threshold (22.1 > 3.0) | BMD/BMDL ratio is greater than threshold (4.65e+02 > 20.0)\nZero degrees of freedom; saturated model | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-g43uren5.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:59 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha 3.33885 \n rho 0 Specified\n a 49.4 \n b 0.00803402 \n c 1.41984 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha 3.64615 13.9949\n a 52 2.76863\n b 0.24124 59.587\n c 1.20962 0.0746004\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 52 5\n 77 5 66.8 7.563\n 153 5 59 4.848\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 52 6.191 -6.114e-008\n 77 62.9 6.191 1.409\n 153 62.9 6.191 -1.409\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -32.54137 4 73.08274\n A2 -31.8825 6 75.765\n A3 -32.54137 4 73.08274\n R -38.77656 2 81.55311\n 4 -34.84609 4 77.69219\n\n\n Additive constant for all log-likelihoods = -13.78. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 13.79 4 0.008003\n Test 2 1.318 2 0.5174\n Test 3 1.318 2 0.5174\n Test 6a 4.609 0 N/A\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n Degrees of freedom for Test 6a are less than or equal to 0.\n The Chi-Square test for fit is not valid.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 3.47892\n\n BMDL = 0.0074798\n\n BMDU = 1.53e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | HDL Cholesterol | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 2.2360679774997898,3.3823069050575527,2.16794833886788,1.3416407864998738,2.5377155080899039 | 2,1,1,2,2 | 1,1,1,1,1 | SD | day | NaN | 165 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: HDL Cholesterol | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 6 | 2 | Exponential-M5 | 9 | 1.11 | True | False | 1.115610e+01 | 3.992100e-02 | 7.537020e+01 | -999 | 99.406180 | 0.000843 | 0.259100 | 0.2591 | -999 | 6.749000 | 0 | -3.169000e-10 | NaN | warning | BMD/BMDL ratio is greater than threshold (2.79e+02 > 5.0)\nMinimum dose/BMD ratio is greater than threshold (6.9 > 3.0) | BMD/BMDL ratio is greater than threshold (2.79e+02 > 20.0)\nZero degrees of freedom; saturated model | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 52.000000 5.000000\n77.000000 5 66.800000 7.563068\n153.000000 5 59.000000 4.847680 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-0fvvr86\_.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:39:57 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha 3.13288 \n rho 0 Specified\n a 49.4 \n b 0.0059263 \n c 1.41984 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha 3.47031 10.1657\n a 52 2.53561\n b 0.0712123 1155.31\n c 1.22949 0.066233\n d 1.90841 18385.7\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 52 5\n 77 5 66.8 7.563\n 153 5 59 4.848\n 306 5 66 3\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 52 5.67 -3.169e-010\n 77 63.93 5.67 1.131\n 153 63.93 5.67 -1.946\n 306 63.93 5.67 0.8151\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -41.32882 5 92.65764\n A2 -39.3177 8 94.6354\n A3 -41.32882 5 92.65764\n R -50.74949 2 105.499\n 5 -44.70309 5 99.40618\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 22.86 6 0.0008435\n Test 2 4.022 3 0.2591\n Test 3 4.022 3 0.2591\n Test 7a 6.749 0 N/A\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n Degrees of freedom for Test 7a are less than or equal to 0.\n The Chi-Square test for fit is not valid.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 11.1561\n\n BMDL = 0.039921\n\n BMDU = 75.3702\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 0 | Linear | 0 | 2.21 | True | False | 6.655900e+02 | 3.303320e+02 | 3.586730e+03 | -999 | 87.750181 | 0.012380 | 0.070000 | 0.2890 | 0.01133 | 11.075300 | 3 | 8.000000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0113 < 0.1)\nBMD/high dose ratio is greater than threshold (1.09 > 1.0) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663\n611.000000 5 10.040000 2.762788 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-oq9o1yg0.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-oq9o1yg0.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:04 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.16654\n rho = 0\n beta\_0 = 13.232\n beta\_1 = -0.00552734\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.023 -0.025\n\n rho -1 1 -0.023 0.026\n\n beta\_0 0.023 -0.023 1 -0.79\n\n beta\_1 -0.025 0.026 -0.79 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -5.3906 6.73968 -18.6001 7.81893\n rho 3.0609 2.71897 -2.26818 8.38998\n beta\_0 13.1589 0.952522 11.292 15.0258\n beta\_1 -0.00523777 0.00249838 -0.0101345 -0.000341029\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 15 13.2 3.36 3.49 1.16\n 77 5 10 12.8 1.26 3.32 -1.83\n 153 5 13.4 12.4 4.45 3.17 0.764\n 306 5 11.3 11.6 1.81 2.86 -0.169\n 611 5 10 9.96 2.76 2.28 0.08\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -36.792409 6 85.584818\n A2 -32.459270 10 84.918540\n A3 -34.337454 7 82.674909\n fitted -39.875091 4 87.750181\n R -42.211766 2 88.423532\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 19.505 8 0.01238\n Test 2 8.66628 4 0.07\n Test 3 3.75637 3 0.289\n Test 4 11.0753 3 0.01133\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 665.59\n\n\n BMDL = 330.332\n\n\n BMDU = 3586.73\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 0 | Polynomial-2 | 1 | 2.21 | True | False | 6.655880e+02 | 3.303320e+02 | 3.586730e+03 | -999 | 87.750181 | 0.012380 | 0.070000 | 0.2890 | 0.01133 | 11.075300 | 3 | 8.000000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0113 < 0.1)\nBMD/high dose ratio is greater than threshold (1.09 > 1.0) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663\n611.000000 5 10.040000 2.762788 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-sb7lspzl.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-sb7lspzl.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:04 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.16654\n rho = 0\n beta\_0 = 13.6192\n beta\_1 = -0.0109135\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.023 -0.025\n\n rho -1 1 -0.023 0.026\n\n beta\_0 0.023 -0.023 1 -0.79\n\n beta\_1 -0.025 0.026 -0.79 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -5.39055 6.73967 -18.6001 7.81896\n rho 3.06088 2.71896 -2.26819 8.38995\n beta\_0 13.1589 0.952521 11.292 15.0258\n beta\_1 -0.00523778 0.00249839 -0.0101345 -0.000341039\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 15 13.2 3.36 3.49 1.16\n 77 5 10 12.8 1.26 3.32 -1.83\n 153 5 13.4 12.4 4.45 3.17 0.764\n 306 5 11.3 11.6 1.81 2.86 -0.169\n 611 5 10 9.96 2.76 2.28 0.08\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -36.792409 6 85.584818\n A2 -32.459270 10 84.918540\n A3 -34.337454 7 82.674909\n fitted -39.875091 4 87.750181\n R -42.211766 2 88.423532\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 19.505 8 0.01238\n Test 2 8.66628 4 0.07\n Test 3 3.75637 3 0.289\n Test 4 11.0753 3 0.01133\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 665.588\n\n\n BMDL = 330.332\n\n\n BMDU = 3586.73\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 0 | Polynomial-3 | 2 | 2.21 | True | False | 6.655880e+02 | 3.303320e+02 | 3.586730e+03 | -999 | 87.750181 | 0.012380 | 0.070000 | 0.2890 | 0.01133 | 11.075300 | 3 | 8.000000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0113 < 0.1)\nBMD/high dose ratio is greater than threshold (1.09 > 1.0) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663\n611.000000 5 10.040000 2.762788 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-qc\_ssd8q.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-qc\_ssd8q.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:04 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.16654\n rho = 0\n beta\_0 = 14.2343\n beta\_1 = -0.0346348\n beta\_2 = 0\n beta\_3 = -1.38164e-007\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.023 -0.025\n\n rho -1 1 -0.023 0.026\n\n beta\_0 0.023 -0.023 1 -0.79\n\n beta\_1 -0.025 0.026 -0.79 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -5.39055 6.73967 -18.6001 7.81896\n rho 3.06088 2.71896 -2.26819 8.38995\n beta\_0 13.1589 0.952521 11.292 15.0258\n beta\_1 -0.00523778 0.00249839 -0.0101345 -0.000341039\n beta\_2 0 NA\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 15 13.2 3.36 3.49 1.16\n 77 5 10 12.8 1.26 3.32 -1.83\n 153 5 13.4 12.4 4.45 3.17 0.764\n 306 5 11.3 11.6 1.81 2.86 -0.169\n 611 5 10 9.96 2.76 2.28 0.08\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -36.792409 6 85.584818\n A2 -32.459270 10 84.918540\n A3 -34.337454 7 82.674909\n fitted -39.875091 4 87.750181\n R -42.211766 2 88.423532\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 19.505 8 0.01238\n Test 2 8.66628 4 0.07\n Test 3 3.75637 3 0.289\n Test 4 11.0753 3 0.01133\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 665.588\n\n\n BMDL = 330.332\n\n\n BMDU = 3586.73\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 0 | Polynomial-4 | 3 | 2.21 | True | False | 3.700200e+03 | 2.235770e+02 | -9.990000e+02 | -999 | 92.423453 | 0.012380 | 0.070000 | 0.2890 | 0.001277 | 15.748500 | 3 | -1.310000e+00 | THE MODEL HAS PROBABLY NOT CONVERGED!!!\nTHIS USUALLY MEANS THE MODEL HAS NOT CONVERGED! | warning | BMD/BMDL ratio is greater than threshold (16.6 > 5.0)\nWarning(s): THE MODEL HAS PROBABLY NOT CONVERGED!!!; THIS USUALLY MEANS THE MODEL HAS NOT CONVERGED! | Goodness of fit p-value is less than threshold (0.00128 < 0.1)\nBMD/high dose ratio is greater than threshold (6.06 > 1.0)\nResidual at lowest dose is greater than threshold (2.04 > 2.0) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663\n611.000000 5 10.040000 2.762788 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-elk831uz.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-elk831uz.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:04 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.16654\n rho = 0\n beta\_0 = 14.96\n beta\_1 = -0.177394\n beta\_2 = 0\n beta\_3 = -6.37535e-006\n beta\_4 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_1 -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_4\n\n lalpha 1 -1 1.4 NA \n\n rho -1 1 -1.4 NA \n\n beta\_0 1.4 -1.4 1 NA \n\n beta\_4 NA NA NA NA \n\n\nNA - This parameter's variance has been estimated as zero or less.\nTHE MODEL HAS PROBABLY NOT CONVERGED!!!\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 81.1034 NA NA NA\n rho -31.7174 NA NA NA\n beta\_0 11.9672 NA NA NA\n beta\_1 -0 NA\n beta\_2 -5.96111e-028 NA\n beta\_3 -3.18265e-031 NA\n beta\_4 -1.74964e-014 NA NA NA\n\nAt least some variance estimates are negative.\nTHIS USUALLY MEANS THE MODEL HAS NOT CONVERGED!\nTry again from another starting point.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 15 12 3.36 3.28 2.04\n 77 5 10 12 1.26 3.28 -1.31\n 153 5 13.4 12 4.45 3.28 1\n 306 5 11.3 12 1.81 3.28 -0.427\n 611 5 10 12 2.76 3.29 -1.31\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -36.792409 6 85.584818\n A2 -32.459270 10 84.918540\n A3 -34.337454 7 82.674909\n fitted -42.211726 4 92.423453\n R -42.211766 2 88.423532\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 19.505 8 0.01238\n Test 2 8.66628 4 0.07\n Test 3 3.75637 3 0.289\n Test 4 15.7485 3 0.001277\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 3700.2\n\n\n BMDL = 223.577\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 0 | Power | 4 | 2.19 | True | False | 6.655890e+02 | 3.303320e+02 | 3.586730e+03 | -999 | 87.750181 | 0.012380 | 0.070000 | 0.2890 | 0.01133 | 11.075300 | 3 | 8.000000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0113 < 0.1)\nBMD/high dose ratio is greater than threshold (1.09 > 1.0) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663\n611.000000 5 10.040000 2.762788 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-mzrvq2ue.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-mzrvq2ue.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:04 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n The power is restricted to be greater than or equal to 1\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.16654\n rho = 0\n control = 10.04\n slope = 3644.99\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho control slope\n\n lalpha 1 -1 0.37 -0.53\n\n rho -1 1 -0.39 0.53\n\n control 0.37 -0.39 1 -0.79\n\n slope -0.53 0.53 -0.79 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -5.39055 7.95474 -20.9816 10.2005\n rho 3.06088 3.21327 -3.23702 9.35878\n control 13.1589 0.951398 11.2942 15.0236\n slope -0.00523778 0.00248422 -0.0101068 -0.000368795\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 15 13.2 3.36 3.49 1.16\n 77 5 10 12.8 1.26 3.32 -1.83\n 153 5 13.4 12.4 4.45 3.17 0.764\n 306 5 11.3 11.6 1.81 2.86 -0.169\n 611 5 10 9.96 2.76 2.28 0.08\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -36.792409 6 85.584818\n A2 -32.459270 10 84.918540\n A3 -34.337454 7 82.674909\n fitted -39.875091 4 87.750181\n R -42.211766 2 88.423532\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 19.505 8 0.01238\n Test 2 8.66628 4 0.07\n Test 3 3.75637 3 0.289\n Test 4 11.0753 3 0.01133\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 665.589 \n\n\n BMDL = 330.332 \n\n\n BMDU = 3586.73 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 0 | Hill | 5 | 2.18 | True | False | 1.973390e-12 | 1.973390e-12 | 1.973390e-12 | -999 | 88.571844 | 0.012380 | 0.070000 | 0.2890 | 0.007094 | 9.896940 | 2 | 2.860000e-08 | NaN | warning | Minimum dose/BMD ratio is greater than threshold (3.9e+13 > 3.0) | Goodness of fit p-value is less than threshold (0.00709 < 0.1) | NaN | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663\n611.000000 5 10.040000 2.762788 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-5vddor24.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-5vddor24.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:04 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n Power parameter restricted to be greater than 1\n The variance is to be modeled as Var(i) = exp(lalpha + rho \* ln(mean(i)))\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.16654\n rho = 0\n intercept = 14.96\n v = -4.92\n n = 0.24702\n k = 38.5\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -k \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho intercept v n\n\n lalpha 1 -1 0.033 -0.04 -6.5e-007\n\n rho -1 1 -0.034 0.04 6.4e-007\n\n intercept 0.033 -0.034 1 -0.9 3.1e-007\n\n v -0.04 0.04 -0.9 1 1.3e-006\n\n n -6.5e-007 6.4e-007 3.1e-007 1.3e-006 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 1.48987 6.08523 -10.437 13.4167\n rho 0.263854 2.4561 -4.55 5.07771\n intercept 14.96 1.34599 12.3219 17.5981\n v -3.745 1.4938 -6.6728 -0.817202\n n 1.2021 52012.2 -101941 101943\n k 6.11e-013 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 15 15 3.36 3.01 2.86e-008\n 77 5 10 11.2 1.26 2.9 -0.907\n 153 5 13.4 11.2 4.45 2.9 1.72\n 306 5 11.3 11.2 1.81 2.9 0.0965\n 611 5 10 11.2 2.76 2.9 -0.907\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -36.792409 6 85.584818\n A2 -32.459270 10 84.918540\n A3 -34.337454 7 82.674909\n fitted -39.285922 5 88.571844\n R -42.211766 2 88.423532\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 19.505 8 0.01238\n Test 2 8.66628 4 0.07\n Test 3 3.75637 3 0.289\n Test 4 9.89694 2 0.007094\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 1.97339e-012\n\n BMDL = 1.97339e-012\n\n BMDU = 1.97339e-012\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 0 | Exponential-M2 | 6 | 1.11 | True | False | 6.589890e+02 | 2.846340e+02 | 3.929860e+03 | -999 | 87.654780 | 0.012380 | 0.070000 | 0.2890 | 0.01184 | 10.980000 | 3 | 8.065000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0118 < 0.1)\nBMD/high dose ratio is greater than threshold (1.08 > 1.0) | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663\n611.000000 5 10.040000 2.762788 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-tn0bflnu.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:04 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha -8.01079 \n rho 3.98161 \n a 10.6576 \n b 0.000447913 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha -5.3312 7.78642\n rho 3.03531 3.14455\n a 13.2476 0.992038\n b 0.000467183 0.000220478\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 14.96 3.365\n 77 5 10.04 1.26\n 153 5 13.44 4.45\n 306 5 11.34 1.815\n 611 5 10.04 2.763\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 13.25 3.51 1.091\n 77 12.78 3.324 -1.843\n 153 12.33 3.15 0.7854\n 306 11.48 2.826 -0.1131\n 611 9.958 2.276 0.08065\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -36.79241 6 85.58482\n A2 -32.45927 10 84.91854\n A3 -34.33745 7 82.67491\n R -42.21177 2 88.42353\n 2 -39.82739 4 87.65478\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 19.5 8 0.01238\n Test 2 8.666 4 0.07\n Test 3 3.756 3 0.289\n Test 4 10.98 3 0.01184\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 658.989\n\n BMDL = 284.634\n\n BMDU = 3929.86\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 0 | Exponential-M3 | 7 | 1.11 | True | False | 6.589890e+02 | 2.846340e+02 | 3.929860e+03 | -999 | 87.654780 | 0.012380 | 0.070000 | 0.2890 | 0.01184 | 10.980000 | 3 | 8.065000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0118 < 0.1)\nBMD/high dose ratio is greater than threshold (1.08 > 1.0) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663\n611.000000 5 10.040000 2.762788 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-59xjhmj6.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:04 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha -8.01079 \n rho 3.98161 \n a 10.6576 \n b 0.000447913 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha -5.3312 7.83043\n rho 3.03532 3.16245\n a 13.2476 1.00365\n b 0.000467184 0.000225113\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 14.96 3.365\n 77 5 10.04 1.26\n 153 5 13.44 4.45\n 306 5 11.34 1.815\n 611 5 10.04 2.763\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 13.25 3.51 1.091\n 77 12.78 3.324 -1.843\n 153 12.33 3.15 0.7854\n 306 11.48 2.826 -0.1131\n 611 9.958 2.276 0.08065\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -36.79241 6 85.58482\n A2 -32.45927 10 84.91854\n A3 -34.33745 7 82.67491\n R -42.21177 2 88.42353\n 3 -39.82739 4 87.65478\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 19.5 8 0.01238\n Test 2 8.666 4 0.07\n Test 3 3.756 3 0.289\n Test 5a 10.98 3 0.01184\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 658.989\n\n BMDL = 284.634\n\n BMDU = 3929.86\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 0 | Exponential-M4 | 8 | 1.11 | True | False | 6.919140e+02 | 1.235390e+00 | 6.110000e+06 | -999 | 89.429580 | 0.012380 | 0.070000 | 0.2890 | 0.00462 | 10.750000 | 2 | -8.157000e-02 | NaN | warning | BMD/BMDL ratio is greater than threshold (5.6e+02 > 5.0) | Goodness of fit p-value is less than threshold (0.00462 < 0.1)\nBMD/BMDL ratio is greater than threshold (5.6e+02 > 20.0)\nBMD/high dose ratio is greater than threshold (1.13 > 1.0) | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663\n611.000000 5 10.040000 2.762788 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-7mj3hsgv.