

Accessory publication

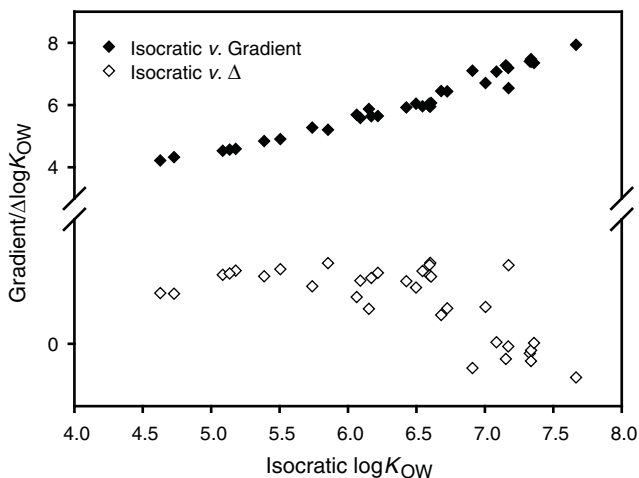
**RP-HPLC Measurement and QSPR Analysis of the *n*-Octanol-Water Partitioning Coefficients of Selected Metabolites of Polybrominated Diphenyl Ethers**

Yijun Yu,<sup>A</sup> Weihua Yang,<sup>A</sup> Zishen Gao,<sup>A</sup> Michael H. W. Lam,<sup>B,C</sup> Xiaohua Liu,<sup>A</sup> Liansheng Wang<sup>A</sup> and Hongxia Yu<sup>A,C</sup>

<sup>A</sup>State Key Laboratory of Pollution Control and Resource Re-use, School of the Environment, Nanjing University, Nanjing 210093, China.

<sup>B</sup>Department of Biology and Chemistry, City University of Hong Kong, Hong Kong SAR, China.

<sup>C</sup>Corresponding authors. Email: yuhx@nju.edu.cn; bhmhwlam@cityu.edu.hk



**Fig. A1.** Correlations between gradient derived and isocratic derived logK<sub>OW</sub>.

**Table A1. Software calculated log $K_{ow}$  of the investigated polybrominated diphenyl ether (PBDE) metabolites**

CASRN, Chemical Abstracts Service Registry Number

	CASRN	<i>AlogP</i>	<i>AclogP</i>	<i>MilogP</i>	<i>KowWin</i>	<i>XlogP</i>	<i>ClogP</i>	<i>MlogP</i>
1	602326-09-0	4.82	4.49	4.74	4.51	4.72	4.82	3.84
2	602326-18-1	4.83	4.49	4.73	4.51	4.69	5.07	3.84
3	602326-10-3	5.54	5.10	5.37	5.15	5.31	5.60	4.09
4A	4656-58-0	5.54	5.19	5.53	5.40	5.49	5.98	4.21
4B	602326-13-5	5.66	5.38	5.83	5.96	5.54	6.31	4.45
5A	102740-06-7	5.54	5.19	5.50	5.40	5.49	5.75	4.21
5B	102740-01-2	5.68	5.38	5.81	5.96	5.54	6.08	4.45
6A	602326-21-6	5.57	5.19	5.50	5.40	5.49	6.00	4.21
6B	602326-27-2	5.67	5.38	6.03	5.96	5.81	6.43	4.45
7A	80246-25-9	6.14	5.88	6.49	6.29	6.29	6.67	4.57
7B	96920-28-4	6.32	6.08	6.71	6.85	6.34	6.99	4.80
8A	79755-43-4	6.15	5.88	6.26	6.29	6.29	6.72	4.57
8B	102739-99-1	6.32	6.08	6.57	6.85	6.34	6.99	4.80
9B	602326-19-2	6.33	6.08	6.77	6.85	6.61	7.11	4.80
10A	602326-23-8	6.17	5.88	6.49	6.29	6.29	6.69	4.57
10B	602326-26-1	6.34	6.08	6.77	6.85	6.61	7.11	4.80
11A	602326-11-4	6.52	6.50	7.10	6.93	6.91	7.19	4.80
11B	678988-39-1	6.67	6.69	7.37	7.50	6.96	7.49	5.30
12A	497069-18-8	6.52	6.50	7.10	6.93	6.91	7.14	4.80
12B	497106-81-7	6.67	6.69	7.37	7.50	6.96	7.49	5.30
13A	35162-01-7	6.55	6.58	7.00	7.18	7.09	7.42	4.92
13B	38926-88-4	6.65	6.78	7.31	7.74	7.14	7.67	5.14
14A	49069-29-1	6.53	6.58	7.23	7.18	7.09	7.34	4.92
14B	497106-82-0	6.65	6.78	7.51	7.74	7.14	7.64	5.14
15A	80246-24-8	6.54	6.58	7.23	7.18	7.09	7.37	4.92
15B	497106-84-0	6.64	6.78	7.51	7.74	7.14	7.67	5.14
16A	602326-24-9	6.55	6.58	7.23	7.18	7.09	7.31	4.92
16B	602326-29-4	6.66	6.78	7.51	7.74	7.41	7.76	5.14
17A	111863-67-3	6.79	7.28	7.97	8.07	7.89	8.21	5.26
17B	169901-73-9	6.91	7.47	8.22	8.63	7.94	8.51	5.47
18A	–	6.54	6.58	7.23	7.18	7.09	7.31	4.92
18B	914670-38-5	6.65	6.78	7.51	7.74	7.41	7.76	5.14
19A	184174-87-6	6.14	5.88	6.49	6.29	6.29	6.47	4.57
20A	–	5.54	5.19	5.73	5.40	5.49	5.70	4.21

