**Supplemental Material**

Identifying Environmental Chemicals as Agonists of the Androgen Receptor by Applying a Quantitative High-throughput Screening Platform

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**Supplementary Table S1.** qHTS primary and follow-up screen data, alongside the binding data of the 75 chosen compounds

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Chemical Name**  **(CAS #, Supplier)** |  | **AR-bla** |  | **AR-luc** |  | **Fluorescence Polarization** |
| **NCGC#**  **[Purity Rating]** | **Structure** | **Primary**  **EC50 (µM)**  **[Efficacy**§ **(%)]** | **Follow-up**  **EC50 (µM)**  **[Efficacy**§ **(%)]** | **Primary**  **EC50 (µM)**  **[Efficacy**§ **(%)]** | **Follow-up**  **EC50 (µM)**  **[Efficacy**§ **(%)]** | **EC50 (µM)**  **[Efficacy (%)]** |
| 1,3-Diiminobenz[f]isoindoline  (65558-69-2, Sigma)  NCGC00090942-03  [A] | 1,3-Diiminobenz[f]isoindoline CASRN: 65558-69-2 | 17.3 ± 4.12  [66.3 ± 18.5] | 10.9 ± 0.00  [51.2 ± 9.40] | Inactive\* | Inactive\* | Inactive° |
| 1,3-Diiminoisoindoline  (3468-11-9, Light Biologicals)  NCGC00256041-01  [Z] | 1,3-Diiminoisoindoline 3468-11-9 | 18.2 ± 2.31  [65.9 ± 16.9] | Inactive\* | Inactive\* | Inactive\* | Inactive° |
| 1,4-Butanediol diacrylate  (1070-70-8, Sigma)  NCGC00254840-01  [A] | 1,4-Butanediol diacrylate (1070-70-8, Sigma) NCGC00254840-01 [A] | 19.6 ± 2.25  [79.5 ± 8.17] | 11.7 ± 0.765  [35.9 ± 2.43] | Inactive\* | Inactive\* | Inactive° |
| 1,6-Hexanediol diacrylate  (13048-33-4, Sigma)  NCGC00257183-01  [Z] | 1,6-Hexanediol diacrylate (13048-33-4, Sigma) NCGC00257183-01 [Z] | 30.0 ± 11.9  [41.3 ± 2.83] | Inactive\* | Inactive\* | Inactive\* | Inactive° |
| 2,2':5',2''-Terthiophene  (1081-34-1, Sigma)  NCGC00254556-01  [A] | 2,2':5',2''-Terthiophene (1081-34-1, Sigma) NCGC00254556-01 [A] | 42.9 ± 10.4  [80.5 ± 15.4] | 33.1 ± 2.16  [82.1 ± 16.5] | 27.4 ± 3.15  [32.8 ± 6.57] | 14.2 ± 2.56  [33.2 ± 2.27] | Inactive° |
| 3,3'-dichlorobenzidine dihydrochloride  (612-83-9, Sigma)  NCGC00256608-01  [A] | 3,3'-dichlorobenzidine dihydrochloride (612-83-9, Sigma) NCGC00256608-01 [A] | Inactive\* | Inactive\* | 20.6 ± 12.3  [109 ± 1.77] | 38.2 ± 0.000  [76.8 ± 2.55] | 3.35 ± 0.626  [-64.2 ± 16.6] |
| 7-Diethylamino-4-methylcoumarin  (91-44-1, Sigma)  NCGC00257038-01  [A] | 7-Diethylamino-4-methylcoumarin (91-44-1, Sigma) NCGC00257038-01 [A] | 23.7 ± 1.54  [285 ± 86.5] | 23.4 ± 1.53  [302 ± 43.2] | 27.4 ± 3.15  [88.7 ± 8.59] | 20.9 ± 8.25  [134 ± 55.0] | 2.24 ± 2.62  [-60.7 ± 4.82] |
| Aclarubicin hydrochloride  (75443-99-1, InterBioScreen)  NCGC00167481-01  [C] | Aclarubicin hydrochloride  (75443-99-1, InterBioScreen) NCGC00167481-01 [C] | 0.127 ± 0.0547  [54.6 ± 11.9] | Inactive\* | Inactive\* | Inactive\* | Inactive° |