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:04 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha -8.01079 \n rho 3.98161 \n a 15.708 \n b 0.00444688 \n c 0.608728 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha -5.26932 8.00239\n rho 3.00696 3.23186\n a 13.5944 1.34036\n b 0.00273583 0.00487945\n c 0.685726 0.243689\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 14.96 3.365\n 77 5 10.04 1.26\n 153 5 13.44 4.45\n 306 5 11.34 1.815\n 611 5 10.04 2.763\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 13.59 3.629 0.8415\n 77 12.78 3.308 -1.854\n 153 12.13 3.059 0.9554\n 306 11.17 2.702 0.1393\n 611 10.13 2.33 -0.08157\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -36.79241 6 85.58482\n A2 -32.45927 10 84.91854\n A3 -34.33745 7 82.67491\n R -42.21177 2 88.42353\n 4 -39.71479 5 89.42958\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 19.5 8 0.01238\n Test 2 8.666 4 0.07\n Test 3 3.756 3 0.289\n Test 6a 10.75 2 0.00462\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is less than .1. Model 4 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 691.914\n\n BMDL = 1.23539\n\n BMDU = 6.11e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 0 | Exponential-M5 | 9 | 1.11 | True | False | 6.919150e+02 | 1.923200e+00 | 6.110000e+06 | -999 | 89.429580 | 0.012380 | 0.070000 | 0.2890 | 0.00462 | 10.750000 | 2 | -8.158000e-02 | NaN | warning | BMD/BMDL ratio is greater than threshold (3.6e+02 > 5.0) | Goodness of fit p-value is less than threshold (0.00462 < 0.1)\nBMD/BMDL ratio is greater than threshold (3.6e+02 > 20.0)\nBMD/high dose ratio is greater than threshold (1.13 > 1.0) | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663\n611.000000 5 10.040000 2.762788 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-rtkk\_i0n.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:04 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha -8.01079 \n rho 3.98161 \n a 15.708 \n b 0.00444688 \n c 0.608728 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha -5.26932 8.0024\n rho 3.00696 3.23187\n a 13.5944 1.34037\n b 0.00273586 0.00487946\n c 0.685727 0.243685\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 14.96 3.365\n 77 5 10.04 1.26\n 153 5 13.44 4.45\n 306 5 11.34 1.815\n 611 5 10.04 2.763\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 13.59 3.629 0.8415\n 77 12.78 3.308 -1.854\n 153 12.13 3.059 0.9554\n 306 11.17 2.702 0.1393\n 611 10.13 2.33 -0.08158\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -36.79241 6 85.58482\n A2 -32.45927 10 84.91854\n A3 -34.33745 7 82.67491\n R -42.21177 2 88.42353\n 5 -39.71479 5 89.42958\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 19.5 8 0.01238\n Test 2 8.666 4 0.07\n Test 3 3.756 3 0.289\n Test 7a 10.75 2 0.00462\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is less than .1. Model 5 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 691.915\n\n BMDL = 1.9232\n\n BMDU = 6.11e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 1 | Linear | 0 | 2.21 | True | False | 6.473860e+02 | 2.201010e+02 | -9.990000e+02 | -999 | 72.763913 | 0.010510 | 0.034890 | 0.6547 | 0.00147 | 13.045000 | 2 | -7.780000e-03 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00147 < 0.1)\nBMD/high dose ratio is greater than threshold (2.12 > 1.0) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 4 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-kuzbz8c2.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-kuzbz8c2.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:07 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.19742\n rho = 0\n beta\_0 = 13.4171\n beta\_1 = -0.00725474\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.41 -0.51\n\n rho -1 1 -0.41 0.51\n\n beta\_0 0.41 -0.41 1 -0.85\n\n beta\_1 -0.51 0.51 -0.85 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -19.3259 19.6431 -57.8257 19.1738\n rho 8.56157 7.7962 -6.7187 23.8418\n beta\_0 13.2798 1.19884 10.9301 15.6294\n beta\_1 -0.00631538 0.00517892 -0.0164659 0.00383513\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 15 13.3 3.36 4.09 0.919\n 77 5 10 12.8 1.26 3.49 -1.77\n 153 5 13.4 12.3 4.45 2.96 0.851\n 306 5 11.3 11.3 1.81 2.09 -0.00778\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -29.742756 5 69.485511\n A2 -25.435927 8 66.871854\n A3 -25.859447 6 63.718895\n fitted -32.381956 4 72.763913\n R -33.778295 2 71.556589\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 16.6847 6 0.01051\n Test 2 8.61366 3 0.03489\n Test 3 0.84704 2 0.6547\n Test 4 13.045 2 0.00147\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 647.386\n\n\n BMDL = 220.101\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 1 | Polynomial-2 | 1 | 2.21 | True | False | 4.714540e+02 | 2.538720e+02 | 4.806980e+03 | -999 | 71.964828 | 0.010510 | 0.034890 | 0.6547 | 0.002192 | 12.245900 | 2 | -1.670000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00219 < 0.1)\nBMD/high dose ratio is greater than threshold (1.54 > 1.0) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 4 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-n7\_lf9s1.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-n7\_lf9s1.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:07 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.19742\n rho = 0\n beta\_0 = 14.047\n beta\_1 = -0.0242755\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_1 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_2\n\n lalpha 1 -1 0.14 -0.19\n\n rho -1 1 -0.14 0.19\n\n beta\_0 0.14 -0.14 1 -0.79\n\n beta\_2 -0.19 0.19 -0.79 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -28.0715 16.2099 -59.8423 3.69933\n rho 12.0073 6.42857 -0.592513 24.607\n beta\_0 12.9987 0.976038 11.0857 14.9117\n beta\_1 0 NA\n beta\_2 -1.75757e-005 1.27466e-005 -4.25586e-005 7.40711e-006\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 15 13 3.36 3.91 1.12\n 77 5 10 12.9 1.26 3.72 -1.71\n 153 5 13.4 12.6 4.45 3.22 0.592\n 306 5 11.3 11.4 1.81 1.73 -0.0167\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -29.742756 5 69.485511\n A2 -25.435927 8 66.871854\n A3 -25.859447 6 63.718895\n fitted -31.982414 4 71.964828\n R -33.778295 2 71.556589\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 16.6847 6 0.01051\n Test 2 8.61366 3 0.03489\n Test 3 0.84704 2 0.6547\n Test 4 12.2459 2 0.002192\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 471.454\n\n\n BMDL = 253.872\n\n\n BMDU = 4806.98\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 1 | Polynomial-3 | 2 | 2.21 | True | False | 4.106350e+02 | 2.742630e+02 | 3.335860e+03 | -999 | 71.598933 | 0.010510 | 0.034890 | 0.6547 | 0.002632 | 11.880000 | 2 | -1.220000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00263 < 0.1)\nBMD/high dose ratio is greater than threshold (1.34 > 1.0) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 4 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-mfe9dgr8.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-mfe9dgr8.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:07 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.19742\n rho = 0\n beta\_0 = 14.96\n beta\_1 = -0.155732\n beta\_2 = 0\n beta\_3 = -3.15462e-006\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_1 -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_3\n\n lalpha 1 -1 0.051 -0.071\n\n rho -1 1 -0.051 0.071\n\n beta\_0 0.051 -0.051 1 -0.79\n\n beta\_3 -0.071 0.071 -0.79 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -29.8588 15.4396 -60.1198 0.402209\n rho 12.7094 6.12338 0.70781 24.711\n beta\_0 12.8987 0.947368 11.0419 14.7555\n beta\_1 0 NA\n beta\_2 -6.11788e-027 NA\n beta\_3 -5.40846e-008 4.10303e-008 -1.34502e-007 2.63332e-008\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 15 12.9 3.36 3.74 1.23\n 77 5 10 12.9 1.26 3.7 -1.71\n 153 5 13.4 12.7 4.45 3.4 0.483\n 306 5 11.3 11.3 1.81 1.66 -0.0122\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -29.742756 5 69.485511\n A2 -25.435927 8 66.871854\n A3 -25.859447 6 63.718895\n fitted -31.799466 4 71.598933\n R -33.778295 2 71.556589\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 16.6847 6 0.01051\n Test 2 8.61366 3 0.03489\n Test 3 0.84704 2 0.6547\n Test 4 11.88 2 0.002632\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 410.635\n\n\n BMDL = 274.263\n\n\n BMDU = 3335.86\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 1 | Polynomial-4 | 3 | 2.21 | True | False | 3.821240e+02 | 2.853380e+02 | 2.904320e+03 | -999 | 71.429361 | 0.010510 | 0.034890 | 0.6547 | 0.002865 | 11.710500 | 2 | -7.430000e-03 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00286 < 0.1)\nBMD/high dose ratio is greater than threshold (1.25 > 1.0) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 4 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-bq09o\_33.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-bq09o\_33.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:07 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.19742\n rho = 0\n beta\_0 = -3.63463\n beta\_1 = -0.138844\n beta\_2 = 0\n beta\_3 = -3.1318e-006\n beta\_4 = -3.85626e-010\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_1 -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_4\n\n lalpha 1 -1 0.02 -0.028\n\n rho -1 1 -0.02 0.028\n\n beta\_0 0.02 -0.02 1 -0.79\n\n beta\_4 -0.028 0.028 -0.79 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -30.384 15.2268 -60.228 -0.540019\n rho 12.9163 6.03987 1.07834 24.7542\n beta\_0 12.8543 0.938267 11.0153 14.6932\n beta\_1 -0 NA\n beta\_2 -0 NA\n beta\_3 -6.86965e-030 NA\n beta\_4 -1.72089e-010 1.34313e-010 -4.35337e-010 9.11591e-011\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 15 12.9 3.36 3.67 1.28\n 77 5 10 12.8 1.26 3.66 -1.72\n 153 5 13.4 12.8 4.45 3.5 0.435\n 306 5 11.3 11.3 1.81 1.64 -0.00743\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -29.742756 5 69.485511\n A2 -25.435927 8 66.871854\n A3 -25.859447 6 63.718895\n fitted -31.714681 4 71.429361\n R -33.778295 2 71.556589\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 16.6847 6 0.01051\n Test 2 8.61366 3 0.03489\n Test 3 0.84704 2 0.6547\n Test 4 11.7105 2 0.002865\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 382.124\n\n\n BMDL = 285.338\n\n\n BMDU = 2904.32\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 1 | Power | 4 | 2.19 | True | False | 3.215670e+02 | 3.061130e+02 | 2.569150e+03 | -999 | 71.264926 | 0.010510 | 0.034890 | 0.6547 | 0.00311 | 11.546000 | 2 | -1.810000e-07 | NaN | warning | BMDL/high dose ratio is greater than threshold (1.0 > 1.0) | Goodness of fit p-value is less than threshold (0.00311 < 0.1)\nBMD/high dose ratio is greater than threshold (1.05 > 1.0) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-kx45ed4e.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-kx45ed4e.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:07 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n The power is restricted to be greater than or equal to 1\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.19742\n rho = 0\n control = 10.04\n slope = 3644.99\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho control slope\n\n lalpha 1 -1 0.63 -0.86\n\n rho -1 1 -0.65 0.86\n\n control 0.63 -0.65 1 -0.79\n\n slope -0.86 0.86 -0.79 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -30.6959 29.7369 -88.9791 27.5874\n rho 13.0396 11.9323 -10.3472 36.4264\n control 12.8133 0.92932 10.9919 14.6348\n slope -2.66266e-045 2.13109e-045 -6.83953e-045 1.51421e-045\n power 18 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 15 12.8 3.36 3.6 1.33\n 77 5 10 12.8 1.26 3.6 -1.72\n 153 5 13.4 12.8 4.45 3.6 0.389\n 306 5 11.3 11.3 1.81 1.62 -1.81e-007\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -29.742756 5 69.485511\n A2 -25.435927 8 66.871854\n A3 -25.859447 6 63.718895\n fitted -31.632463 4 71.264926\n R -33.778295 2 71.556589\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 16.6847 6 0.01051\n Test 2 8.61366 3 0.03489\n Test 3 0.84704 2 0.6547\n Test 4 11.546 2 0.00311\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 321.567 \n\n\n BMDL = 306.113 \n\n\n BMDU = 2569.15 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 1 | Hill | 5 | 2.18 | True | False | 2.346340e-12 | 2.346340e-12 | 2.346350e-12 | -999 | 73.197996 | 0.010510 | 0.034890 | 0.6547 | 0.000704 | 11.479100 | 1 | 1.170000e-06 | NaN | warning | Minimum dose/BMD ratio is greater than threshold (3.28e+13 > 3.0) | Goodness of fit p-value is less than threshold (0.000704 < 0.1) | NaN | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-mbv68ssj.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-mbv68ssj.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:07 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n Power parameter restricted to be greater than 1\n The variance is to be modeled as Var(i) = exp(lalpha + rho \* ln(mean(i)))\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.19742\n rho = 0\n intercept = 14.96\n v = -4.92\n n = 0.24702\n k = 38.5\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -k \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho intercept v n\n\n lalpha 1 -1 0.028 -0.035 -2.3e-006\n\n rho -1 1 -0.028 0.035 2.2e-006\n\n intercept 0.028 -0.028 1 -0.87 2.6e-006\n\n v -0.035 0.035 -0.87 1 2.7e-006\n\n n -2.3e-006 2.2e-006 2.6e-006 2.7e-006 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 1.58128 7.24828 -12.6251 15.7877\n rho 0.230065 2.87921 -5.41307 5.87321\n intercept 14.96 1.34599 12.3219 17.5981\n v -3.35333 1.54315 -6.37786 -0.328807\n n 1.06532 6877.18 -13478 13480.1\n k 3.06e-013 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 15 15 3.36 3.01 1.17e-006\n 77 5 10 11.6 1.26 2.92 -1.2\n 153 5 13.4 11.6 4.45 2.92 1.4\n 306 5 11.3 11.6 1.81 2.92 -0.204\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -29.742756 5 69.485511\n A2 -25.435927 8 66.871854\n A3 -25.859447 6 63.718895\n fitted -31.598998 5 73.197996\n R -33.778295 2 71.556589\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 16.6847 6 0.01051\n Test 2 8.61366 3 0.03489\n Test 3 0.84704 2 0.6547\n Test 4 11.4791 1 0.0007038\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 2.34634e-012\n\n BMDL = 2.34634e-012\n\n BMDU = 2.34635e-012\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 1 | Exponential-M2 | 6 | 1.11 | True | False | 7.304600e+02 | 1.961330e+02 | -9.990000e+02 | -999 | 72.846530 | 0.010510 | 0.034890 | 0.6547 | 0.00141 | 13.130000 | 2 | -3.680000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00141 < 0.1)\nBMD/high dose ratio is greater than threshold (2.39 > 1.0) | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 -1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-ewa4kjj5.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:07 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha -12.8841 \n rho 5.83786 \n a 11.4618 \n b 0.000526989 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha -19.003 28.7325\n rho 8.43778 11.4671\n a 13.2664 1.37197\n b 0.000502655 0.000499149\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 14.96 3.365\n 77 5 10.04 1.26\n 153 5 13.44 4.45\n 306 5 11.34 1.815\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 13.27 4.077 0.9289\n 77 12.76 3.463 -1.758\n 153 12.28 2.947 0.8768\n 306 11.38 2.131 -0.0368\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -29.74276 5 69.48551\n A2 -25.43593 8 66.87185\n A3 -25.85945 6 63.71889\n R -33.77829 2 71.55659\n 2 -32.42327 4 72.84653\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 16.68 6 0.01051\n Test 2 8.614 3 0.03489\n Test 3 0.847 2 0.6547\n Test 4 13.13 2 0.00141\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 730.46\n\n BMDL = 196.133\n\n BMDU = Bad\_Completion\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 1 | Exponential-M3 | 7 | 1.11 | True | False | 3.233570e+02 | 3.061300e+02 | 2.983170e+03 | -999 | 73.264930 | 0.010510 | 0.034890 | 0.6547 | 0.000679 | 11.550000 | 1 | -5.844000e-06 | NaN | warning | BMDL/high dose ratio is greater than threshold (1.0 > 1.0) | Goodness of fit p-value is less than threshold (0.000679 < 0.1)\nBMD/high dose ratio is greater than threshold (1.06 > 1.0) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 -1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-74g0ispa.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:06 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha -12.8841 \n rho 5.83786 \n a 11.4618 \n b 0.000526989 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha -30.696 29.7371\n rho 13.0396 11.9323\n a 12.8133 0.92932\n b 0.00290771 0.000127928\n d 18 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 14.96 3.365\n 77 5 10.04 1.26\n 153 5 13.44 4.45\n 306 5 11.34 1.815\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 12.81 3.599 1.334\n 77 12.81 3.599 -1.723\n 153 12.81 3.599 0.3893\n 306 11.34 1.623 -5.844e-006\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -29.74276 5 69.48551\n A2 -25.43593 8 66.87185\n A3 -25.85945 6 63.71889\n R -33.77829 2 71.55659\n 3 -31.63246 5 73.26493\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 16.68 6 0.01051\n Test 2 8.614 3 0.03489\n Test 3 0.847 2 0.6547\n Test 5a 11.55 1 0.0006789\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 323.357\n\n BMDL = 306.13\n\n BMDU = 2983.17\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 1 | Exponential-M4 | 8 | 1.11 | True | False | 7.304590e+02 | 3.053890e+00 | 3.060000e+06 | -999 | 72.846530 | 0.010510 | 0.034890 | 0.6547 | 0.00141 | 13.130000 | 2 | -3.680000e-02 | NaN | warning | BMD/BMDL ratio is greater than threshold (2.39e+02 > 5.0) | Goodness of fit p-value is less than threshold (0.00141 < 0.1)\nBMD/BMDL ratio is greater than threshold (2.39e+02 > 20.0)\nBMD/high dose ratio is greater than threshold (2.39 > 1.0) | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 -1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-qg6l3ik\_.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:07 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha -12.8841 \n rho 5.83786 \n a 15.708 \n b 0.0020773 \n c 0.319582 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha -19.003 27.4684\n rho 8.43777 10.9594\n a 13.2664 1.30177\n b 0.000502655 0.000463962\n c 0 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 14.96 3.365\n 77 5 10.04 1.26\n 153 5 13.44 4.45\n 306 5 11.34 1.815\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 13.27 4.077 0.9289\n 77 12.76 3.463 -1.758\n 153 12.28 2.947 0.8768\n 306 11.38 2.131 -0.0368\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -29.74276 5 69.48551\n A2 -25.43593 8 66.87185\n A3 -25.85945 6 63.71889\n R -33.77829 2 71.55659\n 4 -32.42327 4 72.84653\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 16.68 6 0.01051\n Test 2 8.614 3 0.03489\n Test 3 0.847 2 0.6547\n Test 6a 13.13 2 0.00141\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is less than .1. Model 4 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 730.459\n\n BMDL = 3.05389\n\n BMDU = 3.06e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 1 | Exponential-M5 | 9 | 1.11 | True | False | 3.233570e+02 | 3.061300e+02 | 3.060000e+06 | -999 | 73.264930 | 0.010510 | 0.034890 | 0.6547 | 0.000679 | 11.550000 | 1 | -7.568000e-07 | NaN | warning | BMDL/high dose ratio is greater than threshold (1.0 > 1.0) | Goodness of fit p-value is less than threshold (0.000679 < 0.1)\nBMD/high dose ratio is greater than threshold (1.06 > 1.0) | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 -1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056\n306.000000 5 11.340000 1.814663 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-1iu5zkx1.