Supporting information for "Experimental determination of poly-parameter linear free energy relationship (pp-LFER) substance descriptors for pesticides and other contaminants: New measurements and recommendations"

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SI-1. Experimental Methods

a) GC retention time measurements

Solutions of the target compounds were prepared in dichloromethane (up to 5 compounds in one mixture, each ≈ 50 mg/l). The injection mode was either split (split ratio, 1:5) or splitless. The injector temperature was isothermal at 210°C or 250°C, and the injected volume was 1 µl. The flow rate of the helium carrier gas was set to 1.5 ml/min and the oven temperature was isothermal at 160°C, 180°C or 250°C. The mass spectra were usually recorded using the scan mode (m/z 50-1050). The net retention time was obtained by subtracting the retention time of the target chemical with the retention time of a non-retained tracer (N_2).

b) organic liquid/liquid partitioning

Concentration measurements necessary for partition coefficient determination were carried out using a GC/MS equipped with the column HP-5MS UI (Agilent). All used solvent pairs were mutually saturated before use and 800 µl of each solvent and 10 µl analyte mixture (≈ 50 mg/l each, solvent: dichloromethane) were filled in a 2 ml screw vial (four replicates for each mixture). In addition, two vials filled with only one solvent (1600 µl) and the analyte mixture (10 µl) were prepared and served as an external standard. All vials were horizontally shaken for 15 min and allowed to stand for 1 h at room temperature. An aliquot of 400 µl was taken from each phase and 5 µl of an internal standard solution (hexachlorobenzene) were added. Prior to GC injection, the aliquots from propylene carbonate and ethylene glycol were extracted with cyclohexane because the former two solvents have relatively low volatility. From each aliquot, 10 µl were injected into the GC. Immediately after the injection, the injector was heated from 50°C to 250°C (rate: 12°C/min), with the purge valve open for a short time to reduce solvent loading on the column. The oven temperature was increased from 50°C to 300°C (rate: 20°C/min) using a flow rate of 1.3 ml/min (helium carrier gas). The mass spectrometer was operated in the SIM mode.

c) PDMS/water partitioning

$K_{PDMS/water}$ values were determined with two different methods depending on the expected log $K_{PDMS/water}$ value. The depletion method was used for log $K_{PDMS/water} < 4$ and the passive-dosing method for log $K_{PDMS/water}$ between 4 and 6. Independent from the method, the pH value of the water phase was adjusted according to the pK_a value of the substance to assure the measurement of the neutral species. Prior to GC injection, an internal standard (hexachlorobenzene, 5 µl) was added to each extract. Calibration curves were established by measuring 4 to 5 external standards at different concentrations. The GC method was identical to the one used for organic liquid/liquid partitioning as mentioned above.

Depletion method

PDMS coated glass fibers (Polymicro Technologies Inc., Phoenix, USA) cleaned in methanol were used for this method (length: 4 cm, coating thickness of PDMS: 30 µm). For each analyte mixture (≈ 50 mg/l each, solvent: dichloromethane), six screw vials were prepared; 10 µl analyte mixture was added to each vial and evaporated under a nitrogen stream. Afterwards, one PDMS fiber for each vial and 6 different volumes of water (200 µl, 400 µl, 800 µl, 1600 µl, 3200 µl and 4000 µl) were added to the vials. All vials were shaken horizontally for 2 days at room temperature (equilibration times were determined by Endo et al.[1]). After equilibration, the fibers were collected with solvent-rinsed tweezers, dried with clean tissue and extracted in 200 µl cyclohexane. The log $K_{PDMS/water}$ were determined from the measured concentrations in PDMS based on the following equation:

$$c_{PDMS} = \frac{m_{tot}}{V_{PDMS} + \frac{V_w}{K_{PDMS/water}}} \quad \text{(S1)}$$

c_{PDMS} is the analyte concentration in PDMS, m_{tot} is the total analyte mass in the system PDMS/water (the initial analyte mass), V_{PDMS} and V_W are the volumes of PDMS and water, respectively, and $K_{PDMS/water}$ is the PDMS/water partition coefficient. $K_{PDMS/water}$ was determined using the nonlinear fit function in OriginPro (version 8G, OriginLab Corporation, Northampton, USA).

Passive-dosing method using preloaded PDMS

This method was carried out with PDMS disks (Specialty Silicone Products Inc., Ballston Spa, USA, diameter: 10 mm, thickness: 0.5 mm) cleaned in isohexane and methanol. The loading of chemicals on PDMS disks was done as follows: 150 µl analyte mixture (up to 10 compounds in dichloromethane) were put into a 20 ml screw vial, evaporated and redissolved in 2 ml 50% water/methanol (v/v). PDMS disks were added, the vial was shaken one night at room temperature, 2 ml of pure water were added and the vial was shaken another night. Loaded disks were transferred into 20 ml glass vials (crimp sealing, aluminum-lined septa, one disk per vial) filled with 20 ml of pure water and a glass-coated stirring bar. The 4 replicate samples for each mixture were stirred (550 rpm) for 2 days (predetermined equilibration time). After equilibration, PDMS disks were extracted in 500 µl cyclohexane. The water was extracted in 2 ml cyclohexane and extracts were evaporated and redissolved in 200 µl cyclohexane. To determine the total analyte concentration loaded on the disks, three additional PDMS disks were prepared for each mixture and extracted in 500 µl cyclohexane directly after loading.

SI-2. Influence of the PDMS/water System on the *B* Descriptor

To investigate the influence of the PDMS/water system on the *B* descriptor (and also its influence on the remaining descriptors) and to underline its necessity for system descriptor determination, we tried to calculate the pp-LFER substance descriptors without the PDMS/water system. This results in overall very large differences for *B*. The rmse between the original and the recalculated *B* is 0.75 and the largest difference is 2.79. Consequently, the prediction accuracy for the water-containing validation systems becomes much worse (rmse for prediction of log K_{ow}: 2.35, log K_{wa}: 3.69, log K_{oc}: 2.57). The influence of the PDMS/water system on the remaining descriptors *S*, *A* and *L* is related to the magnitude of the corresponding system parameter. For instance, *a* is -2.85 for PDMS/water, and thus the influence on *A* is comparably high as well. The rmse between original and recalculated (without PDMS/water) *A* is 0.29 (for those substances whose *A* is not set to 0). The influence on *S* is moderate (rmse 0.17; *s* is -1.55) and there is only a minor influence of the PDMS/water system on *L* (rmse 0.10; *l* is 0.37). All in all, these calculations shows that the PDMS/water partition coefficient is a required system in our calibration data set, and accurate descriptors could not be obtained without this system.

