Supporting information for "Equilibrium Partition Coefficients of Diverse Polar and Nonpolar Organic Compounds to Polyoxymethylene (POM) Passive Sampling Devices"

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Description of GC/MS measurements

Headspace analysis for volatile compounds

The aqueous phase concentrations of volatile compounds were measured by analyzing the headspace of vials using a GC/MS (7890A GC/5975C MS Triple-Axis detector, Agilent Technologies, Inc., Wilmington, DE, US) equipped with an autosampler (MultiPurpose Sampler, Gerstel). The following analytical columns were used for separation: HP-5ms Ultra Inert, 30 m × 0.25 mm i.d., film thickness 0.25 μm (Agilent Technologies); Rtx-VMS, 30 m × 0.25 mm i.d., film thickness 1.4 μm (Restek, Bellefonte, PA, US). The temperatures were as following: injector, 150 °C; transfer line, 280 °C (HP-5ms Ultra Inert) or 230 °C (Rtx-VMS); ion source, 230 °C; quadrupole, 150 °C. The initial oven temperature was 40°C. Different oven temperature programs were used for different analytes. The MS detector was run in the SIM mode for quantification. Sample vials were placed on a sample tray that was temperature-controlled to 25 °C. The headspace (500 μL) was sampled using a gas-tight syringe and was injected into the GC. To establish a calibration curve, 4–5 standard solutions were prepared in vials containing water one day before the analysis and the headspace was sampled and analyzed as for the samples.

Liquid injection method for extracts of organochlorine pesticides (OCPs)

Instrumental quantification was performed using dilutions of the EPA TCL mix for a four point calibration. OCPs quantification was performed on an Agilent 6850 gas chromatograph with an Agilent 5973 mass spectrometer and a fused silica capillary column (HP-5, 60 m x 0.25 mm i.d., 0.25 μm film thickness). A 1 μg mL^{-1} 4,4'-DDT/endrin standard was prepared from a 500 μg mL^{-1} solution in methanol (Sigma Aldrich) in order to monitor the breakdown of both compounds on the gas chromatograph. Compounds were not quantified unless the breakdown was below 15 %.

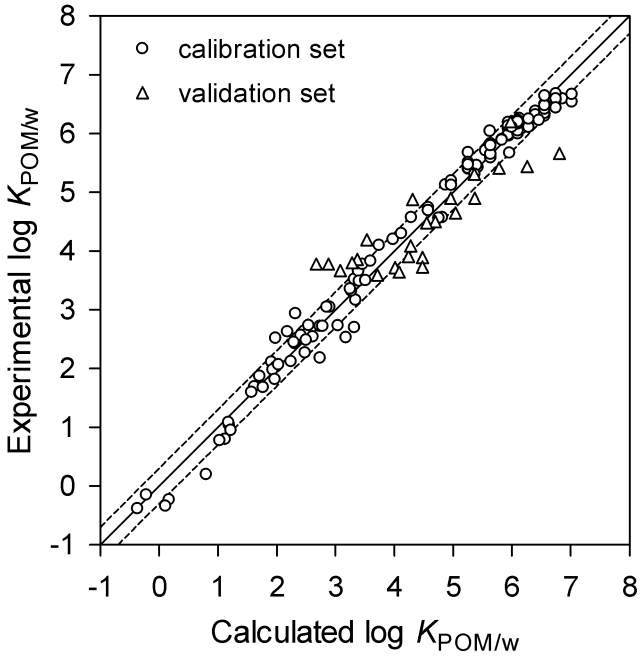

Figure S1. Experimental vs PP-LFER (eq 2)-calculated log $K_{POM/w}$ (L/kg). The solid and dashed lines indicate the 1:1 agreement and 0.3 log unit deviations, respectively. The PP-LFER equation fitted for calibration data (n = 116, R^2 = 0.986) is shown in Table 1.

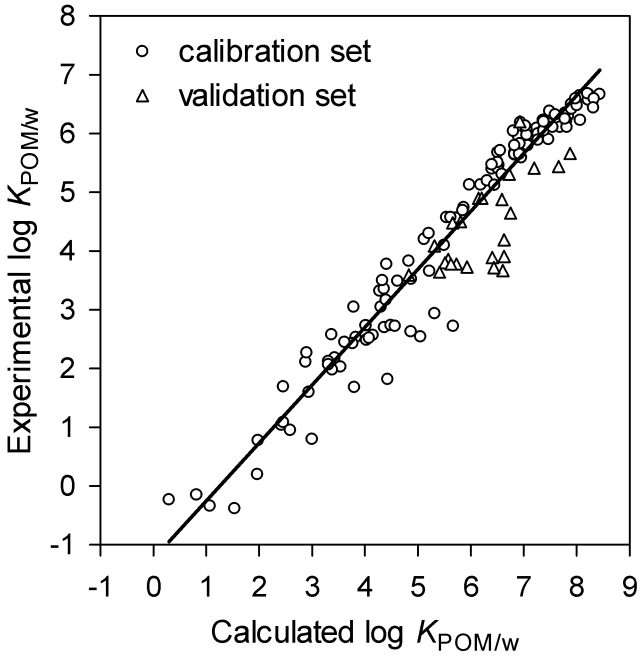

Figure S2. Experimental vs COSMO*thermX*-calculated log $K_{POM/w}$. The combinatorial term was *not* included in the calculation. The line indicates the linear regression for calibration compounds (n = 115, R^2 = 0.96; see Table 2 for the resulting equation).

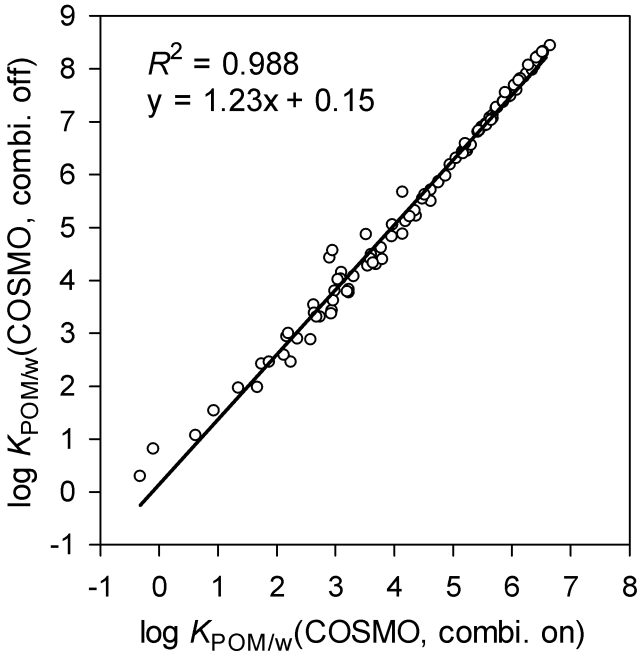

Figure S3. Correlation between the COSMO*thermX*-calculation results for calibration compounds with and without the combinatorial term.

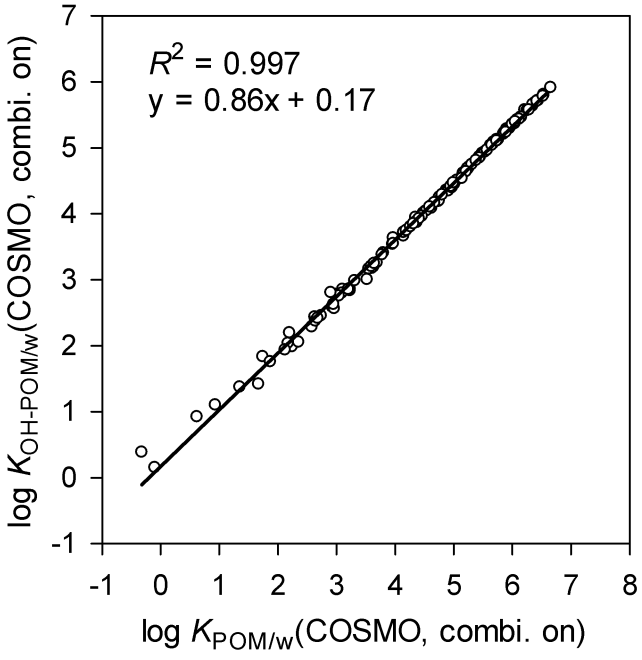

Figure S4. Comparison of partition coefficients to POM and OH-POM calculated using COSMO*thermX* (the combinatorial term was on).