| Ambroxol hydrochloride  (23828-92-4, Labotest)  NCGC00016781-04  [A] | Ambroxol hydrochloride (23828-92-4, Labotest) NCGC00016781-04 [A] | 7.98 ± 2.99  [107 ± 23.7] | 8.10 ± 4.59  [106 ± 22.8] | 2.23 ± 1.38  [134 ± 32.4] | 1.49 ± 0.171  [102 ± 6.01] | Inactive° |
| Arsenic (III) oxide  (1327-53-3, Sigma)  NCGC00164639-01  [A] | Arsenic (III) oxide (1327-53-3, Sigma) NCGC00164639-01 [A] | 5.38 ± 0.618  [87.9 ± 13.3] | 4.73 ± 0.00  [44.5 ± 5.56] | 1.98 ± 0.356  [97.0 ± 13.5] | 1.67 ± 0.192  [77.2 ± 7.09] | Inactive° |
| Atracurium besylate  (64228-81-5, Prestwick Chemical, Inc.)  NCGC00017127-01  [A] | Atracurium besylate  (64228-81-5, Prestwick Chemical, Inc.) NCGC00017127-01 [A] | Inactive\* | Inactive\* | 2.66 ± 0.339  [576 ± 71.3] | Inactive\* | Inactive° |
| Batyl alcohol  (544-62-7, Microsource)  NCGC00095748-01  [A] | Batyl alcohol  (544-62-7, Microsource) NCGC00095748-01 [A] | Inactive\* | Inactive\* | 1.52 ± 0.283  [415 ± 22.2] | Inactive\* | Inactive° |
| Calcium pantothenate  (137-08-6, Sigma)  NCGC00183031-01  [A] | Calcium pantothenate (137-08-6, Sigma) NCGC00183031-01 [A] | 18.4 ± 2.53  [70.7 ± 0.727] | Inactive\* | 8.26 ± 2.06  [355 ± 57.0] | 18.8 ± 3.04  [162 ± 82.9] | Inactive° |
| Canrenone  (976-71-6, Microsource)  NCGC00095148-01  [A] | Canrenone (976-71-6, Microsource) NCGC00095148-01 [A] | 0.786 ± 0.392  [135.7 ± 12.8] | 1.01 ± 0.297  [128 ± 7.98] | 7.87 ± 1.42  [34.4 ± 7.10] | Inactive\* | 1.43 ± 1.06  [-87.4 ± 18.2] |
| Carbamazepineα  (298-46-4, Sigma)  NCGC00015234-11  [A] | Carbamazepineα (298-46-4, Sigma) NCGC00015234-11 [A] | 4.47 ± 0.803  [93.3 ± 7.08] | 3.73 ± 0.513  [57.3 ± 5.52] | 11.0 ± 0.746  [357 ± 10.8] | 12.6 ± 0.851  [561 ± 72.8] | Inactive° |
| Carbamazepineα  (298-46-4, Sigma)  NCGC00253982-01  [A] |  | Inactive\* | N/A | Inactive\* | N/A | N/A |
| Carubicin  (50935-04-1, Vitas)  NCGC00160675-01  [A] | Carubicin  (50935-04-1, Vitas) NCGC00160675-01 [A] | 2.13 ± 0.00  [197 ± 66.6] | 2.41 ± 0.552  [72.5 ± 19.5] | Inactive\* | Inactive\* | Inactive° |
| Cefpodoxime proxetilα  (87239-81-4, Sequoia)  NCGC00164598-01  [I] | Cefpodoxime proxetilα (87239-81-4, Sequoia) NCGC00164598-01 [I] | 16.2 ± 7.26  [33.9 ± 7.63] | Inactive\* | 8.90 ± 2.01  [519 ± 74.9] | 15.4 ± 1.04  [557 ± 14.9] | Inactive° |
| Cefpodoxime proxetilα  (87239-81-4, Sigma DiscoveryCPR)  NCGC00183131-01  [I] |  | 7.20 ± 2.12  [93.3 ± 6.65] | N/A | Inactive\* | N/A | N/A |
| Corticosterone  (50-22-6, Sigma)  NCGC00256539-01  [A] | Corticosterone (50-22-6, Sigma) NCGC00256539-01 [A] | 0.418 ± 0.124  [133 ± 8.49] | 0.646 ± 0.146  [135 ± 3.69] | 0.129 ± 0.0291  [254 ± 46.5] | 1.12 ± 0.695  [281 ± 29.9] | 17.3 ± 2.21  [-80.7 ± 15.7] |
| Daunorubicin  (20830-81-3, InterBioScreen)  NCGC00024246-05  [B] | Daunorubicin  (20830-81-3, InterBioScreen) NCGC00024246-05 [B] | 0.952 ± 0.00  [146 ± 16.6] | 1.25 ± 0.224  [76.7 ± 0.504] | Inactive\* | Inactive\* | Inactive° |