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:07 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha -12.8841 \n rho 5.83786 \n a 15.708 \n b 0.0020773 \n c 0.319582 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha -30.6959 29.7369\n rho 13.0396 11.9323\n a 12.8133 0.92932\n b 0.00290771 0.000127927\n c 0 NA\n d 18 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 14.96 3.365\n 77 5 10.04 1.26\n 153 5 13.44 4.45\n 306 5 11.34 1.815\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 12.81 3.599 1.334\n 77 12.81 3.599 -1.723\n 153 12.81 3.599 0.3893\n 306 11.34 1.623 -7.568e-007\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -29.74276 5 69.48551\n A2 -25.43593 8 66.87185\n A3 -25.85945 6 63.71889\n R -33.77829 2 71.55659\n 5 -31.63246 5 73.26493\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 16.68 6 0.01051\n Test 2 8.614 3 0.03489\n Test 3 0.847 2 0.6547\n Test 7a 11.55 1 0.0006789\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is less than .1. Model 5 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 323.357\n\n BMDL = 306.13\n\n BMDU = 3.06e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 2 | Linear | 0 | 2.21 | True | False | 1.777520e+02 | 4.720730e+01 | -9.990000e+02 | -999 | 60.478257 | 0.014660 | 0.039520 | 0.3598 | 0.001124 | 10.611200 | 1 | 1.060000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00112 < 0.1)\nBMD/high dose ratio is greater than threshold (1.16 > 1.0) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 3 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-qn2nl6s3.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-qn2nl6s3.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:10 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.38919\n rho = 0\n beta\_0 = 13.5841\n beta\_1 = -0.010053\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.52 -0.67\n\n rho -1 1 -0.52 0.67\n\n beta\_0 0.52 -0.52 1 -0.8\n\n beta\_1 -0.67 0.67 -0.8 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 11.3272 14.3806 -16.8583 39.5128\n rho -3.47402 5.6557 -14.559 7.61095\n beta\_0 14.0072 1.48169 11.1031 16.9112\n beta\_1 -0.0165441 0.0206745 -0.0570654 0.0239773\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 15 14 3.36 2.94 0.725\n 77 5 10 12.7 1.26 3.47 -1.74\n 153 5 13.4 11.5 4.45 4.16 1.06\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -23.745355 4 55.490710\n A2 -20.514287 6 53.028574\n A3 -20.933550 5 51.867101\n fitted -26.239129 4 60.478257\n R -26.710818 2 57.421636\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 12.3931 4 0.01466\n Test 2 6.46214 2 0.03952\n Test 3 0.838527 1 0.3598\n Test 4 10.6112 1 0.001124\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 177.752\n\n\n BMDL = 47.2073\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 2 | Polynomial-2 | 1 | 2.21 | True | False | 1.777530e+02 | 4.720730e+01 | -9.990000e+02 | -999 | 60.478257 | 0.014660 | 0.039520 | 0.3598 | 0.001124 | 10.611200 | 1 | 1.060000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00112 < 0.1)\nBMD/high dose ratio is greater than threshold (1.16 > 1.0) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 3 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-o9di3i71.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-o9di3i71.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:11 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.38919\n rho = 0\n beta\_0 = 14.96\n beta\_1 = -0.118568\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.52 -0.67\n\n rho -1 1 -0.52 0.67\n\n beta\_0 0.52 -0.52 1 -0.8\n\n beta\_1 -0.67 0.67 -0.8 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 11.3272 14.3807 -16.8585 39.5129\n rho -3.47401 5.65574 -14.559 7.61103\n beta\_0 14.0072 1.48169 11.1031 16.9112\n beta\_1 -0.016544 0.0206746 -0.0570655 0.0239775\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 15 14 3.36 2.94 0.725\n 77 5 10 12.7 1.26 3.47 -1.74\n 153 5 13.4 11.5 4.45 4.16 1.06\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -23.745355 4 55.490710\n A2 -20.514287 6 53.028574\n A3 -20.933550 5 51.867101\n fitted -26.239129 4 60.478257\n R -26.710818 2 57.421636\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 12.3931 4 0.01466\n Test 2 6.46214 2 0.03952\n Test 3 0.838527 1 0.3598\n Test 4 10.6112 1 0.001124\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 177.753\n\n\n BMDL = 47.2073\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 2 | Polynomial-3 | 2 | 2.21 | True | False | 1.777520e+02 | 4.720730e+01 | -9.990000e+02 | -999 | 60.478257 | 0.014660 | 0.039520 | 0.3598 | 0.001124 | 10.611200 | 1 | 1.060000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00112 < 0.1)\nBMD/high dose ratio is greater than threshold (1.16 > 1.0) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 3 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-099s7n8x.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-099s7n8x.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:11 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.38919\n rho = 0\n beta\_0 = -2621.22\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = -0.000210047\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.52 -0.67\n\n rho -1 1 -0.52 0.67\n\n beta\_0 0.52 -0.52 1 -0.8\n\n beta\_1 -0.67 0.67 -0.8 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 11.3272 14.3806 -16.8583 39.5128\n rho -3.47402 5.6557 -14.559 7.61095\n beta\_0 14.0072 1.48169 11.1031 16.9112\n beta\_1 -0.016544 0.0206745 -0.0570653 0.0239773\n beta\_2 0 NA\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 15 14 3.36 2.94 0.725\n 77 5 10 12.7 1.26 3.47 -1.74\n 153 5 13.4 11.5 4.45 4.16 1.06\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -23.745355 4 55.490710\n A2 -20.514287 6 53.028574\n A3 -20.933550 5 51.867101\n fitted -26.239129 4 60.478257\n R -26.710818 2 57.421636\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 12.3931 4 0.01466\n Test 2 6.46214 2 0.03952\n Test 3 0.838527 1 0.3598\n Test 4 10.6112 1 0.001124\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 177.752\n\n\n BMDL = 47.2073\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 2 | Polynomial-4 | 3 | 2.21 | True | False | 1.777510e+02 | 4.720730e+01 | -9.990000e+02 | -999 | 60.478257 | 0.014660 | 0.039520 | 0.3598 | 0.001124 | 10.611200 | 1 | 1.060000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00112 < 0.1)\nBMD/high dose ratio is greater than threshold (1.16 > 1.0) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 3 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-so2blsmm.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-so2blsmm.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:11 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.38919\n rho = 0\n beta\_0 = 19.7393\n beta\_1 = 0\n beta\_2 = -0.0137691\n beta\_3 = 0\n beta\_4 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.52 -0.67\n\n rho -1 1 -0.52 0.67\n\n beta\_0 0.52 -0.52 1 -0.8\n\n beta\_1 -0.67 0.67 -0.8 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 11.3272 14.3806 -16.8582 39.5127\n rho -3.47402 5.65568 -14.559 7.61091\n beta\_0 14.0072 1.48169 11.1031 16.9112\n beta\_1 -0.0165441 0.0206746 -0.0570655 0.0239773\n beta\_2 0 NA\n beta\_3 0 NA\n beta\_4 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 15 14 3.36 2.94 0.725\n 77 5 10 12.7 1.26 3.47 -1.74\n 153 5 13.4 11.5 4.45 4.16 1.06\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -23.745355 4 55.490710\n A2 -20.514287 6 53.028574\n A3 -20.933550 5 51.867101\n fitted -26.239129 4 60.478257\n R -26.710818 2 57.421636\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 12.3931 4 0.01466\n Test 2 6.46214 2 0.03952\n Test 3 0.838527 1 0.3598\n Test 4 10.6112 1 0.001124\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 177.751\n\n\n BMDL = 47.2073\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 2 | Power | 4 | 2.19 | True | False | 1.777520e+02 | 4.720730e+01 | -9.990000e+02 | -999 | 60.478257 | 0.014660 | 0.039520 | 0.3598 | 0.001124 | 10.611200 | 1 | 1.060000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00112 < 0.1)\nBMD/high dose ratio is greater than threshold (1.16 > 1.0) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-8tqxm8sc.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-8tqxm8sc.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:11 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n The power is restricted to be greater than or equal to 1\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.38919\n rho = 0\n control = 10.04\n slope = 0.0222222\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho control slope\n\n lalpha 1 -1 -0.16 0.25\n\n rho -1 1 0.16 -0.24\n\n control -0.16 0.16 1 -0.75\n\n slope 0.25 -0.24 -0.75 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 11.3272 11.0365 -10.304 32.9584\n rho -3.47402 4.32495 -11.9508 5.00273\n control 14.0072 1.33986 11.3811 16.6333\n slope -0.0165441 0.0174754 -0.0507953 0.0177072\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 15 14 3.36 2.94 0.725\n 77 5 10 12.7 1.26 3.47 -1.74\n 153 5 13.4 11.5 4.45 4.16 1.06\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -23.745355 4 55.490710\n A2 -20.514287 6 53.028574\n A3 -20.933550 5 51.867101\n fitted -26.239129 4 60.478257\n R -26.710818 2 57.421636\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 12.3931 4 0.01466\n Test 2 6.46214 2 0.03952\n Test 3 0.838527 1 0.3598\n Test 4 10.6112 1 0.001124\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 177.752 \n\n\n BMDL = 47.2073 \n\nWarning: optimum may not have been found. Bad completion code in Optimization routine.\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 2 | Hill | 5 | 2.18 | True | False | 2.346340e-12 | 2.346340e-12 | 2.346350e-12 | -999 | 73.197996 | 0.010510 | 0.034890 | 0.6547 | 0.000704 | 11.479100 | 1 | 1.170000e-06 | NaN | warning | Minimum dose/BMD ratio is greater than threshold (3.28e+13 > 3.0) | Goodness of fit p-value is less than threshold (0.000704 < 0.1) | NaN | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-mbv68ssj.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-mbv68ssj.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:07 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n Power parameter restricted to be greater than 1\n The variance is to be modeled as Var(i) = exp(lalpha + rho \* ln(mean(i)))\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.19742\n rho = 0\n intercept = 14.96\n v = -4.92\n n = 0.24702\n k = 38.5\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -k \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho intercept v n\n\n lalpha 1 -1 0.028 -0.035 -2.3e-006\n\n rho -1 1 -0.028 0.035 2.2e-006\n\n intercept 0.028 -0.028 1 -0.87 2.6e-006\n\n v -0.035 0.035 -0.87 1 2.7e-006\n\n n -2.3e-006 2.2e-006 2.6e-006 2.7e-006 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 1.58128 7.24828 -12.6251 15.7877\n rho 0.230065 2.87921 -5.41307 5.87321\n intercept 14.96 1.34599 12.3219 17.5981\n v -3.35333 1.54315 -6.37786 -0.328807\n n 1.06532 6877.18 -13478 13480.1\n k 3.06e-013 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 15 15 3.36 3.01 1.17e-006\n 77 5 10 11.6 1.26 2.92 -1.2\n 153 5 13.4 11.6 4.45 2.92 1.4\n 306 5 11.3 11.6 1.81 2.92 -0.204\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -29.742756 5 69.485511\n A2 -25.435927 8 66.871854\n A3 -25.859447 6 63.718895\n fitted -31.598998 5 73.197996\n R -33.778295 2 71.556589\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 16.6847 6 0.01051\n Test 2 8.61366 3 0.03489\n Test 3 0.84704 2 0.6547\n Test 4 11.4791 1 0.0007038\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 2.34634e-012\n\n BMDL = 2.34634e-012\n\n BMDU = 2.34635e-012\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 2 | Exponential-M2 | 6 | 1.11 | True | False | 1.557190e+02 | 3.841930e+01 | 1.530000e+06 | -999 | 60.351410 | 0.014660 | 0.039520 | 0.3598 | 0.001204 | 10.480000 | 1 | 1.135000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0012 < 0.1)\nBMD/high dose ratio is greater than threshold (1.02 > 1.0) | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 -1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-v23kzame.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:11 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha -12.5268 \n rho 5.71019 \n a 11.9686 \n b 0.000710113 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha 10.8644 9.66865\n rho -3.29922 3.79448\n a 14.1609 1.29232\n b 0.00146368 0.00129272\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 14.96 3.365\n 77 5 10.04 1.26\n 153 5 13.44 4.45\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 14.16 2.886 0.6191\n 77 12.65 3.476 -1.68\n 153 11.32 4.176 1.135\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -23.74536 4 55.49071\n A2 -20.51429 6 53.02857\n A3 -20.93355 5 51.8671\n R -26.71082 2 57.42164\n 2 -26.17571 4 60.35141\n\n\n Additive constant for all log-likelihoods = -13.78. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 12.39 4 0.01466\n Test 2 6.462 2 0.03952\n Test 3 0.8385 1 0.3598\n Test 4 10.48 1 0.001204\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 155.719\n\n BMDL = 38.4193\n\n BMDU = 1.53e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 2 | Exponential-M3 | 7 | 1.11 | True | False | 1.557190e+02 | 3.841930e+01 | -9.990000e+02 | -999 | 60.351410 | 0.014660 | 0.039520 | 0.3598 | 0.001204 | 10.480000 | 1 | 1.135000e+00 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0012 < 0.1)\nBMD/high dose ratio is greater than threshold (1.02 > 1.0) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 -1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-0z3ox9jc.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:11 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha -12.5268 \n rho 5.71019 \n a 11.9686 \n b 0.000710113 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha 10.8644 9.74022\n rho -3.29924 3.81981\n a 14.1609 1.37132\n b 0.00146367 0.00145826\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 14.96 3.365\n 77 5 10.04 1.26\n 153 5 13.44 4.45\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 14.16 2.886 0.6191\n 77 12.65 3.476 -1.68\n 153 11.32 4.176 1.135\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -23.74536 4 55.49071\n A2 -20.51429 6 53.02857\n A3 -20.93355 5 51.8671\n R -26.71082 2 57.42164\n 3 -26.17571 4 60.35141\n\n\n Additive constant for all log-likelihoods = -13.78. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 12.39 4 0.01466\n Test 2 6.462 2 0.03952\n Test 3 0.8385 1 0.3598\n Test 5a 10.48 1 0.001204\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 155.719\n\n BMDL = 38.4193\n\n BMDU = Bad\_Completion\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 2 | Exponential-M4 | 8 | 1.11 | True | False | 9.438520e+00 | 2.839400e-02 | 1.530000e+06 | -999 | 60.395220 | 0.014660 | 0.039520 | 0.3598 | -999 | 8.528000 | 0 | -1.023000e-06 | NaN | warning | BMD/BMDL ratio is greater than threshold (3.32e+02 > 5.0)\nMinimum dose/BMD ratio is greater than threshold (8.16 > 3.0) | BMD/BMDL ratio is greater than threshold (3.32e+02 > 20.0)\nZero degrees of freedom; saturated model | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 -1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-x01o6qcd.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:11 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha -12.5268 \n rho 5.71019 \n a 15.708 \n b 0.00198947 \n c 0.000639165 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha 4.8154 8.24411\n rho -0.965376 3.23626\n a 14.96 1.34598\n b 0.289098 631.124\n c 0.784759 0.100498\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 14.96 3.365\n 77 5 10.04 1.26\n 153 5 13.44 4.45\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 14.96 3.01 -1.023e-006\n 77 11.74 3.383 -1.124\n 153 11.74 3.383 1.124\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -23.74536 4 55.49071\n A2 -20.51429 6 53.02857\n A3 -20.93355 5 51.8671\n R -26.71082 2 57.42164\n 4 -25.19761 5 60.39522\n\n\n Additive constant for all log-likelihoods = -13.78. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 12.39 4 0.01466\n Test 2 6.462 2 0.03952\n Test 3 0.8385 1 0.3598\n Test 6a 8.528 0 N/A\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n Degrees of freedom for Test 6a are less than or equal to 0.\n The Chi-Square test for fit is not valid.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 9.43852\n\n BMDL = 0.028394\n\n BMDU = 1.53e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Sorbitol dehydrogenase | IU/L | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | 1.5048587973627294,.56356011214421464,1.9901256241755194,.81154174261093937,1.2355565547557907 | 0,1,0,0,0 | 1,1,1,1,1 | SD | day | NaN | 230 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Sorbitol dehydrogenase | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 7 | 2 | Exponential-M5 | 9 | 1.11 | True | False | 3.233570e+02 | 3.061300e+02 | 3.060000e+06 | -999 | 73.264930 | 0.010510 | 0.034890 | 0.6547 | 0.000679 | 11.550000 | 1 | -7.568000e-07 | NaN | warning | BMDL/high dose ratio is greater than threshold (2.0 > 1.0) | Goodness of fit p-value is less than threshold (0.000679 < 0.1)\nBMD/high dose ratio is greater than threshold (2.11 > 1.0) | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 -1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 14.960000 3.364967\n77.000000 5 10.040000 1.260159\n153.000000 5 13.440000 4.450056 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-1iu5zkx1.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:07 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha -12.8841 \n rho 5.83786 \n a 15.708 \n b 0.0020773 \n c 0.319582 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha -30.6959 29.7369\n rho 13.0396 11.9323\n a 12.8133 0.92932\n b 0.00290771 0.000127927\n c 0 NA\n d 18 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 14.96 3.365\n 77 5 10.04 1.26\n 153 5 13.44 4.45\n 306 5 11.34 1.815\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 12.81 3.599 1.334\n 77 12.81 3.599 -1.723\n 153 12.81 3.599 0.3893\n 306 11.34 1.623 -7.568e-007\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -29.74276 5 69.48551\n A2 -25.43593 8 66.87185\n A3 -25.85945 6 63.71889\n R -33.77829 2 71.55659\n 5 -31.63246 5 73.26493\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 16.68 6 0.01051\n Test 2 8.614 3 0.03489\n Test 3 0.847 2 0.6547\n Test 7a 11.55 1 0.0006789\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is less than .1. Model 5 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 323.357\n\n BMDL = 306.13\n\n BMDU = 3.06e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 0 | Linear | 0 | 2.21 | True | False | 4.117740e+03 | 4.900110e+02 | 3.733210e+09 | -999 | 78.652884 | 0.002059 | 0.000453 | 0.2948 | 0.000332 | 18.594600 | 3 | -4.890000e-01 | NaN | warning | BMD/BMDL ratio is greater than threshold (8.4 > 5.0) | Goodness of fit p-value is less than threshold (0.000332 < 0.1)\nBMD/high dose ratio is greater than threshold (6.74 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (5.78 > 1.5) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575\n611.000000 5 11.200000 1.643168 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-s0y3pggk.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-s0y3pggk.