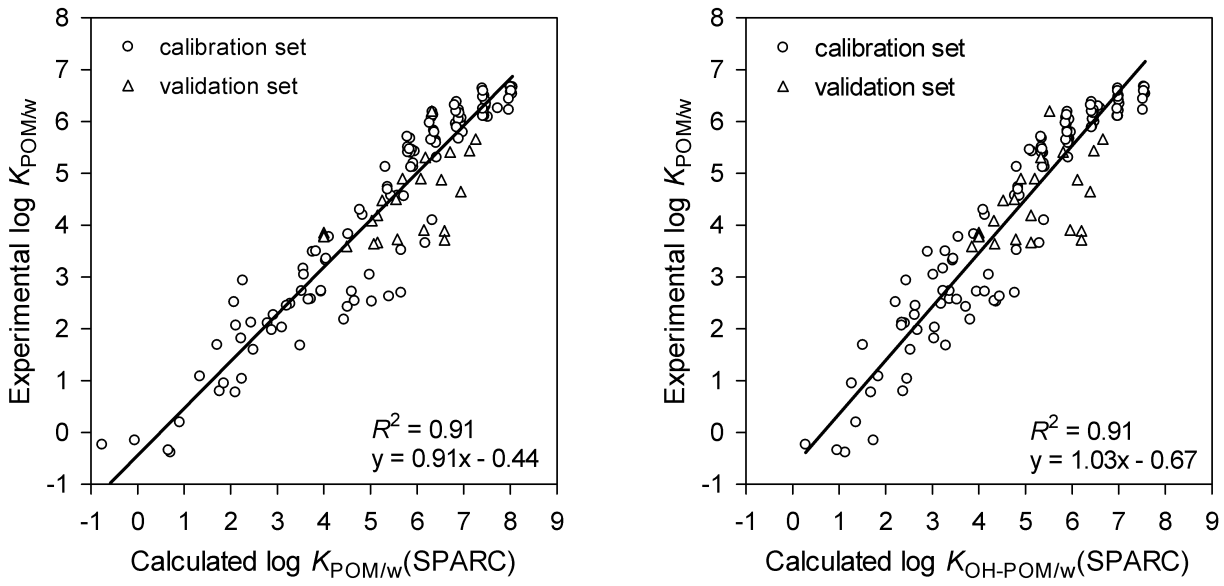

Figure S5. Experimental log $K_{POM/w}$ vs SPARC-calculated log $K_{POM/w}$ (left) and log $K_{OH-POM/w}$ (right). The line indicates the linear regression for calibration compounds (see Table 2 for the resulting equation).

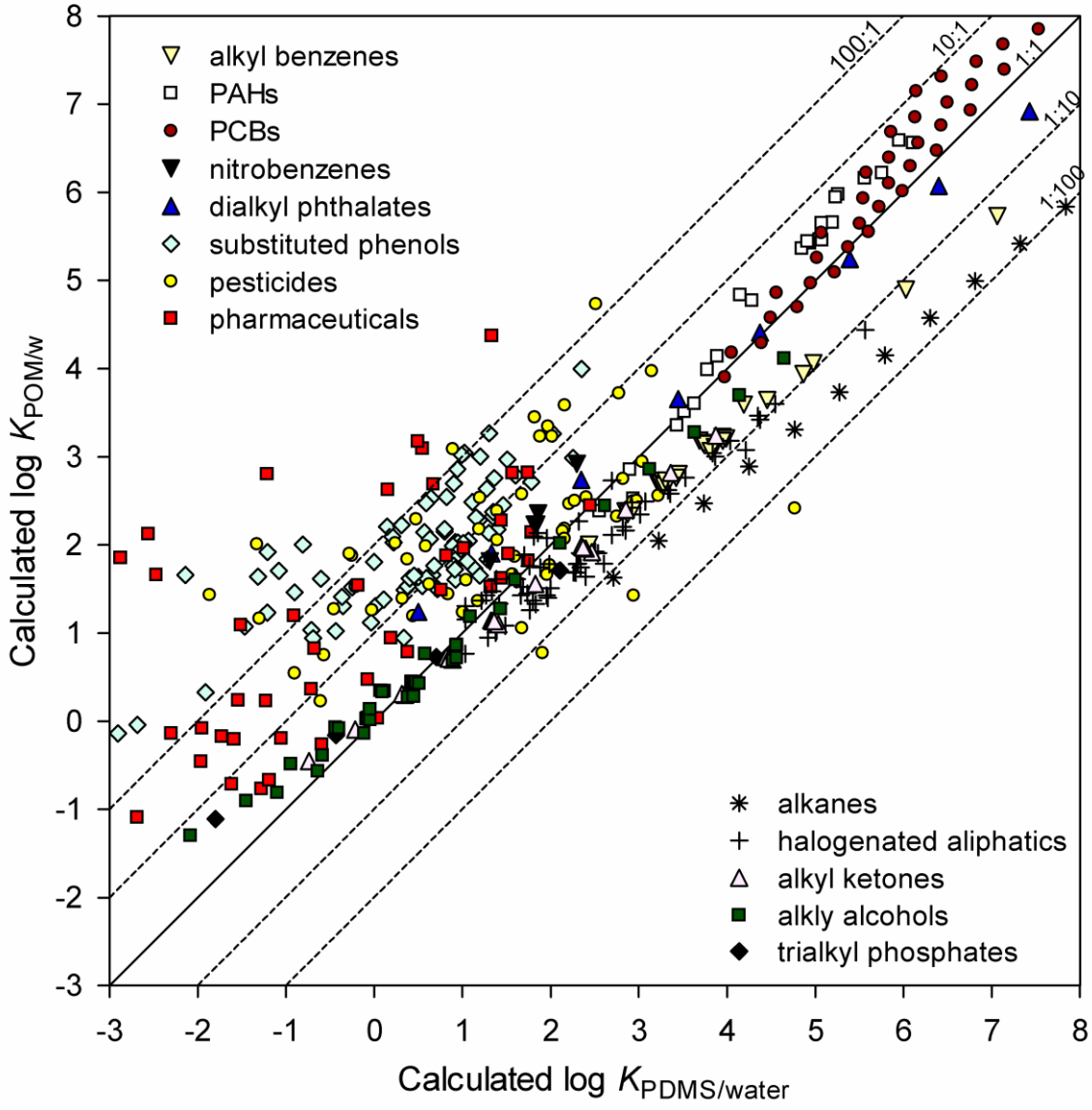

Figure S6. Comparison of sampler–water partition coefficients of POM with PDMS using the PP-LFER models in Table 3. "Pesticides" and "pharmaceuticals" are those listed in ref *1* and ref *2*, respectively, and also include some compounds that are not used as pesticides or pharmaceuticals.

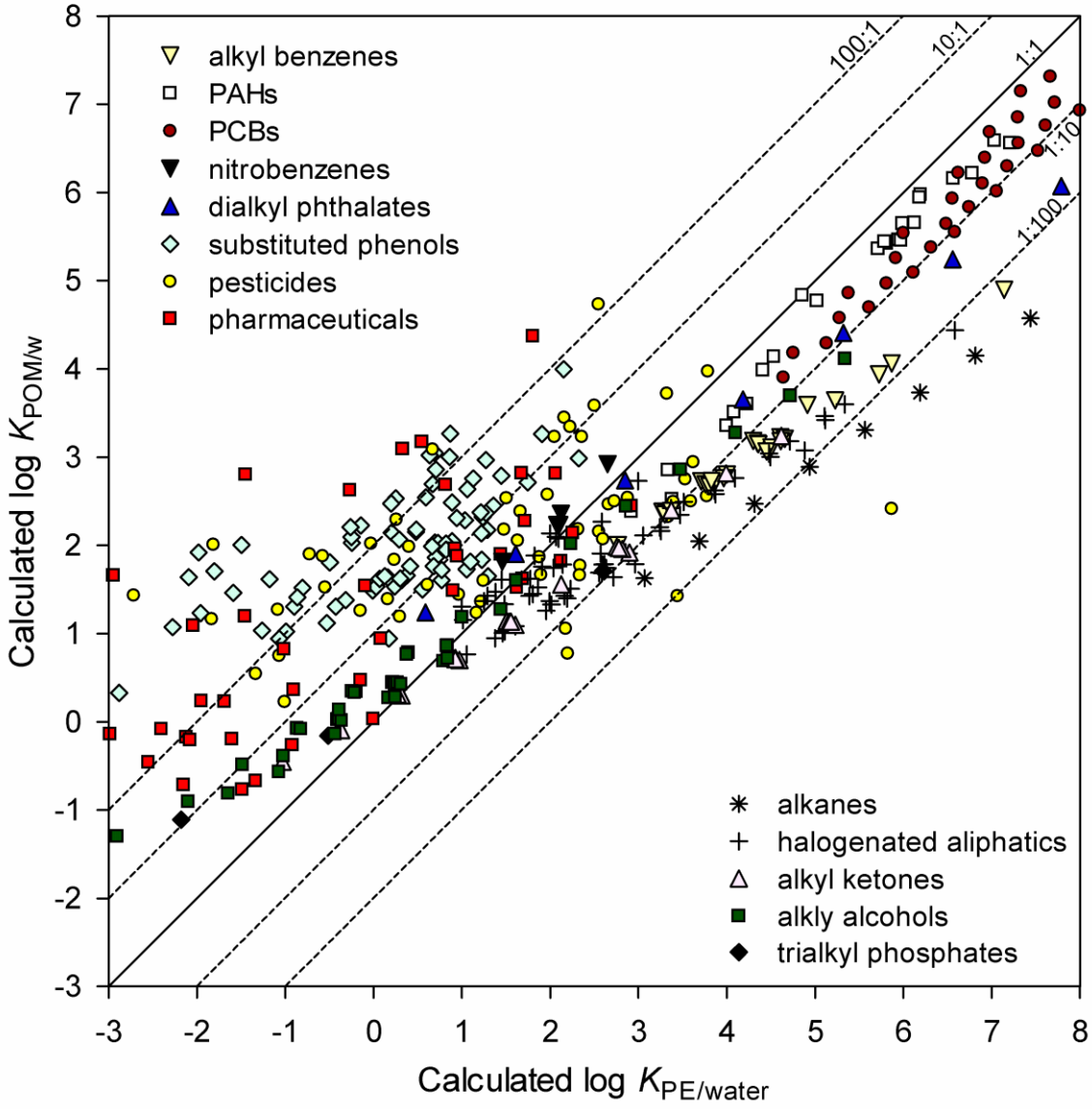

Figure S7. Comparison of sampler–water partition coefficients of POM with PE using the PP-LFER models in Table 3. "Pesticides" and "pharmaceuticals" are those listed in ref *1* and ref *2*, respectively, and also include some compounds that are not used as pesticides or pharmaceuticals.

