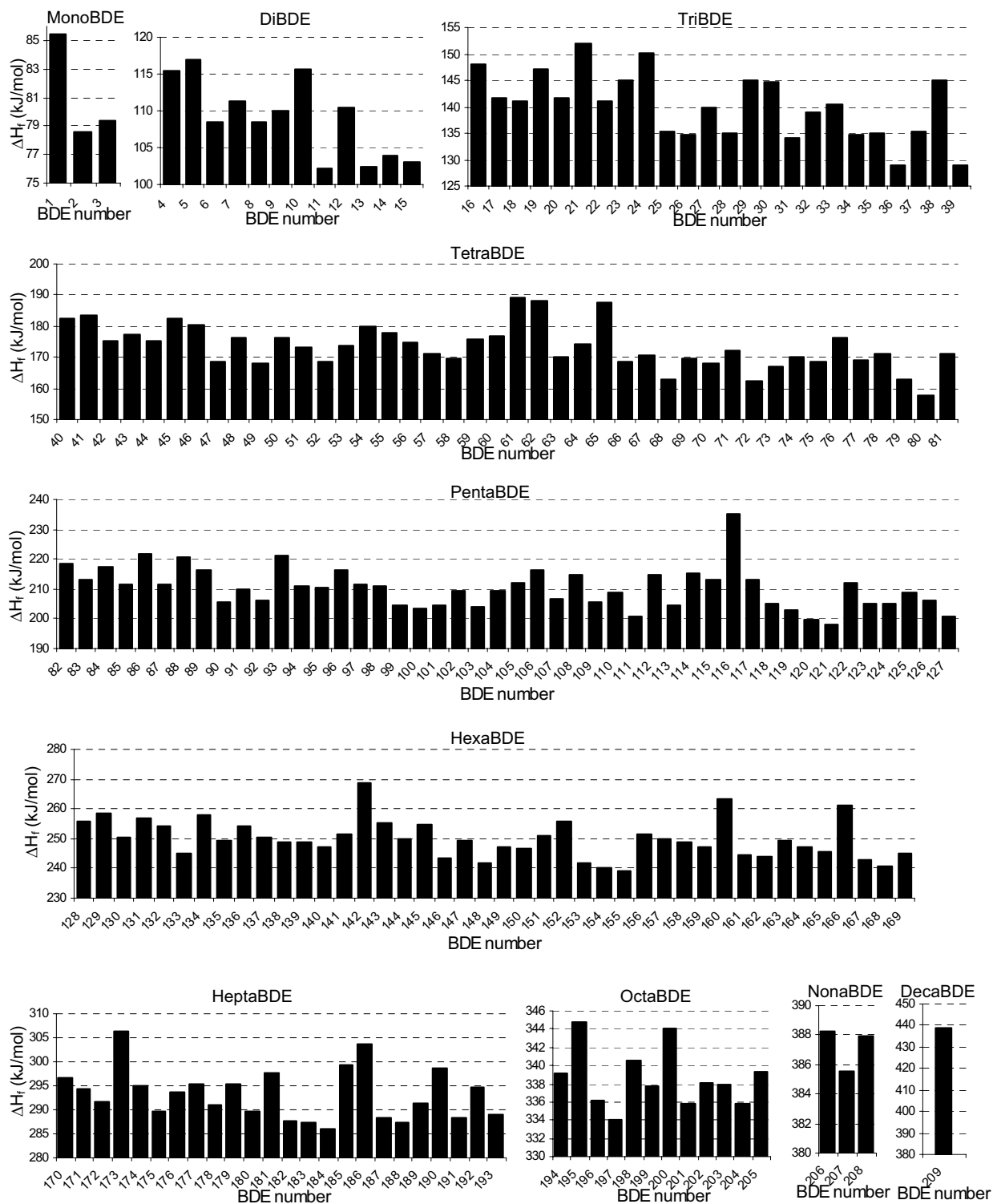


1 **Table S-1.** Experimental and multiple linear fit GC retention times for PBDE congeners