**Table A2. Peaks of analytes when MeOH/H<sub>2</sub>O = 95/5**

	RetTime	Area	Height	Width	log <i>k'</i>
1	2.96	1107.6	255.0	0.067	0.55
2	3.05	349.0	82.3	0.071	0.60
3	3.07	66.7	15.4	0.072	0.61
4A	3.41	386.5	74.1	0.079	0.79
4B	4.47	268.0	45.8	0.092	1.35
5A	3.13	255.5	57.7	0.074	0.64
5B	3.94	450.6	85.7	0.088	1.06
6A	3.45	165.0	33.1	0.078	0.81
6B	4.83	644.5	102.3	0.098	1.53
7A	4.20	332.9	57.0	0.092	1.20
7B	7.31	481.4	51.9	0.146	2.83
8A	4.63	1300.7	198.4	0.102	1.43
8B	7.18	241.4	24.6	0.153	2.76
9B	5.55	263.7	35.9	0.114	1.91
10A	4.18	318.8	52.1	0.093	1.19
10B	5.73	460.2	59.9	0.118	2.00
11A	4.16	1218.8	201.4	0.093	1.18
11B	7.94	992.5	96.5	0.162	3.16
12A	4.54	186.5	23.6	0.118	1.38
12B	7.94	183.0	17.7	0.159	3.16
13A	4.70	377.0	54.1	0.109	1.46
13B	8.72	30.1	2.7	0.175	3.57
14A	4.62	694.6	105.3	0.103	1.42
14B	7.93	344.4	32.9	0.162	3.16
15A	4.70	755.8	111.8	0.107	1.46
15B	8.58	294.8	26.7	0.173	3.50
16A	4.71	232.4	33.7	0.107	1.47
16B	7.51	174.7	17.6	0.156	2.94
17A	5.57	2633.9	318.7	0.128	1.92
17B	7.60	536.7	47.0	0.177	2.98
18A	4.47	624.5	94.1	0.103	1.34
18B	6.85	856.3	93.1	0.143	2.59
19	3.58	681.9	130.0	0.081	0.88
20	3.14	1865.4	401.2	0.072	0.65