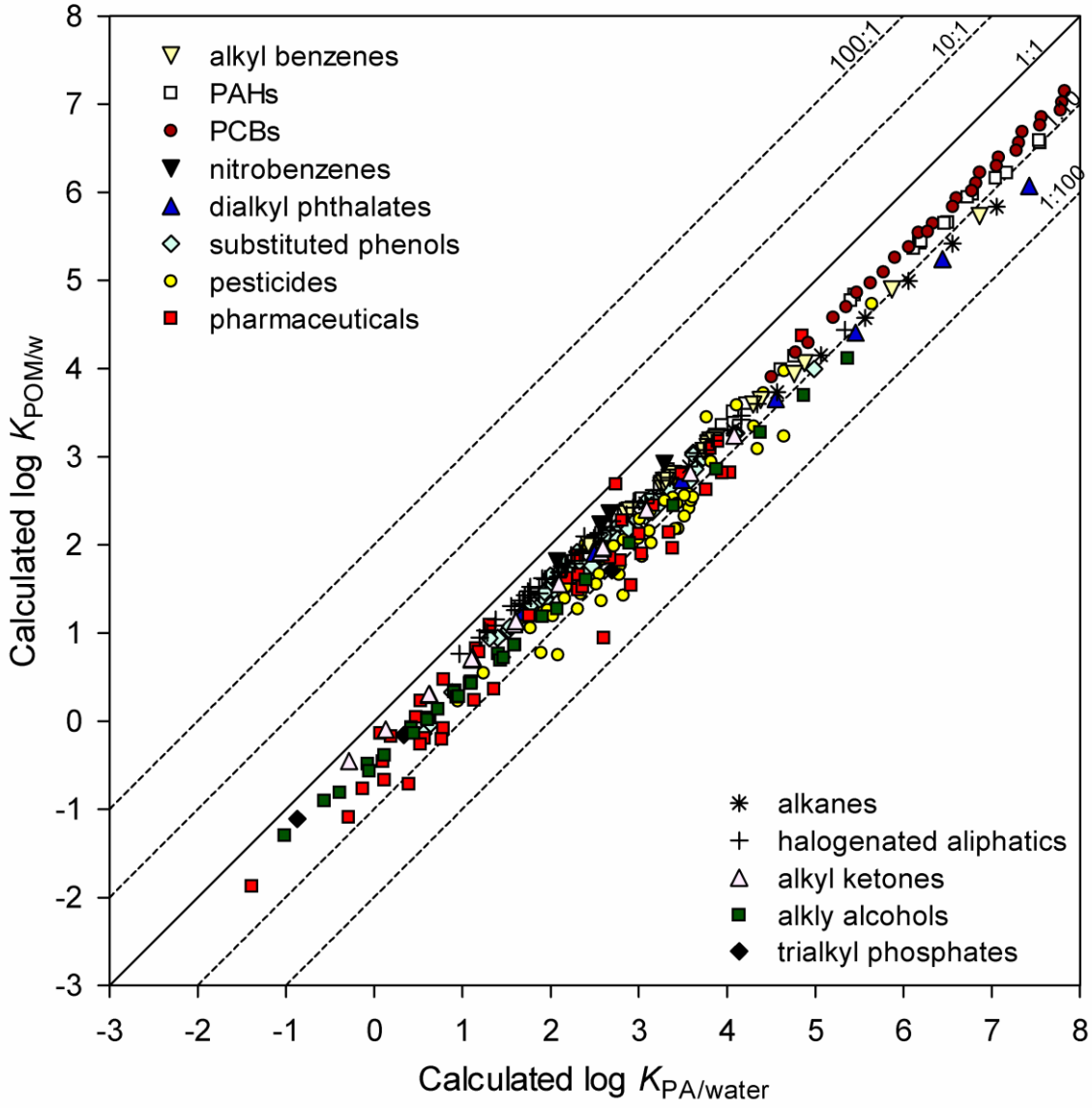

Figure S8. Comparison of sampler–water partition coefficients of POM with polyacrylate (PA) using the PP-LFER models in Table 3. "Pesticides" and "pharmaceuticals" are those listed in ref *1* and ref *2*, respectively, and also include some compounds that are not used as pesticides or pharmaceuticals.

Table S1. Experimental log $K_{POM/w}$ from this study and from the literature and log K_{ow} from the literature.

		experimental log $K_{POM/w}$	ref	log K_{ow}	calculated log $K_{POM/w}$	calc - exp
calibration compounds						
142-82-5	n-heptane	3.05	this study	4.66	4.12	1.08
111-65-9	n-octane	3.52	this study	5.18	4.65	1.13
111-84-2	n-nonane	4.10	this study	5.65	5.13	1.03
540-84-1	2,2,4-trimethylpentane	2.70	this study			
291-64-5	cycloheptane	2.18	this study	4.00	3.46	1.28
292-64-8	cyclooctane	2.53	this study	4.45	3.91	1.38
124-11-8	1-nonene	3.66	this study	5.15	4.62	0.96
628-71-7	1-heptyne	2.43	this study			
67-66-3	trichloromethane	1.69	this study	1.97	1.40	-0.30
79-01-6	trichloroethene	2.11	this study	2.42	1.85	-0.26
127-18-4	tetrachloroethene	2.58	this study	3.40	2.85	0.27
142-96-1	di-n-butyl ether	1.68	this study	3.21	2.65	0.97
693-65-2	di-n-pentyl ether	2.54	this study			
111-13-7	2-octanone	1.60	this study	2.37	1.80	0.20
821-55-6	2-nonanone	2.03	this study	3.14	2.58	0.56
693-54-9	2-decanone	2.57	this study	3.73	3.18	0.61
1193-82-4	methyl phenyl sulfoxide	-0.23	this study	0.55	-0.04	0.18
126-73-8	tri-n-butyl phosphate	1.87	this study	4.00	3.46	1.58
111-70-6	1-heptanol	1.04	this study	2.62	2.06	1.02
597-76-2	3-ethyl-3-hexanol	0.80	this study			
111-76-2	2-butoxyethanol	-0.38	this study	0.83	0.24	0.62
106-37-6	1,4-dibromobenzene	3.17	this study	3.79	3.24	0.07
93-89-0	ethyl benzoate	1.98	this study	2.64	2.08	0.09
1009-14-9	valerophenone	2.49	this study			
119-61-9	benzophenone	2.73	this study	3.18	2.62	-0.10
131-16-8	di-n-propyl phthalate	2.72	this study	3.27	2.71	0.00
88-72-2	2-nitrotoluene	2.12	this study	2.30	1.73	-0.39
121-14-2	2,4-dinitrotoluene	2.52	this study	1.98	1.41	-1.11
118-96-7	2,4,6-trinitrotoluene	2.94	this study	1.60	1.02	-1.92
100-17-4	4-nitroanisole	2.07	this study	2.03	1.46	-0.61
123-32-0	2,5-dimethylpyrazine	-0.34	this study	0.63	0.04	0.38
58-08-2	caffeine	-0.15	this study	0.07	-0.53	-0.38
439-14-5	diazepam	1.82	this study	2.82	2.26	0.43
873-76-7	4-chlorobenzyl alcohol	1.09	this study	1.96	1.39	0.30
108-95-2	phenol	0.78	this study	1.46	0.88	0.10
540-38-5	4-iodophenol	2.27	this study	2.91	2.35	0.08
90-15-3	1-naphthol	2.45	this study	2.85	2.29	-0.16
90-43-7	2-phenylphenol	2.74	this study	3.09	2.53	-0.21
80-05-7	bisphenol A	2.63	this study	3.32	2.77	0.13