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:14 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 1.96571\n rho = 0\n beta\_0 = 10.7185\n beta\_1 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.49 -0.74\n\n rho -1 1 -0.49 0.74\n\n beta\_0 0.49 -0.49 1 -0.64\n\n beta\_1 -0.74 0.74 -0.64 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 76.0958 81.8984 -84.4221 236.614\n rho -30.6606 33.8088 -96.9246 35.6035\n beta\_0 11.0967 0.61246 9.89626 12.2971\n beta\_1 0.000769568 0.00119774 -0.00157796 0.00311709\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 9.6 11.1 0.548 3.17 -1.06\n 77 5 10.8 11.2 2.77 2.92 -0.273\n 153 5 11.8 11.2 4.76 2.7 0.486\n 306 5 12.6 11.3 1.52 2.3 1.23\n 611 5 11.2 11.6 1.64 1.68 -0.489\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -34.282116 6 80.564232\n A2 -24.175143 10 68.350287\n A3 -26.029119 7 66.058238\n fitted -35.326442 4 78.652884\n R -36.313603 2 76.627205\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 24.2769 8 0.002059\n Test 2 20.2139 4 0.0004531\n Test 3 3.70795 3 0.2948\n Test 4 18.5946 3 0.0003316\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 4117.74\n\n\n BMDL = 490.011\n\n\n BMDU = 3.73321e+009\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 0 | Polynomial-2 | 1 | 2.21 | True | False | 3.182970e+03 | 6.293740e+02 | -9.990000e+02 | -999 | 77.816962 | 0.002059 | 0.000453 | 0.2948 | 0.000493 | 17.758700 | 3 | -1.930000e-01 | NaN | warning | BMD/BMDL ratio is greater than threshold (5.06 > 5.0)\nBMDL/high dose ratio is greater than threshold (1.03 > 1.0) | Goodness of fit p-value is less than threshold (0.000493 < 0.1)\nBMD/high dose ratio is greater than threshold (5.21 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (5.4 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575\n611.000000 5 11.200000 1.643168 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-ls0\_kgtc.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-ls0\_kgtc.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:15 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 1.96571\n rho = 0\n beta\_0 = 9.62462\n beta\_1 = 0\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_1 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_2\n\n lalpha 1 -1 0.24 -0.26\n\n rho -1 1 -0.24 0.26\n\n beta\_0 0.24 -0.24 1 -0.94\n\n beta\_2 -0.26 0.26 -0.94 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 355.547 193.789 -24.2727 735.366\n rho -146.178 80.0773 -303.127 10.7706\n beta\_0 11.2172 1.26837 8.73124 13.7031\n beta\_1 0 NA\n beta\_2 2.91939e-007 6.00834e-006 -1.14842e-005 1.20681e-005\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 9.6 11.2 0.548 2.96 -1.22\n 77 5 10.8 11.2 2.77 2.92 -0.32\n 153 5 11.8 11.2 4.76 2.83 0.455\n 306 5 12.6 11.2 1.52 2.48 1.22\n 611 5 11.2 11.3 1.64 1.46 -0.193\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -34.282116 6 80.564232\n A2 -24.175143 10 68.350287\n A3 -26.029119 7 66.058238\n fitted -34.908481 4 77.816962\n R -36.313603 2 76.627205\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 24.2769 8 0.002059\n Test 2 20.2139 4 0.0004531\n Test 3 3.70795 3 0.2948\n Test 4 17.7587 3 0.0004932\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 3182.97\n\n\n BMDL = 629.374\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 0 | Polynomial-3 | 2 | 2.21 | True | False | 2.300870e+03 | 7.234280e+02 | -9.990000e+02 | -999 | 79.807900 | 0.002059 | 0.000453 | 0.2948 | 0.00014 | 17.749700 | 2 | -1.180000e-01 | NaN | warning | BMDL/high dose ratio is greater than threshold (1.18 > 1.0) | Goodness of fit p-value is less than threshold (0.00014 < 0.1)\nBMD/high dose ratio is greater than threshold (3.77 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (5.27 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575\n611.000000 5 11.200000 1.643168 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-4zjod\_0e.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-4zjod\_0e.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:15 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 1.96571\n rho = 0\n beta\_0 = 9.583\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_1 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_2 beta\_3\n\n lalpha 1 -1 0.022 -0.052 -0.054\n\n rho -1 1 -0.022 0.052 0.054\n\n beta\_0 0.022 -0.022 1 0.35 -0.23\n\n beta\_2 -0.052 0.052 0.35 1 -1.2\n\n beta\_3 -0.054 0.054 -0.23 -1.2 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 564.666 290.272 -4.25667 1133.59\n rho -232.765 120.036 -468.031 2.50114\n beta\_0 11.2098 0.45857 10.3111 12.1086\n beta\_1 9.0198e-025 NA\n beta\_2 4.63751e-008 1.17654e-006 -2.25961e-006 2.35236e-006\n beta\_3 2.17058e-010 1.12195e-009 -1.98192e-009 2.41604e-009\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 9.6 11.2 0.548 2.89 -1.25\n 77 5 10.8 11.2 2.77 2.88 -0.319\n 153 5 11.8 11.2 4.76 2.83 0.464\n 306 5 12.6 11.2 1.52 2.59 1.19\n 611 5 11.2 11.3 1.64 1.45 -0.118\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -34.282116 6 80.564232\n A2 -24.175143 10 68.350287\n A3 -26.029119 7 66.058238\n fitted -34.903950 5 79.807900\n R -36.313603 2 76.627205\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 24.2769 8 0.002059\n Test 2 20.2139 4 0.0004531\n Test 3 3.70795 3 0.2948\n Test 4 17.7497 2 0.0001399\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 2300.87\n\n\n BMDL = 723.428\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 0 | Polynomial-4 | 3 | 2.21 | True | False | 2.303440e+03 | 7.039870e+02 | -9.990000e+02 | -999 | 79.807896 | 0.002059 | 0.000453 | 0.2948 | 0.00014 | 17.749700 | 2 | -1.180000e-01 | NaN | warning | BMDL/high dose ratio is greater than threshold (1.15 > 1.0) | Goodness of fit p-value is less than threshold (0.00014 < 0.1)\nBMD/high dose ratio is greater than threshold (3.77 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (5.27 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575\n611.000000 5 11.200000 1.643168 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-zw55ys\_r.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-zw55ys\_r.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:14 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 1.96571\n rho = 0\n beta\_0 = 9.6\n beta\_1 = 0\n beta\_2 = 0\n beta\_3 = 0\n beta\_4 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_1 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_2 beta\_3\n\n lalpha 1 -1 0.022 -0.052 -0.054\n\n rho -1 1 -0.022 0.052 0.054\n\n beta\_0 0.022 -0.022 1 0.35 -0.23\n\n beta\_2 -0.052 0.052 0.35 1 -1.2\n\n beta\_3 -0.054 0.054 -0.23 -1.2 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 566.959 291.436 -4.24494 1138.16\n rho -233.713 120.517 -469.922 2.49629\n beta\_0 11.2099 0.458963 10.3104 12.1095\n beta\_1 6.78595e-026 NA\n beta\_2 4.60285e-008 1.1723e-006 -2.25164e-006 2.34369e-006\n beta\_3 2.16432e-010 1.11938e-009 -1.97752e-009 2.41038e-009\n beta\_4 -0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 9.6 11.2 0.548 2.89 -1.25\n 77 5 10.8 11.2 2.77 2.88 -0.319\n 153 5 11.8 11.2 4.76 2.83 0.464\n 306 5 12.6 11.2 1.52 2.59 1.19\n 611 5 11.2 11.3 1.64 1.45 -0.118\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -34.282116 6 80.564232\n A2 -24.175143 10 68.350287\n A3 -26.029119 7 66.058238\n fitted -34.903948 5 79.807896\n R -36.313603 2 76.627205\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 24.2769 8 0.002059\n Test 2 20.2139 4 0.0004531\n Test 3 3.70795 3 0.2948\n Test 4 17.7497 2 0.0001399\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 2303.44\n\n\n BMDL = 703.987\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 0 | Power | 4 | 2.19 | True | False | 2.705350e+03 | 6.331420e+02 | -9.990000e+02 | -999 | 79.777065 | 0.002059 | 0.000453 | 0.2948 | 0.000142 | 17.718800 | 2 | -1.380000e-01 | NaN | warning | BMDL/high dose ratio is greater than threshold (1.04 > 1.0) | Goodness of fit p-value is less than threshold (0.000142 < 0.1)\nBMD/high dose ratio is greater than threshold (4.43 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (5.31 > 1.5) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575\n611.000000 5 11.200000 1.643168 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-8r94bv\_1.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-8r94bv\_1.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:14 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n The power is restricted to be greater than or equal to 1\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 1.96571\n rho = 0\n control = 9.6\n slope = 0.758912\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n lalpha rho control slope power\n\n lalpha 1 -1 0.71 -0.66 0.15\n\n rho -1 1 -0.71 0.66 -0.15\n\n control 0.71 -0.71 1 -0.35 -0.044\n\n slope -0.66 0.66 -0.35 1 -0.84\n\n power 0.15 -0.15 -0.044 -0.84 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 496.183 5927.74 -11122 12114.3\n rho -204.402 2449.02 -5004.39 4595.58\n control 11.2128 0.647098 9.94448 12.4811\n slope 1.20873e-008 2.64643e-007 -5.06603e-007 5.30778e-007\n power 2.44182 2.58606 -2.62675 7.5104\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 9.6 11.2 0.548 2.91 -1.24\n 77 5 10.8 11.2 2.77 2.89 -0.319\n 153 5 11.8 11.2 4.76 2.84 0.461\n 306 5 12.6 11.2 1.52 2.55 1.2\n 611 5 11.2 11.3 1.64 1.45 -0.138\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -34.282116 6 80.564232\n A2 -24.175143 10 68.350287\n A3 -26.029119 7 66.058238\n fitted -34.888532 5 79.777065\n R -36.313603 2 76.627205\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 24.2769 8 0.002059\n Test 2 20.2139 4 0.0004531\n Test 3 3.70795 3 0.2948\n Test 4 17.7188 2 0.000142\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 2705.35 \n\n\n BMDL = 633.142 \n\nWarning: optimum may not have been found. Bad completion code in Optimization routine.\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 0 | Hill | 5 | 2.18 | True | False | 6.417830e+01 | -9.990000e+02 | -9.990000e+02 | -999 | 66.067046 | 0.002059 | 0.000453 | 0.2948 | 0.1112 | 6.008810 | 3 | -5.830000e-01 | BMDL computation failed. | failure | Warning(s): BMDL computation failed. | NaN | BMDL does not exist | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575\n611.000000 5 11.200000 1.643168 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-hu6\_s6p9.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-hu6\_s6p9.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:14 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n Power parameter restricted to be greater than 1\n The variance is to be modeled as Var(i) = exp(lalpha + rho \* ln(mean(i)))\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 1.96571\n rho = 0\n intercept = 9.6\n v = 3\n n = 0.178184\n k = 206.2\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -n \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha intercept v k\n\n lalpha 1 -0.47 -0.65 0.14\n\n intercept -0.47 1 -0.12 -0.027\n\n v -0.65 -0.12 1 0.14\n\n k 0.14 -0.027 0.14 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -42.0957 0.610729 -43.2927 -40.8987\n rho 18 NA\n intercept 9.59313 0.209194 9.18312 10.0031\n v 2.04834 0.381158 1.30129 2.7954\n n 18 NA\n k 68.3643 8.88357 50.9528 85.7757\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 9.6 9.59 0.548 0.497 0.0309\n 77 5 10.8 11.4 2.77 2.4 -0.583\n 153 5 11.8 11.6 4.76 2.84 0.125\n 306 5 12.6 11.6 1.52 2.84 0.755\n 611 5 11.2 11.6 1.64 2.84 -0.348\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -34.282116 6 80.564232\n A2 -24.175143 10 68.350287\n A3 -26.029119 7 66.058238\n fitted -29.033523 4 66.067046\n R -36.313603 2 76.627205\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 24.2769 8 0.002059\n Test 2 20.2139 4 0.0004531\n Test 3 3.70795 3 0.2948\n Test 4 6.00881 3 0.1112\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 64.1783\n\n\nBMDL computation failed.\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 0 | Exponential-M2 | 6 | 1.11 | True | False | 3.582190e+03 | 5.393310e+02 | 6.110000e+06 | -999 | 78.636360 | 0.002059 | 0.000453 | 0.2948 | 0.000334 | 18.580000 | 3 | -4.970000e-01 | NaN | warning | BMD/BMDL ratio is greater than threshold (6.64 > 5.0) | Goodness of fit p-value is less than threshold (0.000334 < 0.1)\nBMD/high dose ratio is greater than threshold (5.86 > 1.0) | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575\n611.000000 5 11.200000 1.643168 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-rr81f3cm.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:14 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha -21.8138 \n rho 9.52437 \n a 10.6612 \n b 0.00019702 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha 73.7932 220.95\n rho -29.7158 90.9685\n a 11.0872 0.851116\n b 7.00637e-005 0.000185812\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 9.6 0.5477\n 77 5 10.8 2.775\n 153 5 11.8 4.764\n 306 5 12.6 1.517\n 611 5 11.2 1.643\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 11.09 3.163 -1.051\n 77 11.15 2.919 -0.2659\n 153 11.21 2.697 0.4918\n 306 11.33 2.3 1.237\n 611 11.57 1.674 -0.497\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -34.28212 6 80.56423\n A2 -24.17514 10 68.35029\n A3 -26.02912 7 66.05824\n R -36.3136 2 76.62721\n 2 -35.31818 4 78.63636\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 24.28 8 0.002059\n Test 2 20.21 4 0.0004531\n Test 3 3.708 3 0.2948\n Test 4 18.58 3 0.0003342\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 3582.19\n\n BMDL = 539.331\n\n BMDU = 6.11e+006\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 0 | Exponential-M3 | 7 | 1.11 | True | False | 2.703320e+03 | 6.313080e+02 | -9.990000e+02 | -999 | 79.777630 | 0.002059 | 0.000453 | 0.2948 | 0.000142 | 17.720000 | 2 | -1.319000e-01 | NaN | warning | BMDL/high dose ratio is greater than threshold (1.03 > 1.0) | Goodness of fit p-value is less than threshold (0.000142 < 0.1)\nBMD/high dose ratio is greater than threshold (4.42 > 1.0) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575\n611.000000 5 11.200000 1.643168 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-2rk3c14p.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:15 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha -21.8138 \n rho 9.52437 \n a 10.6612 \n b 0.00019702 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha 556.988 8950.24\n rho -229.524 3699.21\n a 11.2169 0.664928\n b 0.000202849 0.00144432\n d 2.44382 9.1048\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 9.6 0.5477\n 77 5 10.8 2.775\n 153 5 11.8 4.764\n 306 5 12.6 1.517\n 611 5 11.2 1.643\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 11.22 2.905 -1.244\n 77 11.22 2.892 -0.3226\n 153 11.22 2.837 0.4578\n 306 11.23 2.554 1.2\n 611 11.29 1.446 -0.1319\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -34.28212 6 80.56423\n A2 -24.17514 10 68.35029\n A3 -26.02912 7 66.05824\n R -36.3136 2 76.62721\n 3 -34.88881 5 79.77763\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 24.28 8 0.002059\n Test 2 20.21 4 0.0004531\n Test 3 3.708 3 0.2948\n Test 5a 17.72 2 0.000142\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 2703.32\n\n BMDL = 631.308\n\n BMDU = Bad\_Completion\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 0 | Exponential-M4 | 8 | 1.11 | True | False | 7.084260e+00 | 4.135940e-02 | 3.440090e+01 | -999 | 68.182340 | 0.002059 | 0.000453 | 0.2948 | 0.04679 | 6.124000 | 2 | 2.156000e-02 | NaN | warning | BMD/BMDL ratio is greater than threshold (1.71e+02 > 5.0)\nMinimum dose/BMD ratio is greater than threshold (10.9 > 3.0) | Goodness of fit p-value is less than threshold (0.0468 < 0.1)\nBMD/BMDL ratio is greater than threshold (1.71e+02 > 20.0) | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575\n611.000000 5 11.200000 1.643168 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-06thzifp.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:15 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha -21.8138 \n rho 9.52437 \n a 9.12 \n b 0.00243177 \n c 1.45066 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha -42.1116 0.607716\n rho 18 NA\n a 9.59523 0.0439833\n b 0.0393136 0.0402095\n c 1.21196 0\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 9.6 0.5477\n 77 5 10.8 2.775\n 153 5 11.8 4.764\n 306 5 12.6 1.517\n 611 5 11.2 1.643\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 9.595 0.4944 0.02156\n 77 11.53 2.584 -0.6323\n 153 11.62 2.779 0.1416\n 306 11.63 2.789 0.7784\n 611 11.63 2.789 -0.344\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -34.28212 6 80.56423\n A2 -24.17514 10 68.35029\n A3 -26.02912 7 66.05824\n R -36.3136 2 76.62721\n 4 -29.09117 5 68.18234\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 24.28 8 0.002059\n Test 2 20.21 4 0.0004531\n Test 3 3.708 3 0.2948\n Test 6a 6.124 2 0.04679\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is less than .1. Model 4 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 7.08426\n\n BMDL = 0.0413594\n\n BMDU = 34.4009\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 0 | Exponential-M5 | 9 | 1.11 | True | False | 4.790060e+01 | 7.312840e-02 | 7.509100e+01 | -999 | 70.067040 | 0.002059 | 0.000453 | 0.2948 | 0.01423 | 6.009000 | 1 | -5.834000e-01 | NaN | warning | BMD/BMDL ratio is greater than threshold (6.55e+02 > 5.0) | Goodness of fit p-value is less than threshold (0.0142 < 0.1)\nBMD/BMDL ratio is greater than threshold (6.55e+02 > 20.0) | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575\n611.000000 5 11.200000 1.643168 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-19kx5fra.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:15 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha -21.8138 \n rho 9.52437 \n a 9.12 \n b 0.00243177 \n c 1.45066 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha -42.0957 0.610729\n rho 18 NA\n a 9.59313 2.3084\n b 0.0156148 0.0405674\n c 1.21352 3535.01\n d 4.40627 0\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 9.6 0.5477\n 77 5 10.8 2.775\n 153 5 11.8 4.764\n 306 5 12.6 1.517\n 611 5 11.2 1.643\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 9.593 0.4974 0.03089\n 77 11.43 2.399 -0.5834\n 153 11.64 2.839 0.1249\n 306 11.64 2.839 0.7551\n 611 11.64 2.839 -0.3478\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -34.28212 6 80.56423\n A2 -24.17514 10 68.35029\n A3 -26.02912 7 66.05824\n R -36.3136 2 76.62721\n 5 -29.03352 6 70.06704\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 24.28 8 0.002059\n Test 2 20.21 4 0.0004531\n Test 3 3.708 3 0.2948\n Test 7a 6.009 1 0.01423\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is less than .1. Model 5 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 47.9006\n\n BMDL = 0.0731284\n\n BMDU = 75.091\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 1 | Linear | 0 | 2.21 | True | False | 1.323430e+02 | 3.840030e+01 | 1.167860e+03 | -999 | 65.114830 | 0.001352 | 0.000392 | 0.1593 | 0.000939 | 13.941400 | 2 | 2.130000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.000939 < 0.1)\nRatio of modeled to actual stdev. at control is greater than threshold (2.96 > 1.5) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-\_43ft6er.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-\_43ft6er.