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## **Supplemental Material**

# **Serum Metabolomic Profiles in Neonatal Mice following Oral Brominated Flame Retardant Exposures to Hexabromocyclododecane (HBCD) Alpha, Gamma, and Commercial Mixture**

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**Table S1.** Mean (SD) concentrations of 40 endogenous metabolites and formate (internal control) with SD according to treatment group.

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Metabolite	Control	Commercial	$\alpha$ -HBCD			$\gamma$ -HBCD	
	0 mg/kg n = 6	30 mg/kg n = 6	3 mg/kg n = 3	10 mg/kg n = 3	30 mg/kg n = 6	3 mg/kg n = 3	30 mg/kg n = 6
<b>2-HYDROXYISOBUTYRATE</b>							
Mean	0.0060	0.0062	0.0064	0.0071	0.0070	0.0063	0.0076
SD	0.0003	0.0009	0.0019	0.0014	0.0009	0.0015	0.0011
<b>3-HYDROXYBUTYRATE</b>							
Mean	0.1688	0.1921	0.1766	0.2286	0.1781	0.2148	0.2028
SD	0.0153	0.0219	0.0240	0.0402	0.0227	0.0416	0.0248
<b>ACETATE</b>							
Mean	0.0086	0.0103	0.0074	0.0083	0.0086	0.0069	0.0081
SD	0.0009	0.0020	0.0013	0.0015	0.0006	0.0012	0.0010
<b>ACETOACETATE</b>							
Mean	0.0169	0.0157	0.0178	0.0282*	0.0209	0.0178	0.0180
SD	0.0021	0.0020	0.0024	0.0028	0.0044	0.0049	0.0019
<b>ACETONE</b>							
Mean	0.0046	0.0047	0.0045	0.0055	0.0036**	0.0048	0.0046
SD	0.0003	0.0006	0.0006	0.0009	0.0001	0.0003	0.0003
<b>ALANINE</b>							
Mean	0.0921	0.0856	0.0723	0.0862	0.0832	0.0810	0.0913
SD	0.0079	0.0057	0.0089	0.0089	0.0040	0.0058	0.0047
<b>ARGININE</b>							
Mean	0.0998	0.0912	0.0769**	0.0948	0.0983	0.0674**	0.0974
SD	0.0056	0.0145	0.0054	0.0084	0.0120	0.0025	0.0102
<b>ASPARAGINE</b>							
Mean	0.0197	0.0244	0.0174	0.0218	0.0202	0.0158	0.0247
SD	0.0010	0.0034	0.0019	0.0026	0.0025	0.0022	0.0026
<b>CHOLINE</b>							
Mean	0.0163	0.0190	0.0154	0.0169	0.0114**	0.0170	0.0146
SD	0.0009	0.0025	0.0012	0.0007	0.0009	0.0003	0.0005
<b>CITRATE</b>							
Mean	0.0301	0.0337	0.0277	0.0299	0.0271	0.0488	0.0356
SD	0.0017	0.0024	0.0021	0.0007	0.0012	0.0187	0.0026
<b>CREATINE</b>							
Mean	0.0795	0.0847	0.0861	0.0861	0.0829	0.1324	0.0842
SD	0.0034	0.0067	0.0147	0.0003	0.0026	0.0536	0.0054
<b>CYSTEINE</b>							
Mean	0.0309	0.0361	0.0269	0.0269	0.0292	0.0269	0.0293
SD	0.0021	0.0063	0.0000	0.0000	0.0024	0.0000	0.0015
<b>DIMETHYLAMINE</b>							
Mean	0.0022	0.0027	0.0021	0.0026	0.0021	0.0039	0.0023
SD	0.0001	0.0004	0.0001	0.0002	0.0002	0.0018	0.0001
<b>FORMATE</b>							
Mean	1.0346	1.0372	1.0372	1.0372	1.0372	1.0372	1.0372
SD	0.0026	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
<b>GLUCOSE</b>							
Mean	0.9253	0.8910	0.9298	0.9267	0.8986	0.9149	1.0007
SD	0.0703	0.0604	0.0763	0.0164	0.0295	0.0931	0.0963
<b>GLUTAMATE</b>							
Mean	0.0669	0.0701	0.0585	0.0560**	0.0523**	0.0716	0.0565
SD	0.0046	0.0067	0.0048	0.0052	0.0010	0.0053	0.0035
<b>GLUTAMINE</b>							
Mean	0.0803	0.0871	0.0786	0.0877	0.0834	0.0835	0.0899