| Daunorubicin hydrochloride  (23541-50-6, LKT Lab)  NCGC00258711-01  [A] | Daunorubicin hydrochloride  (23541-50-6, LKT Lab) NCGC00258711-01 [A] | 0.259 ± 0.127  [153 ± 49.9] | 0.585 ± 0.172  [73.6 ± 6.70] | Inactive\* | Inactive\* | Inactive° |
| Dibekacin  (34493-98-6, Microsource)  NCGC00095276-01  [A] | Dibekacin (34493-98-6, Microsource) NCGC00095276-01 [A] | Inactive\* | Inactive\* | 28.8 ± 1.87  [34.6 ± 8.92] | 19.4 ± 1.31  [44.7 ± 0.430] | Inactive° |
| Diethylcarbamazine citrate  (1642-54-2, Prestwick Chemical, Inc.)  NCGC00017034-01  [Z] | Diethylcarbamazine citrate  (1642-54-2, Prestwick Chemical, Inc.) NCGC00017034-01 [Z] | Inactive\* | Inactive\* | 4.54 ± 0.522  [329 ± 42.2] | Inactive\* | Inactive° |
| Difloxacin hydrochloride  (91296-86-5, Riedel)  NCGC00166308-01  [A] | Difloxacin hydrochloride (91296-86-5, Riedel) NCGC00166308-01 [A] | Inactive\* | Inactive\* | 27.7 ± 1.87  [51.0 ± 1.61] | Inactive\* | 5.39 ± 2.02  [-150 ± 51.7] |
| Doxorubicin hydrochloride  (25316-40-9, Biomol)  NCGC00163543-01  [A] | Doxorubicin hydrochloride  (25316-40-9, Biomol) NCGC00163543-01 [A] | 0.760 ± 0.0873  [103 ± 14.7] | Inactive\* | Inactive\* | Inactive\* | Inactive° |
| Drospirenone  (67392-87-4, Sequoia)  NCGC00164590-01  [A] | Drospirenone (67392-87-4, Sequoia) NCGC00164590-01 [A] | 0.0403 ± 0.0386  [164 ± 31.3] | 0.0387 ± 0.0141  [119 ± 10.7] | 4.39 ± 0.297  [86.2 ± 4.85] | 3.98 ± 0.269  [59.7 ± 7.60] | 0.310 ± 0.0557  [-68.1 ± 8.16] |
| Dutasteride  (164656-23-9, Sequoia)  NCGC00164571-01  [A] | Dutasteride (164656-23-9, Sequoia) NCGC00164571-01 [A] | Inactive\* | Inactive\* | 21.2 ± 2.44  [164 ± 10.9] | 18.7 ± 0.00  [261 ± 41.4] | Inactive° |
| Equilin  (474-86-2, Sigma)  NCGC00256728-01  [A] | Equilin (474-86-2, Sigma) NCGC00256728-01 [A] | 19.5 ± 0.00  [31.5 ± 3.88] | Inactive\* | 6.31 ± 2.03  [89.3 ± 18.9] | 4.30 ± 0.495  [80.4 ± 12.1] | 14.7 ± 11.2  [-89.8 ± 13.2] |
| Estramustine phosphate  (4891-15-0, APAC)  NCGC00184995-01  [A] | Estramustine phosphate (4891-15-0, APAC) NCGC00184995-01 [A] | Inactive\* | Inactive\* | Inactive\* | Inactive\* | Inactive° |
| Ethidium bromide  (1239-45-8, NIEHS)  NCGC00091387-01  [A] | Ethidium bromide (1239-45-8, NIEHS) NCGC00091387-01 [A] | 2.82 ± 0.507  [91.8 ± 5.79] | 3.91 ± 0.265  [64.1 ± 4.69] | Inactive\* | 1.43 ± 0.0930  [70.4 ± 21.7] | Inactive° |
| Ethynodiol diacetate  (297-76-7, ACC)  NCGC00186466-01  [A] | Ethynodiol diacetate (297-76-7, ACC) NCGC00186466-01 [A] | 0.0832 ± 0.0455  [59.8 ± 6.90] | 0.377 ± 0.124  [78.7 ± 3.46] | 0.233 ± 0.0581  [51.3 ± 3.72] | 0.326 ± 0.0813  [37.2 ± 5.24] | 4.78 ± 0.860  [-53.2 ± 2.93] |
| Exemestane  (107868-30-4, Microsource)  NCGC00095289-01  [A] | Exemestane  (107868-30-4, Microsource) NCGC00095289-01 [A] | 0.611 ± 0.140  [215 ± 17.9] | 0.787 ± 0.142  [155 ± 5.59] | 0.0313 ± 0.00564  [108 ± 7.03] | 0.0398 ± 0.0117  [102 ± 12.2] | 2.73 ± 1.59  [-110 ± 21.0] |