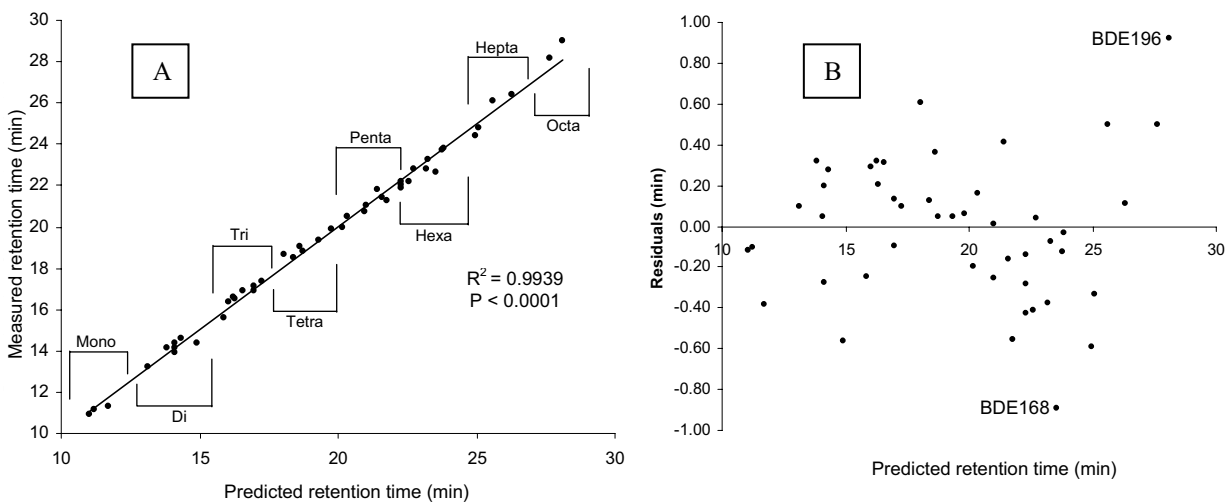
PBDE number	Retention time exp (min)	Retention time fit (min)	Residual	PBDE number	Retention time exp (min)	Retention time fit (min)	Residual
BDE-1	10.92	11.04	-0.12	BDE-153	22.83	23.20	-0.37
BDE-2	11.12	11.22	-0.10	BDE-154	22.18	22.59	-0.41
BDE-3	11.32	11.70	-0.38	BDE-155	21.87	22.29	-0.42
BDE-7	13.87	14.14	-0.27	BDE-166	23.82	23.85	-0.03
BDE-8	14.15	14.10	0.05	BDE-168	22.67	23.56	-0.89
BDE-10	13.25	13.15	0.10	BDE-181	26.13	25.63	0.50
BDE-11	14.15	13.83	0.32	BDE-183	24.77	25.10	-0.33
BDE-12	14.33	14.89	-0.56	BDE-184	24.38	24.97	-0.59
BDE-13	14.33	14.14	0.19	BDE-190	26.43	26.32	0.11
BDE-15	14.62	14.35	0.27	BDE-196	29.03	28.11	0.92
BDE-17	16.52	16.32	0.20	BDE-197	28.15	27.65	0.50
BDE-25	16.58	16.26	0.32				
BDE-28	16.88	16.57	0.31				
BDE-30	15.62	15.87	-0.25				
BDE-32	16.35	16.06	0.29				
BDE-33	16.88	16.98	-0.10				
BDE-35	17.12	16.99	0.13				
BDE-37	17.37	17.27	0.10				
BDE-47	19.02	18.66	0.36				
BDE-49	18.67	18.06	0.61				
BDE-66	19.37	19.32	0.05				
BDE-71	18.78	18.73	0.05				
BDE-75	18.52	18.39	0.13				
BDE-77	19.87	19.81	0.06				
BDE-85	21.83	21.42	0.41				
BDE-99	21.02	21.01	0.01				
BDE-100	20.53	20.37	0.16				
BDE-116	21.23	21.78	-0.55				
BDE-118	21.42	21.58	-0.16				
BDE-119	20.73	20.98	-0.25				
BDE-121	20.00	20.20	-0.20				
BDE-126	22.02	22.30	-0.28				
BDE-138	23.68	23.81	-0.13				
BDE-140	23.22	23.30	-0.08				
BDE-146	22.78	22.74	0.04				
BDE-148	22.17	22.31	-0.14				

3 **Table S-2.** Calculated reaction rate constants relative to BDE-209 for all the 209 PBDEs