95-53-4	2-methylaniline	0.95	this study	1.32	0.74	-0.21
103-84-4	acetanilide	0.20	this study	1.16	0.57	0.38
86-74-8	carbazole	3.49	this study	3.72	3.17	-0.32
53-16-7	estrone	2.72	this study	3.13	2.57	-0.15
91-20-3	naphthalene	3.05	(*3*)	3.30	2.75	-0.30
90-12-0	1-methylnaphthalene	3.32	(*3*)	3.87	3.32	0.00
91-57-6	2-methylnaphthalene	3.36	(*3*)	3.86	3.31	-0.05
208-96-8	acenaphthylene	3.78	(*3*)	3.94	3.39	-0.38
83-32-9	acenaphthene	3.50	(*3*)	3.92	3.37	-0.13
86-73-7	fluorene	3.83	(*3*)	4.18	3.64	-0.19
85-01-8	phenanthrene	4.20	(*3*)	4.46	3.92	-0.28
120-12-7	anthracene	4.30	(*3*)	4.45	3.91	-0.39
129-00-0	pyrene	4.57	(*3*)	4.88	4.35	-0.22
206-44-0	fluoranthene	4.56	(*3*)	5.16	4.63	0.07
218-01-9	chrysene	5.43	(*3*)	5.81	5.29	-0.14
56-55-3	benz[a]anthracene	5.46	(*3*)	5.76	5.24	-0.22
205-99-2	benzo[b]fluoranthene	5.80	(*3*)	5.78	5.26	-0.54
207-08-9	benzo[k]fluoranthene	5.97	(*3*)	6.11	5.60	-0.37
50-32-8	benzo[a]pyrene	5.96	(*3*)	6.13	5.62	-0.34
192-97-2	benzo[e]pyrene	5.67	(*3*)	6.44	5.93	0.26
198-55-0	perylene	6.04	(*3*)	6.25	5.74	-0.30
193-39-5	indeno[123cd]pyrene	6.26	(*3*)			
191-24-2	dibenz[a,h]anthracene	6.30	(*3*)	6.75	6.24	-0.06
191-24-2	benzo[ghi]perylene	6.09	(*3*)	6.63	6.12	0.03
13029-08-8	PCB 4	4.57	(*4*)	4.87	4.34	-0.23
25569-80-6	PCB 6	4.74	(*4*)	5.06	4.53	-0.21
34883-43-7	PCB 8	4.69	(*4*)	5.07	4.54	-0.15
2050-68-2	PCB 15	5.13	(*4*)	5.28	4.75	-0.38
	PCB 16/32	5.13	(*4*)	5.45	4.93	-0.21
37680-66-3	PCB 17	5.20	(*4*)	5.42	4.89	-0.31
37680-65-2	PCB 18	5.12	(*4*)	5.40	4.88	-0.24
38444-85-8	PCB 22	5.40	(*4*)	5.66	5.13	-0.26
38444-81-4	PCB 26	5.41	(*4*)	5.59	5.07	-0.34
7012-37-5	PCB 28	5.68	(*4*)	5.62	5.10	-0.59
16606-02-3	PCB 31	5.51	(*4*)	5.61	5.09	-0.42
38444-86-9	PCB 33	5.47	(*4*)	5.65	5.13	-0.34
38444-90-5	PCB 37	5.71	(*4*)	5.85	5.34	-0.37
36559-22-5	PCB 42	5.64	(*4*)	5.96	5.45	-0.20
41464-39-5	PCB 44	5.65	(*4*)	5.95	5.43	-0.21
70362-45-7	PCB 45	5.31	(*4*)	5.85	5.33	0.02
	PCB 47/48	5.59	(*4*)	5.93	5.41	-0.18
41464-40-8	PCB 49	5.83	(*4*)	5.91	5.40	-0.44
35693-99-3	PCB 52	5.65	(*4*)	5.90	5.38	-0.27
	PCB 56/60	6.19	(*4*)	6.20	5.68	-0.51
52663-58-8	PCB 64	5.80	(*4*)	5.96	5.44	-0.36

32598-10-0	PCB 66	6.08	(*4*)	6.16	5.65	-0.43
32598-11-1	PCB 70	5.98	(*4*)	6.15	5.64	-0.34
32690-93-0	PCB 74	6.13	(*4*)	6.12	5.61	-0.52
52663-62-4	PCB 82	6.00	(*4*)	6.52	6.01	0.01
	PCB 84/101	5.90	(*4*)	6.42	5.91	0.01
65510-45-4	PCB 85	6.07	(*4*)	6.48	5.97	-0.09
38380-02-8	PCB 87	6.05	(*4*)	6.47	5.96	-0.09
38379-99-6	PCB 95	5.89	(*4*)	6.35	5.84	-0.06
41464-51-1	PCB 97	6.23	(*4*)	6.46	5.95	-0.27
38380-01-7	PCB 99	6.17	(*4*)	6.43	5.92	-0.25
32598-14-4	PCB 105	6.38	(*4*)	6.72	6.21	-0.16
38380-03-9	PCB 110	6.20	(*4*)	6.50	5.99	-0.21
31508-00-6	PCB 118	6.32	(*4*)	6.66	6.16	-0.16
38380-07-3	PCB 128	6.35	(*4*)	7.04	6.54	0.18
38380-05-1	PCB 132	6.11	(*4*)	6.92	6.41	0.30
52744-13-5	PCB 135	6.21	(*4*)	6.84	6.34	0.13
38411-22-2	PCB 136	6.11	(*4*)	6.79	6.29	0.18
	PCB 138/163	6.50	(*4*)	6.98	6.48	-0.01
52712-04-6	PCB 141	6.42	(*4*)	6.95	6.45	0.03
51908-16-8	PCB 146	6.48	(*4*)	6.91	6.41	-0.07
38380-04-0	PCB 149	6.11	(*4*)	6.86	6.36	0.25
52663-63-5	PCB 151	6.25	(*4*)	6.80	6.30	0.05
35065-27-1	PCB 153	6.64	(*4*)	6.93	6.43	-0.21
38380-08-4	PCB 156	6.59	(*4*)	7.20	6.70	0.12
35065-30-6	PCB 170	6.54	(*4*)	7.52	7.03	0.49
52663-71-5	PCB 171	6.67	(*4*)	7.36	6.87	0.20
38411-25-5	PCB 174	6.57	(*4*)	7.40	6.90	0.34
52663-70-4	PCB 177	6.68	(*4*)	7.38	6.88	0.20
52663-64-6	PCB 179	6.23	(*4*)	7.24	6.74	0.51
35065-29-3	PCB 180	6.67	(*4*)	7.48	6.98	0.31
52663-69-1	PCB 183	6.59	(*4*)	7.31	6.81	0.23
52663-68-0	PCB 187	6.44	(*4*)	7.32	6.82	0.38
validation compounds						
319-84-6	α-HCH	3.86	this study	3.80	3.25	-0.61
319-85-7	β-HCH	3.78	this study	3.78	3.23	-0.55
58-89-9	γ-HCH	3.80	this study	3.72	3.17	-0.63
319-86-8	δ-HCH	3.78	this study	4.14	3.60	-0.18
309-00-2	aldrin	4.65	this study	6.50	5.99	1.34
60-57-1	dieldrin	3.89	this study	5.40	4.88	0.98
50-29-3	4,4-DDT	5.66	this study	6.91	6.41	0.74
72-55-9	4,4-DDE	5.44	this study	6.51	6.00	0.56
959-98-8	endosulfan I	4.19	this study	3.83	3.28	-0.90
33213-65-9	endosulfan II	3.67	this study	3.83	3.28	-0.39
72-20-8	endrin	3.72	this study	5.20	4.67	0.95

76-44-8	heptachlor	4.88	this study	6.10	5.59	0.71
1024-57-3	heptachlor epoxide	3.91	this study	4.98	4.45	0.54
	C2 naphthalenes	3.59	(*3*)	4.37	3.83	0.24
	C3 naphthalenes	3.64	(*3*)	4.73	4.20	0.56
	C4 naphthalenes	3.73	(*3*)			
	C1 fluorenes	4.09	(*3*)	4.97	4.44	0.35
	C2 fluorenes	4.50	(*3*)			
	C1 phenanthrenes/anthracenes	4.48	(*3*)	5.04	4.51	0.03
	C2 phenanthrenes/anthracenes	4.90	(*3*)	5.77	5.25	0.35
	C3 phenanthrenes/anthracenes	5.31	(*3*)			
	C4 phenanthrenes/anthracenes	5.41	(*3*)			
	C1 fluoranthenes/pyrenes	4.90	(*3*)			

Log K_{ow} values are from ref *5*, except for PCBs, values of which were estimated using the PP-LFER. Log K_{ow} values of alkyl-PAHs are the mean of the values available for respective isomers. For non-unique PCBs, descriptors of the following congeners were used: PCB 16 for PCB 16/32, PCB 47 for PCB 47/48, PCB 56 for PCB 56/60, PCB 101 for PCB 84/101, PCB 138 for PCB 138/163.

Table S2. PP-LFER descriptors of calibration and validation compounds and values of PP-LFER-calculated log $K_{POM/w}$.