SI-3. Extended Method Comparison

Applicability

The applicability of the different methods for the desired target compounds is a crucial point for the final method decision. The known restrictions for GC and HPLC analyses apply as well for descriptor determination, i.e., GC measurements are not possible for very big and/or polar compounds or for thermally unstable compounds. We were still able to measure compounds such as the brominated diphenylether 183 (BDE 183) and estriol, but BDE 209 and tetrabromopbisphenol A diallyl ether were not measurable. Too strong retentions are particularly a big problem with polar stationary phases because of their relatively low maximal operating temperatures and unstable results at high temperatures, as explained in the manuscript.

HPLC is better suited for polar and/or big compounds and less suited for nonpolar compounds. A limiting factor for HPLC is the detection method. Most common for HPLC is an ultraviolet (UV) detector being only applicable to UV-active compounds whereas the most common GC detector for retention time measurements (the flame ionization detector, FID) is applicable to practically all organic compounds.

Partitioning experiments are possible for polar as well as nonpolar compounds. The limiting point for these measurements is the log *K* dimension in the chosen system. Measurements are usually easy and accurate for log *K* values between -3 and +3. Outside this range, measurements can be difficult due to a very low concentration in one of the two phases, which requires sensitive analysis as well as careful experimental work. In most cases, the log *K* in completely organic systems are within the range of -3 to +3 (e.g., our log *K* range was -2.97 to 1.15 for heptane/propylene carbonate and -2.29 to 0.73 for ethylene glycol/dichloroethane). However, the log *K* in aqueous systems might span over a larger range. For example, the log $K_{PDMS/water}$ measured by us were between -0.79 and 6.13. Theoretically, any solvent-water or sorbent-water partition coefficient can serve as a calibration system that is sensitive to *B*. We decided on PDMS/water because our compound set contained moderately to highly hydrophobic compounds, and the system PDMS/water offers the possibility of an easy phase separation which is advantageous in determining high log $K_{PDMS/water}$. Moreover, the measurement of relatively hydrophilic compounds in our compound set such as bromophenols was still possible with this system. Alternative polymers for rather hydrophilic compounds would be polyacrylate (PA) or polyoxymethylene (POM), for which calibrated pp-LFER equations are available.[1, 2]

Table S1. Measured logarithmic net retention times on columns SPB Octyl and DB-200 at different temperatures.

		SPB Octyl		DB-200		
CAS	compound	180°C	250°C	160°C	180°C	250°C
3424-82-6	2,4'-DDE	-	0.38	-	-	-0.14
72-55-9	4,4'-DDE	-	0.48	-	-	-0.06
50-29-3	4,4'-DDT	-	0.70	-	-	0.16
15972-60-8	alachlor	0.96	-	-	0.82	-
309-00-2	aldrin	1.19	-	-	0.61	-
71626-11-4	benalaxyl	-	0.54	-	-	0.28
82657-04-3	bifenthrin	-	0.69	-	1.45	0.25
4824-78-6	bromophos-ethyl	1.38	-	-	0.96	-0.06
2104-96-3	bromophos-methyl	1.23	-	-	0.84	-0.11
786-19-6	carbophenothion	-	0.61	-	-	0.19
5103-71-9	cis-chlordane	1.44	-	1.25	-	-
470-90-6	chlorfenvinfos 1[a]	1.18	-	-	1.05	-
470-90-6	chlorfenvinfos 2[a]	1.21	-	-	1.10	-
1897-45-6	chlorothalonil	0.89	-	-	0.87	-
2921-88-2	chlorpyrifos-ethyl	1.14	-	-	0.78	-
5598-13-0	chlorpyrifos-methyl	0.96	-	-	0.66	-
1861-32-1	chlorthal-dimethyl	1.11	-	-	0.95	-
60238-56-4	chlorthiophos 1[a]	-	0.49	-	-	0.13
60238-56-4	chlorthiophos 2[a]	-	0.51	-	-	0.16
56-72-4	coumaphos	-	1.00	-	-	0.96
1194-65-6	dichlobenil	0.01	-	-	0.01	-
97-17-6	dichlofenthion	0.94	-	-	0.63	-
1085-98-9	dichlofluanid	1.02	-	-	1.00	-
62-73-7	dichlorvos	-0.35	-	-	-0.20	-
60-57-1	dieldrin	1.49	-	-	1.06	-
87674-68-8	dimethenamid	0.91	-	-	0.81	-
298-04-4	disulfoton	0.80	-	-	0.52	-
115-29-7	endosulfan	1.43	-	-	0.98	-
1031-07-8	endosulfan-sulfate	-	0.62	-	-	0.48
72-20-8	endrin	1.58	-	-	1.13	-
66230-04-4	esfenvalerate	-	1.33	-	-	0.96
563-12-2	ethion	-	0.45	-	-	0.19
299-84-3	fenchlorphos	1.03	-	-	0.70	-
122-14-5	fenitrothion	0.99	-	-	1.01	-
39515-41-8	fenpropathrin	-	0.73	-	-	0.45
55-38-9	fenthion	1.10	-	-	0.82	-
62924-70-3	flumetralin	-	0.27	-	-	0.19
85509-19-9	flusilazole	1.43	-	-	1.37	-
944-22-9	fonofos	0.80	-	-	0.50	-
1024-57-3	heptachlor epoxide	1.30	-	1.15	-	-
23560-59-0	heptenophos	0.29	-	0.64	-	-
118-74-1	hexachlorobenzene	0.86	-	-	0.22	-
121-75-5	malathion	0.96	-	-	0.97	-
67129-08-2	metazachlor	-	0.22	-	-	0.04