PBDE Number	relative $\sum k$	PBDE Number	relative $\sum k$	PBDE Number	relative $\sum k$	PBDE Number	relative $\sum k$	PBDE Number	relative $\sum k$
BDE1	9.25E-06	BDE44	1.26E-03	BDE87	7.34E-03	BDE130	1.62E-02	BDE173	1.46E-01
BDE2	5.80E-07	BDE45	1.58E-03	BDE88	1.04E-02	BDE131	1.97E-02	BDE174	5.15E-02
BDE3	7.98E-07	BDE46	1.36E-03	BDE89	7.00E-03	BDE132	1.40E-02	BDE175	3.65E-02
BDE4	3.03E-05	BDE47	1.23E-04	BDE90	2.77E-03	BDE133	1.10E-02	BDE176	3.14E-02
BDE5	4.79E-04	BDE48	4.05E-04	BDE91	1.87E-03	BDE134	1.66E-02	BDE177	3.46E-02
BDE6	1.47E-05	BDE49	1.35E-04	BDE92	3.70E-03	BDE135	9.47E-03	BDE178	3.01E-02
BDE7	3.46E-05	BDE50	2.27E-04	BDE93	8.90E-03	BDE136	7.69E-03	BDE179	2.80E-02
BDE8	1.10E-05	BDE51	1.49E-04	BDE94	3.95E-03	BDE137	2.66E-02	BDE180	4.56E-02
BDE9	2.88E-05	BDE52	1.43E-04	BDE95	2.48E-03	BDE138	1.03E-02	BDE181	1.16E-01
BDE10	3.35E-05	BDE53	1.59E-04	BDE96	2.65E-03	BDE139	1.39E-02	BDE182	3.84E-02
BDE11	2.18E-06	BDE54	1.80E-04	BDE97	1.95E-03	BDE140	9.07E-03	BDE183	2.48E-02
BDE12	5.63E-05	BDE55	4.67E-03	BDE98	1.72E-03	BDE141	3.27E-02	BDE184	2.17E-02
BDE13	2.12E-06	BDE56	9.42E-04	BDE99	5.94E-04	BDE142	8.47E-02	BDE185	1.43E-01
BDE14	4.60E-06	BDE57	2.21E-03	BDE100	3.19E-04	BDE143	2.88E-02	BDE186	1.24E-01
BDE15	2.27E-06	BDE58	1.13E-03	BDE101	6.94E-04	BDE144	1.77E-02	BDE187	1.72E-02
BDE16	8.05E-04	BDE59	1.46E-03	BDE102	6.31E-04	BDE145	1.63E-02	BDE188	1.71E-02
BDE17	7.17E-05	BDE60	3.63E-03	BDE103	3.85E-04	BDE146	5.07E-03	BDE189	5.93E-02
BDE18	6.98E-05	BDE61	1.40E-02	BDE104	4.20E-04	BDE147	1.03E-02	BDE190	1.40E-01
BDE19	7.98E-05	BDE62	6.76E-03	BDE105	6.30E-03	BDE148	4.74E-03	BDE191	3.17E-02
BDE20	7.31E-04	BDE63	1.63E-03	BDE106	2.30E-02	BDE149	3.56E-03	BDE192	1.69E-01
BDE21	2.82E-03	BDE64	1.07E-03	BDE107	7.85E-03	BDE150	3.31E-03	BDE193	2.06E-02
BDE22	5.37E-04	BDE65	5.45E-03	BDE108	1.14E-02	BDE151	1.38E-02	BDE194	1.49E-01
BDE23	1.44E-03	BDE66	1.63E-04	BDE109	2.72E-03	BDE152	1.46E-02	BDE195	2.23E-01
BDE24	9.49E-04	BDE67	4.45E-04	BDE110	1.82E-03	BDE153	1.64E-03	BDE196	1.05E-01
BDE25	5.33E-05	BDE68	8.87E-05	BDE111	3.42E-03	BDE154	1.04E-03	BDE197	7.23E-02
BDE26	4.55E-05	BDE69	1.90E-04	BDE112	8.43E-03	BDE155	7.09E-04	BDE198	2.54E-01
BDE27	5.16E-05	BDE70	1.71E-04	BDE113	2.26E-03	BDE156	3.18E-02	BDE199	1.04E-01
BDE28	3.99E-05	BDE71	1.47E-04	BDE114	1.90E-02	BDE157	1.44E-02	BDE200	2.16E-01
BDE29	2.75E-04	BDE72	8.00E-05	BDE115	9.01E-03	BDE158	1.57E-02	BDE201	7.14E-02
BDE30	1.25E-04	BDE73	8.58E-05	BDE116	5.92E-02	BDE159	3.82E-02	BDE202	6.84E-02
BDE31	3.36E-05	BDE74	3.70E-04	BDE117	6.24E-03	BDE160	9.95E-02	BDE203	2.00E-01
BDE32	3.75E-05	BDE75	1.41E-04	BDE118	7.79E-04	BDE161	1.96E-02	BDE204	1.69E-01
BDE33	8.63E-05	BDE76	1.76E-03	BDE119	3.47E-04	BDE162	8.32E-03	BDE205	2.47E-01
BDE34	2.77E-05	BDE77	2.79E-04	BDE120	7.40E-04	BDE163	1.00E-02	BDE206	4.51E-01
BDE35	9.63E-05	BDE78	2.40E-03	BDE121	2.98E-04	BDE164	5.81E-03	BDE207	3.51E-01
BDE36	1.07E-05	BDE79	1.74E-04	BDE122	4.02E-03	BDE165	1.31E-02	BDE208	3.97E-01
BDE37	8.46E-05	BDE80	3.25E-05	BDE123	2.59E-03	BDE166	8.18E-02	BDE209	1.00E+0
BDE38	1.52E-03	BDE81	2.19E-03	BDE124	2.84E-03	BDE167	4.98E-03		
BDE39	8.95E-06	BDE82	8.60E-03	BDE125	2.09E-03	BDE168	3.23E-03		
BDE40	2.38E-03	BDE83	5.40E-03	BDE126	3.69E-03	BDE169	1.10E-02		
BDE41	4.43E-03	BDE84	4.30E-03	BDE127	3.83E-03	BDE170	6.03E-02		
BDE42	9.55E-04	BDE85	5.71E-03	BDE128	1.89E-02	BDE171	3.82E-02		
BDE43	2.38E-03	BDE86	1.98E-02	BDE129	3.46E-02	BDE172	6.06E-02		