	E	*S*	*A*	*B*	*V*	*L*	calculated log $K_{POM/w}$ (eq 2)	calc - exp	calculated log $K_{POM/w}$ (eq 3)	calc - exp
calibration compounds										
n-heptane	0.00	0.00	0.00	0.00	1.09	3.17	2.90	-0.15	2.91	-0.14
n-octane	0.00	0.00	0.00	0.00	1.24	3.68	3.32	-0.20	3.34	-0.18
n-nonane	0.00	0.00	0.00	0.00	1.38	4.18	3.74	-0.36	3.77	-0.33
2,2,4-trimethylpentane	0.00	0.00	0.00	0.00	1.24	3.11	3.32	0.62	3.18	0.49
cycloheptane	0.35	0.10	0.00	0.00	0.99	3.70	2.74	0.56	2.84	0.66
cyclooctane	0.41	0.10	0.00	0.00	1.13	4.33	3.18	0.65	3.30	0.77
1-nonene	0.09	0.08	0.00	0.07	1.33	4.07	3.39	-0.27	3.38	-0.28
1-heptyne	0.16	0.23	0.13	0.10	1.01	3.00	2.31	-0.12	2.24	-0.19
trichloromethane	0.43	0.49	0.15	0.02	0.62	2.48	1.62	-0.07	1.63	-0.06
trichloroethene	0.52	0.37	0.08	0.03	0.71	3.00	1.91	-0.20	1.96	-0.15
tetrachloroethene	0.64	0.44	0.00	0.00	0.84	3.58	2.50	-0.08	2.55	-0.03
di-n-butyl ether	0.00	0.25	0.00	0.45	1.29	3.92	1.77	0.09	1.75	0.07
di-n-pentyl ether	0.00	0.25	0.00	0.45	1.58	4.88	2.61	0.07	2.60	0.06
2-octanone	0.11	0.68	0.00	0.51	1.25	4.26	1.57	-0.03	1.58	-0.02
2-nonanone	0.12	0.68	0.00	0.51	1.39	4.74	1.99	-0.04	2.01	-0.02
2-decanone	0.11	0.68	0.00	0.51	1.53	5.25	2.41	-0.16	2.44	-0.13
methyl phenyl sulfoxide	1.10	1.80	0.00	0.91	1.08	5.58	0.17	0.39	0.16	0.38
tri-n-butyl phosphate	-0.10	0.90	0.00	1.21	2.24	7.37	1.71	-0.16	1.70	-0.17
1-heptanol	0.21	0.42	0.37	0.48	1.15	4.12	1.19	0.15	1.19	0.15
3-ethyl-3-hexanol	0.20	0.30	0.31	0.60	1.29	4.29	1.12	0.32	1.06	0.27
2-butoxyethanol	0.20	0.53	0.26	0.83	1.07	3.66	-0.37	0.01	-0.43	-0.06
1,4-dibromobenzene	1.15	0.86	0.00	0.04	1.07	5.32	3.34	0.17	3.41	0.24
ethyl benzoate	0.69	0.85	0.00	0.46	1.21	5.08	1.93	-0.06	1.95	-0.03
valerophenone	0.80	0.95	0.00	0.50	1.44	5.90	2.50	0.01	2.50	0.00
benzophenone	1.45	1.50	0.00	0.50	1.48	6.96	3.04	0.31	2.97	0.24
di-n-propyl phthalate	0.71	1.40	0.00	0.88	1.99	7.70	2.74	0.03	2.69	-0.03
2-nitrotoluene	0.87	1.11	0.00	0.28	1.03	4.88	2.24	0.12	2.29	0.17
2,4-dinitrotoluene	1.17	1.27	0.07	0.51	1.21	6.27	1.98	-0.54	2.08	-0.43

2,4,6-trinitrotoluene	1.57	1.71	0.11	0.62	1.38	7.03	2.32	-0.62	2.26	-0.68
4-nitroanisole	0.97	1.29	0.00	0.40	1.09	5.85	2.03	-0.04	2.22	0.15
2,5-dimethylpyrazine	0.63	0.90	0.00	0.69	0.92	4.09	0.11	0.46	0.15	0.49
caffeine	1.50	1.82	0.08	1.25	1.36	7.84	-0.22	-0.07	-0.06	0.09
diazepam	2.08	1.55	0.00	1.28	2.07	10.48	1.97	0.15	2.02	0.19
4-chlorobenzyl alcohol	0.91	0.96	0.40	0.50	1.04	5.07	1.18	0.09	1.20	0.11
phenol	0.81	0.89	0.60	0.30	0.78	3.77	1.03	0.26	0.97	0.19
4-iodophenol	1.38	1.22	0.68	0.20	1.03	5.49	2.48	0.21	2.38	0.11
1-naphthol	1.52	1.10	0.66	0.34	1.14	6.28	2.29	-0.17	2.25	-0.20
2-phenylphenol	1.55	1.40	0.56	0.49	1.38	7.23	2.54	-0.19	2.51	-0.22
bisphenol A	1.61	1.56	0.99	0.91	1.86	9.60	2.18	-0.46	2.23	-0.41
2-methylaniline	0.97	0.92	0.23	0.45	0.96	4.44	1.22	0.27	1.16	0.21
acetanilide	0.90	1.37	0.48	0.67	1.11	5.57	0.80	0.60	0.82	0.62
carbazole	1.79	1.42	0.47	0.26	1.32	7.98	3.40	-0.09	3.56	0.07
estrone	1.73	2.05	0.50	1.08	2.16	10.78	2.78	0.06	2.85	0.13
naphthalene	1.34	0.92	0.00	0.20	1.09	5.16	2.85	-0.19	2.77	-0.28
1-methylnaphthalene	1.34	0.90	0.00	0.20	1.23	5.79	3.27	-0.05	3.23	-0.09
2-methylnaphthalene	1.30	0.88	0.00	0.20	1.23	5.77	3.25	-0.11	3.22	-0.14
acenaphthylene	1.75	1.14	0.00	0.20	1.22	6.18	3.46	-0.31	3.35	-0.42
acenaphthene	1.60	1.04	0.00	0.20	1.26	6.47	3.51	0.01	3.50	0.00
fluorene	1.59	1.06	0.00	0.25	1.36	6.92	3.60	-0.23	3.63	-0.20
phenanthrene	2.06	1.29	0.00	0.29	1.45	7.63	3.98	-0.22	3.90	-0.30
anthracene	2.29	1.34	0.00	0.28	1.45	7.57	4.12	-0.18	3.94	-0.36
pyrene	2.81	1.71	0.00	0.28	1.58	8.83	4.82	0.25	4.61	0.04
fluoranthene	2.38	1.55	0.00	0.24	1.58	8.83	4.76	0.20	4.74	0.18
chrysene	3.03	1.73	0.00	0.33	1.82	10.33	5.42	-0.01	5.32	-0.11
benz[a]anthracene	2.99	1.70	0.00	0.33	1.82	10.29	5.40	-0.06	5.30	-0.16
benzo[b]fluoranthene	3.19	1.82	0.00	0.40	1.95	11.63	5.62	-0.18	5.67	-0.13
benzo[k]fluoranthene	3.19	1.91	0.00	0.33	1.95	11.61	5.93	-0.04	5.96	-0.01
benzo[a]pyrene	3.63	1.96	0.00	0.37	1.95	11.74	5.95	-0.01	5.84	-0.12
benzo[e]pyrene	3.63	1.99	0.00	0.37	1.95	11.66	5.96	0.29	5.83	0.16
perylene	3.26	1.76	0.00	0.40	1.95	12.05	5.63	-0.41	5.77	-0.27
indeno[123cd]pyrene	3.61	1.93	0.00	0.42	2.08	12.70	6.13	-0.13	6.17	-0.09

dibenz[a,h]anthracene	4.00	2.04	0.00	0.44	2.19	12.96	6.56	0.26	6.40	0.10
benzo[ghi]perylene	4.07	1.90	0.00	0.45	2.08	13.26	6.18	0.09	6.19	0.10
PCB 4	1.60	1.22	0.00	0.20	1.57	6.82	4.29	-0.28	4.25	-0.32
PCB 6	1.63	1.20	0.00	0.18	1.57	7.15	4.58	-0.16	4.54	-0.20
PCB 8	1.62	1.20	0.00	0.18	1.57	7.20	4.58	-0.12	4.56	-0.14
PCB 15	1.64	1.18	0.00	0.16	1.57	7.58	4.87	-0.26	4.87	-0.26
PCB 16/32	1.75	1.35	0.00	0.17	1.69	7.65	4.97	-0.17	4.97	-0.16
PCB 17	1.74	1.35	0.00	0.17	1.69	7.52	4.97	-0.23	4.94	-0.26
PCB 18	1.75	1.35	0.00	0.17	1.69	7.48	4.97	-0.15	4.93	-0.19
PCB 22	1.77	1.33	0.00	0.15	1.69	8.03	5.26	-0.14	5.28	-0.12
PCB 26	1.78	1.33	0.00	0.15	1.69	7.81	5.26	-0.15	5.23	-0.18
PCB 28	1.76	1.33	0.00	0.15	1.69	7.90	5.26	-0.43	5.25	-0.43
PCB 31	1.77	1.33	0.00	0.15	1.69	7.86	5.26	-0.25	5.24	-0.27
PCB 33	1.77	1.33	0.00	0.15	1.69	8.01	5.26	-0.22	5.28	-0.19
PCB 37	1.79	1.31	0.00	0.13	1.69	8.39	5.55	-0.16	5.59	-0.11
PCB 42	1.89	1.48	0.00	0.15	1.81	8.35	5.64	0.00	5.66	0.02
PCB 44	1.90	1.48	0.00	0.15	1.81	8.31	5.64	0.00	5.65	0.01
PCB 45	1.87	1.48	0.00	0.15	1.81	7.97	5.37	0.06	5.36	0.05
PCB 47/48	1.88	1.48	0.00	0.15	1.81	8.23	5.64	0.05	5.63	0.04
PCB 49	1.89	1.48	0.00	0.15	1.81	8.19	5.64	-0.19	5.62	-0.21
PCB 52	1.90	1.48	0.00	0.15	1.81	8.14	5.64	-0.01	5.61	-0.05
PCB 56/60	1.92	1.46	0.00	0.13	1.81	8.84	5.94	-0.25	6.01	-0.18
PCB 64	1.89	1.48	0.00	0.15	1.81	8.35	5.64	-0.16	5.66	-0.14
PCB 66	1.91	1.46	0.00	0.13	1.81	8.72	5.94	-0.14	5.97	-0.10
PCB 70	1.89	1.46	0.00	0.13	1.81	8.69	5.94	-0.05	5.97	-0.01
PCB 74	1.91	1.46	0.00	0.13	1.81	8.58	5.94	-0.19	5.94	-0.19
PCB 82	2.04	1.61	0.00	0.13	1.94	9.22	6.10	0.10	6.18	0.18
PCB 84/101	2.02	1.61	0.00	0.13	1.94	8.80	5.83	-0.06	5.86	-0.04
PCB 85	2.03	1.61	0.00	0.13	1.94	9.09	6.10	0.04	6.14	0.08
PCB 87	2.04	1.61	0.00	0.13	1.94	9.05	6.10	0.05	6.13	0.08
PCB 95	2.02	1.61	0.00	0.13	1.94	8.63	5.83	-0.06	5.82	-0.08
PCB 97	2.04	1.61	0.00	0.13	1.94	9.03	6.10	-0.12	6.13	-0.10
PCB 99	2.03	1.61	0.00	0.13	1.94	8.91	6.10	-0.07	6.09	-0.08