		SPB Octyl		DB-200		
CAS	compound	180°C	250°C	160°C	180°C	250°C
51218-45-2	metolachlor	1.09	-	1.31	-	-
15299-99-7	napropamide	1.41	-	-	1.23	-
1836-75-5	nitrofen	1.57	-	-	1.32	-
26530-20-1	octhilinone	0.86	-	-	0.74	-
34622-58-7	orbencarb	1.09	-	-	0.67	-
56-38-2	parathion-ethyl	1.08	-	-	1.09	-
1825-21-4	pentachloroanisole	0.82	-	-	0.30	-
52645-53-1	permethrin 1[a]	-	1.02	-	-	0.47
52645-53-1	permethrin 2[a]	-	1.05	-	-	0.52
298-02-2	phorate	0.61	-	-	0.33	-
2310-17-0	phosalone	-	0.82	-	-	0.63
32809-16-8	procymidone	1.30	-	-	1.30	-
2312-35-8	propargite	-	0.63	-	-	0.24
13457-18-6	pyrazophos	-	0.86	-	-	0.65
3689-24-5	sulfotep	0.47	-	-	0.40	-
117-18-0	tecnazene	0.55	-	-	0.26	-
13071-79-9	terbufos	0.75	-	-	0.47	-
640-15-3	thiometon	0.64	-	-	0.40	-
731-27-1	tolylfluanid	1.20	-	-	1.15	-
50471-44-8	vinclozolin	0.97	-	-	0.93	-
2051-60-7	PCB 1	0.37	-	-	-0.11	-
2051-61-8	PCB 2	0.53	-	-	0.05	-
2051-62-9	PCB 3	0.54	-	-	0.06	-
13029-08-8	PCB 4	0.56	-	0.36	-	-
2050-68-2	PCB 15	0.91	-	-	0.41	-
7012-37-5	PCB 28	1.07	-	0.81	-	-
15862-07-4	PCB 29	1.03	-	-	0.41	-
35693-99-3	PCB 52	1.16	-	0.91	-	-
37680-73-2	PCB 101	1.49	-	1.19	-	-
35065-27-1	PCB 153	-	0.68	-	-	0.10
486-25-9	9-fluorenone	0.80	-	-	0.55	-
119-65-3	isoquinoline	-0.06	-	-	-0.27	-
91-22-5	quinoline	-0.10	-	-0.12	-	-
92-83-1	xanthene	0.68	-	-	0.22	-
86-57-7	1-nitronaphthalene	0.53	-	-	0.40	-
121-14-2	2,4-dinitrotoluene	0.30	-	-	0.48	-
91-23-6	2-nitroanisole	-0.08	-	-	0.06	-
555-03-3	3-nitroanisole	-0.06	-	0.20	-	-
100-17-4	4-nitroanisole	0.07	-	-	0.12	-
602-60-8	9-nitroanthracene	1.44	-	-	1.20	-
81-15-2	musk xylene	0.91	-	-	0.81	-0.15
57-83-0	progesterone	-	1.22	-	-	1.15
53-19-0	2,4'-DDD	-	0.49	-	-	0.01
834-12-8	ametryn	1.02	-	-	0.67	-0.27
1912-24-9	atrazine	0.71	-	-	0.47	-0.43
314-40-9	bromacil	0.96	-	-	1.03	-

		SPB Octyl		DB-200		
CAS	compound	180°C	250°C	160°C	180°C	250°C
18181-80-1	bromopropylate	-	0.79	-	-	0.35
63-25-2	carbaryl	0.95	-	-	0.93	-
1563-66-2	carbofuran	0.58	-	-	0.54	-
510-15-6	chlorobenzilate	-	0.50	-	-	0.12
101-21-3	chlorpropham	0.51	-	-	0.32	-
99-30-9	dicloran	0.71	-	-	0.60	-
122-39-4	diphenylamine	0.55	-	-	0.14	-
319-84-6	α-HCH	0.75	-	-	0.34	-
319-85-7	β-HCH	0.84	-	-	0.52	-
58-89-9	γ-HCH (lindane)	0.86	-	-	0.46	-
319-86-8	δ-HCH	0.88	-	-	0.57	-
21087-64-9	metribuzin	0.91	-	-	0.61	-
40487-42-1	pendimethalin	1.23	-	-	1.07	-
527-20-8	pentachloroaniline	1.02	-	-	0.52	-
7287-19-6	prometryn	1.04	-	-	0.67	-
122-42-9	propham	0.15	-	-	-0.01	-
23950-58-5	propyzamide	0.81	-	-	0.56	-
886-50-0	terbutryn	1.07	-	-	0.71	-
86-74-8	carbazole	0.92	-	-	0.65	-
120-72-9	indole	-0.13	-	-	-0.26	-
3380-34-5	triclosan	1.40	-	-	0.90	-

[a]isomers in the order of peak appearance in the GC

Table S2. Measured logarithmic partition coefficients and standard deviations (sd) of the target compounds for the systems heptane/propylene carbonate (PC), ethylene glycol (EG)/1,2-dichloroethane (DCE) and PDMS/water.

compound	log $K_{hep/PC}$	sd	log $K_{EG/DCE}$	sd	log $K_{PDMS/w}$	sd
2,4'-DDE	-0.11	0.01	-1.10	0.23	5.82[b]	-
4,4'-DDE	0.03	0.01	-1.90	0.18	6.17[b]	-
4,4'-DDT	-0.77	0.03	-0.54	0.17	5.79[b]	-
alachlor	-1.33	0.11	-0.22	0.09	2.03	0.05[c]
aldrin	0.50	0.01	-0.53	0.06	5.88[b]	-
benalaxyl	-1.50	0.08	-	-	2.88	0.12
bifenthrin	-0.03	0.02	-2.29	0.12	5.97[b]	-
bromophos-ethyl	-0.07	0.01	-2.39	0.26	4.58	0.04
bromophos-methyl	-0.71	0.01	-1.31	0.15	4.31	0.07
carbophenothion	-0.83	0.02	-1.15	0.06	3.85	0.06
cis-chlordane	-0.42	0.02	-	-	5.52[b]	-
chlorfenvinfos 1[a]	-0.96	0.08	-1.78	0.10	3.05	0.05[c]
chlorfenvinfos 2[a]	-1.27	0.11	-1.81	0.06	2.83	0.06[c]
chlorothalonil	-2.10	0.04	-1.20	0.07	2.52	0.09[c]
chlorpyrifos-ethyl	-0.42	0.01	-0.96	0.09	4.36	0.15
chlorpyrifos-methyl	-0.84	0.02	-1.53	0.20	3.65	0.04[c]
chlorthal-dimethyl	-0.70	0.01	-1.39	0.16	3.38	0.04[c]
chlorthiophos 1[a]	-1.40	0.09	-1.70	0.10	4.13	0.10