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:20 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.11021\n rho = 0\n beta\_0 = 9.9179\n beta\_1 = 0.00956794\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 -0.95 0.97\n\n rho -1 1 0.95 -0.97\n\n beta\_0 -0.95 0.95 1 -0.96\n\n beta\_1 0.97 -0.97 -0.96 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -12.6873 63.166 -136.49 111.116\n rho 6.01431 26.0782 -45.098 57.1266\n beta\_0 9.67033 1.8212 6.10086 13.2398\n beta\_1 0.0122086 0.0207575 -0.0284753 0.0528925\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 9.6 9.67 0.548 1.62 -0.0973\n 77 5 10.8 10.6 2.77 2.14 0.199\n 153 5 11.8 11.5 4.76 2.75 0.213\n 306 5 12.6 13.4 1.52 4.31 -0.418\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -28.870697 5 67.741394\n A2 -19.749872 8 55.499744\n A3 -21.586694 6 55.173388\n fitted -28.557415 4 65.114830\n R -30.617866 2 65.235733\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 21.736 6 0.001352\n Test 2 18.2416 3 0.0003921\n Test 3 3.67364 2 0.1593\n Test 4 13.9414 2 0.000939\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 132.343\n\n\n BMDL = 38.4003\n\n\n BMDU = 1167.86\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 1 | Polynomial-2 | 1 | 2.21 | True | False | 1.323430e+02 | 3.840030e+01 | 1.167860e+03 | -999 | 65.114830 | 0.001352 | 0.000392 | 0.1593 | 0.000939 | 13.941400 | 2 | 2.130000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.000939 < 0.1)\nRatio of modeled to actual stdev. at control is greater than threshold (2.96 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-wu7qekvg.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-wu7qekvg.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:20 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.11021\n rho = 0\n beta\_0 = 9.58225\n beta\_1 = 0.0186386\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 -0.95 0.97\n\n rho -1 1 0.95 -0.97\n\n beta\_0 -0.95 0.95 1 -0.96\n\n beta\_1 0.97 -0.97 -0.96 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -12.6872 63.1554 -136.47 111.095\n rho 6.01429 26.0738 -45.0894 57.118\n beta\_0 9.67034 1.82092 6.1014 13.2393\n beta\_1 0.0122086 0.020754 -0.0284685 0.0528857\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 9.6 9.67 0.548 1.62 -0.0973\n 77 5 10.8 10.6 2.77 2.14 0.199\n 153 5 11.8 11.5 4.76 2.75 0.213\n 306 5 12.6 13.4 1.52 4.31 -0.418\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -28.870697 5 67.741394\n A2 -19.749872 8 55.499744\n A3 -21.586694 6 55.173388\n fitted -28.557415 4 65.114830\n R -30.617866 2 65.235733\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 21.736 6 0.001352\n Test 2 18.2416 3 0.0003921\n Test 3 3.67364 2 0.1593\n Test 4 13.9414 2 0.000939\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 132.343\n\n\n BMDL = 38.4003\n\n\n BMDU = 1167.86\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 1 | Polynomial-3 | 2 | 2.21 | True | False | 1.323430e+02 | 3.840030e+01 | 1.167860e+03 | -999 | 65.114830 | 0.001352 | 0.000392 | 0.1593 | 0.000939 | 13.941400 | 2 | 2.130000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.000939 < 0.1)\nRatio of modeled to actual stdev. at control is greater than threshold (2.96 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-e91ar49f.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-e91ar49f.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:20 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.11021\n rho = 0\n beta\_0 = 9.6\n beta\_1 = 0.0160831\n beta\_2 = 0\n beta\_3 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 -0.95 0.97\n\n rho -1 1 0.95 -0.97\n\n beta\_0 -0.95 0.95 1 -0.96\n\n beta\_1 0.97 -0.97 -0.96 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -12.6873 63.1669 -136.492 111.118\n rho 6.01431 26.0785 -45.0987 57.1273\n beta\_0 9.67033 1.82122 6.10082 13.2399\n beta\_1 0.0122086 0.0207578 -0.0284758 0.0528931\n beta\_2 0 NA\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 9.6 9.67 0.548 1.62 -0.0973\n 77 5 10.8 10.6 2.77 2.14 0.199\n 153 5 11.8 11.5 4.76 2.75 0.213\n 306 5 12.6 13.4 1.52 4.31 -0.418\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -28.870697 5 67.741394\n A2 -19.749872 8 55.499744\n A3 -21.586694 6 55.173388\n fitted -28.557415 4 65.114830\n R -30.617866 2 65.235733\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 21.736 6 0.001352\n Test 2 18.2416 3 0.0003921\n Test 3 3.67364 2 0.1593\n Test 4 13.9414 2 0.000939\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 132.343\n\n\n BMDL = 38.4003\n\n\n BMDU = 1167.86\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 1 | Polynomial-4 | 3 | 2.21 | True | False | 3.448870e+02 | 2.884530e+02 | 6.586990e+02 | -999 | 64.486316 | 0.001352 | 0.000392 | 0.1593 | 0.001286 | 13.312900 | 2 | -1.510000e-02 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.00129 < 0.1)\nBMD/high dose ratio is greater than threshold (1.13 > 1.0)\nRatio of modeled to actual stdev. at control is greater than threshold (5.58 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-lunkmfh0.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-lunkmfh0.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:20 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.11021\n rho = 0\n beta\_0 = -10.4385\n beta\_1 = 0.0289688\n beta\_2 = 0.000169933\n beta\_3 = 0\n beta\_4 = 1.52158e-009\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_1 -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_4\n\n lalpha 1 -1 0.13 -0.16\n\n rho -1 1 -0.13 0.16\n\n beta\_0 0.13 -0.13 1 -0.76\n\n beta\_4 -0.16 0.16 -0.76 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 24.6395 11.8722 1.37035 47.9086\n rho -9.44666 4.9138 -19.0775 0.184217\n beta\_0 10.7133 0.756604 9.23037 12.1962\n beta\_1 3.26028e-024 NA\n beta\_2 4.9144e-026 NA\n beta\_3 2.77359e-029 NA\n beta\_4 2.16281e-010 1.0935e-010 1.9599e-012 4.30602e-010\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 9.6 10.7 0.548 3.06 -0.814\n 77 5 10.8 10.7 2.77 3.05 0.058\n 153 5 11.8 10.8 4.76 2.91 0.745\n 306 5 12.6 12.6 1.52 1.42 -0.0151\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -28.870697 5 67.741394\n A2 -19.749872 8 55.499744\n A3 -21.586694 6 55.173388\n fitted -28.243158 4 64.486316\n R -30.617866 2 65.235733\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 21.736 6 0.001352\n Test 2 18.2416 3 0.0003921\n Test 3 3.67364 2 0.1593\n Test 4 13.3129 2 0.001286\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 344.887\n\n\n BMDL = 288.453\n\n\n BMDU = 658.699\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 1 | Power | 4 | 2.19 | True | False | 1.323420e+02 | 3.840030e+01 | 1.167860e+03 | -999 | 65.114830 | 0.001352 | 0.000392 | 0.1593 | 0.000939 | 13.941400 | 2 | 2.130000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.000939 < 0.1)\nRatio of modeled to actual stdev. at control is greater than threshold (2.96 > 1.5) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-8nnqpodk.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-8nnqpodk.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:20 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n The power is restricted to be greater than or equal to 1\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.11021\n rho = 0\n control = 9.6\n slope = 0.0671804\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho control slope\n\n lalpha 1 -1 -0.077 -0.026\n\n rho -1 1 0.071 0.012\n\n control -0.077 0.071 1 -0.66\n\n slope -0.026 0.012 -0.66 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -12.6873 13.8283 -39.7904 14.4158\n rho 6.01431 5.70278 -5.16293 17.1916\n control 9.67033 0.669511 8.35811 10.9825\n slope 0.0122087 0.00660608 -0.000739023 0.0251563\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 9.6 9.67 0.548 1.62 -0.0973\n 77 5 10.8 10.6 2.77 2.14 0.199\n 153 5 11.8 11.5 4.76 2.75 0.213\n 306 5 12.6 13.4 1.52 4.31 -0.418\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -28.870697 5 67.741394\n A2 -19.749872 8 55.499744\n A3 -21.586694 6 55.173388\n fitted -28.557415 4 65.114830\n R -30.617866 2 65.235733\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 21.736 6 0.001352\n Test 2 18.2416 3 0.0003921\n Test 3 3.67364 2 0.1593\n Test 4 13.9414 2 0.000939\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 132.342 \n\n\n BMDL = 38.4003 \n\n\n BMDU = 1167.86 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 1 | Hill | 5 | 2.18 | True | False | 6.612310e+01 | -9.990000e+02 | -9.990000e+02 | -999 | 53.637159 | 0.001352 | 0.000392 | 0.1593 | 0.2917 | 2.463770 | 2 | -5.720000e-01 | BMDL computation failed. | failure | Warning(s): BMDL computation failed. | NaN | BMDL does not exist | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-bd4347rs.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-bd4347rs.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:20 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n Power parameter restricted to be greater than 1\n The variance is to be modeled as Var(i) = exp(lalpha + rho \* ln(mean(i)))\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.11021\n rho = 0\n intercept = 9.6\n v = 3\n n = 0.205811\n k = 206.2\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -n \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha intercept v k\n\n lalpha 1 -0.5 -0.64 0.17\n\n intercept -0.5 1 -0.054 -0.02\n\n v -0.64 -0.054 1 0.17\n\n k 0.17 -0.02 0.17 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -42.0759 0.65618 -43.362 -40.7898\n rho 18 NA\n intercept 9.58995 0.213457 9.17158 10.0083\n v 2.22978 0.433877 1.37939 3.08016\n n 18 NA\n k 70.8351 5.52633 60.0037 81.6665\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 9.6 9.59 0.548 0.501 0.0449\n 77 5 10.8 11.4 2.77 2.4 -0.572\n 153 5 11.8 11.8 4.76 3.29 -0.0134\n 306 5 12.6 11.8 1.52 3.29 0.531\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -28.870697 5 67.741394\n A2 -19.749872 8 55.499744\n A3 -21.586694 6 55.173388\n fitted -22.818580 4 53.637159\n R -30.617866 2 65.235733\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 21.736 6 0.001352\n Test 2 18.2416 3 0.0003921\n Test 3 3.67364 2 0.1593\n Test 4 2.46377 2 0.2917\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 66.1231\n\n\nBMDL computation failed.\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 1 | Exponential-M2 | 6 | 1.11 | True | False | 2.016290e+02 | 6.484990e+01 | 2.238270e+03 | -999 | 65.720560 | 0.001352 | 0.000392 | 0.1593 | 0.000694 | 14.550000 | 2 | 3.779000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.000694 < 0.1) | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-01ig4a82.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:20 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha -21.8235 \n rho 9.54946 \n a 9.93001 \n b 0.000859812 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha -8.09577 16.0009\n rho 4.13857 6.63177\n a 9.87133 0.74415\n b 0.000912396 0.000503747\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 9.6 0.5477\n 77 5 10.8 2.775\n 153 5 11.8 4.764\n 306 5 12.6 1.517\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 9.871 1.994 -0.3043\n 77 10.59 2.306 0.2039\n 153 11.35 2.661 0.3779\n 306 13.05 3.553 -0.2835\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -28.8707 5 67.74139\n A2 -19.74987 8 55.49974\n A3 -21.58669 6 55.17339\n R -30.61787 2 65.23573\n 2 -28.86028 4 65.72056\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 21.74 6 0.001352\n Test 2 18.24 3 0.0003921\n Test 3 3.674 2 0.1593\n Test 4 14.55 2 0.0006936\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 201.629\n\n BMDL = 64.8499\n\n BMDU = 2238.27\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 1 | Exponential-M3 | 7 | 1.11 | True | False | 2.016290e+02 | 6.484990e+01 | 2.238270e+03 | -999 | 65.720560 | 0.001352 | 0.000392 | 0.1593 | 0.000694 | 14.550000 | 2 | 3.779000e-01 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.000694 < 0.1) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-zvakd8lj.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:20 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha -21.8235 \n rho 9.54946 \n a 9.93001 \n b 0.000859812 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha -8.09576 16.0009\n rho 4.13857 6.63176\n a 9.87132 0.744149\n b 0.000912397 0.000503747\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 9.6 0.5477\n 77 5 10.8 2.775\n 153 5 11.8 4.764\n 306 5 12.6 1.517\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 9.871 1.994 -0.3043\n 77 10.59 2.306 0.2039\n 153 11.35 2.661 0.3779\n 306 13.05 3.553 -0.2835\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -28.8707 5 67.74139\n A2 -19.74987 8 55.49974\n A3 -21.58669 6 55.17339\n R -30.61787 2 65.23573\n 3 -28.86028 4 65.72056\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 21.74 6 0.001352\n Test 2 18.24 3 0.0003921\n Test 3 3.674 2 0.1593\n Test 5a 14.55 2 0.0006936\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 201.629\n\n BMDL = 64.8499\n\n BMDU = 2238.27\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 1 | Exponential-M4 | 8 | 1.11 | True | False | 8.931990e+00 | 2.255360e-02 | 4.042340e+01 | -999 | 55.916960 | 0.001352 | 0.000392 | 0.1593 | 0.09765 | 2.744000 | 1 | 3.547000e-02 | NaN | warning | BMD/BMDL ratio is greater than threshold (3.96e+02 > 5.0)\nMinimum dose/BMD ratio is greater than threshold (8.62 > 3.0) | Goodness of fit p-value is less than threshold (0.0977 < 0.1)\nBMD/BMDL ratio is greater than threshold (3.96e+02 > 20.0) | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-gsj47itm.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:20 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha -21.8235 \n rho 9.54946 \n a 9.12 \n b 0.00630935 \n c 1.45066 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha -42.0978 0.654235\n rho 18 NA\n a 9.59213 0.0225644\n b 0.0284242 0.0464545\n c 1.23079 0\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 9.6 0.5477\n 77 5 10.8 2.775\n 153 5 11.8 4.764\n 306 5 12.6 1.517\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 9.592 0.4964 0.03547\n 77 11.56 2.657 -0.6377\n 153 11.78 3.148 0.01614\n 306 11.81 3.216 0.5524\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -28.8707 5 67.74139\n A2 -19.74987 8 55.49974\n A3 -21.58669 6 55.17339\n R -30.61787 2 65.23573\n 4 -22.95848 5 55.91696\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 21.74 6 0.001352\n Test 2 18.24 3 0.0003921\n Test 3 3.674 2 0.1593\n Test 6a 2.744 1 0.09765\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is less than .1. Model 4 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 8.93199\n\n BMDL = 0.0225536\n\n BMDU = 40.4234\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 1 | Exponential-M5 | 9 | 1.11 | True | False | 4.615570e+01 | 4.258470e-02 | 7.559920e+01 | -999 | 57.637150 | 0.001352 | 0.000392 | 0.1593 | -999 | 2.464000 | 0 | -5.718000e-01 | NaN | warning | BMD/BMDL ratio is greater than threshold (1.08e+03 > 5.0) | BMD/BMDL ratio is greater than threshold (1.08e+03 > 20.0)\nZero degrees of freedom; saturated model | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452\n306.000000 5 12.600000 1.516575 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-p56ltww9.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:20 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha -21.8235 \n rho 9.54946 \n a 9.12 \n b 0.00630935 \n c 1.45066 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha -42.0759 0.65618\n rho 18 NA\n a 9.58995 0.76867\n b 0.0149883 0.0458135\n c 1.23251 1329.43\n d 3.71523 0\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 9.6 0.5477\n 77 5 10.8 2.775\n 153 5 11.8 4.764\n 306 5 12.6 1.517\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 9.59 0.5008 0.04487\n 77 11.41 2.4 -0.5718\n 153 11.82 3.287 -0.01342\n 306 11.82 3.287 0.5308\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -28.8707 5 67.74139\n A2 -19.74987 8 55.49974\n A3 -21.58669 6 55.17339\n R -30.61787 2 65.23573\n 5 -22.81857 6 57.63715\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 21.74 6 0.001352\n Test 2 18.24 3 0.0003921\n Test 3 3.674 2 0.1593\n Test 7a 2.464 0 N/A\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n Degrees of freedom for Test 7a are less than or equal to 0.\n The Chi-Square test for fit is not valid.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 46.1557\n\n BMDL = 0.0425847\n\n BMDU = 75.5992\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 2 | Linear | 0 | 2.21 | True | False | 3.511350e+01 | 1.475370e+01 | 1.048480e+02 | -999 | 39.068072 | 0.002417 | 0.000530 | 0.1361 | <0.0001 | -0.604779 | 2 | 6.620000e-02 | Warning: Likelihood for fitted model larger than the Likelihood for model A3. | valid | Warning(s): Warning: Likelihood for fitted model larger than the Likelihood for model A3. | NaN | NaN | True | AIC | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 3 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-i0rxus4c.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-i0rxus4c.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:24 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.32565\n rho = 0\n beta\_0 = 9.63073\n beta\_1 = 0.0143817\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha beta\_0 beta\_1\n\n lalpha 1 -0.017 0.095\n\n beta\_0 -0.017 1 -0.1\n\n beta\_1 0.095 -0.1 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -41.6966 0.366826 -42.4156 -40.9777\n rho 18 NA\n beta\_0 9.5822 0.254781 9.08284 10.0816\n beta\_1 0.017116 0.00605784 0.00524287 0.0289892\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 9.6 9.58 0.548 0.601 0.0662\n 77 5 10.8 10.9 2.77 1.92 -0.117\n 153 5 11.8 12.2 4.76 5.29 -0.17\n \n Warning: Likelihood for fitted model larger than the Likelihood for model A3.\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -23.268801 4 54.537603\n A2 -15.725458 6 43.450916\n A3 -16.836426 5 43.672851\n fitted -16.534036 3 39.068072\n R -23.975480 2 51.950960\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 16.5 4 0.002417\n Test 2 15.0867 2 0.0005296\n Test 3 2.22194 1 0.1361\n Test 4 -0.604779 2 <.0001\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 35.1135\n\n\n BMDL = 14.7537\n\n\n BMDU = 104.848\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 2 | Polynomial-2 | 1 | 2.21 | True | False | 3.511350e+01 | 1.475370e+01 | 1.048480e+02 | -999 | 39.068072 | 0.002417 | 0.000530 | 0.1361 | <0.0001 | -0.604779 | 2 | 6.620000e-02 | Warning: Likelihood for fitted model larger than the Likelihood for model A3. | valid | Warning(s): Warning: Likelihood for fitted model larger than the Likelihood for model A3. | NaN | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 3 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-lchbbjas.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-lchbbjas.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:24 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.32565\n rho = 0\n beta\_0 = 9.6\n beta\_1 = 0.0168056\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha beta\_0 beta\_1\n\n lalpha 1 -0.017 0.095\n\n beta\_0 -0.017 1 -0.1\n\n beta\_1 0.095 -0.1 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -41.6966 0.366826 -42.4156 -40.9777\n rho 18 NA\n beta\_0 9.5822 0.254781 9.08284 10.0816\n beta\_1 0.017116 0.00605785 0.00524286 0.0289892\n beta\_2 2.63703e-026 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 9.6 9.58 0.548 0.601 0.0662\n 77 5 10.8 10.9 2.77 1.92 -0.117\n 153 5 11.8 12.2 4.76 5.29 -0.17\n \n Warning: Likelihood for fitted model larger than the Likelihood for model A3.