PCB 105	2.04	1.59	0.00	0.11	1.94	9.59	6.40	0.02	6.49	0.12
PCB 110	2.04	1.61	0.00	0.13	1.94	9.16	6.10	-0.10	6.16	-0.04
PCB 118	2.06	1.59	0.00	0.11	1.94	9.40	6.40	0.08	6.44	0.12
PCB 128	2.18	1.74	0.00	0.11	2.06	9.96	6.56	0.21	6.65	0.30
PCB 132	2.16	1.74	0.00	0.11	2.06	9.54	6.29	0.18	6.34	0.22
PCB 135	2.17	1.74	0.00	0.11	2.06	9.29	6.29	0.09	6.27	0.06
PCB 136	2.14	1.74	0.00	0.11	2.06	9.12	6.00	-0.10	6.02	-0.09
PCB 138/163	2.18	1.74	0.00	0.11	2.06	9.77	6.56	0.06	6.60	0.11
PCB 141	2.19	1.74	0.00	0.11	2.06	9.67	6.56	0.14	6.58	0.15
PCB 146	2.19	1.74	0.00	0.11	2.06	9.53	6.56	0.08	6.54	0.06
PCB 149	2.16	1.74	0.00	0.11	2.06	9.35	6.29	0.18	6.29	0.17
PCB 151	2.17	1.74	0.00	0.11	2.06	9.14	6.29	0.05	6.23	-0.01
PCB 153	2.18	1.74	0.00	0.11	2.06	9.59	6.56	-0.07	6.55	-0.08
PCB 156	2.21	1.72	0.00	0.09	2.06	10.27	6.86	0.27	6.96	0.37
PCB 170	2.33	1.87	0.00	0.09	2.18	10.58	7.02	0.48	7.10	0.56
PCB 171	2.30	1.87	0.00	0.09	2.18	10.03	7.02	0.35	6.95	0.29
PCB 174	2.31	1.87	0.00	0.09	2.18	10.16	6.75	0.19	6.78	0.22
PCB 177	2.28	1.87	0.00	0.09	2.18	10.07	6.75	0.08	6.76	0.08
PCB 179	2.32	1.87	0.00	0.09	2.18	9.61	6.46	0.23	6.42	0.20
PCB 180	2.29	1.87	0.00	0.09	2.18	10.42	7.02	0.35	7.06	0.38
PCB 183	2.30	1.87	0.00	0.09	2.18	9.85	6.75	0.17	6.70	0.11
PCB 187	2.31	1.87	0.00	0.09	2.18	9.86	6.75	0.31	6.70	0.26
validation compounds										
α-HCH	1.45	1.20	0.00	0.47	1.58	7.34	3.37	-0.49	3.35	-0.51
β-HCH	1.45	1.18	0.12	0.58	1.58	7.63	2.88	-0.91	2.90	-0.88
γ-HCH	1.45	1.28	0.00	0.50	1.58	7.57	3.28	-0.52	3.30	-0.50
δ-HCH	1.45	0.94	0.00	0.63	1.58	7.63	2.67	-1.11	2.73	-1.04
aldrin	2.07	0.95	0.00	0.42	2.01	8.58	5.04	0.39	4.75	0.10
dieldrin	2.09	2.05	0.03	0.63	2.01	8.49	4.48	0.59	4.03	0.14
4,4-DDT	1.81	1.76	0.00	0.16	2.22	10.02	6.81	1.14	6.75	1.08
4,4-DDE	1.80	1.40	0.06	0.14	2.05	9.73	6.26	0.82	6.31	0.87
endosulfan I	2.23	0.98	0.00	0.87	2.08	8.56	3.53	-0.66	3.08	-1.11

endosulfan II	2.23	0.94	0.00	0.98	2.08	9.28	3.08	-0.60	2.82	-0.86
endrin	2.09	1.60	0.09	0.71	2.01	7.69	4.01	0.29	3.38	-0.34
heptachlor	2.08	0.85	0.00	0.56	1.96	8.05	4.31	-0.57	3.92	-0.96
heptachlor epoxide	2.22	1.20	0.00	0.61	1.96	8.51	4.24	0.33	3.88	-0.03
C2 naphthalenes	1.38	0.91	0.00	0.20	1.37	6.28	3.71	0.12	3.66	0.07
C3 naphthalenes	1.39	0.88	0.00	0.21	1.51	6.67	4.08	0.44	4.01	0.37
C4 naphthalenes	1.34	0.86	0.00	0.21	1.65	6.83	4.48	0.75	4.35	0.61
C1 fluorenes	1.59	1.27	0.00	0.20	1.50	7.32	4.28	0.18	4.27	0.18
C2 fluorenes	1.59	1.27	0.00	0.20	1.64	7.46	4.70	0.19	4.60	0.10
C1 phenanthrenes/anthracenes	2.14	1.26	0.00	0.26	1.60	8.34	4.55	0.07	4.51	0.03
C2 phenanthrenes/anthracenes	2.09	1.30	0.00	0.26	1.74	8.96	4.96	0.06	4.97	0.08
C3 phenanthrenes/anthracenes	2.06	1.30	0.00	0.26	1.88	9.27	5.36	0.06	5.35	0.05
C4 phenanthrenes/anthracenes	2.06	1.30	0.00	0.26	2.02	9.88	5.78	0.37	5.81	0.40
C1 fluoranthenes/pyrenes	2.81	1.60	0.00	0.24	1.73	9.51	5.37	0.47	5.23	0.33

Major source of PP-LFER descriptors are refs *6-12*.

Note: There exist two descriptor sets for PCBs (*13, 14*). In the preliminary fitting, it was found that for PCBs, the solute descriptor values from van Noort et al. (*14*) fit better to the experimental data than the solute descriptor values from Abraham and Al-Hussaini (*13*), regardless of whether eq 2 or 3 is used. Hence, the values from the former reference were used for PCBs. For non-unique PCBs, descriptors of the following congeners were used: PCB 16 for PCB 16/32, PCB 47 for PCB 47/48, PCB 56 for PCB 56/60, PCB 101 for PCB 84/101, PCB 138 for PCB 138/163.

PP-LFER descriptors of alkyl-PAHs (underlined above) were estimated from the available descriptor values of isomers that belong to each compound class and from the values of parent PAHs. This approach may be justified, as the descriptors only weakly depend on the alkyl substitution pattern, although these estimated descriptors may be subject to relatively large estimation error.

Table S3. Log $K_{POM/w}$ values calculated using COSMO*thermX* and SPARC.