compound	log $K_{hep/PC}$	sd	log $K_{EG/DCE}$	sd	log $K_{PDMS/w}$	sd
chlorthiophos 2[a]	-0.90	0.04	-1.44	0.14	3.96	0.06
coumaphos	-2.24	0.03	-	-	2.82	0.08[c]
dichlobenil	-1.15	0.06	-0.92	0.11	1.84	0.04[c]
dichlofenthion	-0.39	0.01	-1.26	0.15	3.76	0.14
dichlofluanid	-2.04	0.14	-1.31	0.08	2.84	0.02[c]
dichlorvos	-1.78	0.03	-	-	1.88[b]	-
dieldrin	-0.61	0.06	-0.17	0.11	4.93[b]	-
dimethenamid	-0.86	0.04	-1.78	0.15	1.42	0.02[c]
disulfoton	-0.61	0.02	-1.72	0.15	2.96	0.03[c]
endosulfan	-0.35	0.00	-0.83	0.08	4.22	0.12
endosulfan-sulfate	-1.43	0.01	-1.35	0.15	2.60[b]	-
endrin	-0.48	0.02	-	-	4.64[b]	-
esfenvalerate	-1.89	0.17	-	-	5.80[b]	-
ethion	-1.06	0.03	-	-	3.17[b]	-
fenchlorphos	-0.73	0.16	-	-	3.97	0.02[c]
fenitrothion	-2.29	0.00	-0.78	0.21	2.53	0.03[c]
fenpropathrin	-1.04	0.02	-0.67	0.14	5.51[b]	-
fenthion	-1.40	0.01	-1.04	0.13	3.18	0.02[c]
flumetralin	-0.91	0.05	-1.51	0.08	4.48	0.08
flusilazole	-2.32	0.12	-	-	2.58	0.10[c]
fonofos	-0.74	0.01	-0.99	0.09	3.14	0.02[c]
heptachlor epoxide	-0.58	0.02	-	-	4.59[b]	-
heptenophos	-1.42	0.10	-	-	1.40	0.06[c]
hexachlorobenzene	0.66	0.03	-	-	4.79[b]	-
malathion	-1.89	0.01	-1.31	0.22	1.71	0.10[c]
metazachlor	-1.53	0.06	-0.22	0.04	1.29	0.02[c]
metolachlor	-0.96	0.03	-	-	2.01	0.03[c]
napropamide	-1.32	0.06	-	-	2.13	0.03[c]
nitrofen	-1.05	0.05	-	-	2.83	0.05[c]
octhilinone	-1.21	0.05	-1.23	0.02	1.26	0.06[c]
orbencarb	-0.50	0.01	-1.20	0.14	3.07	0.03[c]
parathion-ethyl	-0.77	0.02	-1.50	0.15	2.73	0.05[c]
pentachloroanisole	0.32	0.01	-1.40	0.14	4.13	0.01[c]
permethrin 1[a]	-0.16	0.01	-	-	5.42[b]	-
permethrin 2[a]	-0.17	0.01	-	-	5.42[b]	-
phorate	-0.52	0.05	-1.01	0.16	2.94	0.04[c]
phosalone	-2.12	0.02	-	-	3.07	0.04[c]
procymidone	-1.19	0.10	-1.36	0.10	2.05	0.01[c]
propargite	-0.59	0.01	-	-	4.11	0.02[c]
pyrazophos	-1.53	0.08	-	-	2.89	0.09[c]
sulfotep	-0.95	0.04	-	-	3.06	0.05[c]
tecnazene	-0.36	0.01	-1.28	0.11	3.41	0.01[c]
terbufos	-0.26	0.01	-	-	3.27	0.03[c]
thiometon	-1.06	0.04	-0.76	0.05	2.31	0.07[c]
tolylfluanid	-1.39	0.09	-	-	2.83	0.06[c]
vinclozolin	-1.56	0.01	-1.27	0.11	2.07	0.04[c]

compound	log $K_{hep/PC}$	sd	log $K_{EG/DCE}$	sd	log $K_{PDMS/w}$	sd
PCB 1	-0.19	0.01	-0.44	0.12	3.76	0.03[c]
PCB 2	-0.11	0.00	-	-	4.16[b]	-
PCB 3	-0.16	0.01	-1.22	0.13	3.58	0.07[c]
PCB 4	-0.30	0.00	-1.38	0.20	4.52[b]	-
PCB 15	-0.16	0.01	-1.32	0.05	4.75[b]	-
PCB 28	0.14	0.01	-	-	5.37[b]	-
PCB 29	0.29	0.00	-	-	5.33[b]	-
PCB 52	0.06	0.00	-	-	5.51[b]	-
PCB 101	0.35	0.04	-	-	6.08[b]	-
PCB 153	0.59	0.02	-	-	6.40[b]	-
9-fluorenone	-1.03	0.05	-1.10	0.19	2.72	0.04[c]
isoquinoline	-0.93	0.03	-	-	1.62	0.05[c]
quinoline	-0.75	0.04	-	-	1.11	0.06[c]
xanthene	-0.30	0.06	-1.11	0.19	3.32	0.02[c]
1-nitronaphthalene	-1.06	0.07	-1.33	0.11	1.88	0.03[c]
2,4-dinitrotoluene	-2.01	0.04	-1.11	0.11	0.62	0.05[c]
2-nitroanisole	-1.72	0.02	-0.87	0.11	0.26	0.08[c]
3-nitroanisole	-0.79	0.06	-1.16	0.14	1.36	0.06[c]
4-nitroanisole	-1.30	0.10	-1.20	0.12	1.10	0.04[c]
9-nitroanthracene	-1.03	0.06	-1.63	0.25	2.90	0.07[c]
musk xylene	-0.77	0.01	-1.45	0.05	3.77	0.18
progesterone	-1.20	0.18	-	-	2.49	0.08[c]
2,4'-DDD	-0.96	0.02	-1.69	0.10	5.28[b]	-
ametryn	-1.01	0.05	-0.28	0.07	0.98	0.06[c]
atrazine	-1.49	0.06	0.15	0.04	0.22	0.03[c]
bromacil	-1.91	0.20	-0.08	0.04	0.56	0.07[c]
bromopropylate	-1.14	0.03	-1.86	0.19	3.67	0.08
carbaryl	-1.05	0.43	-1.38	0.14	1.09[b]	-
carbofuran	-1.35	0.16	-0.74	0.11	0.77[b]	-
chlorobenzilate	-1.28	0.06	-0.24	0.02	3.01	0.07[c]
chlorpropham	-1.39	0.06	-0.67	0.04	2.06	0.06[c]
dicloran	-2.10	0.16	-0.51	0.10	1.34	0.02[c]
diphenylamine	-1.54	0.06	-0.09	0.15	2.41	0.05[c]
α-HCH	-1.05	0.13	-1.03	0.09	2.59	0.04[c]
β-HCH	-2.18	0.02	-0.46	0.01	1.57	0.09[c]
γ-HCH (lindane)	-1.10	0.04	-1.00	0.08	2.67	0.05[c]
δ-HCH	-1.96	0.04	-0.78	0.09	2.08	0.04[c]
metribuzin	-1.40	0.09	0.73	0.02	-0.79	0.14[c]
pendimethalin	-0.85	0.02	-1.27	0.15	3.60	0.05[c]
pentachloroaniline	-0.61	0.02	-0.80	0.06	2.91	0.05[c]
prometryn	-1.03	0.08	-0.66	0.03	2.23	0.09[c]
propham	-1.14	0.06	-0.49	0.04	1.27	0.01[c]
propyzamide	-2.15	0.03	-0.72	0.03	1.03	0.03[c]
terbutryn	-1.12	0.03	-0.74	0.04	2.31	0.05[c]
carbazole	-2.97	0.08	-0.39	0.12	1.55	0.06[c]
indole	-2.15	0.08	-0.05	0.15	0.28	0.04[c]