| Feprazone  (30748-29-9, Sequoia)  NCGC00164582-01  [A] | Feprazone  (30748-29-9, Sequoia) NCGC00164582-01 [A] | Inactive\* | Inactive\* | 3.95 ± 0.710  [217 ± 8.35] | 5.56 ± 1.26  [210 ± 15.6] | Inactive° |
| Formestane  (566-48-3, Sigma)  NCGC00255321-01  [A] | Formestane (566-48-3, Sigma) NCGC00255321-01 [A] | 0.479 ± 0.256  [135 ± 5.75] | 1.38 ± 0.259  [126 ± 5.83] | 0.0910 ± 0.0569  [123 ± 8.65] | 0.466 ± 0.0641  [114 ± 14.9] | 2.86 ± 1.35  [-92.5 ± 16.9] |
| Gestrinone  (16320-04-0, Bosche)  NCGC00167457-01  [A] | Gestrinone (16320-04-0, Bosche) NCGC00167457-01 [A] | 0.00338 ± 0.00291  [63.4 ± 14.9] | 0.00183 ± 0.000311  [39.7 ± 4.04] | 0.0125 ± 0.0150  [125 ± 14.5] | 0.00482 ± 0.00134  [123 ± 4.73] | 0.0194 ± 0.00872  [-87.8 ± 4.33] |
| Glycyrrhizin  (1405-86-3, Sigma DiscoveryCPR)  NCGC00183128-01  [A] | Glycyrrhizin (1405-86-3, Sigma DiscoveryCPR) NCGC00183128-01 [A] | 18.2 ± 12.2  [35.2 ± 4.13] | Inactive\* | 9.48 ± 3.45  [88.5 ± 8.41] | 7.64 ± 3.59  [134 ± 39.4] | 9.77 ± 2.36  [-50.4 ± 4.24] |
| GSK232420A  (864283-48-7, GlaxoSmithKline)  NCGC00254089-01  [A] | GSK232420A (864283-48-7, GlaxoSmithKline) NCGC00254089-01 [A] | 5.87 ± 3.41  [38.0 ± 5.31] | 9.37 ± 1.29  [56.3 ± 5.28] | 0.0155 ± 0.00986  [96.6 ± 11.6] | 0.167 ± 0.0418  [118 ± 9.03] | 0.0889 ± 0.0452  [-71.3 ± 10.1] |
| Idarubicin  (57852-57-0, Sequoia)  NCGC00093976-031  [A]  (58957-92-9, Sigma)  NCGC00093976-042  [A] | Idarubicin (57852-57-0, Sequoia) NCGC00093976-031 [A]  (58957-92-9, Sigma) NCGC00093976-042 [A] | 0.849 ± 0.001  [166 ± 37.1]1 | 0.977 ± 0.4652  [53.0 ± 13.8]2 | Inactive1\* | Inactive2\* | Inactive2° |
| Isepamicin sulfate  (67814-76-0, Sequoia)  NCGC00164587-01  [A] | Isepamicin sulfate (67814-76-0, Sequoia) NCGC00164587-01 [A] | Inactive\* | Inactive\* | 15.4 ± 4.97  [397 ± 73.4] | 16.6 ± 0.00  [327 ± 29.9] | Inactive° |
| Lasalocid sodium  (25999-20-6, Microsource)  NCGC00095029-01  [A] | Lasalocid sodium  (25999-20-6, Microsource) NCGC00095029-01 [A] | Inactive\* | Inactive\* | 1.89 ± 0.217  [164 ± 15.2] | Inactive\* | Inactive° |
| Levodopa  (59-92-7, BIOMOL)  NCGC00016270-04  [Z] | Levodopa  (59-92-7, BIOMOL) NCGC00016270-04 [Z] | 4.43 ± 3.39  [80.9 ± 78.7] | Inactive\* | Inactive\* | Inactive\* | Inactive° |
| Melengestrol acetate  (2919-66-6, Sigma)  NCGC00257329-01  [A] | Melengestrol acetate  (2919-66-6, Sigma) NCGC00257329-01 [A] | Inactive\* | Inactive\* | 0.0170 ± 0.0124  [288 ± 44.8] | 0.0426 ± 0.00725  [266 ± 14.7] | 1.17 ± 0.199  [-124 ± 3.58] |
| Methenolone enanthate  (303-42-4, Bosche)  NCGC00167979-01  [A] | Methenolone enanthate (303-42-4, Bosche) NCGC00167979-01 [A] | 0.0361 ± 0.0184  [72.5 ± 15.5] | 0.0396 ± 0.0148  [83.2 ± 10.1] | 0.00311 ± 0.000210  [121 ± 12.2] | 0.00966 ± 0.00311  [169 ± 25.0] | 1.20 ± 0.216  [-75.1 ± 17.7] |