\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -23.268801 4 54.537603\n A2 -15.725458 6 43.450916\n A3 -16.836426 5 43.672851\n fitted -16.534036 3 39.068072\n R -23.975480 2 51.950960\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 16.5 4 0.002417\n Test 2 15.0867 2 0.0005296\n Test 3 2.22194 1 0.1361\n Test 4 -0.604779 2 <.0001\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 35.1135\n\n\n BMDL = 14.7537\n\n\n BMDU = 104.848\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 2 | Polynomial-3 | 2 | 2.21 | True | False | 3.511350e+01 | 1.475370e+01 | 1.048710e+02 | -999 | 39.068072 | 0.002417 | 0.000530 | 0.1361 | <0.0001 | -0.604779 | 2 | 6.620000e-02 | Warning: Likelihood for fitted model larger than the Likelihood for model A3. | valid | Warning(s): Warning: Likelihood for fitted model larger than the Likelihood for model A3. | NaN | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 3 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-reio41vv.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-reio41vv.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:24 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.32565\n rho = 0\n beta\_0 = -2345.34\n beta\_1 = 5.88281\n beta\_2 = 0.0619812\n beta\_3 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha beta\_0 beta\_1\n\n lalpha 1 -0.017 0.095\n\n beta\_0 -0.017 1 -0.1\n\n beta\_1 0.095 -0.1 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -41.6966 0.366826 -42.4156 -40.9777\n rho 18 NA\n beta\_0 9.5822 0.254781 9.08284 10.0816\n beta\_1 0.017116 0.00605784 0.00524286 0.0289892\n beta\_2 1.42805e-026 NA\n beta\_3 -0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 9.6 9.58 0.548 0.601 0.0662\n 77 5 10.8 10.9 2.77 1.92 -0.117\n 153 5 11.8 12.2 4.76 5.29 -0.17\n \n Warning: Likelihood for fitted model larger than the Likelihood for model A3.\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -23.268801 4 54.537603\n A2 -15.725458 6 43.450916\n A3 -16.836426 5 43.672851\n fitted -16.534036 3 39.068072\n R -23.975480 2 51.950960\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 16.5 4 0.002417\n Test 2 15.0867 2 0.0005296\n Test 3 2.22194 1 0.1361\n Test 4 -0.604779 2 <.0001\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 35.1135\n\n\n BMDL = 14.7537\n\n\n BMDU = 104.871\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 2 | Polynomial-4 | 3 | 2.21 | True | False | 3.511350e+01 | 1.475370e+01 | 1.048710e+02 | -999 | 39.068072 | 0.002417 | 0.000530 | 0.1361 | <0.0001 | -0.604779 | 2 | 6.620000e-02 | Warning: Likelihood for fitted model larger than the Likelihood for model A3. | valid | Warning(s): Warning: Likelihood for fitted model larger than the Likelihood for model A3. | NaN | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 3 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-6n5nqv8c.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-6n5nqv8c.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:23 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be positive\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.32565\n rho = 0\n beta\_0 = 13.5124\n beta\_1 = 1.0925\n beta\_2 = 0\n beta\_3 = 3.51467e-005\n beta\_4 = 4.95929e-008\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha beta\_0 beta\_1\n\n lalpha 1 -0.017 0.095\n\n beta\_0 -0.017 1 -0.1\n\n beta\_1 0.095 -0.1 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -41.6966 0.366826 -42.4156 -40.9777\n rho 18 NA\n beta\_0 9.5822 0.254781 9.08284 10.0816\n beta\_1 0.017116 0.00605781 0.00524293 0.0289891\n beta\_2 0 NA\n beta\_3 0 NA\n beta\_4 4.05082e-029 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 9.6 9.58 0.548 0.601 0.0662\n 77 5 10.8 10.9 2.77 1.92 -0.117\n 153 5 11.8 12.2 4.76 5.29 -0.17\n \n Warning: Likelihood for fitted model larger than the Likelihood for model A3.\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -23.268801 4 54.537603\n A2 -15.725458 6 43.450916\n A3 -16.836426 5 43.672851\n fitted -16.534036 3 39.068072\n R -23.975480 2 51.950960\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 16.5 4 0.002417\n Test 2 15.0867 2 0.0005296\n Test 3 2.22194 1 0.1361\n Test 4 -0.604779 2 <.0001\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 35.1135\n\n\n BMDL = 14.7537\n\n\n BMDU = 104.871\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 2 | Power | 4 | 2.19 | True | False | 3.511350e+01 | 1.475370e+01 | 1.048480e+02 | -999 | 39.068072 | 0.002417 | 0.000530 | 0.1356 | <0.0001 | -0.609471 | 2 | 6.620000e-02 | Warning: Likelihood for fitted model larger than the Likelihood for model A3. | valid | Warning(s): Warning: Likelihood for fitted model larger than the Likelihood for model A3. | NaN | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-70gwwxxe.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-70gwwxxe.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:23 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n The power is restricted to be greater than or equal to 1\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.32565\n rho = 0\n control = 9.6\n slope = 0.0259329\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha control slope\n\n lalpha 1 -0.54 -0.67\n\n control -0.54 1 -0.027\n\n slope -0.67 -0.027 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -41.6966 0.754561 -43.1756 -40.2177\n rho 18 NA\n control 9.5822 0.252931 9.08647 10.0779\n slope 0.017116 0.00441639 0.00846005 0.025772\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 9.6 9.58 0.548 0.601 0.0662\n 77 5 10.8 10.9 2.77 1.92 -0.117\n 153 5 11.8 12.2 4.76 5.29 -0.17\n \n Warning: Likelihood for fitted model larger than the Likelihood for model A3.\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -23.268801 4 54.537603\n A2 -15.725458 6 43.450916\n A3 -16.838772 5 43.677543\n fitted -16.534036 3 39.068072\n R -23.975480 2 51.950960\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 16.5 4 0.002417\n Test 2 15.0867 2 0.0005296\n Test 3 2.22663 1 0.1356\n Test 4 -0.609471 2 <.0001\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 35.1135 \n\n\n BMDL = 14.7537 \n\n\n BMDU = 104.848 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 2 | Hill | 5 | 2.18 | True | False | 6.612310e+01 | -9.990000e+02 | -9.990000e+02 | -999 | 53.637159 | 0.001352 | 0.000392 | 0.1593 | 0.2917 | 2.463770 | 2 | -5.720000e-01 | BMDL computation failed. | failure | Warning(s): BMDL computation failed. | NaN | BMDL does not exist | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-bd4347rs.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-bd4347rs.plt\n \t\t\t\t\t\t\tTue Jul 06 12:40:20 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n Power parameter restricted to be greater than 1\n The variance is to be modeled as Var(i) = exp(lalpha + rho \* ln(mean(i)))\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 2.11021\n rho = 0\n intercept = 9.6\n v = 3\n n = 0.205811\n k = 206.2\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -n \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha intercept v k\n\n lalpha 1 -0.5 -0.64 0.17\n\n intercept -0.5 1 -0.054 -0.02\n\n v -0.64 -0.054 1 0.17\n\n k 0.17 -0.02 0.17 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -42.0759 0.65618 -43.362 -40.7898\n rho 18 NA\n intercept 9.58995 0.213457 9.17158 10.0083\n v 2.22978 0.433877 1.37939 3.08016\n n 18 NA\n k 70.8351 5.52633 60.0037 81.6665\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 9.6 9.59 0.548 0.501 0.0449\n 77 5 10.8 11.4 2.77 2.4 -0.572\n 153 5 11.8 11.8 4.76 3.29 -0.0134\n 306 5 12.6 11.8 1.52 3.29 0.531\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -28.870697 5 67.741394\n A2 -19.749872 8 55.499744\n A3 -21.586694 6 55.173388\n fitted -22.818580 4 53.637159\n R -30.617866 2 65.235733\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 21.736 6 0.001352\n Test 2 18.2416 3 0.0003921\n Test 3 3.67364 2 0.1593\n Test 4 2.46377 2 0.2917\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 66.1231\n\n\nBMDL computation failed.\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 2 | Exponential-M2 | 6 | 1.11 | True | False | 4.122630e+01 | 1.829100e+01 | 1.166520e+02 | -999 | 41.525380 | 0.002417 | 0.000530 | 0.1356 | -999 | -0.152200 | 1 | -1.358000e-02 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-ghwcnhvx.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:23 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha -49.2044 \n rho 21.32 \n a 9.64442 \n b 0.001349 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha -41.6063 0.759946\n rho 18 NA\n a 9.59208 0.000379675\n b 0.00155397 0\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 9.6 0.5477\n 77 5 10.8 2.775\n 153 5 11.8 4.764\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 9.592 0.6346 0.0279\n 77 10.81 1.863 -0.01358\n 153 12.17 5.393 -0.152\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -23.2688 4 54.5376\n A2 -15.72546 6 43.45092\n A3 -16.83877 5 43.67754\n R -23.97548 2 51.95096\n 2 -16.76269 4 41.52538\n\n\n Additive constant for all log-likelihoods = -13.78. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 16.5 4 0.002417\n Test 2 15.09 2 0.0005296\n Test 3 2.227 1 0.1356\n Test 4 -0.1522 1 N/A\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 41.2263\n\n BMDL = 18.291\n\n BMDU = 116.652\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 2 | Exponential-M3 | 7 | 1.11 | True | False | 4.122630e+01 | 1.829100e+01 | 1.166520e+02 | -999 | 41.525380 | 0.002417 | 0.000530 | 0.1356 | -999 | -0.152200 | 1 | -1.358000e-02 | NaN | valid | NaN | NaN | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-qesz5o7g.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:23 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha -49.2044 \n rho 21.32 \n a 9.64442 \n b 0.001349 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha -41.6063 0.759946\n rho 18 NA\n a 9.59208 0.000379675\n b 0.00155397 0\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 9.6 0.5477\n 77 5 10.8 2.775\n 153 5 11.8 4.764\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 9.592 0.6346 0.0279\n 77 10.81 1.863 -0.01358\n 153 12.17 5.393 -0.152\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -23.2688 4 54.5376\n A2 -15.72546 6 43.45092\n A3 -16.83877 5 43.67754\n R -23.97548 2 51.95096\n 3 -16.76269 4 41.52538\n\n\n Additive constant for all log-likelihoods = -13.78. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 16.5 4 0.002417\n Test 2 15.09 2 0.0005296\n Test 3 2.227 1 0.1356\n Test 5a -0.1522 1 N/A\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 41.2263\n\n BMDL = 18.291\n\n BMDU = 116.652\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 2 | Exponential-M4 | 8 | 1.11 | True | False | 1.700570e+01 | 9.211880e-02 | 7.441510e+01 | -999 | 41.788650 | 0.002417 | 0.000530 | 0.1356 | -999 | -1.889000 | 0 | 1.471000e-01 | NaN | warning | BMD/BMDL ratio is greater than threshold (1.85e+02 > 5.0)\nMinimum dose/BMD ratio is greater than threshold (4.53 > 3.0) | BMD/BMDL ratio is greater than threshold (1.85e+02 > 20.0)\nZero degrees of freedom; saturated model | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-17myoa4u.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:23 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 3\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha -49.2044 \n rho 21.32 \n a 9.12 \n b 0.0108229 \n c 1.35855 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha -41.9264 0.733619\n rho 18 NA\n a 9.56531 0.0125834\n b 0.0112271 0.170434\n c 1.31719 0\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 9.6 0.5477\n 77 5 10.8 2.775\n 153 5 11.8 4.764\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 9.565 0.5273 0.1471\n 77 11.32 2.403 -0.4849\n 153 12.05 4.229 -0.1347\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -23.2688 4 54.5376\n A2 -15.72546 6 43.45092\n A3 -16.83877 5 43.67754\n R -23.97548 2 51.95096\n 4 -15.89433 5 41.78865\n\n\n Additive constant for all log-likelihoods = -13.78. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 16.5 4 0.002417\n Test 2 15.09 2 0.0005296\n Test 3 2.227 1 0.1356\n Test 6a -1.889 0 N/A\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n Degrees of freedom for Test 6a are less than or equal to 0.\n The Chi-Square test for fit is not valid.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 17.0057\n\n BMDL = 0.0921188\n\n BMDU = 74.4151\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Urea Nitrogen | mg/dL | Male | PA41 | Clinical Chemistry | SD | 4 | X-C10866B|Male|Clinical Chemistry|PA41|4 | 1, 2, 3, 4, 5 | mg/kg | .24494897427831783,1.2409673645990857,2.1307275752662518,.6782329983125267,.73484692283495334 | 0,0,0,1,0 | 1,1,1,1,1 | SD | day | NaN | 10 | Clinical Chemistry Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Urea Nitrogen | Dose (mg/kg) | X-C10866B|Male|Clinical Chemistry|PA41|4 | 8 | 2 | Exponential-M5 | 9 | 1.11 | True | False | 4.615570e+01 | 4.258470e-02 | 7.559920e+01 | -999 | 57.637150 | 0.001352 | 0.000392 | 0.1593 | -999 | 2.464000 | 0 | -5.718000e-01 | NaN | warning | BMD/BMDL ratio is greater than threshold (1.08e+03 > 5.0) | BMD/BMDL ratio is greater than threshold (1.08e+03 > 20.0)\nZero degrees of freedom; saturated model | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 3 1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 9.600000 0.547723\n77.000000 5 10.800000 2.774887\n153.000000 5 11.800000 4.764452 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-p56ltww9.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:40:20 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha -21.8235 \n rho 9.54946 \n a 9.12 \n b 0.00630935 \n c 1.45066 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha -42.0759 0.65618\n rho 18 NA\n a 9.58995 0.76867\n b 0.0149883 0.0458135\n c 1.23251 1329.43\n d 3.71523 0\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 9.6 0.5477\n 77 5 10.8 2.775\n 153 5 11.8 4.764\n 306 5 12.6 1.517\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 9.59 0.5008 0.04487\n 77 11.41 2.4 -0.5718\n 153 11.82 3.287 -0.01342\n 306 11.82 3.287 0.5308\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -28.8707 5 67.74139\n A2 -19.74987 8 55.49974\n A3 -21.58669 6 55.17339\n R -30.61787 2 65.23573\n 5 -22.81857 6 57.63715\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 21.74 6 0.001352\n Test 2 18.24 3 0.0003921\n Test 3 3.674 2 0.1593\n Test 7a 2.464 0 N/A\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n Degrees of freedom for Test 7a are less than or equal to 0.\n The Chi-Square test for fit is not valid.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 46.1557\n\n BMDL = 0.0425847\n\n BMDU = 75.5992\n | NaN | NaN |

## Hormone Data
| DEPOSITOR\_STUDY\_NUMBER | study\_id | CHEMICAL | ENDPOINT | ENDPOINT\_UNIT | SEX | table\_id | OUTPUT\_TYPE | PHASE\_TYPE | PHASE\_START | id | GROUP\_NAME | Converted\_Dose\_Units | STE | MULT\_COMP\_SIGNIF | NUM\_DECIMAL\_DIGIT | DEATH\_PHASE\_TYPE | DEATH\_PHASE\_TIME\_UNIT | LEGEND\_ID | SORT\_ORDER | TABLE\_HEADER | DEATH\_PHASE\_TIME | DOSE\_UNIT | original\_doses | dataset\_name | xlabel | ylabel | dataset\_index | doses\_dropped | model\_name | model\_index | model\_version | has\_output | execution\_halted | BMD | BMDL | BMDU | CSF | AIC | pvalue1 | pvalue2 | pvalue3 | pvalue4 | Chi2 | df | residual\_of\_interest | warnings | logic\_bin | logic\_cautions | logic\_warnings | logic\_failures | recommended | recommended\_variable | dfile | outfile | stdout | stderr |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 0 | Linear | 0 | 2.21 | True | False | 662.63500 | 388.79000 | 1451.4500 | -999 | 207.555349 | <0.0001 | 0.01947 | 0.1856 | <0.0001 | 28.596700 | 3 | 0.21800 | NaN | warning | NaN | BMD/high dose ratio is greater than threshold (1.08 > 1.0)\nResidual at lowest dose is greater than threshold (3.31 > 2.0)\nRatio of modeled to actual stdev. at control is greater than threshold (2.11 > 1.5) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037\n611.000000 5 104.000000 8.631338 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-d5\_g1k\_h.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-d5\_g1k\_h.plt\n \t\t\t\t\t\t\tTue Jul 06 12:41:41 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 6.33796\n rho = 0\n beta\_0 = 216.268\n beta\_1 = -0.229068\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.14 -0.14\n\n rho -1 1 -0.15 0.14\n\n beta\_0 0.14 -0.15 1 -0.98\n\n beta\_1 -0.14 0.14 -0.98 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -39.2095 6.69994 -52.3412 -26.0779\n rho 9.28625 1.34627 6.64762 11.9249\n beta\_0 173.186 15.9185 141.986 204.385\n beta\_1 -0.114334 0.0276065 -0.168442 -0.0602264\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 285 173 36 75.8 3.31\n 77 5 166 164 17.8 59.5 0.0759\n 153 5 146 156 30.9 46.2 -0.45\n 306 5 116 138 13.8 26.6 -1.83\n 611 5 104 103 8.63 6.89 0.218\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -88.935179 6 189.870357\n A2 -83.070045 10 186.140089\n A3 -85.479305 7 184.958611\n fitted -99.777674 4 207.555349\n R -118.020849 2 240.041699\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 69.9016 8 <.0001\n Test 2 11.7303 4 0.01947\n Test 3 4.81852 3 0.1856\n Test 4 28.5967 3 <.0001\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 662.635\n\n\n BMDL = 388.79\n\n\n BMDU = 1451.45\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 0 | Polynomial-2 | 1 | 2.21 | True | False | 662.63400 | 388.79000 | 1451.4500 | -999 | 207.555349 | <0.0001 | 0.01947 | 0.1856 | <0.0001 | 28.596700 | 3 | 0.21800 | NaN | warning | NaN | BMD/high dose ratio is greater than threshold (1.08 > 1.0)\nResidual at lowest dose is greater than threshold (3.31 > 2.0)\nRatio of modeled to actual stdev. at control is greater than threshold (2.11 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037\n611.000000 5 104.000000 8.631338 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-e28mjr7l.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-e28mjr7l.plt\n \t\t\t\t\t\t\tTue Jul 06 12:41:41 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 6.33796\n rho = 0\n beta\_0 = 259.485\n beta\_1 = -0.830218\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.14 -0.14\n\n rho -1 1 -0.15 0.14\n\n beta\_0 0.14 -0.15 1 -0.98\n\n beta\_1 -0.14 0.14 -0.98 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -39.2095 6.69994 -52.3412 -26.0779\n rho 9.28625 1.34627 6.64761 11.9249\n beta\_0 173.186 15.9185 141.986 204.385\n beta\_1 -0.114334 0.0276064 -0.168442 -0.0602266\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 285 173 36 75.8 3.31\n 77 5 166 164 17.8 59.5 0.0759\n 153 5 146 156 30.9 46.2 -0.45\n 306 5 116 138 13.8 26.6 -1.83\n 611 5 104 103 8.63 6.89 0.218\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -88.935179 6 189.870357\n A2 -83.070045 10 186.140089\n A3 -85.479305 7 184.958611\n fitted -99.777674 4 207.555349\n R -118.020849 2 240.041699\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 69.9016 8 <.0001\n Test 2 11.7303 4 0.01947\n Test 3 4.81852 3 0.1856\n Test 4 28.5967 3 <.0001\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 662.634\n\n\n BMDL = 388.79\n\n\n BMDU = 1451.45\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 0 | Polynomial-3 | 2 | 2.21 | True | False | 662.63500 | 388.79000 | 1451.4500 | -999 | 207.555349 | <0.0001 | 0.01947 | 0.1856 | <0.0001 | 28.596700 | 3 | 0.21800 | NaN | warning | NaN | BMD/high dose ratio is greater than threshold (1.08 > 1.0)\nResidual at lowest dose is greater than threshold (3.31 > 2.0)\nRatio of modeled to actual stdev. at control is greater than threshold (2.11 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037\n611.000000 5 104.000000 8.631338 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-31fe3rhu.