compound	log $K_{hep/PC}$	sd	log $K_{EG/DCE}$	sd	log $K_{PDMS/w}$	sd
triclosan	-0.96	0.07	-0.51	0.05	2.83	0.03[c]

[a]isomers in the order of peak appearance in the GC
[b]value taken from DiFilippo and Eganhouse[3], only log K considered reliable by the authors were taken into account, a mean log K is used when there is more than one value given
[c]for depletion experiments the standard error is given

Table S3. Comparison of log $K_{PDMS/water}$ from this work and from DiFilippo and Eganhouse.[3]

compound	log $K_{PDMS/water}$ from this work	log $K_{PDMS/water}$ from DiFilippo and Eganhouse
chlorfenvinfos 1	3.05	3.38
chlorfenvinfos 2	2.83	3.38
chlorpyrifos-ethyl	4.36	4.18
chlorpyrifos-methyl	3.65	3.45
fenitrothion	2.53	3.05
fenthion	3.18	3.33
fonofos	3.14	3.44
malathion	1.71	2.21
parathion-ethyl	2.73	2.83
phorate	2.94	3.21
phosalone	3.07	3.50
PCB 1	3.76	4.20
α-HCH	2.59	2.66
β-HCH	1.57	2.59
γ-HCH (lindane)	2.67	2.59
δ-HCH	2.08	2.03
terbutryn	2.31	3.10

Table S4. Experimental and pp-LFER predicted logarithmic partition coefficients of the target compounds for the systems octanol/water (K_{ow}), water/air[a] (K_{wa}) and organic carbon/water (K_{oc}). The given experimental value is the mean value of the literature values found (n indicates the number of literature values).

	exp. log K_{ow}	n	ref	pred. log K_{ow}	exp. log K_{wa}	n	ref	pred. log K_{wa}	exp. log K_{oc}	n	ref	pred. log K_{oc}
2,4'-DDE	6.96	1	[4]	6.55	3.14[b]	1	[5]	2.39	5.49	1	[5]	5.36
4,4'-DDE	6.74	2	[5, 6]	6.87	2.78	1	[5]	2.28	4.76	2	[5, 7]	5.71
4,4'-DDT	6.64	2	[5, 6]	6.64	3.48	1	[5]	3.39	5.24	2	[5, 7]	5.52
alachlor	3.31	2	[5, 7]	3.08	6.19	2	[5, 7]	6.45	2.22	3	[5, 7, 8]	1.89
aldrin	6.50	1	[5]	6.56	2.47	2	[5, 7]	1.87	4.47	2	[5, 7]	5.23
benalaxyl	3.47	2	[5, 7]	4.13	5.47[b]	2	[5, 7]	7.33	3.62	2	[5, 7]	2.74
bifenthrin	6.30	2	[6, 7]	7.13	5.96[b]	2	[5, 7]	4.32	5.36	2	[5, 7]	5.02
bromophos-ethyl	6.15	1	[5]	5.51	3.19	1	[7]	4.23	-	-	-	4.12
bromophos-methyl	5.05	2	[5, 6]	5.05	2.09	1	[7]	3.95	1.23	1	[7]	4.01
carbophenothion	5.25	3	[5-7]	4.86	4.36[b]	2	[5, 7]	6.17	4.68	2	[5, 7]	3.60
cis-chlordane	6.10	1	[5]	6.29	4.77	2	[5, 7]	2.83	4.54	2	[5, 7]	5.07
chlorfenvinfos 1[c]	3.81	2	[6, 7]	4.16	5.94[b]	1	[5]	5.81	2.65	2	[5, 7]	2.78
chlorfenvinfos 2[c]	3.81	2	[6, 7]	3.96	5.94[b]	1	[5]	6.09	2.65	2	[5, 7]	2.65