**Table A3. Peaks of analytes when MeOH/H<sub>2</sub>O = 90/10**

	RetTime	Area	Height	Width	log <i>k'</i>
1	3.59	1031.6	203.8	0.084	0.87
2	3.73	350.9	66.2	0.084	0.95
3	3.86	66.5	12.2	0.086	1.01
4A	4.53	337.9	53.0	0.098	1.36
4B	6.65	265.2	31.0	0.134	2.47
5A	3.98	250.0	43.3	0.096	1.08
5B	5.53	433.5	59.5	0.121	1.88
6A	4.57	159.8	24.2	0.103	1.38
6B	7.35	632.0	67.4	0.145	2.83
7A	6.26	328.3	37.9	0.135	2.26
7B	12.84	479.0	30.3	0.247	5.70
8A	7.34	1285.8	124.7	0.160	2.83
8B	12.95	242.8	14.3	0.264	5.75
9B	9.18	258.6	21.9	0.184	3.78
10A	6.20	316.6	35.0	0.139	2.23
10B	9.56	446.6	36.6	0.190	3.99
11A	6.21	1184.5	134.5	0.137	2.24
11B	14.84	994.9	53.9	0.289	6.74
12A	7.16	169.5	14.4	0.175	2.74
12B	14.81	138.2	8.5	0.266	6.73
13A	7.46	356.0	33.6	0.166	2.89
13B	16.82	35.6	1.6	0.344	7.77
14A	7.35	688.2	66.6	0.161	2.83
14B	14.81	336.9	18.3	0.287	6.72
15A	7.44	735.3	70.8	0.161	2.88
15B	15.98	279.6	14.6	0.300	7.33
16A	7.43	226.5	21.5	0.163	2.87
16B	13.57	175.4	9.9	0.274	6.08
17A	9.70	2589.7	186.4	0.216	4.06
17B	14.69	541.1	26.1	0.324	6.66
18A	6.89	610.7	60.7	0.155	2.59
18B	12.11	825.3	53.3	0.241	5.32
19	5.00	645.5	90.9	0.109	1.61
20	3.99	1780.2	303.7	0.092	1.08

**Table A4. Peaks of analytes when MeOH/H<sub>2</sub>O = 85/15**

	RetTime	Area	Height	Width	logk'
1	4.59	1060.3	160.9	0.103	1.37
2	4.87	364.3	51.8	0.110	1.51
3	5.21	68.0	9.0	0.118	1.69
4A	6.55	345.7	37.5	0.144	2.38
4B	10.70	275.0	20.0	0.214	4.52
5A	5.45	240.2	30.1	0.125	1.81
5B	8.41	421.4	38.4	0.172	3.34
6A	6.53	158.8	17.0	0.147	2.37
6B	12.04	647.2	42.8	0.236	5.21
7A	10.08	338.8	23.2	0.224	4.20
7B	23.72	460.5	16.5	0.436	11.23
8A	12.67	1256.8	72.6	0.270	5.53
8B	24.92	226.8	7.4	0.472	11.85
9B	16.37	254.0	12.3	0.320	7.44
10A	9.90	308.8	22.2	0.216	4.10
10B	16.93	449.8	21.6	0.347	7.73
11A	10.09	1173.1	84.8	0.215	4.20
11B	29.14	992.1	28.7	0.533	14.03
12A	12.27	145.2	8.7	0.259	5.33
12B	29.18	154.3	4.7	0.498	14.05
13A	13.05	378.7	20.9	0.282	5.73
13B	21.59	50.4	1.8	0.470	10.13
14A	12.79	664.5	38.5	0.270	5.59
14B	29.41	326.2	9.3	0.531	14.16
15A	12.94	725.9	41.4	0.273	5.67
15B	31.65	266.4	7.6	0.519	15.32
16A	12.76	225.0	13.1	0.269	5.58
16B	26.18	152.9	5.2	0.442	12.50
17A	18.38	2500.0	102.1	0.382	8.48
17B	30.19	477.9	12.7	0.575	14.57
18A	11.69	568.5	34.8	0.253	5.03
18B	23.20	761.1	27.2	0.438	10.96
19	7.56	623.9	59.3	0.165	2.90
20	5.47	1629.8	210.9	0.120	1.82