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-31fe3rhu.plt\n \t\t\t\t\t\t\tTue Jul 06 12:41:41 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 6.33796\n rho = 0\n beta\_0 = 280.158\n beta\_1 = -1.62749\n beta\_2 = 0\n beta\_3 = -4.64369e-006\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1\n\n lalpha 1 -1 0.14 -0.14\n\n rho -1 1 -0.15 0.14\n\n beta\_0 0.14 -0.15 1 -0.98\n\n beta\_1 -0.14 0.14 -0.98 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -39.2095 6.69996 -52.3412 -26.0778\n rho 9.28624 1.34627 6.6476 11.9249\n beta\_0 173.186 15.9185 141.986 204.385\n beta\_1 -0.114334 0.0276065 -0.168442 -0.0602265\n beta\_2 0 NA\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 285 173 36 75.8 3.31\n 77 5 166 164 17.8 59.5 0.0759\n 153 5 146 156 30.9 46.2 -0.45\n 306 5 116 138 13.8 26.6 -1.83\n 611 5 104 103 8.63 6.89 0.218\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -88.935179 6 189.870357\n A2 -83.070045 10 186.140089\n A3 -85.479305 7 184.958611\n fitted -99.777674 4 207.555349\n R -118.020849 2 240.041699\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 69.9016 8 <.0001\n Test 2 11.7303 4 0.01947\n Test 3 4.81852 3 0.1856\n Test 4 28.5967 3 <.0001\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 662.635\n\n\n BMDL = 388.79\n\n\n BMDU = 1451.45\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 0 | Polynomial-4 | 3 | 2.21 | True | False | -9999.00000 | 51.02260 | -999.0000 | -999 | 294.496541 | <0.0001 | 0.01947 | 0.1856 | <0.0001 | 113.538000 | 2 | -999.00000 | BMD = 100\*(maximum dose) | warning | Warning(s): BMD = 100\*(maximum dose) | Residual of Interest does not exist\nResidual at lowest dose is greater than threshold (3.45 > 2.0)\nRatio of modeled to actual stdev. at control is greater than threshold (5.31 > 1.5) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 5 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037\n611.000000 5 104.000000 8.631338 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-fmausaji.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-fmausaji.plt\n \t\t\t\t\t\t\tTue Jul 06 12:41:41 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n The polynomial coefficients are restricted to be negative\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 6.33796\n rho = 0\n beta\_0 = 285.4\n beta\_1 = -2.65865\n beta\_2 = 0\n beta\_3 = -4.96952e-005\n beta\_4 = 0\n\n\n!!! Warning: optimum may not have been found. !!!\n!!! You may want to try choosing different initial values. !!!\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -beta\_2 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho beta\_0 beta\_1 beta\_3\n\n lalpha 1 -1 -1.4 0.023 0.13\n\n rho -1 1 1.4 -0.026 -0.13\n\n beta\_0 -1.4 1.4 1 1 -0.6\n\n beta\_1 0.023 -0.026 1 1 -0.94\n\n beta\_3 0.13 -0.13 -0.6 -0.94 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha 17.7584 5.87511 6.24337 29.2734\n rho -3.30719 2.65765 -8.51609 1.90171\n beta\_0 -8.97702 1.27838 -11.4826 -6.47144\n beta\_1 -0 0.00605742 -0.0118723 0.0118723\n beta\_2 -2.87233e-006 NA\n beta\_3 -2.43452e-009 2.60381e-008 -5.34683e-008 4.85992e-008\n beta\_4 -0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 285 -8.98 36 191 3.45\n 77 5 166 -9 17.8 190 2.06\n 153 5 146 -9.05 30.9 188 1.85\n 306 5 116 -9.32 13.8 179 1.57\n 611 5 104 -10.6 8.63 145 1.77\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -88.935179 6 189.870357\n A2 -83.070045 10 186.140089\n A3 -85.479305 7 184.958611\n fitted -142.248271 5 294.496541\n R -118.020849 2 240.041699\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 69.9016 8 <.0001\n Test 2 11.7303 4 0.01947\n Test 3 4.81852 3 0.1856\n Test 4 113.538 2 <.0001\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n\nBMD computation failed for BMR = -1.#IND\nSetting BMD = 100\*(maximum dose) \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = -9999\n\n\n BMDL = 51.0226\n\n \nBMDU computation failed. | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 0 | Power | 4 | 2.19 | True | False | 662.63500 | 388.79000 | 1451.4500 | -999 | 207.555349 | <0.0001 | 0.01947 | 0.1856 | <0.0001 | 28.596700 | 3 | 0.21800 | NaN | warning | NaN | BMD/high dose ratio is greater than threshold (1.08 > 1.0)\nResidual at lowest dose is greater than threshold (3.31 > 2.0)\nRatio of modeled to actual stdev. at control is greater than threshold (2.11 > 1.5) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037\n611.000000 5 104.000000 8.631338 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-qyvz92oa.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-qyvz92oa.plt\n \t\t\t\t\t\t\tTue Jul 06 12:41:41 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n The power is restricted to be greater than or equal to 1\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 6.33796\n rho = 0\n control = 285.4\n slope = -334228\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho control slope\n\n lalpha 1 -1 0.85 -0.87\n\n rho -1 1 -0.86 0.88\n\n control 0.85 -0.86 1 -0.98\n\n slope -0.87 0.88 -0.98 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -39.2095 13.9 -66.4529 -11.9661\n rho 9.28625 2.89168 3.61866 14.9538\n control 173.186 16.8405 140.179 206.192\n slope -0.114334 0.0288676 -0.170914 -0.0577547\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 285 173 36 75.8 3.31\n 77 5 166 164 17.8 59.5 0.0759\n 153 5 146 156 30.9 46.2 -0.45\n 306 5 116 138 13.8 26.6 -1.83\n 611 5 104 103 8.63 6.89 0.218\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -88.935179 6 189.870357\n A2 -83.070045 10 186.140089\n A3 -85.479305 7 184.958611\n fitted -99.777674 4 207.555349\n R -118.020849 2 240.041699\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 69.9016 8 <.0001\n Test 2 11.7303 4 0.01947\n Test 3 4.81852 3 0.1856\n Test 4 28.5967 3 <.0001\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 662.635 \n\n\n BMDL = 388.79 \n\n\n BMDU = 1451.45 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 0 | Hill | 5 | 2.18 | True | False | 14.17710 | -999.00000 | -999.0000 | -999 | 182.799081 | <0.0001 | 0.01947 | 0.1856 | 0.3984 | 1.840470 | 2 | 0.17300 | BMDL computation failed. | failure | Warning(s): BMDL computation failed.\nMinimum dose/BMD ratio is greater than threshold (5.43 > 3.0) | NaN | BMDL does not exist | False | NaN | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037\n611.000000 5 104.000000 8.631338 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-6br7qt4o.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-6br7qt4o.plt\n \t\t\t\t\t\t\tTue Jul 06 12:41:41 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n Power parameter restricted to be greater than 1\n The variance is to be modeled as Var(i) = exp(lalpha + rho \* ln(mean(i)))\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n lalpha = 6.33796\n rho = 0\n intercept = 285.4\n v = -181.4\n n = 1.73272\n k = 58.6882\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -n \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n lalpha rho intercept v k\n\n lalpha 1 -1 0.29 -0.21 -0.28\n\n rho -1 1 -0.29 0.22 0.28\n\n intercept 0.29 -0.29 1 -0.87 -0.59\n\n v -0.21 0.22 -0.87 1 0.16\n\n k -0.28 0.28 -0.59 0.16 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n lalpha -4.89056 5.24386 -15.1683 5.38721\n rho 2.14698 1.04072 0.107206 4.18676\n intercept 282.525 16.8892 249.423 315.627\n v -197.251 17.4659 -231.483 -163.018\n n 1 NA\n k 61.2262 17.4527 27.0196 95.4328\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 285 283 36 37.1 0.173\n 77 5 166 173 17.8 21.9 -0.639\n 153 5 146 142 30.9 17.7 0.601\n 306 5 116 118 13.8 14.5 -0.271\n 611 5 104 103 8.63 12.6 0.135\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + rho\*ln(Mu(i)))\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -88.935179 6 189.870357\n A2 -83.070045 10 186.140089\n A3 -85.479305 7 184.958611\n fitted -86.399541 5 182.799081\n R -118.020849 2 240.041699\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 69.9016 8 <.0001\n Test 2 11.7303 4 0.01947\n Test 3 4.81852 3 0.1856\n Test 4 1.84047 2 0.3984\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is less than .1. A non-homogeneous variance \nmodel appears to be appropriate\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 14.1771\n\n\nBMDL computation failed.\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 0 | Exponential-M2 | 6 | 1.11 | True | False | 569.47200 | 274.19000 | 1560.7700 | -999 | 204.420200 | <0.0001 | 0.01947 | 0.1856 | <0.0001 | 25.460000 | 3 | 0.43860 | NaN | warning | NaN | Residual at lowest dose is greater than threshold (3.13 > 2.0) | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037\n611.000000 5 104.000000 8.631338 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-9\_vhc1rc.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:41:41 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha -6.47735 \n rho 2.4539 \n a 111.686 \n b 0.00137539 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha -34.3684 11.6531\n rho 8.26848 2.40111\n a 181.125 15.7659\n b 0.000930096 0.00016028\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 285.4 35.96\n 77 5 166.4 17.78\n 153 5 146.4 30.88\n 306 5 116.4 13.81\n 611 5 104 8.631\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 181.1 74.48 3.131\n 77 168.6 55.39 -0.08907\n 153 157.1 41.35 -0.5785\n 306 136.3 22.96 -1.934\n 611 102.6 7.107 0.4386\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -88.93518 6 189.8704\n A2 -83.07004 10 186.1401\n A3 -85.47931 7 184.9586\n R -118.0208 2 240.0417\n 2 -98.21011 4 204.4202\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 69.9 8 < 0.0001\n Test 2 11.73 4 0.01947\n Test 3 4.819 3 0.1856\n Test 4 25.46 3 < 0.0001\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 569.472\n\n BMDL = 274.19\n\n BMDU = 1560.77\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 0 | Exponential-M3 | 7 | 1.11 | True | False | 569.47300 | 274.19000 | 1560.7700 | -999 | 204.420200 | <0.0001 | 0.01947 | 0.1856 | <0.0001 | 25.460000 | 3 | 0.43860 | NaN | warning | NaN | Residual at lowest dose is greater than threshold (3.13 > 2.0) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037\n611.000000 5 104.000000 8.631338 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-082uyixt.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:41:41 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha -6.47735 \n rho 2.4539 \n a 111.686 \n b 0.00137539 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha -34.3684 12.7451\n rho 8.26849 2.6308\n a 181.125 17.604\n b 0.000930096 0.00018085\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 285.4 35.96\n 77 5 166.4 17.78\n 153 5 146.4 30.88\n 306 5 116.4 13.81\n 611 5 104 8.631\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 181.1 74.48 3.131\n 77 168.6 55.39 -0.08907\n 153 157.1 41.35 -0.5785\n 306 136.3 22.96 -1.934\n 611 102.6 7.107 0.4386\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -88.93518 6 189.8704\n A2 -83.07004 10 186.1401\n A3 -85.47931 7 184.9586\n R -118.0208 2 240.0417\n 3 -98.21011 4 204.4202\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 69.9 8 < 0.0001\n Test 2 11.73 4 0.01947\n Test 3 4.819 3 0.1856\n Test 5a 25.46 3 < 0.0001\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 569.473\n\n BMDL = 274.19\n\n BMDU = 1560.77\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 0 | Exponential-M4 | 8 | 1.11 | True | False | 28.98150 | 11.43230 | 117.0850 | -999 | 185.787200 | <0.0001 | 0.01947 | 0.1856 | 0.08943 | 4.829000 | 2 | 0.74970 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0894 < 0.1) | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037\n611.000000 5 104.000000 8.631338 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-tejfggxq.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:41:41 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha -6.47735 \n rho 2.4539 \n a 299.67 \n b 0.00668069 \n c 0.330522 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha -6.37574 7.48455\n rho 2.46563 1.48745\n a 271.551 21.9377\n b 0.00984649 0.00253926\n c 0.387289 0.0304773\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 285.4 35.96\n 77 5 166.4 17.78\n 153 5 146.4 30.88\n 306 5 116.4 13.81\n 611 5 104 8.631\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 271.6 41.31 0.7497\n 77 183.1 25.41 -1.471\n 153 142.1 18.58 0.5231\n 306 113.3 14.07 0.4855\n 611 105.6 12.89 -0.2732\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -88.93518 6 189.8704\n A2 -83.07004 10 186.1401\n A3 -85.47931 7 184.9586\n R -118.0208 2 240.0417\n 4 -87.89362 5 185.7872\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 69.9 8 < 0.0001\n Test 2 11.73 4 0.01947\n Test 3 4.819 3 0.1856\n Test 6a 4.829 2 0.08943\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is less than .1. Model 4 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 28.9815\n\n BMDL = 11.4323\n\n BMDU = 117.085\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 0 | Exponential-M5 | 9 | 1.11 | True | False | 28.98150 | 11.43230 | 117.0850 | -999 | 185.787200 | <0.0001 | 0.01947 | 0.1856 | 0.08943 | 4.829000 | 2 | 0.74970 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.0894 < 0.1) | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 5 -1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 0 0.95\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037\n611.000000 5 104.000000 8.631338 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-ebdvui\_b.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:41:41 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n The variance is to be modeled as Var(i) = exp(lalpha + log(mean(i)) \* rho)\n\n Total number of dose groups = 5\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha -6.47735 \n rho 2.4539 \n a 299.67 \n b 0.00668069 \n c 0.330522 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha -6.37574 7.48455\n rho 2.46563 1.48745\n a 271.551 21.9377\n b 0.00984649 0.00253926\n c 0.387289 0.0304773\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 285.4 35.96\n 77 5 166.4 17.78\n 153 5 146.4 30.88\n 306 5 116.4 13.81\n 611 5 104 8.631\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 271.6 41.31 0.7497\n 77 183.1 25.41 -1.471\n 153 142.1 18.58 0.5231\n 306 113.3 14.07 0.4855\n 611 105.6 12.89 -0.2732\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -88.93518 6 189.8704\n A2 -83.07004 10 186.1401\n A3 -85.47931 7 184.9586\n R -118.0208 2 240.0417\n 5 -87.89362 5 185.7872\n\n\n Additive constant for all log-likelihoods = -22.97. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 69.9 8 < 0.0001\n Test 2 11.73 4 0.01947\n Test 3 4.819 3 0.1856\n Test 7a 4.829 2 0.08943\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is less than .1. A non-homogeneous\n variance model appears to be appropriate.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is less than .1. Model 5 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 28.9815\n\n BMDL = 11.4323\n\n BMDU = 117.085\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 1 | Linear | 0 | 2.21 | True | False | 82.82960 | 60.03360 | 131.2420 | -999 | 173.917426 | <0.0001 | 0.13720 | 0.1372 | <0.0001 | 21.692200 | 2 | -2.22000 | NaN | warning | NaN | Residual at lowest dose is greater than threshold (2.3 > 2.0) | NaN | False | NaN | Linear\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1\n1 4 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999\n0\n-9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-15hd36g2.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-15hd36g2.plt\n \t\t\t\t\t\t\tTue Jul 06 12:41:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 688.425\n rho = 0 Specified\n beta\_0 = 243.95\n beta\_1 = -0.487312\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 1.6e-006 -1.9e-006\n\n beta\_0 1.6e-006 1 -0.76\n\n beta\_1 -1.9e-006 -0.76 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 1629.24 515.211 619.447 2639.04\n beta\_0 243.95 13.9946 216.521 271.379\n beta\_1 -0.487312 0.0798151 -0.643747 -0.330878\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 285 244 36 40.4 2.3\n 77 5 166 206 17.8 40.4 -2.22\n 153 5 146 169 30.9 40.4 -1.27\n 306 5 116 94.8 13.8 40.4 1.19\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -73.112628 5 156.225257\n A2 -70.350906 8 156.701812\n A3 -73.112628 5 156.225257\n fitted -83.958713 3 173.917426\n R -94.480419 2 192.960838\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 48.259 6 <.0001\n Test 2 5.52344 3 0.1372\n Test 3 5.52344 3 0.1372\n Test 4 21.6922 2 <.0001\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 82.8296\n\n\n BMDL = 60.0336\n\n\n BMDU = 131.242\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 1 | Polynomial-2 | 1 | 2.21 | True | False | 82.82970 | 60.03360 | 131.2420 | -999 | 173.917426 | <0.0001 | 0.13720 | 0.1372 | <0.0001 | 21.692200 | 2 | -2.22000 | NaN | warning | NaN | Residual at lowest dose is greater than threshold (2.3 > 2.0) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n2\n1 4 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-qpqg8dy1.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-qpqg8dy1.plt\n \t\t\t\t\t\t\tTue Jul 06 12:41:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 688.425\n rho = 0 Specified\n beta\_0 = 277.75\n beta\_1 = -1.40075\n beta\_2 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 7.3e-007 -3.8e-007\n\n beta\_0 7.3e-007 1 -0.76\n\n beta\_1 -3.8e-007 -0.76 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 1629.24 515.212 619.447 2639.04\n beta\_0 243.95 13.9946 216.521 271.379\n beta\_1 -0.487312 0.0798151 -0.643747 -0.330877\n beta\_2 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 285 244 36 40.4 2.3\n 77 5 166 206 17.8 40.4 -2.22\n 153 5 146 169 30.9 40.4 -1.27\n 306 5 116 94.8 13.8 40.4 1.19\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -73.112628 5 156.225257\n A2 -70.350906 8 156.701812\n A3 -73.112628 5 156.225257\n fitted -83.958713 3 173.917426\n R -94.480419 2 192.960838\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 48.259 6 <.0001\n Test 2 5.52344 3 0.1372\n Test 3 5.52344 3 0.1372\n Test 4 21.6922 2 <.0001\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 82.8297\n\n\n BMDL = 60.0336\n\n\n BMDU = 131.242\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 1 | Polynomial-3 | 2 | 2.21 | True | False | 82.82970 | 60.03360 | 131.2420 | -999 | 173.917426 | <0.0001 | 0.13720 | 0.1372 | <0.0001 | 21.692200 | 2 | -2.22000 | NaN | warning | NaN | Residual at lowest dose is greater than threshold (2.3 > 2.0) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n3\n1 4 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-m8j5bs3j.