	exp. log K_{ow}	n	ref	pred. log K_{ow}	exp. log K_{wa}	n	ref	pred. log K_{wa}	exp. log K_{oc}	n	ref	pred. log K_{oc}
chlorothalonil	2.96	3	[5-7]	3.26	4.56	2	[5, 7]	5.00	3.05	3	[5, 7, 8]	2.86
chlorpyrifos-ethyl	4.98	3	[4, 6, 7]	5.22	3.83	2	[5, 7]	3.86	3.81	2	[5, 7]	3.90
chlorpyrifos-methyl	4.16	2	[6, 7]	4.44	3.93[b]	2	[5, 7]	4.06	3.59	2	[5, 7]	3.44
chlorthal-dimethyl	4.34	2	[5, 6]	4.26	3.97[b]	2	[5, 7]	4.95	3.59	2	[5, 7]	3.27
chlorthiophos 1[c]	4.34	1	[7]	5.14	-	-	-	5.23	-	-	-	3.90
chlorthiophos 2[c]	4.34	1	[7]	4.98	-	-	-	5.72	-	-	-	3.68
coumaphos	4.00	2	[5, 7]	4.16	5.64[b]	2	[5, 7]	8.63	4.26	1	[7]	3.30
dichlobenil	2.72	2	[6, 7]	2.37	3.34[b]	2	[5, 7]	3.73	2.45	2	[5, 7]	1.95
dichlofenthion	5.14	1	[5]	4.57	1.43[b]	1	[5]	4.27	1.26	1	[7]	3.27
dichlofluanid	3.70	1	[5]	3.73	5.84[b]	2	[5, 7]	5.47	2.40	2	[7, 8]	2.76
dichlorvos	1.67	2	[5, 7]	2.40	4.82[b]	2	[5, 7]	3.01	1.68	2	[5, 7]	1.74
dieldrin	5.30	2	[4, 5]	5.75	4.00	2	[5, 7]	3.65	4.08	1	[5]	4.73
dimethenamid	2.18	2	[5, 7]	2.53	5.48	2	[5, 7]	7.18	1.75	1	[8]	1.34
disulfoton	3.99	2	[6, 7]	3.91	4.14[b]	2	[5, 7]	4.74	3.17	2	[5, 7]	2.62
endosulfan	4.23	4	[5-7, 9]	5.13	2.91	2	[5, 7]	4.56	3.68	3	[5, 7, 8]	3.98
endosulfan-sulfate	3.66	1	[5]	3.76	4.89[b]	1	[5]	7.54	-	-	-	2.89
endrin	5.20	1	[5]	5.51	3.82	2	[5, 7]	4.25	4.04	2	[5, 7]	4.52
esfenvalerate	6.23	2	[5, 7]	7.15	6.29[b]	2	[5, 7]	6.41	3.73	2	[5, 7]	5.51
ethion	5.07	1	[5]	4.42	4.82	1	[5]	6.92	4.03	2	[5, 7]	2.81
fenchlorphos	4.88	1	[5]	4.76	2.90[b]	1	[5]	3.83	-	-	-	3.72
fenitrothion	3.31	2	[5, 7]	3.42	4.92	2	[5, 7]	5.49	2.97	2	[5, 7]	2.72
fenpropathrin	5.87	2	[5, 7]	6.62	2.83[b]	2	[5, 7]	4.80	4.00	2	[5, 7]	5.03
fenthion	4.47	2	[6, 7]	3.99	4.63[b]	2	[5, 7]	5.16	3.31	2	[5, 8]	3.00
flumetralin	5.45	1	[5]	5.48	4.13[b]	2	[5, 7]	4.99	4.39	2	[5, 7]	3.87
flusilazole	3.79	2	[6, 7]	3.70	6.98	1	[7]	6.81	3.12	2	[7, 8]	2.64
fonofos	3.92	2	[5, 7]	3.88	3.58[b]	2	[5, 7]	4.53	2.94	1	[5]	2.81
heptachlor epoxide	5.19	2	[5, 9]	5.37	3.08	1	[5]	3.55	4.19	2	[5, 7]	4.33
heptenophos	2.32	1	[5]	2.23	6.41[b]	2	[5, 7]	5.41	2.21	1	[7]	1.40
hexachloro-benzene	5.52	2	[5, 6]	5.33	1.78	2	[5, 7]	1.97	4.22	2	[5, 7]	4.49
malathion	2.56	2	[6, 7]	2.83	6.56	2	[5, 7]	7.06	2.81	2	[5, 7]	1.55
metazachlor	2.31	2	[5, 7]	2.46	7.64	2	[5, 7]	7.91	1.71	2	[7, 8]	1.46
metolachlor	3.27	2	[6, 7]	3.16	6.24	2	[5, 7]	7.00	2.14	3	[5, 7, 8]	1.81
napropamide	3.33	2	[5, 7]	3.30	7.49[b]	2	[5, 7]	7.40	2.79	3	[5, 7, 8]	2.15
nitrofen	4.02	2	[6, 7]	3.82	-	-	-	6.38	3.99	2	[5, 8]	3.18
octhilinone	2.45	1	[5]	2.29	6.09[b]	1	[5]	6.85	2.44	2	[7, 8]	1.45
orbencarb	3.80	2	[5, 7]	3.95	4.28[b]	2	[5, 7]	5.24	3.19	1	[8]	2.83
parathion-ethyl	3.83	1	[5]	3.75	4.93	1	[5]	5.85	3.44	3	[5, 7, 8]	2.70
pentachloro-anisole	5.45	1	[5]	4.75	-	-	-	2.86	-	-	-	3.87
permethrin 1[c]	6.30	2	[6, 7]	6.64	4.13	1	[5]	5.73	4.90	2	[5, 7]	4.95
permethrin 2[c]	6.30	2	[6, 7]	6.65	4.13	1	[5]	5.82	4.90	2	[5, 7]	4.98
phorate	3.71	2	[5, 7]	3.69	3.70[b]	2	[5, 7]	4.45	2.96	2	[5, 7]	2.48
phosalone	4.20	2	[5, 7]	4.30	6.10	1	[7]	7.61	2.97	2	[5, 7]	3.35