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5 **Figure S-1.** Enthalpy of formation of 209 PBDEs calculated using the GAM model [1].

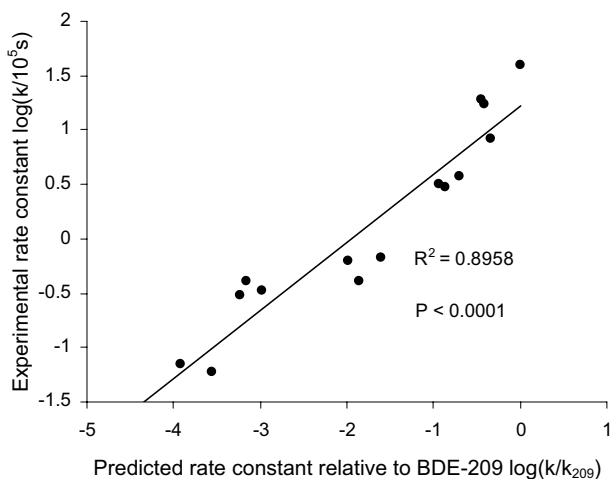


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7 **Figure S-2.** Correlation between measured and predicted GC retention time (A) and plot of
8 residuals (B).

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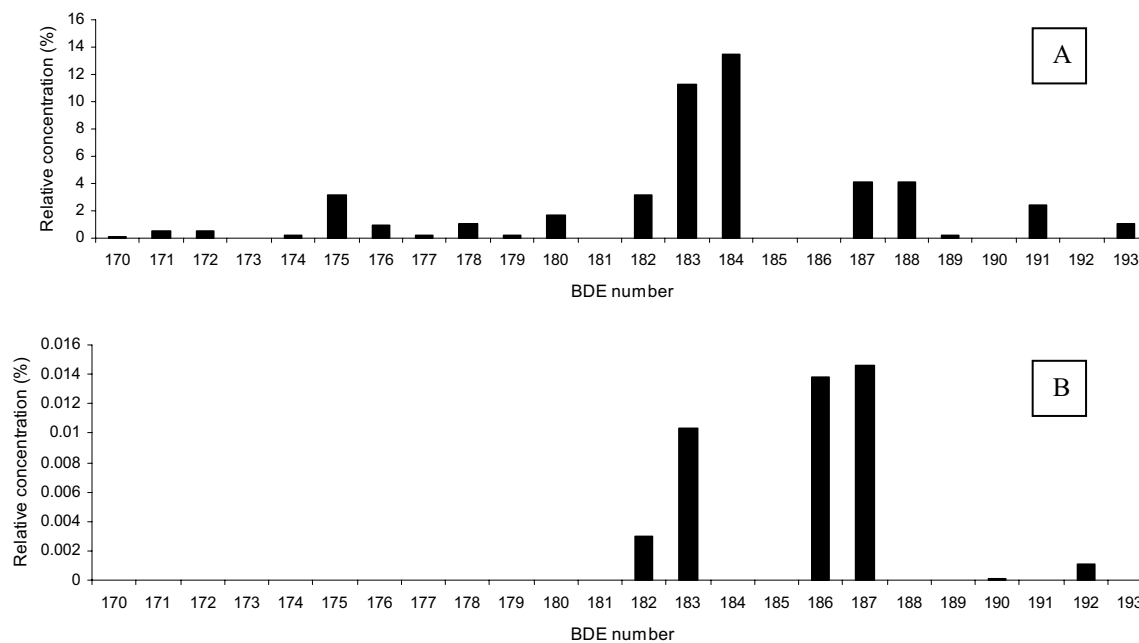


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12 **Figure S-3.** Correlation between predicted photodegradation rates (relative to BDE-209) and
13 experimental rates [2].