| Methylthiouracilα  (56-04-2, Microsource)  NCGC00091124-02  [A] | Methylthiouracil (56-04-2) | 16.0 ± 13.8  [74.1 ± 66.6] | Inactive\* | 28.8 ± 1.87  [116 ± 31.4] | 23.8 ± 4.44  [122 ± 11.2] | Inactive° |
| Methylthiouracilα  (56-04-2, Light Biologicals)  NCGC00254505-01  [A] |  | Inactive\* | N/A | Inactive\* | N/A | N/A |
| Moclobemideα  (71320-77-9, Toronto Research)  NCGC00027930-04  [A] | Moclobemide (71320-77-9) | 4.72 ± 1.32  [157 ± 22.1] | 5.65 ± 1.60  [140 ± 14.4] | 2.05 ± 0.282  [136 ± 14.5] | 2.74 ± 1.79  [136 ± 42.9] | Inactive° |
| Moclobemideα  (71320-77-9, Vitas)  NCGC00027930-02  [A] |  | Inactive\* | N/A | Inactive\* | N/A | N/A |
| Moxidectinα  (113507-06-5, Fluka)  NCGC00183118-01  [B] | Moxidectin (113507-06-5) | 23.0 ± 9.66  [203 ± 26.4] | 1.44 ± 0.0939  [62.4 ± 1.78] | 0.538 ± 0.100  [108 ± 10.5] | 0.521 ± 0.359  [101 ± 24.3] | 4.02 ± 2.88  [-78.7 ± 10.6] |
| Moxidectinα  (113507-06-5, Sigma)  NCGC00182083-02  [A] |  | 26.8 ± 0.00  [242 ± 29.6] | N/A | Inactive\* | N/A | N/A |
| Nandrolone phenylproprionate  (62-90-8, Pharmeks)  NCGC00159356-02  [A] | Nandrolone phenylproprionate (62-90-8, Pharmeks) NCGC00159356-02 [A] | 0.0104 ± 0.00177  [163 ± 1.14] | 0.0134 ± 0.00154  [99.5 ± 3.77] | 0.00189 ± 0.000217  [134 ± 5.15] | 0.00239 ± 0.000547  [121 ± 17.5] | 3.28 ± 2.14  [-67.6 ± 27.8] |
| Nimetazepam  (2011-67-8, Sequoia)  NCGC00164577-01  [A] | Nimetazepam  (2011-67-8, Sequoia) NCGC00164577-01 [A] | Inactive\* | Inactive\* | 4.38 ± 2.86  [470 ± 106] | 9.88 ± 2.75  [506 ± 60.8] | Inactive° |
| Norethindrone  (68-22-4, Sigma)  NCGC00255187-01  [A] | Norethindrone (68-22-4, Sigma) NCGC00255187-01 [A] | 0.00261 ± 0.00198  [60.6 ± 16.6] | 0.00926 ± 0.00624  [69.3 ± 5.54] | 0.0454 ± 0.0367  [112 ± 17.9] | 0.0429 ± 0.00  [73.3 ± 8.95] | 0.0991 ± 0.0754  [-87.4 ± 25.0] |
| Norethisterone enanthate  (3836-23-5, APAC)  NCGC00182712-01  [A] | Norethisterone enanthate (3836-23-5, APAC) NCGC00182712-01 [A] | 0.198 ± 0.0134  [61.3 ± 3.79] | 0.610 ± 0.398  [58.1 ± 11.5] | 0.230 ± 0.0911  [61.6 ± 5.94] | 0.755 ± 0.493  [58.1 ± 19.1] | 1.62 ± 0.187  [-83.2 ± 7.27] |
| Norgestimate  (35189-28-7, APAC)  NCGC00181353-01  [A] | Norgestimate (35189-28-7, APAC) NCGC00181353-01 [A] | 0.0270 ± 0.00438  [70.9 ± 6.13] | 0.117 ± 0.0291  [74.0 ± 2.77] | 0.0531 ± 0.00  [85.8 ± 4.25] | 0.0788 ± 0.00641  [83.0 ± 0.728] | 2.72 ± 1.92  [-76.9 ± 32.1] |
| Orbifloxacin  (113617-63-3, InterBioScreen)  NCGC00160518-01  [A] | Orbifloxacin (113617-63-3, InterBioScreen) NCGC00160518-01 [A] | 22.3 ± 2.84  [38.8 ± 8.09] | 37.1 ± 2.42  [37.8 ± 3.44] | 25.6 ± 1.67  [59.4 ± 7.23] | 42.9 ± 0.00  [64.1 ± 6.02] | Inactive° |
| Oryzalin  (19044-88-3, Light Biologicals)  NCGC00163815-04  [A] | Oryzalin (19044-88-3, Light Biologicals) NCGC00163815-04 [A] | 7.39 ± 10.5  [52.7 ± 25.3] | 5.29 ± 2.09  [69.3 ± 15.6] | Inactive\* | Inactive\* | Inactive° |