	log $K_{POM/w}$(COSMO, combi on)	calibrated log $K_{POM/w}$[a]	calibrated - exp	log $K_{POM/w}$(COSMO, combi off)	calibrated log $K_{POM/w}$[a]	calibrated - exp	log $K_{POM/w}$(SPARC)	calibrated log $K_{POM/w}$[a]	calibrated - exp
calibration compounds									
n-heptane	3.69	3.35	0.31	4.30	2.99	-0.05	4.98	4.08	1.04
n-octane	4.14	3.91	0.39	4.88	3.57	0.05	5.66	4.70	1.18
n-nonane	4.62	4.48	0.39	5.50	4.18	0.08	6.33	5.31	1.21
2,2,4-trimethylpentane	3.63	3.28	0.59	4.37	3.06	0.37	5.66	4.70	2.01
cycloheptane	2.94	2.44	0.26	3.43	2.14	-0.04	4.43	3.58	1.41
cyclooctane	3.23	2.79	0.26	3.83	2.53	0.00	5.03	4.13	1.60
1-nonene	4.37	4.18	0.52	5.22	3.90	0.24	6.18	5.17	1.52
1-heptyne	3.23	2.79	0.36	3.77	2.48	0.05	4.51	3.66	1.23
trichloromethane	2.24	1.59	-0.11	2.46	1.18	-0.51	1.71	1.11	-0.58
trichloroethene	2.58	2.00	-0.11	2.88	1.60	-0.51	2.79	2.10	-0.01
tetrachloroethene	2.93	2.43	-0.15	3.37	2.08	-0.50	3.72	2.94	0.36
di-n-butyl ether	2.99	2.49	0.81	3.80	2.50	0.82	3.49	2.73	1.05
di-n-pentyl ether	3.97	3.69	1.15	5.05	3.74	1.20	4.66	3.79	1.25
2-octanone	2.17	1.49	-0.11	2.94	1.66	0.06	2.49	1.82	0.22
2-nonanone	2.63	2.05	0.03	3.54	2.24	0.22	3.10	2.38	0.35
2-decanone	3.10	2.63	0.06	4.15	2.85	0.28	3.67	2.89	0.33
methyl phenyl sulfoxide	-0.32	-1.54	-1.32	0.30	-0.94	-0.71	-0.76	-1.13	-0.90
tri-n-butyl phosphate[b]	4.50[b]	4.34	2.47	6.27[b]	4.94	3.07	7.75[b]	6.60	4.73
1-heptanol	1.74	0.97	-0.07	2.42	1.14	0.11	2.24	1.60	0.56
3-ethyl-3-hexanol	2.20	1.53	0.73	3.00	1.71	0.91	1.76	1.16	0.36
2-butoxyethanol	0.93	-0.02	0.36	1.54	0.28	0.65	0.70	0.20	0.57
1,4-dibromobenzene	3.80	3.49	0.32	4.40	3.10	-0.07	3.56	2.79	-0.38
ethyl benzoate	2.64	2.08	0.09	3.38	2.09	0.11	2.88	2.18	0.19
valerophenone	3.09	2.62	0.13	4.03	2.73	0.23	3.28	2.54	0.05
benzophenone	3.04	2.56	-0.17	4.02	2.72	-0.01	3.52	2.76	0.03
di-n-propyl phthalate	4.14	3.91	1.19	5.67	4.35	1.63	3.94	3.14	0.42
2-nitrotoluene	2.74	2.20	0.08	3.31	2.02	-0.10	2.44	1.78	-0.34
2,4-dinitrotoluene	3.31	2.89	0.37	4.08	2.78	0.26	2.07	1.44	-1.08

2,4,6-trinitrotoluene	4.35	4.16	1.22	5.32	4.00	1.05	2.26	1.61	-1.33
4-nitroanisole	2.68	2.12	0.05	3.31	2.02	-0.04	2.11	1.48	-0.59
2,5-dimethylpyrazine	0.62	-0.40	-0.06	1.07	-0.19	0.15	0.66	0.16	0.51
caffeine	-0.10	-1.27	-1.12	0.82	-0.43	-0.28	-0.06	-0.49	-0.34
diazepam	2.90	2.39	0.56	4.43	3.13	1.30	2.22	1.58	-0.25
4-chlorobenzyl alcohol	1.87	1.13	0.04	2.46	1.18	0.09	1.34	0.78	-0.31
phenol	1.67	0.88	0.11	1.98	0.71	-0.07	2.10	1.47	0.69
4-iodophenol	2.35	1.71	-0.56	2.90	1.62	-0.65	2.92	2.21	-0.06
1-naphthol	2.96	2.46	0.01	3.62	2.32	-0.13	3.20	2.47	0.02
2-phenylphenol	3.61	3.25	0.51	4.49	3.18	0.44	3.94	3.14	0.40
bisphenol A	3.52	3.15	0.51	4.87	3.55	0.92	5.40	4.47	1.83
2-methylaniline	2.12	1.44	0.49	2.59	1.31	0.36	1.85	1.24	0.29
acetanilide	1.35	0.49	0.29	1.97	0.70	0.51	0.90	0.38	0.18
carbazole	3.78	3.46	-0.02	4.62	3.31	-0.18	3.76	2.98	-0.51
estrone	2.95	2.45	-0.27	4.57	3.27	0.54	4.60	3.74	1.02
naphthalene	3.20	2.75	-0.29	3.79	2.50	-0.55	3.57	2.80	-0.24
1-methylnaphthalene	3.55	3.19	-0.14	4.28	2.98	-0.35	4.04	3.23	-0.09
2-methylnaphthalene	3.63	3.28	-0.08	4.36	3.06	-0.30	4.05	3.24	-0.12
acenaphthylene	3.59	3.23	-0.55	4.41	3.11	-0.67	4.11	3.29	-0.48
acenaphthene	3.64	3.29	-0.21	4.33	3.03	-0.47	3.83	3.04	-0.46
fluorene	3.96	3.68	-0.15	4.83	3.52	-0.31	4.52	3.67	-0.16
phenanthrene	4.19	3.96	-0.24	5.12	3.81	-0.39	4.83	3.95	-0.25
anthracene	4.26	4.04	-0.26	5.21	3.89	-0.41	4.77	3.89	-0.41
pyrene	4.48	4.32	-0.25	5.54	4.22	-0.35	5.57	4.62	0.05
fluoranthene	4.62	4.49	-0.07	5.71	4.39	-0.17	5.72	4.76	0.20
chrysene	5.16	5.15	-0.28	6.44	5.11	-0.32	5.95	4.96	-0.47
benz[a]anthracene	5.23	5.24	-0.22	6.53	5.19	-0.27	5.89	4.91	-0.55
benzo[b]fluoranthene	5.63	5.72	-0.08	7.08	5.73	-0.07	6.98	5.90	0.10
benzo[k]fluoranthene	5.68	5.78	-0.19	7.12	5.77	-0.20	6.88	5.81	-0.16
benzo[a]pyrene	5.49	5.55	-0.41	6.90	5.56	-0.40	6.83	5.76	-0.19
benzo[e]pyrene	5.44	5.49	-0.18	6.83	5.49	-0.18	6.89	5.82	0.15
perylene	5.42	5.46	-0.58	6.81	5.47	-0.57	6.89	5.82	-0.22
indeno[123cd]pyrene	5.90	6.06	-0.20	7.46	6.12	-0.14	7.73	6.58	0.32

dibenz[a,h]anthracene	6.21	6.43	0.13	7.85	6.49	0.19	7.47	6.34	0.04
benzo[ghi]perylene	5.73	5.85	-0.24	7.25	5.91	-0.18	7.52	6.39	0.30
PCB 4	4.52	4.36	-0.21	5.62	4.30	-0.27	5.44	4.50	-0.07
PCB 6	4.76	4.66	-0.08	5.87	4.54	-0.20	5.37	4.44	-0.30
PCB 8	4.75	4.65	-0.05	5.85	4.53	-0.17	5.37	4.44	-0.26
PCB 15	4.87	4.79	-0.33	5.98	4.65	-0.48	5.32	4.39	-0.73
PCB 16/32	4.95	4.89	-0.25	6.19	4.86	-0.28	5.92	4.94	-0.20
PCB 17	5.05	5.02	-0.18	6.31	4.98	-0.22	5.92	4.94	-0.26
PCB 18	5.24	5.25	0.13	6.45	5.11	0.00	5.87	4.89	-0.23
PCB 22	5.16	5.15	-0.25	6.40	5.07	-0.33	5.86	4.88	-0.52
PCB 26	5.26	5.27	-0.14	6.51	5.18	-0.23	5.80	4.83	-0.58
PCB 28	5.26	5.27	-0.42	6.51	5.17	-0.51	5.85	4.87	-0.81
PCB 31	5.26	5.27	-0.24	6.51	5.18	-0.33	5.80	4.83	-0.68
PCB 33	5.17	5.16	-0.32	6.40	5.07	-0.41	5.84	4.86	-0.61
PCB 37	5.31	5.33	-0.37	6.56	5.22	-0.48	5.79	4.82	-0.89
PCB 42	5.45	5.50	-0.15	6.83	5.49	-0.15	6.40	5.37	-0.27
PCB 44	5.44	5.49	-0.16	6.83	5.49	-0.16	6.35	5.33	-0.32
PCB 45	5.21	5.20	-0.11	6.59	5.25	-0.06	6.42	5.39	0.08
PCB 47/48	5.56	5.63	0.04	6.96	5.62	0.03	6.41	5.38	-0.21
PCB 49	5.54	5.61	-0.22	6.93	5.59	-0.24	6.36	5.34	-0.50
PCB 52	5.53	5.60	-0.05	6.92	5.58	-0.07	6.30	5.28	-0.37
PCB 56/60	5.57	5.65	-0.54	6.94	5.60	-0.59	6.33	5.31	-0.88
PCB 64	5.44	5.49	-0.32	6.83	5.49	-0.32	6.37	5.35	-0.46
PCB 66	5.67	5.77	-0.31	7.06	5.71	-0.37	6.31	5.29	-0.79
PCB 70	5.68	5.78	-0.20	7.06	5.72	-0.26	6.27	5.26	-0.73
PCB 74	5.65	5.74	-0.38	7.03	5.69	-0.44	6.35	5.33	-0.80
PCB 82	5.76	5.88	-0.12	7.27	5.93	-0.07	6.94	5.86	-0.14
PCB 84/101	5.95	6.11	0.21	7.47	6.12	0.22	6.85	5.78	-0.12
PCB 85	5.86	6.00	-0.07	7.38	6.03	-0.03	6.95	5.87	-0.19
PCB 87	5.85	6.00	-0.06	7.38	6.03	-0.02	6.89	5.82	-0.24
PCB 95	5.74	5.85	-0.04	7.27	5.92	0.03	6.85	5.78	-0.11
PCB 97	5.85	5.99	-0.24	7.37	6.03	-0.20	6.90	5.83	-0.40
PCB 99	5.94	6.10	-0.07	7.48	6.13	-0.05	6.91	5.84	-0.33