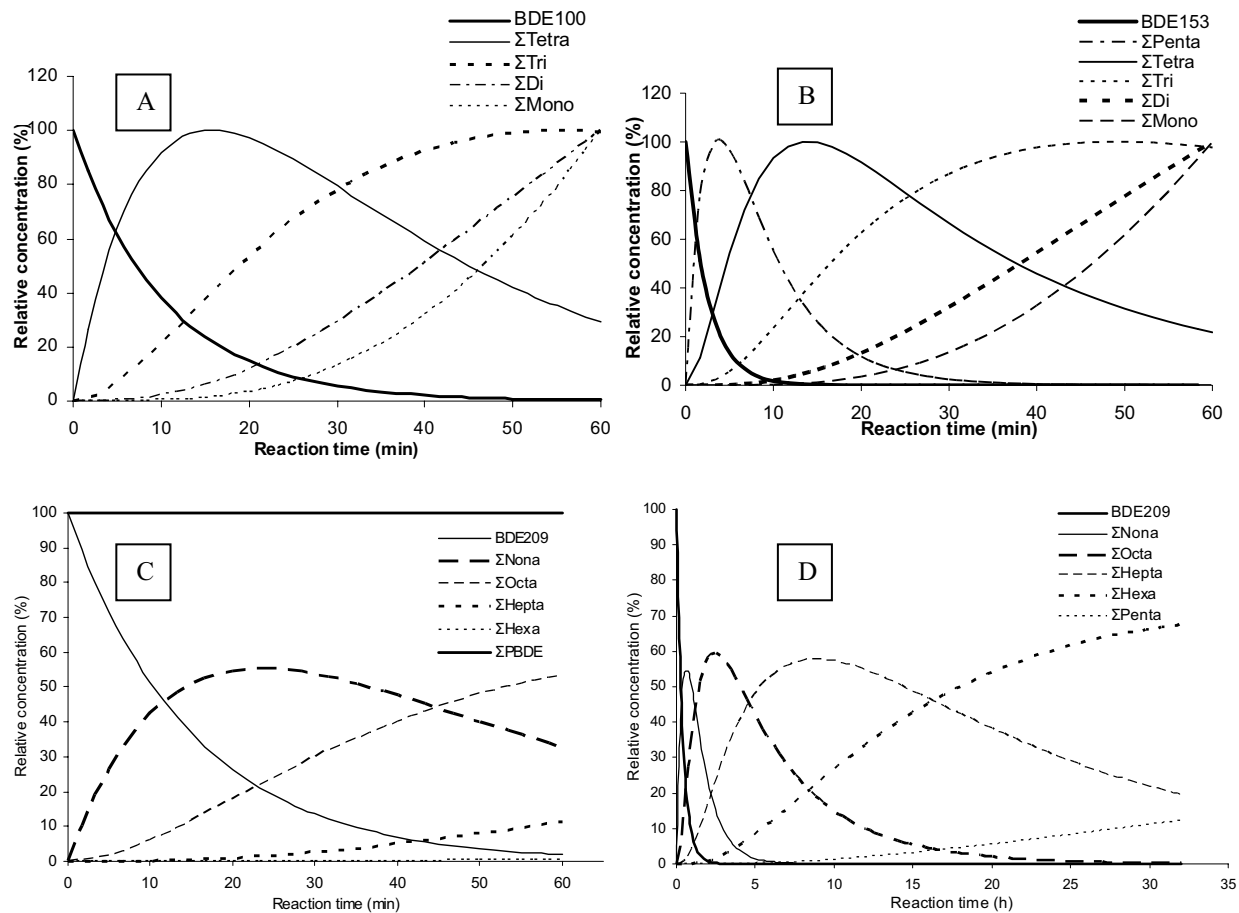
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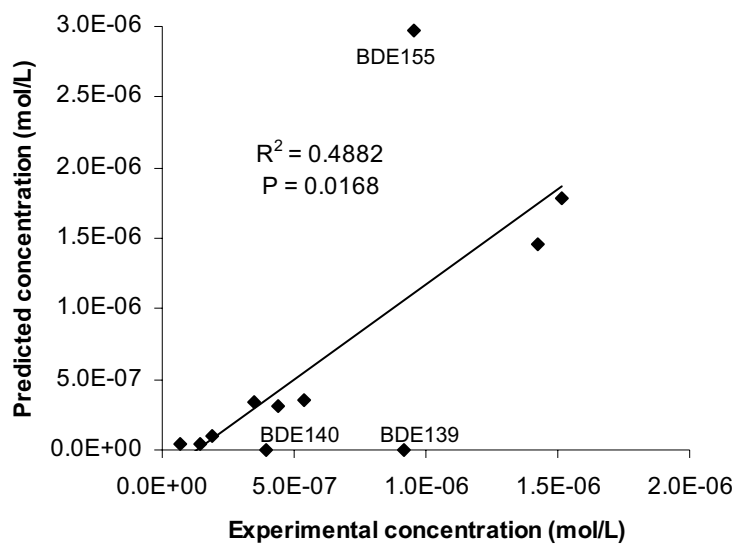
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17 **Figure S-4.** Predicted hepta-BDE products from BDE-209 photodegradation in methanol/water
18 (80/20) and UV light. A is the product profile at 1×10^5 sec reaction time and B is the product
19 profile at 1.4×10^6 sec. The concentrations are relative to the total BDE concentration.