| Ouabain  (630-60-4, Light Biologicals)  NCGC00255970-01  [A] | Ouabain (630-60-4, Light Biologicals) NCGC00255970-01 [A] | 0.0248 ± 0.0144  [40.2 ± 13.6] | Inactive\* | Inactive\* | Inactive\* | Inactive° |
| Oxabolone cypionate  (1254-35-9, NCI)  NCGC00181156-01  [Ac] | Oxabolone cypionate (1254-35-9, NCI) NCGC00181156-01 [Ac] | 0.0165 ± 0.00280  [138 ± 10.0] | 0.0291 ± 0.0158  [121 ± 10.4] | 0.00475 ± 0.000546  [134 ± 9.16] | 0.0178 ± 0.0135  [186 ± 27.8] | 2.49 ± 1.27  [-59.8 ± 14.5] |
| Oxiglutathione  (27025-41-8, Sigma DiscoveryCPR)  NCGC00164484-02  [A] | Oxiglutathione (27025-41-8, Sigma DiscoveryCPR) NCGC00164484-02 [A] | 0.0579 ± 0.00377  [99.9 ± 2.09] | 0.222 ± 0.0399  [76.8 ± 1.60] | 0.0109 ± 0.00304  [106 ± 6.49] | 0.0253 ± 0.0191  [122 ± 49.3] | 1.89 ± 0.242  [-95.6 ± 13.0] |
| Parbendazole  (14255-87-9, Prestwick Chemical, Inc.)  NCGC00016706-01  [A] | Parbendazole  (14255-87-9, Prestwick Chemical, Inc.) NCGC00016706-01 [A] | 0.287 ± 0.312  [34.5 ± 1.86] | Inactive\* | 4.71 ± 0.319  [487 ± 81.2] | 7.10 ± 0.00  [342 ± 19.1] | Inactive° |
| Phenyl salicylateα  (118-55-8, Sigma)  NCGC00090887-02  [A] | Phenyl salicylateα (118-55-8) | Inactive\* | 13.9 ± 0.939  [38.0 ± 3.51] | 2.71 ± 0.619  [87.7 ± 12.1] | 2.16 ± 0.905  [138 ± 27.3] | 8.10  [-33.7 ± 16.4] |
| Phenyl salicylateα  (118-55-8, Sigma)  NCGC00256612-01  [A] |  | Inactive\* | N/A | Inactive\* | N/A | N/A |
| Pregnanolone  (128-20-1, BIOMOL)  NCGC00163287-01  [A] | Pregnanolone (128-20-1, BIOMOL) NCGC00163287-01 [A] | 1.08 ± 0.608  [45.2 ± 20.7] | 2.38 ± 0.782  [38.9 ± 11.2] | Inactive\* | Inactive\* | 1.71 ± 2.09  [-79.9 ± 15.0] |
| Pregnenolone acetate  (1778-02-5, SALOR)  NCGC00160652-02  [A] | Pregnenolone acetate (1778-02-5, SALOR) NCGC00160652-02 [A] | Inactive\* | Inactive\* | 25.6 ± 1.67  [52.5 ± 5.10] | Inactive\* | 9.15 ± 1.48  [-44.8 ± 19.3] |
| Proflavin hydrochloride  (952-23-8, Sigma)  NCGC00258067-01  [A] | Proflavin hydrochloride  (952-23-8, Sigma) NCGC00258067-01 [A] | 3.61 ± 0.244  [180 ± 60.5] | 3.73 ± 0.513  [76.4 ± 7.40] | Inactive\* | Inactive\* | Inactive° |
| Prulifloxacin  (123447-62-1, InterBioScreen)  NCGC00164615-01  [A] | Prulifloxacin (123447-62-1, InterBioScreen) NCGC00164615-01 [A] | 1.26 ± 0.435  [135 ± 17.2] | 1.65 ± 0.411  [107 ± 14.0] | 0.277 ± 0.0187  [116 ± 8.01] | 0.254 ± 0.0165  [108 ± 5.45] | 5.23 ± 2.79  [-72.4 ± 7.67] |
| Quinine ethyl carbonate  (83-75-0, Microsource)  NCGC00095256-01  [A] | Quinine ethyl carbonate (83-75-0, Microsource) NCGC00095256-01 [A] | 21.7 ± 4.96  [37.5 ± 8.41] | Inactive\* | 26.7 ± 3.07  [78.4 ± 1.78] | 16.6 ± 0.00  [54.0 ± 5.47] | Inactive° |
| Resveratrol  (501-36-0, Light Biologicals)  NCGC00257465-01  [A] | Resveratrol (501-36-0, Light Biologicals) NCGC00257465-01 [A] | Inactive\* | Inactive\* | Inactive\* | Inactive\* | Inactive° |