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-m8j5bs3j.plt\n \t\t\t\t\t\t\tTue Jul 06 12:41:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 688.425\n rho = 0 Specified\n beta\_0 = 285.4\n beta\_1 = -2.50219\n beta\_2 = 0\n beta\_3 = -2.64317e-005\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -2.7e-008 -5e-008\n\n beta\_0 -2.7e-008 1 -0.76\n\n beta\_1 -5e-008 -0.76 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 1629.24 515.212 619.447 2639.04\n beta\_0 243.95 13.9946 216.521 271.379\n beta\_1 -0.487312 0.0798151 -0.643747 -0.330877\n beta\_2 0 NA\n beta\_3 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 285 244 36 40.4 2.3\n 77 5 166 206 17.8 40.4 -2.22\n 153 5 146 169 30.9 40.4 -1.27\n 306 5 116 94.8 13.8 40.4 1.19\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -73.112628 5 156.225257\n A2 -70.350906 8 156.701812\n A3 -73.112628 5 156.225257\n fitted -83.958713 3 173.917426\n R -94.480419 2 192.960838\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 48.259 6 <.0001\n Test 2 5.52344 3 0.1372\n Test 3 5.52344 3 0.1372\n Test 4 21.6922 2 <.0001\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 82.8297\n\n\n BMDL = 60.0336\n\n\n BMDU = 131.242\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 1 | Polynomial-4 | 3 | 2.21 | True | False | 82.82970 | 60.03360 | 131.2420 | -999 | 173.917426 | <0.0001 | 0.13720 | 0.1372 | <0.0001 | 21.692200 | 2 | -2.22000 | NaN | warning | NaN | Residual at lowest dose is greater than threshold (2.3 > 2.0) | NaN | False | NaN | Polynomial\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n4\n1 4 0\n500 1e-08 1e-08 0 -1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037 | \n\n ==================================================================== \n \t Polynomial Model. (Version: 2.21; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-89lnmwv6.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-89lnmwv6.plt\n \t\t\t\t\t\t\tTue Jul 06 12:41:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = beta\_0 + beta\_1\*dose + beta\_2\*dose^2 + ...\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The polynomial coefficients are restricted to be negative\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 688.425\n rho = 0 Specified\n beta\_0 = 90.6797\n beta\_1 = -2.38956\n beta\_2 = 0\n beta\_3 = -3.3211e-005\n beta\_4 = 0\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -beta\_2 -beta\_3 -beta\_4 \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha beta\_0 beta\_1\n\n alpha 1 -3.4e-009 4.3e-009\n\n beta\_0 -3.4e-009 1 -0.76\n\n beta\_1 4.3e-009 -0.76 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 1629.24 515.212 619.447 2639.04\n beta\_0 243.95 13.9946 216.521 271.379\n beta\_1 -0.487312 0.0798151 -0.643747 -0.330877\n beta\_2 0 NA\n beta\_3 0 NA\n beta\_4 0 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 285 244 36 40.4 2.3\n 77 5 166 206 17.8 40.4 -2.22\n 153 5 146 169 30.9 40.4 -1.27\n 306 5 116 94.8 13.8 40.4 1.19\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -73.112628 5 156.225257\n A2 -70.350906 8 156.701812\n A3 -73.112628 5 156.225257\n fitted -83.958713 3 173.917426\n R -94.480419 2 192.960838\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 48.259 6 <.0001\n Test 2 5.52344 3 0.1372\n Test 3 5.52344 3 0.1372\n Test 4 21.6922 2 <.0001\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean\n\nConfidence level = 0.95\n\n BMD = 82.8297\n\n\n BMDL = 60.0336\n\n\n BMDU = 131.242\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 1 | Power | 4 | 2.19 | True | False | 82.82970 | 60.03360 | 131.2420 | -999 | 173.917426 | <0.0001 | 0.13720 | 0.1372 | <0.0001 | 21.692200 | 2 | -2.22000 | NaN | warning | NaN | Residual at lowest dose is greater than threshold (2.3 > 2.0) | NaN | False | NaN | Power\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037 | \n\n ==================================================================== \n \t Power Model. (Version: 2.19; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-svuuj259.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-svuuj259.plt\n \t\t\t\t\t\t\tTue Jul 06 12:41:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = control + slope \* dose^power\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n The power is restricted to be greater than or equal to 1\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 688.425\n rho = 0 Specified\n control = 285.4\n slope = -11944.2\n power = -9999\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -power \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha control slope\n\n alpha 1 -2e-007 6.9e-008\n\n control -2e-007 1 -0.76\n\n slope 6.9e-008 -0.76 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 1629.24 515.212 619.447 2639.04\n control 243.95 13.9946 216.521 271.379\n slope -0.487312 0.0798151 -0.643747 -0.330877\n power 1 NA\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 285 244 36 40.4 2.3\n 77 5 166 206 17.8 40.4 -2.22\n 153 5 146 169 30.9 40.4 -1.27\n 306 5 116 94.8 13.8 40.4 1.19\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -73.112628 5 156.225257\n A2 -70.350906 8 156.701812\n A3 -73.112628 5 156.225257\n fitted -83.958713 3 173.917426\n R -94.480419 2 192.960838\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 48.259 6 <.0001\n Test 2 5.52344 3 0.1372\n Test 3 5.52344 3 0.1372\n Test 4 21.6922 2 <.0001\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is less than .1. You may want to try a different \nmodel\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 82.8297 \n\n\n BMDL = 60.0336 \n\n\n BMDU = 131.242 \n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 1 | Hill | 5 | 2.18 | True | False | 7.27554 | 3.42945 | 40.7938 | -999 | 154.707710 | <0.0001 | 0.13720 | 0.1372 | 0.4873 | 0.482454 | 1 | 0.01780 | NaN | valid | Minimum dose/BMD ratio is greater than threshold (10.6 > 3.0) | NaN | NaN | True | AIC | Hill\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 0\n500 1e-08 1e-08 0 1 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037 | \n\n ==================================================================== \n \t Hill Model. (Version: 2.18; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-2x4x97oc.(d) \n \t Gnuplot Plotting File: C:\Windows\TEMP\bmds-2x4x97oc.plt\n \t\t\t\t\t\t\tTue Jul 06 12:41:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function is: \n\n Y[dose] = intercept + v\*dose^n/(k^n + dose^n)\n\n\n Dependent variable = Response\n Independent variable = Dose\n rho is set to 0\n Power parameter restricted to be greater than 1\n A constant variance model is fit\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n\n\n Default Initial Parameter Values \n alpha = 688.425\n rho = 0 Specified\n intercept = 285.4\n v = -169\n n = 2.01134\n k = 54.6765\n\n\n Asymptotic Correlation Matrix of Parameter Estimates\n\n ( \*\*\* The model parameter(s) -rho -n \n have been estimated at a boundary point, or have been specified by the user,\n and do not appear in the correlation matrix )\n\n alpha intercept v k\n\n alpha 1 -8.6e-007 8.8e-007 -3.6e-007\n\n intercept -8.6e-007 1 -0.38 -0.24\n\n v 8.8e-007 -0.38 1 -0.74\n\n k -3.6e-007 -0.24 -0.74 1\n\n\n\n Parameter Estimates\n\n 95.0% Wald Confidence Interval\n Variable Estimate Std. Err. Lower Conf. Limit Upper Conf. Limit\n alpha 564.187 178.412 214.507 913.867\n intercept 285.211 10.6345 264.368 306.054\n v -194.089 23.8154 -240.766 -147.411\n n 1 NA\n k 52.1748 23.7256 5.67351 98.6761\n\nNA - Indicates that this parameter has hit a bound\n implied by some inequality constraint and thus\n has no standard error.\n\n\n\n Table of Data and Estimated Values of Interest\n\n Dose N Obs Mean Est Mean Obs Std Dev Est Std Dev Scaled Res.\n------ --- -------- -------- ----------- ----------- ----------\n\n 0 5 285 285 36 23.8 0.0178\n 77 5 166 170 17.8 23.8 -0.293\n 153 5 146 140 30.9 23.8 0.558\n 306 5 116 119 13.8 23.8 -0.282\n\n\n\n Model Descriptions for likelihoods calculated\n\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n Model A3 uses any fixed variance parameters that\n were specified by the user\n\n Model R: Yi = Mu + e(i)\n Var{e(i)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) # Param's AIC\n A1 -73.112628 5 156.225257\n A2 -70.350906 8 156.701812\n A3 -73.112628 5 156.225257\n fitted -73.353855 4 154.707710\n R -94.480419 2 192.960838\n\n\n Explanation of Tests \n\n Test 1: Do responses and/or variances differ among Dose levels? \n (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A1 vs A2)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does the Model for the Mean Fit? (A3 vs. fitted)\n (Note: When rho=0 the results of Test 3 and Test 2 will be the same.)\n\n Tests of Interest \n\n Test -2\*log(Likelihood Ratio) Test df p-value \n\n Test 1 48.259 6 <.0001\n Test 2 5.52344 3 0.1372\n Test 3 5.52344 3 0.1372\n Test 4 0.482454 1 0.4873\n\nThe p-value for Test 1 is less than .05. There appears to be a\ndifference between response and/or variances among the dose levels\nIt seems appropriate to model the data\n\nThe p-value for Test 2 is greater than .1. A homogeneous variance \nmodel appears to be appropriate here\n\n\nThe p-value for Test 3 is greater than .1. The modeled variance appears \n to be appropriate here\n\nThe p-value for Test 4 is greater than .1. The model chosen seems \nto adequately describe the data\n \n\n Benchmark Dose Computation\n\nSpecified effect = 1\n\nRisk Type = Estimated standard deviations from the control mean \n\nConfidence level = 0.95\n\n BMD = 7.27554\n\n BMDL = 3.42945\n\n BMDU = 40.7938\n\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 1 | Exponential-M2 | 6 | 1.11 | True | False | 39.61620 | 27.34300 | 65.9210 | -999 | 167.124700 | <0.0001 | 0.13720 | 0.1372 | 0.000582 | 14.900000 | 2 | -2.28000 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.000582 < 0.1) | NaN | False | NaN | Exponential-M2\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 -1 1000 11 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-x\_7ag3ww.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:41:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 2\n -------- --------\n lnalpha 6.31126 \n rho 0 Specified\n a 118.052 \n b 0.0026626 \n c 0 Specified\n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 2 Std. Err.\n -------- ------- ---------\n lnalpha 7.05623 366.846\n a 263.271 13.2416\n b 0.00349706 0.000457701\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 285.4 35.96\n 77 5 166.4 17.78\n 153 5 146.4 30.88\n 306 5 116.4 13.81\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 263.3 34.06 1.453\n 77 201.1 34.06 -2.28\n 153 154.2 34.06 -0.5109\n 306 90.3 34.06 1.714\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -73.11263 5 156.2253\n A2 -70.35091 8 156.7018\n A3 -73.11263 5 156.2253\n R -94.48042 2 192.9608\n 2 -80.56234 3 167.1247\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n Test 4: Does Model 2 fit the data? (A3 vs. 2)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 48.26 6 < 0.0001\n Test 2 5.523 3 0.1372\n Test 3 5.523 3 0.1372\n Test 4 14.9 2 0.0005816\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 4 is less than .1. Model 2 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 39.6162\n\n BMDL = 27.343\n\n BMDU = 65.921\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 1 | Exponential-M3 | 7 | 1.11 | True | False | 39.61610 | 27.34300 | 65.9210 | -999 | 167.124700 | <0.0001 | 0.13720 | 0.1372 | 0.000582 | 14.900000 | 2 | -2.28000 | NaN | warning | NaN | Goodness of fit p-value is less than threshold (0.000582 < 0.1) | NaN | False | NaN | Exponential-M3\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 -1 0100 22 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-\_x1erzig.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:41:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 3\n -------- --------\n lnalpha 6.31126 \n rho 0 Specified\n a 118.052 \n b 0.0026626 \n c 0 Specified\n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 3 Std. Err.\n -------- ------- ---------\n lnalpha 7.05623 366.845\n a 263.271 14.0916\n b 0.00349706 0.000536834\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 285.4 35.96\n 77 5 166.4 17.78\n 153 5 146.4 30.88\n 306 5 116.4 13.81\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 263.3 34.06 1.453\n 77 201.1 34.06 -2.28\n 153 154.2 34.06 -0.5109\n 306 90.3 34.06 1.714\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -73.11263 5 156.2253\n A2 -70.35091 8 156.7018\n A3 -73.11263 5 156.2253\n R -94.48042 2 192.9608\n 3 -80.56234 3 167.1247\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 5a: Does Model 3 fit the data? (A3 vs 3)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 48.26 6 < 0.0001\n Test 2 5.523 3 0.1372\n Test 3 5.523 3 0.1372\n Test 5a 14.9 2 0.0005816\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 5a is less than .1. Model 3 may not adequately\n describe the data; you may want to consider another model.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 39.6161\n\n BMDL = 27.343\n\n BMDU = 65.921\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 1 | Exponential-M4 | 8 | 1.11 | True | False | 10.68890 | 6.72560 | 18.5598 | -999 | 155.580700 | <0.0001 | 0.13720 | 0.1372 | 0.2443 | 1.355000 | 1 | 0.07699 | NaN | valid | Minimum dose/BMD ratio is greater than threshold (7.2 > 3.0) | NaN | NaN | False | NaN | Exponential-M4\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 -1 0010 33 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-h8gw5mz7.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:41:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 4\n -------- --------\n lnalpha 6.31126 \n rho 0 Specified\n a 299.67 \n b 0.0116234 \n c 0.369931 \n d 1 Specified\n\n\n\n Parameter Estimates\n\n Variable Model 4 Std. Err.\n -------- ------- ---------\n lnalpha 6.37903 186.371\n a 284.564 10.8877\n b 0.0149034 0.0039809\n c 0.420675 0.0439046\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 285.4 35.96\n 77 5 166.4 17.78\n 153 5 146.4 30.88\n 306 5 116.4 13.81\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 284.6 24.28 0.07699\n 77 172 24.28 -0.5191\n 153 136.6 24.28 0.9057\n 306 121.4 24.28 -0.4636\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -73.11263 5 156.2253\n A2 -70.35091 8 156.7018\n A3 -73.11263 5 156.2253\n R -94.48042 2 192.9608\n 4 -73.79033 4 155.5807\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 6a: Does Model 4 fit the data? (A3 vs 4)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 48.26 6 < 0.0001\n Test 2 5.523 3 0.1372\n Test 3 5.523 3 0.1372\n Test 6a 1.355 1 0.2443\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 6a is greater than .1. Model 4 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 10.6889\n\n BMDL = 6.7256\n\n BMDU = 18.5598\n | NaN | NaN |
| X-C10866B | 1472 | Isopropylated Phenyl Phosphate | Cholinesterase | IU/L | Male | R07 | Hormone Data | SD | 4 | X-C10866B|Male|Hormone Data|R07|4 | 1, 2, 3, 4, 5 | mg/kg | 16.079800993793423,7.9536155300592704,13.811589336495636,6.1773780845921999,3.8600518131237562 | 2,2,2,2,2 | 1,1,1,1,1 | SD | day | NaN | 11 | Hormone Summary | 4 | mMol/kg | 0.0, 0.169, 0.338, 0.675, 1.35 | BMD Results for Table: Cholinesterase | Dose (mg/kg) | X-C10866B|Male|Hormone Data|R07|4 | 0 | 1 | Exponential-M5 | 9 | 1.11 | True | False | 10.68890 | 6.72560 | 69.2941 | -999 | 155.580700 | <0.0001 | 0.13720 | 0.1372 | 0.2443 | 1.355000 | 1 | 0.07699 | NaN | valid | Minimum dose/BMD ratio is greater than threshold (7.2 > 3.0) | NaN | NaN | False | NaN | Exponential-M5\nBMDS\_Model\_Run\n/temp/bmd/datafile.dax\n/temp/bmd/output.out\n1 4 -1 0001 44 0 1\n500 1e-08 1e-08 0 1 0 0\n1 1.0 1 0.95\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\n-9999 0 -9999 -9999 -9999 -9999\n0\n-9999 -9999 -9999 -9999 -9999 -9999\nDose NumAnimals Response Stdev\n0.000000 5 285.400000 35.955528\n77.000000 5 166.400000 17.784825\n153.000000 5 146.400000 30.883653\n306.000000 5 116.400000 13.813037 | \n\n ==================================================================== \n \t Exponential Model. (Version: 1.11; Date: 03/14/2017) \n \t Input Data File: C:\Windows\TEMP\bmds-qur0ip92.(d) \n \t Gnuplot Plotting File: \n \t\t\t\t\t\t\tTue Jul 06 12:41:45 2021\n ==================================================================== \n\n BMDS\_Model\_Run \n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~\n \n The form of the response function by Model: \n Model 2: Y[dose] = a \* exp{sign \* b \* dose}\n Model 3: Y[dose] = a \* exp{sign \* (b \* dose)^d}\n Model 4: Y[dose] = a \* [c-(c-1) \* exp{-b \* dose}]\n Model 5: Y[dose] = a \* [c-(c-1) \* exp{-(b \* dose)^d}]\n\n Note: Y[dose] is the median response for exposure = dose;\n sign = +1 for increasing trend in data;\n sign = -1 for decreasing trend.\n\n Model 2 is nested within Models 3 and 4.\n Model 3 is nested within Model 5.\n Model 4 is nested within Model 5.\n\n\n Dependent variable = Response\n Independent variable = Dose\n Data are assumed to be distributed: normally\n Variance Model: exp(lnalpha +rho \*ln(Y[dose]))\n rho is set to 0.\n A constant variance model is fit.\n\n Total number of dose groups = 4\n Total number of records with missing values = 0\n Maximum number of iterations = 500\n Relative Function Convergence has been set to: 1e-008\n Parameter Convergence has been set to: 1e-008\n\n MLE solution provided: Exact\n\n\n Initial Parameter Values\n\n Variable Model 5\n -------- --------\n lnalpha 6.31126 \n rho 0 Specified\n a 299.67 \n b 0.0116234 \n c 0.369931 \n d 1 \n\n\n\n Parameter Estimates\n\n Variable Model 5 Std. Err.\n -------- ------- ---------\n lnalpha 6.37903 186.371\n a 284.564 10.8877\n b 0.0149034 0.0039809\n c 0.420675 0.0439046\n d 1 NA\n\n NC = No Convergence\n\n\n Table of Stats From Input Data\n\n Dose N Obs Mean Obs Std Dev\n ----- --- ---------- -------------\n 0 5 285.4 35.96\n 77 5 166.4 17.78\n 153 5 146.4 30.88\n 306 5 116.4 13.81\n\n\n Estimated Values of Interest\n\n Dose Est Mean Est Std Scaled Residual\n ------ ---------- --------- ----------------\n 0 284.6 24.28 0.07699\n 77 172 24.28 -0.5191\n 153 136.6 24.28 0.9057\n 306 121.4 24.28 -0.4636\n\n\n\n Other models for which likelihoods are calculated:\n\n Model A1: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma^2\n\n Model A2: Yij = Mu(i) + e(ij)\n Var{e(ij)} = Sigma(i)^2\n\n Model A3: Yij = Mu(i) + e(ij)\n Var{e(ij)} = exp(lalpha + log(mean(i)) \* rho)\n\n Model R: Yij = Mu + e(i)\n Var{e(ij)} = Sigma^2\n\n\n Likelihoods of Interest\n\n Model Log(likelihood) DF AIC\n ------- ----------------- ---- ------------\n A1 -73.11263 5 156.2253\n A2 -70.35091 8 156.7018\n A3 -73.11263 5 156.2253\n R -94.48042 2 192.9608\n 5 -73.79033 4 155.5807\n\n\n Additive constant for all log-likelihoods = -18.38. This constant added to the\n above values gives the log-likelihood including the term that does not\n depend on the model parameters.\n\n\n Explanation of Tests\n\n Test 1: Does response and/or variances differ among Dose levels? (A2 vs. R)\n Test 2: Are Variances Homogeneous? (A2 vs. A1)\n Test 3: Are variances adequately modeled? (A2 vs. A3)\n\n Test 7a: Does Model 5 fit the data? (A3 vs 5)\n\n\n Tests of Interest\n\n Test -2\*log(Likelihood Ratio) D. F. p-value\n -------- ------------------------ ------ --------------\n Test 1 48.26 6 < 0.0001\n Test 2 5.523 3 0.1372\n Test 3 5.523 3 0.1372\n Test 7a 1.355 1 0.2443\n\n\n The p-value for Test 1 is less than .05. There appears to be a\n difference between response and/or variances among the dose\n levels, it seems appropriate to model the data.\n\n The p-value for Test 2 is greater than .1. A homogeneous\n variance model appears to be appropriate here.\n\n The p-value for Test 3 is greater than .1. The modeled\n variance appears to be appropriate here.\n\n The p-value for Test 7a is greater than .1. Model 5 seems\n to adequately describe the data.\n\n\n Benchmark Dose Computations:\n\n Specified Effect = 1.000000\n\n Risk Type = Estimated standard deviations from control\n\n Confidence Level = 0.950000\n\n BMD = 10.6889\n\n BMDL = 6.7256\n\n BMDU = 69.2941\n | NaN | NaN |