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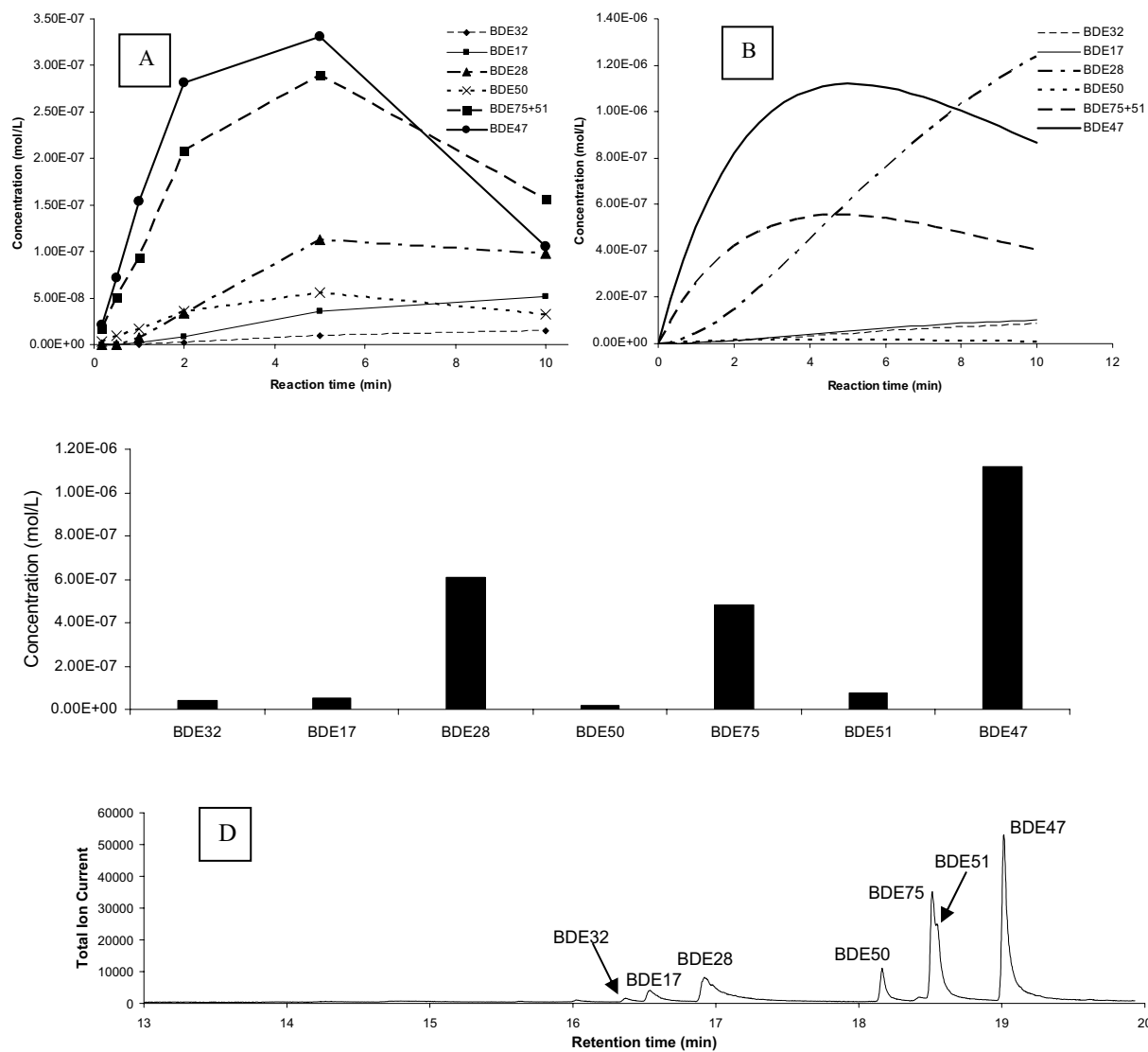
21 **Figure S-5.** Predicted PBDE photodegradation time profiles. A and B are the predicted
 22 photodegradation of BDE-100 and BDE-153, respectively, after SPME fiber exposure to sunlight
 23 simulated irradiation normalized to the maximum concentration of each homologous group [3].
 24 C is the predicted solar photodecomposition of BDE-209 in hexane relative to total PBDE
 25 concentration [4]. D is the predicted photodegradation of BDE-209 on silica gel under UV-light
 26 relative to total PBDE concentration [5].