| Rocuronium bromide  (119302-91-9, Bosche)  NCGC00167433-01  [Z] | Rocuronium bromide (119302-91-9, Bosche) NCGC00167433-01 [Z] | 8.83 ± 0.598  [125 ± 4.91] | 8.44 ± 0.970  [84.4 ± 1.68] | 2.34 ± 0.654  [129 ± 12.1] | 2.33 ± 0.998  [182 ± 31.3] | Inactive° |
| Sivelestat sodium tetrahydrate  (201677-61-4, Bosche)  NCGC00167577-01  [A] | Sivelestat sodium tetrahydrate  (201677-61-4, Bosche) NCGC00167577-01 [A] | 5.38 ± 0.618  [144 ± 11.1] | Inactive\* | 1.05 ± 0.292  [122 ± 11.4] | Inactive\* | 11.0 ± 2.65  [-59.3 ± 16.0] |
| Sparfloxacin  (110871-86-8, InterBioScreen)  NCGC00159333-02  [A] | Sparfloxacin (110871-86-8, InterBioScreen) NCGC00159333-02 [A] | Inactive\* | Inactive\* | 19.9 ± 4.50  [82.7 ± 10.3] | 17.3 ± 1.17  [63.4 ± 8.04] | Inactive° |
| Spironolactone  (52-01-7, Acros)  NCGC00255229-01  [A] | Spironolactone (52-01-7, Acros) NCGC00255229-01 [A] | 0.0279 ± 0.00521  [82.3 ± 3.26] | 0.0737 ± 0.0218  [74.3 ± 10.9] | 0.181 ± 0.218  [55.0 ± 15.8] | 0.360 ± 0.0813  [41.1 ± 3.17] | 1.11 ± 1.32  [-71.1 ± 15.7] |
| SR271425  (155990-20-8, Pharma)  NCGC00253949-01  [A] | SR271425 (155990-20-8, Pharma) NCGC00253949-01 [A] | 4.90 ± 1.75  [93.8 ± 30.3] | 7.19 ± 1.29  [73.7 ± 3.29] | Inactive\* | Inactive\* | Inactive° |
| Sulfacarbamide  (547-44-4, InnovaPharm)  NCGC00164541-01  [C] | Sulfacarbamide (547-44-4, InnovaPharm) NCGC00164541-01 [C] | 11.6 ± 1.60  [88.4 ± 1.39] | Inactive\* | 9.91 ± 1.78  [134 ± 17.8] | Inactive\* | Inactive° |
| Thimerosal  (54-64-8, Acros)  NCGC00255169-01  [A] | Thimerosal  (54-64-8, Acros) NCGC00255169-01 [A] | 8.33 ± 11.7  [81.1 ± 21.4] | Inactive\* | Inactive\* | Inactive\* | Inactive° |
| Tosufloxacin tosylate  (115964-29-9, Sequoia)  NCGC00167536-01  [A] | Tosufloxacin tosylate (115964-29-9, Sequoia) NCGC00167536-01 [A] | 24.9 ± 1.68  [61.1 ± 12.4] | Inactive\* | Inactive\* | Inactive\* | 12.9 ± 2.09  [-56.9 ± 16.1] |
| Tri(propylene glycol) diacrylate  (42978-66-5, Sigma)  NCGC00255375-01  [I] | Tri(propylene glycol) diacrylate (42978-66-5, Sigma) NCGC00255375-01 [I] | 18.2 ± 2.31  [64.2 ± 10.5] | Inactive\* | Inactive\* | Inactive\* | Inactive° |
| Tris[2-(acryloyloxy)ethyl] isocyanurate  (40220-08-4, Sigma)  NCGC00256218-01  [B] | Tris[2-(acryloyloxy)ethyl] isocyanurate  (40220-08-4, Sigma) NCGC00256218-01 [B] | 2.22 ± 0.414  [51.8 ± 6.92] | Inactive\* | Inactive\* | Inactive\* | Inactive° |
| Trenbolone  (10161-33-8, Toronto Research)  NCGC00257511-01  [A] | Trenbolone (10161-33-8, Toronto Research) NCGC00257511-01 [A] | 0.00370 ± 0.00247  [73.5 ± 19.2] | 0.00316 ± 0.00102  [82.6 ± 7.45] | 0.001#  [122]# | 0.001#  [167]# | 0.0182 ± 0.0131  [-72.3 ± 7.27] |
| Trovafloxacin mesylate  (147059-75-4, InterBioScreen)  NCGC00064532-02  [A] | Trovafloxacin mesylate (147059-75-4, InterBioScreen) NCGC00064532-02 [A] | 20.5 ± 1.34  [119 ± 25.3] | 15.0 ± 2.44  [32.0 ± 2.62] | Inactive\* | Inactive\* | Inactive° |