**Table A5. Peaks of analytes when MeOH/H<sub>2</sub>O = 80/20**

	RetTime	Area	Height	Width	log <i>k'</i>
1	6.36	1024.6	114.3	0.139	2.23
2	6.85	347.5	36.2	0.150	2.48
3	7.68	64.7	6.0	0.167	2.91
4A	10.19	334.9	23.1	0.225	4.18
4B	18.37	266.7	11.6	0.359	8.34
5A	8.20	236.0	20.5	0.179	3.17
5B	13.92	411.2	23.8	0.267	6.08
6A	10.19	156.6	11.1	0.218	4.18
6B	21.18	600.4	24.6	0.383	9.77
7A	17.80	321.1	14.0	0.354	8.05
7B	46.51	383.0	9.2	0.639	22.64
8A	23.59	1232.1	41.6	0.466	10.99
8B	50.23	184.4	3.7	0.659	24.53
9B	31.02	237.6	6.8	0.520	14.77
10A	17.15	299.5	13.2	0.349	7.72
10B	31.84	421.9	11.6	0.558	15.19
11A	17.71	1165.8	50.1	0.361	8.00
11B	59.45	910.8	14.2	0.917	29.22
12A	22.57	128.1	4.8	0.423	10.47
12B	59.62	136.7	2.2	1.051	29.31
13A	24.38	345.3	11.1	0.468	11.39
13B	43.34	43.8	1.0	0.757	21.03
14A	23.54	662.1	22.2	0.464	10.97
14B	59.95	319.7	5.0	1.071	29.47
15A	24.00	720.4	23.8	0.469	11.20
15B	64.69	289.2	4.0	1.192	31.88
16A	23.29	221.2	7.4	0.455	10.84
16B	52.31	129.9	2.6	0.844	25.59
17A	36.85	2491.6	54.6	0.705	17.73
17B	64.44	554.4	6.6	1.395	31.75
18A	21.09	591.7	21.5	0.426	9.72
18B	46.02	786.2	15.1	0.789	22.39
19	12.55	622.5	37.4	0.258	5.38
20	8.11	1646.6	148.1	0.174	3.12

**Table A6. Peaks of analytes when MeOH/H<sub>2</sub>O = 75/25**

	RetTime	Area	Height	Width	log <i>k'</i>
1	9.43	1040.2	81.1	0.200	3.80
2	10.35	352.3	25.5	0.215	4.27
3	12.24	55.1	3.7	0.246	5.23
4A	17.74	370.1	15.7	0.358	8.02
4B	34.07	279.4	7.3	0.544	16.33
5A	13.17	237.1	13.6	0.273	5.70
5B	24.36	497.8	15.9	0.477	11.39
6A	16.93	234.2	7.4	0.455	7.61
6B	38.99	572.8	13.6	0.659	18.84
7A	32.78	306.4	8.2	0.565	15.67
7B			ND <sup>A</sup>		
8A	46.10	1209.4	22.7	0.810	22.45
8B			ND		
9B	61.42	260.3	3.8	1.153	30.25
10A	31.46	271.9	7.4	0.569	15.00
10B	62.47	380.6	6.1	0.743	30.78
11A	33.34	1140.8	28.2	0.625	15.96
11B			ND		
12A	43.99	155.2	3.0	0.864	21.38
12B			ND		
13A	48.55	446.4	6.2	1.193	23.70
13B			ND		
14A	46.23	625.0	12.0	0.779	22.52
14B			ND		
15A	46.99	704.3	13.0	0.778	22.90
15B			ND		
16A	44.92	302.3	4.4	0.863	21.85
16B			ND		
17A	77.62	2439.8	27.4	1.257	38.49
17B			ND		
18A	40.50	572.5	11.9	0.678	19.60
18B			ND		
19	22.47	664.2	22.9	0.444	10.43
20	13.02	1689.0	98.1	0.267	5.62

<sup>A</sup>Retention time too long to afford.