27

28 **Figure S-6.** Correlation between experimental concentration and model predicted concentration

29 for BDE-184 photodegradation products at 120 min.



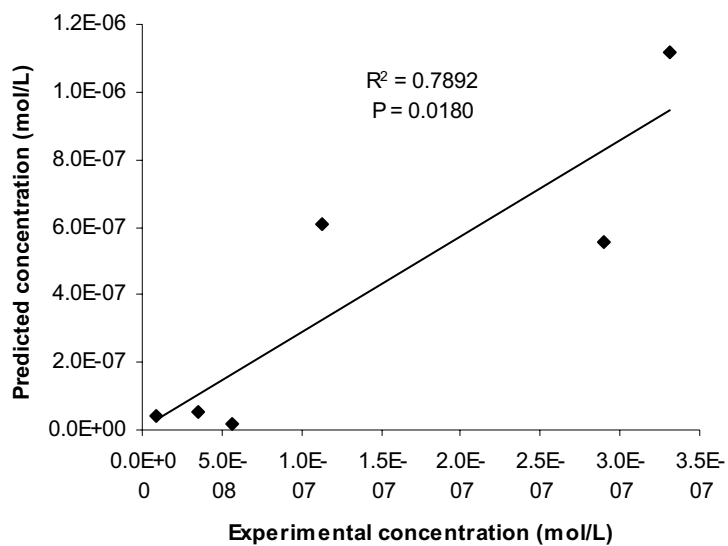
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31 **Figure S-7.** Photodegradation of BDE-100 in isoctane under UV. A is the experimental results

32 and B is the model prediction for BDE-100. C is the model prediction and D is experimental

33 results of BDE-100 photodegradation at 5 min.