§: The % efficacy is based on the maximal efficacy produced by R1881.

\*: Compound was identified as inactive if the efficacy was below 30% of R1881’s activity.

°: Compound was identified as inactive if the efficacy was below 20% of R1881’s activity.

#: At our lowest concentration, the efficacy is already higher than 100% and therefore we generated an estimate based on the lowest test concentration.

Purity Ratings: A = MW Confirmed, Purity > 90%; B = MW Confirmed, Purity 75 – 90%; C = MW Confirmed, Purity 50 – 75%; I = MW Confirmed, Two or more isomers detected; Z = MW Confirmed, No Purity Info; Ac = Purity > 90%, Low concentration of sample

1: This compound was used in the primary screen and picked for the follow-up screen; however, we ran out of the sample and therefore, had to buy a new one.

2: This is the compound we bought to replace 1 for the follow-up screens.

α: These samples had conflicting data through different suppliers, so we listed the data from two sources.

**Supplementary Table S2. Definition of curve rank as a numeric measure of compound activity**

|  |  |  |  |
| --- | --- | --- | --- |
| Curve class | Efficacy | Curve rank | Activity Category |
| 1.1 |  | 9 | Active activator |
| 1.2 | >50% | 8 | Active activator |
| 2.1 |  | 7 | Active activator |
| 1.2 | ≤50% | 6 | Active activator |
| 2.2 | >50% | 5 | Active activator |
| 2.2 | ≤50% | 4 | Inconclusive activator |
| 1.3 |  | 3 | Inconclusive activator |
| 1.4 |  | 3 | Inconclusive activator |
| 2.3 |  | 2 | Inconclusive activator |
| 2.4 |  | 2 | Inconclusive activator |
| 3 |  | 2 | Inconclusive activator |
| 5 |  | 1 | Inconclusive activator |
| 4 |  | 0 | Inactive |
| -2.3 |  | -2 | Inconclusive inhibitor |
| -2.4 |  | -2 | Inconclusive inhibitor |
| -3 |  | -2 | Inconclusive inhibitor |
| -1.3 |  | -3 | Inconclusive inhibitor |
| -1.4 |  | -3 | Inconclusive inhibitor |
| -2.2 | ≤50% | -4 | Inconclusive inhibitor |
| -2.2 | >50% | -5 | Active inhibitor |
| -1.2 | ≤50% | -6 | Active inhibitor |
| -2.1 |  | -7 | Active inhibitor |
| -1.2 | >50% | -8 | Active inhibitor |
| -1.1 |  | -9 | Active inhibitor |

**Supplementary Figures**

Concentration response curves were acquired on well-known AR agonists using AR-bla and AR-luc assays

**Figure S1.** Concentration response curves were acquired on well-known AR agonists using AR-bla and AR-luc assays. Fifteen point dilutions of Androstenedione (A), Spironolactone (B), and Testosterone (C) were performed. Data were collected from the primary screening and expressed as mean ± SD from three replicate experiments.

Concentration dependent translocation of GFP-AR protein for the positive control (A) and eight (B – I) of the top 17 compounds. 

**Figure S2.** Concentration dependent translocation of GFP-AR protein for the positive control (A) and eight (B – I) of the top 17 compounds. An automated image analysis of localization was performed for each concentration and the mean GFP-AR intensity for both the nucleus and the cytoplasm was identified. The ratio of both intensities was calculated and the triplicate values were then normalized to the corresponding control (DMSO) values. Data represents the mean ± SD (n = 3).

Concentration dependent translocation of GFP-AR protein for 9 (J – R) of the top 17 compounds. 

**Figure S2 cont.** Concentration dependent translocation of GFP-AR protein for 9 (J – R) of the top 17 compounds. An automated image analysis of localization was performed for each concentration and the mean GFP-AR intensity for both the nucleus and the cytoplasm was identified. The ratio of both intensities was calculated and the triplicate values were then normalized to the corresponding control (DMSO) values. Data represents the mean ± SD (n = 3).