	exp. log K_{ow}	n	ref	pred. log K_{ow}	exp. log K_{wa}	n	ref	pred. log K_{wa}	exp. log K_{oc}	n	ref	pred. log K_{oc}
procymidone	3.13	3	5-7	3.13	4.66[b]	2	5, 7	6.98	2.66	3	5, 7, 8	2.38
propargite	5.35	2	5, 7	5.34	4.60	1	7	6.28	4.20	1	5	3.63
pyrazophos	3.80	1	5	4.25	7.00	1	7	8.34	2.81	1	7	2.99
sulfotep	3.99	1	5	3.95	3.75[b]	2	5, 7	4.28	2.87	1	7	2.38
tecnazene	4.22	3	5-7	3.99	7.84	1	7	3.08	4.08	2	5, 7	3.32
terbufos	4.50	2	5, 7	4.19	3.00[b]	2	5, 7	4.54	2.76	2	5, 7	2.67
thiometon	3.15	1	5	3.05	5.46[b]	2	5, 7	5.16	2.76	1	7	2.10
tolylfluanid	3.93	2	5, 6	3.88	4.52	1	7	6.07	-	-	-	2.72
vinclozolin	3.06	2	5, 7	3.02	6.22[b]	2	5, 7	6.15	2.59	2	5, 7	2.21
PCB 1	4.50	2	5, 10	4.28	1.54	1	5	2.15	3.47	1	5	3.40
PCB 2	4.64	2	6, 10	4.68	1.62	1	5	2.01	-	-	-	3.85
PCB 3	4.65	2	6, 10	4.13	1.64	1	5	2.84	-	-	-	3.32
PCB 4	4.78	3	5, 6, 10	5.00	2.04	1	5	1.77	3.92	1	5	4.06
PCB 15	5.37	3	5, 6, 10	5.27	2.10	1	5	2.31	-	-	-	4.45
PCB 28	5.67	3	5, 6, 10	5.96	2.10	1	5	1.86	4.63	1	5	5.00
PCB 29	5.71	2	6, 10	5.92	2.10	1	5	1.84	-	-	-	4.92
PCB 52	5.91	3	5, 6, 10	6.14	2.10	1	5	1.98	5.12	1	5	5.09
PCB 101	6.59	2	5, 10	6.77	2.45	1	5	2.09	5.22	1	5	5.64
PCB 153	7.16	3	5, 6, 10	7.17	3.04	1	5	2.61	5.58	1	5	6.00
9-fluorenone	3.58	1	5	3.39	-	-	-	4.45	-	-	-	2.93
isoquinoline	2.08	1	5	2.14	-	-	-	3.62	-	-	-	1.72
quinoline	2.03	1	5	1.69	4.18[b]	1	5	4.21	3.10	1	5	1.22
xanthene	4.23	1	5	3.91	-	-	-	3.45	-	-	-	3.21
1-nitro-naphthalene	3.19	1	5	2.62	4.16	1	5	4.76	-	-	-	2.21
2,4-dinitrotoluene	1.98	1	5	1.41	5.67	1	5	5.89	2.23	1	8	1.17
2-nitroanisole	1.73	1	5	0.96	4.77[b]	1	5	5.47	1.89	1	8	0.65
3-nitroanisole	2.17	2	5, 6	2.00	-	-	-	4.17	2.11	1	8	1.55
4-nitroanisole	2.03	1	5	1.78	4.29	1	11	4.66	2.28	1	8	1.46
9-nitroanthracene	4.78	1	5	3.85	-	-	-	5.74	-	-	-	3.35
musk xylene	4.90	1	12	4.61	4.63	1	12	4.25	4.19	1	13	3.38
progesterone	3.87	1	5	4.03	-	-	-	10.15	3.02	1	8	2.92
2,4'-DDD	6.22	1	4	6.44	3.49[b]	1	5	3.36	-	-	-	5.29
ametryn	2.81	2	5, 7	2.78	6.91[b]	2	5, 7	7.81	2.54	2	5, 7	1.69
atrazine	2.66	2	6, 7	2.43	7.13[b]	2	5, 7	7.85	2.02	3	5, 7, 8	1.40
bromacil	2.00	2	6, 7	2.58	8.26[b]	2	5, 7	8.07	1.50	3	5, 7, 8	1.81
bromopropylate	5.40	1	5	4.90	4.74	1	5	6.76	3.80	1	7	3.60
carbaryl	2.36	1	5	2.14	7.17[b]	2	5, 7	7.03	2.40	3	5, 7, 8	1.60
carbofuran	2.06	2	5, 7	2.01	7.31[b]	2	5, 7	6.90	1.75	1	5	1.13
chlorobenzilate	4.66	2	5, 7	5.73	5.30[b]	2	5, 7	6.87	3.34	3	5, 7, 8	4.13
chlorpropham	3.64	2	6, 7	3.54	4.69[b]	2	5, 7	4.91	2.60	1	5	2.60
dicloran	2.80	1	5	2.75	5.61[b]	2	5, 7	5.83	3.00	1	5	2.41
diphenylamine	3.66	2	6, 7	4.58	3.94[b]	2	5, 7	4.31	3.20	2	5, 7	3.58
α-HCH	3.81	3	6, 7, 14	3.72	3.64	2	5, 14	4.59	3.16	2	5, 7	2.88
β-HCH	3.81	3	5, 6, 14	3.39	4.26	2	5, 14	6.04	3.04	1	5	2.59
γ-HCH (lindane)	3.64	3	5, 7, 14	3.85	3.83	2	5, 14	4.74	3.07	2	5, 7	3.05

	exp. log K_{ow}	n	ref	pred. log K_{ow}	exp. log K_{wa}	n	ref	pred. log K_{wa}	exp. log K_{oc}	n	ref	pred. log K_{oc}
δ-HCH	4.14	1	[5]	3.56	3.69	1	[5]	5.48	3.04	1	[5]	2.83
metribuzin	1.68	2	[6, 7]	1.96	8.22[b]	2	[5, 7]	9.64	1.60	2	[5, 8]	0.88
pendimethalin	5.19	2	[6, 7]	4.95	5.22	2	[5, 7]	5.17	3.97	2	[5, 7]	3.65
pentachloroaniline	4.82	1	[5]	4.20	-	-	-	4.69	4.32	2	[5, 7]	3.50
prometryn	3.43	2	[6, 7]	4.01	6.33	1	[5]	6.18	2.73	2	[5, 7]	2.75
propham	2.60	1	[5]	2.68	5.48[b]	2	[5, 7]	5.06	1.91	2	[5, 7]	1.72
propyzamide	3.31	3	[5-7]	2.63	6.47[b]	2	[5, 7]	6.94	2.62	2	[5, 7]	1.65
terbutryn	3.70	2	[5, 7]	4.01	6.15[b]	2	[5, 7]	6.13	2.93	3	[5, 7, 8]	2.80
carbazole	3.72	1	[5]	3.38	5.34	1	[5]	5.85	3.40	1	[5]	3.00
indole	2.14	1	[5]	1.84	4.68[b]	1	[5]	5.07	2.04	1	[8]	1.42
triclosan	4.76	1	[5]	4.79	-	-	-	6.03	4.02	1	[8]	3.72

[a]Units were converted to [m^3_{air}/m^3_{water}].
[b]At least one value is from water solubility/vapor pressure.
[c]isomers in the order of peak appearance in the GC

Table S5. Rmse values resulting from the comparison between predicted[a] log *K* and experimental log *K* from different databases.

	log K_{ow}		log K_{wa}		log K_{oc}	
	rmse	n	rmse	n	rmse	n
mean values (used for figures)	0.39	111	1.19	99	0.71	94
EPI Suite™ (experimental database)[5]	0.42	105	1.10	92	0.62	72
The Pesticide Properties Database (PPDB)[7]	0.68	80	1.55	70	0.76	70
LOGKOW[©,6]	0.50	108	-	-	-	-

[a]prediction based on substance descriptors from this work

Table S6. Experimental and pp-LFER predicted logarithmic partition coefficients for structurally similar target compounds for the systems octanol/water (K_{ow}), water/air[a] (K_{wa}) and organic carbon/water (K_{oc}) (extracted from Table S4).