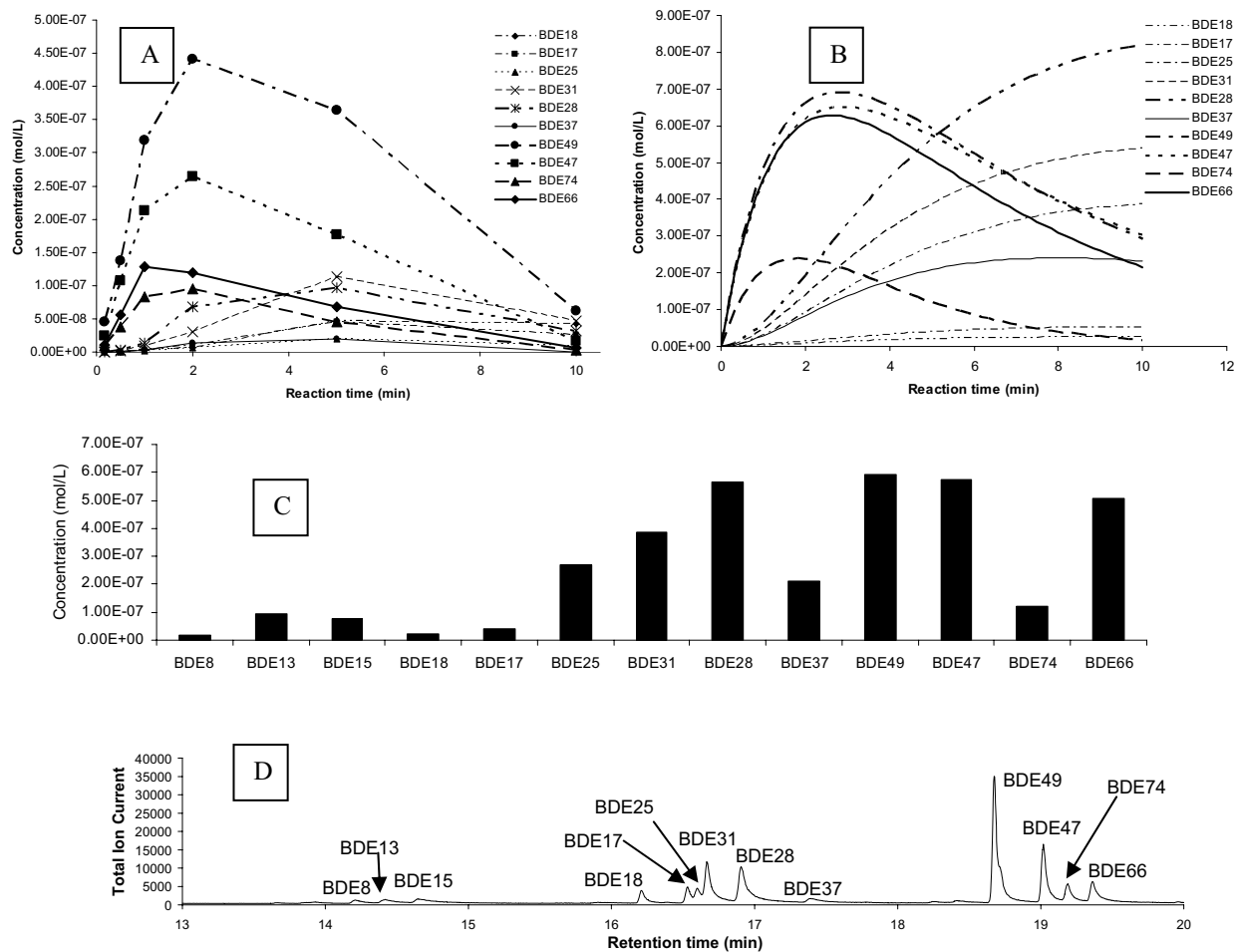
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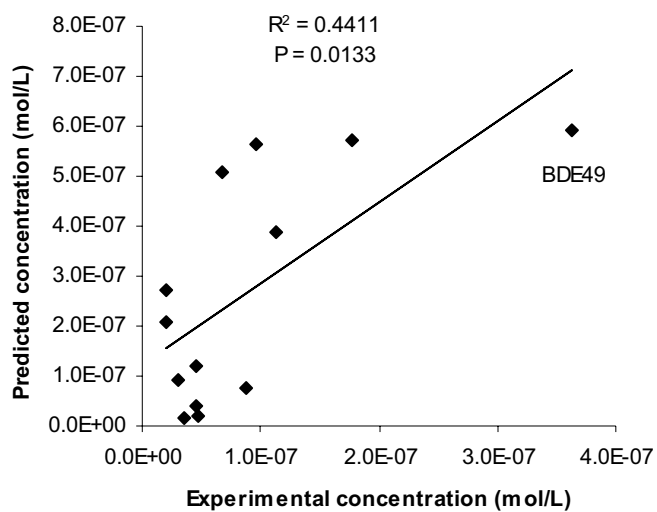
36 **Figure S-8.** Correlation between experimental result and model simulation for BDE-100

37 photodegradation products at 5 min.



38
 39 **Figure S-9.** Photodegradation of BDE-99 in isooctane under UV. A is the experimental results
 40 and B is the model prediction for BDE-99. C is the model prediction and D is experimental
 41 results of BDE-99 photodegradation at 5 min.

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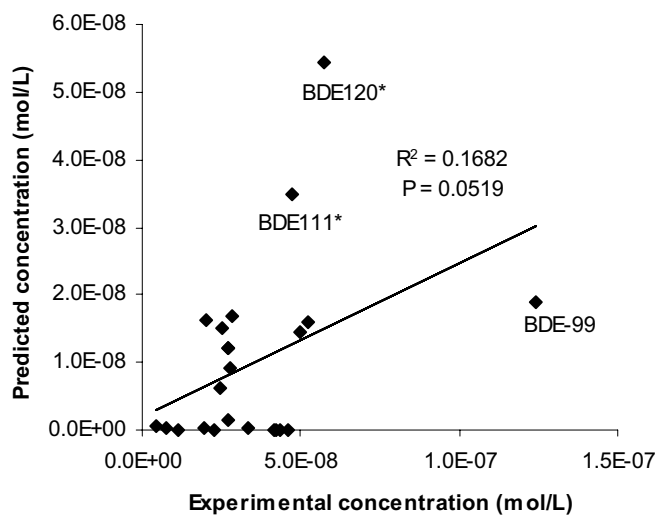


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44 **Figure S-10.** Correlation between experimental result and model simulation for BDE-99

45 photodegradation products at 5 min.

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48 **Figure S-11.** Correlation between experimental result and model simulation for tetra-BDEs and

49 penta-BDEs in BDE-209 photodegradation products at 120 min.

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51 **References**

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