PCB 105	5.98	6.15	-0.23	7.49	6.14	-0.24	6.85	5.78	-0.59
PCB 110	5.86	6.00	-0.20	7.38	6.04	-0.16	6.84	5.77	-0.43
PCB 118	6.08	6.27	-0.04	7.60	6.25	-0.07	6.81	5.75	-0.57
PCB 128	6.15	6.35	0.00	7.79	6.44	0.09	7.48	6.35	0.00
PCB 132	6.04	6.22	0.11	7.69	6.34	0.22	7.44	6.32	0.20
PCB 135	6.14	6.35	0.14	7.81	6.45	0.24	7.43	6.31	0.10
PCB 136	5.89	6.04	-0.07	7.55	6.20	0.09	7.41	6.29	0.18
PCB 138/163	6.25	6.48	-0.02	7.90	6.54	0.05	7.44	6.32	-0.18
PCB 141	6.25	6.48	0.06	7.91	6.55	0.13	7.46	6.34	-0.09
PCB 146	6.34	6.59	0.11	8.01	6.65	0.17	7.41	6.29	-0.19
PCB 149	6.15	6.36	0.24	7.82	6.46	0.35	7.41	6.29	0.18
PCB 151	6.12	6.32	0.07	7.78	6.43	0.18	7.41	6.29	0.05
PCB 153	6.39	6.65	0.01	8.06	6.70	0.06	7.40	6.28	-0.35
PCB 156	6.35	6.60	0.02	7.98	6.63	0.04	7.42	6.30	-0.29
PCB 170	6.53	6.82	0.29	8.31	6.95	0.41	8.04	6.86	0.33
PCB 171	6.44	6.71	0.04	8.23	6.87	0.20	8.05	6.87	0.20
PCB 174	6.43	6.70	0.14	8.22	6.86	0.30	8.01	6.84	0.27
PCB 177	6.42	6.69	0.01	8.21	6.85	0.17	8.00	6.83	0.15
PCB 179	6.28	6.52	0.29	8.07	6.71	0.48	7.97	6.80	0.57
PCB 180	6.65	6.97	0.29	8.44	7.07	0.40	8.01	6.84	0.16
PCB 183	6.53	6.81	0.23	8.33	6.97	0.38	8.02	6.84	0.26
PCB 187	6.52	6.81	0.37	8.32	6.96	0.52	7.97	6.80	0.36
validation compounds									
α-HCH	4.40	4.22	0.36	5.57	4.24	0.38	4.00	3.19	-0.67
β-HCH	4.54	4.39	0.61	5.73	4.40	0.62	4.00	3.19	-0.59
γ-HCH	4.34	4.15	0.35	5.51	4.19	0.39	4.00	3.19	-0.61
δ-HCH	4.46	4.29	0.51	5.63	4.31	0.53	4.00	3.19	-0.58
aldrin	5.14	5.12	0.47	6.75	5.41	0.76	6.94	5.86	1.21
dieldrin	4.74	4.64	0.74	6.41	5.07	1.18	6.59	5.55	1.65
4,4-DDT	6.00	6.17	0.50	7.88	6.52	0.86	7.26	6.15	0.49
4,4-DDE	6.05	6.24	0.80	7.66	6.31	0.87	7.13	6.04	0.60
endosulfan I	4.91	4.84	0.66	6.63	5.29	1.11	5.15	4.24	0.05

endosulfan II	4.91	4.84	1.16	6.61	5.27	1.60	5.15	4.24	0.56
endrin	4.75	4.65	0.93	6.44	5.10	1.38	6.59	5.55	1.82
heptachlor	5.01	4.97	0.09	6.59	5.25	0.38	6.52	5.48	0.61
heptachlor epoxide	4.97	4.91	1.00	6.63	5.29	1.38	6.15	5.15	1.23
C2 naphthalenes	3.97	3.69	0.11	4.83	3.52	-0.07	4.49	3.64	0.05
C3 naphthalenes	4.41	4.23	0.59	5.41	4.09	0.45	5.07	4.17	0.53
C4 naphthalenes	4.80	4.71	0.98	5.93	4.61	0.88	5.58	4.63	0.90
C1 fluorenes	4.31	4.11	0.01	5.31	4.00	-0.10	5.03	4.13	0.04
C2 fluorenes	4.67	4.54	0.04	5.81	4.48	-0.02	5.55	4.60	0.10
C1 phenanthrenes/anthracenes	4.59	4.45	-0.03	5.66	4.34	-0.14	5.25	4.33	-0.15
C2 phenanthrenes/anthracenes	4.95	4.89	-0.01	6.15	4.82	-0.08	5.69	4.73	-0.17
C3 phenanthrenes/anthracenes	5.38	5.42	0.11	6.73	5.39	0.08	6.18	5.17	-0.14
C4 phenanthrenes/anthracenes	5.73	5.84	0.43	7.20	5.86	0.45	6.71	5.65	0.24
C1 fluoranthenes/pyrenes	4.99	4.94	0.04	6.21	4.88	-0.02	6.08	5.08	0.18

[a] "Calibrated" values are those calculated from linear regression equations given in Table 3.

[b] Tri-n-butyl phosphate was not used for calibration.

For non-unique PCBs, descriptors of the following congeners were used: PCB 16 for PCB 16/32, PCB 47 for PCB 47/48, PCB 56 for PCB 56/60, PCB 101 for PCB 84/101, PCB 138 for PCB 138/163.

Values for alkyl PAHs were calculated as the log-mean of the following isomeric compounds: C2 naphthalenes (1,2-dimethylnaphthalene, 2,6-dimethylnaphthalene), C3 naphthalenes (1,2,6-trimethylnaphthalene, 1-ethyl-6-methylnaphthalene, 2-propylnaphthalene), C4 naphthalenes (2-butyl naphthalene, 2-ethyl-6,8-dimethlynaphthalene, 1,2,6,8-tetramethylnaphthalene), C1 fluorenes (9-methylfluorene, 1-methylfluorene), C2 fluorenes (1,9-dimethylfluorene, 2-ethylfluorene, 9-ethylfluorene), C1 phenanthrenes/anthracenes (3-methylphenanthrene, 4-methylphenanthrene, 2-methylanthracene), C2 phenanthrenes/anthracenes (9-ethylphenanthrene, 1,7-dimethylanthracene, 1,5-dimethylphenanthrene), C3 phenanthrenes/anthracenes (1-propylanthracene, 1,7,10-trimethylanthracene, 2-ethyl-10-methylphenanthrene), C4 phenanthrenes/anthracenes (1-butly anthracene, 1,7,8,10-anthracene, 2,10-diethylphenanthrene), C1 fluoranthenes/pyrenes (2-methylfluoranthene, 2-methylpyrene, 4-methylpyrene), C1 chrysenes (3-methylchrysene, 5-methylchrysene).

Table 4. The total recovery of analytes from the batch experiment.

	Recovery	SD
n-heptane	83%	26%
n-octane	82%	20%
n-nonane	87%	4%
2,2,4-trimethylpentane	76%	24%
cycloheptane	77%	2%
cyclooctane	87%	3%
1-nonene	84%	3%
1-heptyne	68%	7%
trichloromethane	87%	17%
trichloroethene	65%	7%
tetrachloroethene	69%	18%
di-n-butyl ether	107%	13%
di-n-pentyl ether	97%	6%
2-octanone	96%	6%
2-nonanone	97%	6%
2-decanone	104%	2%
methyl phenyl sulfoxide	101%	2%
tri-n-butyl phosphate	99%	2%
1-heptanol	102%	1%
3-ethyl-3-hexanol	104%	1%
2-butoxyethanol	100%	1%
1,4-dibromobenzene	81%	5%
ethyl benzoate	94%	3%
valerophenone	95%	3%
benzophenone	96%	3%
di-n-propyl phthalate	76%	4%
2-nitrotoluene	96%	3%
2,4-dinitrotoluene	98%	3%
2,4,6-trinitrotoluene	98%	3%
4-nitroanisole	83%	6%
2,5-dimethylpyrazine	100%	1%
caffeine	103%	4%
diazepam	95%	2%
4-chlorobenzyl alcohol	98%	2%
phenol	99%	0%
4-iodophenol	92%	1%
1-naphthol	86%	2%
2-phenylphenol	103%	3%
bisphenol A	92%	2%
2-methylaniline	99%	1%
acetanilide	98%	2%
carbazole	105%	1%
estrone	99%	2%
α-HCH	111%	34%
β-HCH	109%	34%
γ-HCH	103%	25%
δ-HCH	116%	40%
aldrin	106%	27%
dieldrin	108%	15%
4,4-DDT	119%	24%

4,4-DDE	108%	22%
endosulfan I	123%	29%
endosulfan II	114%	26%
endrin	124%	36%
heptachlor	69%	17%
heptachlor epoxide	122%	26%

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