Metabolite	Control	Commercial	$\alpha$ -HBCD			$\gamma$ -HBCD	
	0 mg/kg n = 6	30 mg/kg n = 6	3 mg/kg n = 3	10 mg/kg n = 3	30 mg/kg n = 6	3 mg/kg n = 3	30 mg/kg n = 6
SD	0.0036	0.0074	0.0036	0.0049	0.0028	0.0024	0.0046
<b>GLYCEROL</b>							
Mean	0.1004	0.1225*	0.0908	0.1085	0.0979	0.1257	0.1114
SD	0.0058	0.0048	0.0095	0.0138	0.0048	0.0138	0.0092
<b>GLYCINE</b>							
Mean	0.0880	0.0910	0.0825	0.0985	0.0911	0.1017	0.1024
SD	0.0044	0.0058	0.0106	0.0075	0.0095	0.0066	0.0061
<b>HOMOSERINE</b>							
Mean	0.1677	0.1591	0.1591	0.1591	0.1591	0.1591	0.1591
SD	0.0086	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
<b>ISOBUTYRATE</b>							
Mean	0.0046	0.0046	0.0039	0.0037	0.0044	0.0040	0.0041
SD	0.0002	0.0004	0.0005	0.0006	0.0002	0.0005	0.0003
<b>ISOLEUCINE</b>							
Mean	0.0220	0.0238	0.0204	0.0257	0.0237	0.0230	0.0222
SD	0.0019	0.0029	0.0030	0.0021	0.0022	0.0020	0.0015
<b>LACTATE</b>							
Mean	0.9056	1.0190	0.7690	0.6941	0.7012	0.8190	0.8231
SD	0.0745	0.0752	0.0780	0.1154	0.0472	0.0451	0.0590
<b>LEUCINE</b>							
Mean	0.0354	0.0361	0.0394	0.0408	0.0395	0.0372	0.0389
SD	0.0028	0.0040	0.0085	0.0022	0.0033	0.0055	0.0022
<b>N LYSINE</b>							
Mean	0.0509	0.0549	0.0549	0.0496	0.0502	0.0491	0.0464
SD	0.0053	0.0082	0.0036	0.0021	0.0041	0.0088	0.0041
<b>METHANOL</b>							
Mean	0.0101	0.0055	0.0241	0.0049	0.0050	0.0057	0.0067
SD	0.0033	0.0009	0.0106	0.0007	0.0009	0.0012	0.0015
<b>METHIONINE</b>							
Mean	0.0252	0.0296	0.0256	0.0310	0.0245	0.0274	0.0259
SD	0.0021	0.0041	0.0003	0.0033	0.0011	0.0014	0.0027
<b>METHYLSUCCINATE</b>							
Mean	0.0205	0.0191	0.0192	0.0231	0.0214	0.0204	0.0191
SD	0.0030	0.0018	0.0036	0.0021	0.0025	0.0040	0.0018
<b>N,N-DIMETHYLGLYCINE</b>							
Mean	0.0052	0.0044	0.0043	0.0045	0.0041	0.0058	0.0046
SD	0.0005	0.0003	0.0005	0.0008	0.0003	0.0017	0.0004
<b>O-PHOSPHOCHOLINE</b>							
Mean	0.0375	0.0478	0.0369	0.0527*	0.0371	0.0370	0.0343
SD	0.0039	0.0052	0.0032	0.0056	0.0022	0.0062	0.0034
<b>PHENYLALANINE</b>							
Mean	0.0204	0.0168	0.0205	0.0198	0.0177	0.0150**	0.0144**
SD	0.0013	0.0014	0.0024	0.0014	0.0010	0.0007	0.0018
<b>PYRUVATE</b>							
Mean	0.0447	0.0447	0.0407	0.0394	0.0321*	0.0413	0.0398
SD	0.0019	0.0040	0.0030	0.0040	0.0024	0.0001	0.0011
<b>SARCOSINE</b>							
Mean	0.0120	0.0126	0.0118	0.0121	0.0119	0.0179	0.0121
SD	0.0001	0.0005	0.0002	0.0002	0.0001	0.0063	0.0002
<b>SERINE</b>							
Mean	0.0623	0.0628	0.0446	0.0665	0.0597	0.0772	0.0526
SD	0.0061	0.0065	0.0056	0.0072	0.0030	0.0139	0.0037
<b>SUCCINATE</b>							
Mean	0.0148	0.0153	0.0109	0.0092	0.0115	0.0128	0.0141

Metabolite	Control	Commercial	$\alpha$ -HBCD			$\gamma$ -HBCD	
	0 mg/kg n = 6	30 mg/kg n = 6	3 mg/kg n = 3	10 mg/kg n = 3	30 mg/kg n = 6	3 mg/kg n = 3	30 mg/kg n = 6
SD	0.0021	0.0019	0.0014	0.0012	0.0011	0.0020	0.0010
<b>TAURINE</b>							
Mean	0.1697	0.1913*	0.1769	0.1854	0.1691	0.2440	0.1825
SD	0.0055	0.0012	0.0128	0.0043	0.0075	0.0823	0.0091
<b>THREONINE</b>							
Mean	0.0665	0.0700	0.0459	0.0635	0.0543	0.0634	0.0525
SD	0.0103	0.0139	0.0037	0.0064	0.0064	0.0085	0.0065
<b>TYROSINE</b>							
Mean	0.0324	0.0294	0.0354	0.0373	0.0310	0.0328	0.0278
SD	0.0042	0.0021	0.0024	0.0005	0.0020	0.0029	0.0033
<b>VALINE</b>							
Mean	0.0258	0.0298	0.0262	0.0315	0.0320	0.0268	0.0283
SD	0.0022	0.0028	0.0030	0.0007	0.0030	0.0038	0.0015
<b>MYO-INOSITOL</b>							
Mean	0.0278	0.0300	0.0172	0.0190	0.0227	0.0369	0.0242
SD	0.0035	0.0043	0.0051	0.0021	0.0023	0.0173	0.0034
<b>METHYLHISTIDINE</b>							
Mean	0.0200	0.0203	0.0168	0.0199	0.0196	0.0185	0.0196
SD	0.0015	0.0033	0.0015	0.0004	0.0012	0.0012	0.0005

\*Significantly higher than control,  $p < 0.05$

\*\* Significantly lower than control,  $p < 0.05$