	log K_{ow}		log K_{wa}		log K_{oc}	
	exp.	pred.	exp.	pred.	exp.	pred.
bromopropylate	5.40	4.90	4.74	6.76	3.80	3.60
chlorobenzilate	4.66	5.73	5.30[b]	6.87	3.34	4.13
bromophos-ethyl	6.15	5.51	3.19	4.23	-	4.12
bromophos-methyl	5.05	5.05	2.09	3.95	1.23	4.01
chlorthiophos 1[c]	4.34	5.14	-	5.23	-	3.90
chlorthiophos 2[c]	4.34	4.98	-	5.72	-	3.68
dichlofenthion	5.14	4.57	1.43[b]	4.27	1.26	3.27
fenchlorphos	4.88	4.76	2.90[b]	3.83	-	3.72

[a]Units were converted to [m^3_{air}/m^3_{water}].
[b]At least one value is from water solubility/vapor pressure.
[c]isomers in the order of peak appearance in the GC

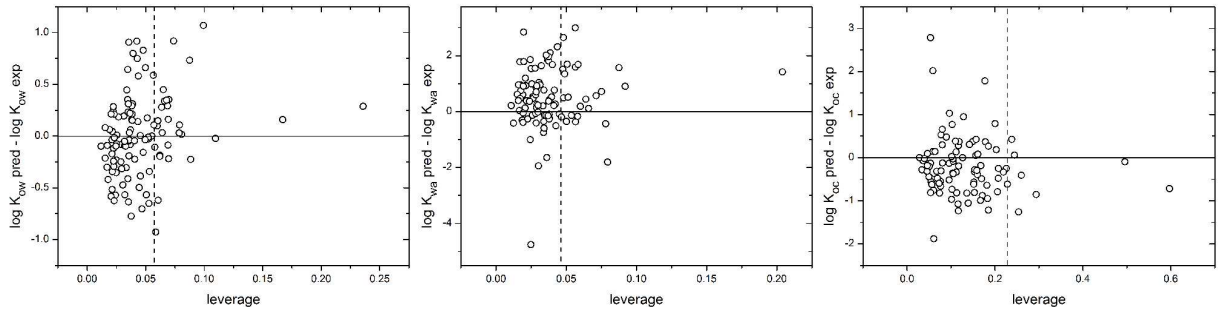

Figure S1. Comparison between target compound leverages (x-axis) and prediction error (log *K* predicted – log *K* experimental; y-axis) for the systems K_{ow}, K_{wa}, and K_{oc} (from left to right). The vertical line indicates three times the mean of the leverages of the calibration compounds.

Table S7. Rmse values resulting from the comparison between experimental and predicted log *K* or log t_{net} for different HPLC columns. Experimental values are from Tülp et al.[11]

system	descriptors from this work		descriptors from Tülp et al.[11]	
	rmse	n	rmse	n
heptane/methanol	0.30	26	0.19	67
C18	0.33	29	0.16	76
Ph	0.16	29	0.11	74
CN-RP	0.50	29	0.24	74
OH-RP	0.22	29	0.38	74
CN-NP	0.14	29	0.19	75
OH-NP	0.40	29	0.50	75
NH_2-NP	0.38	29	0.25	75
HILIC	0.12	27	0.13	69

Table S8. Comparison of substance descriptors from this work and the literature (excluding descriptors from Tülp et al.[11] and Bronner et al.[17]). A comparison for HCHs and PCBs is provided separately in Tables S9 and S10.

compound	V^a	*L*	*S*	*B*	*A*	ref
4,4'-DDE	2.05	9.42	1.36	0.16	0.00	this work
	2.05	9.73	1.40	0.14	0.06	Sprunger et al.[18]
4,4'-DDT	2.22	9.98	1.78	0.24	0.00	this work

compound	V^a	L	S	B	A	ref
	2.22	10.02	1.76	0.16	0.00	Sprunger et al.[18]
aldrin	2.01	8.69	1.03	0.26	0.00	this work
	2.01	8.58	0.95	0.42	0.00	Sprunger et al.[18]
dichlobenil	1.12	5.63	1.40	0.32	0.00	this work
	1.12	5.57	1.22	0.27	0.00	Abraham et al.[19]
dieldrin	2.01	9.23	1.59	0.33	0.00	this work
	2.01	8.49	2.05	0.63	0.03	Sprunger et al.[18]
endrin	2.01	9.48	1.53	0.46	0.00	this work
	2.01	7.69	1.60	0.71	0.09	Sprunger et al.[18]
heptachlor epoxide	1.96	8.70	1.49	0.38	0.00	this work
	1.96	8.51	1.20	0.61	0.00	Sprunger et al.[18]
hexachloro-benzene	1.45	7.64	0.85	0.17	0.00	this work
	1.45	7.67	0.88	0.00	0.00	Karunasekara and Poole[20]
	1.45	7.74	0.82	0.00	0.00	Atapattu et al.[21]
	1.45	7.39	0.99	0.00	0.00	Sprunger et al.[18]
pentachloro-anisole	1.53	7.63	0.96	0.35	0.00	this work
	1.53	7.57	1.06	0.00	0.00	Abraham[22]
9-fluorenone	1.37	7.41	1.55	0.37	0.00	this work
	1.37	7.47	1.49	0.63	0.00	Sprunger et al.[18]
	1.37	7.47	1.49	0.35	0.00	Abraham et al.[23]
isoquinoline	1.04	5.31	1.25	0.36	0.00	this work
	1.04	5.60	1.00	0.54	0.00	Abraham and Acree[24]
quinoline	1.04	5.27	1.11	0.54	0.00	this work
	1.04	5.46	0.97	0.54	0.00	Abraham et al.[25]
	1.04	5.34	1.12	0.54	0.00	Atapattu et al.[21]
1-nitro-naphthalene	1.26	6.79	1.49	0.46	0.00	this work
	1.26	6.84	1.48	0.29	0.00	Karunasekara and Poole[20]
	1.26	6.82	1.49	0.29	0.00	Atapattu et al.[21]
	1.26	6.81	1.51	0.27	0.00	Poole et al.[26]
	1.26	7.06	1.59	0.29	0.00	Sprunger et al.[18]
2,4-dinitrotoluene	1.21	6.27	1.84	0.56	0.00	this work
	1.21	6.26	1.60	0.47	0.00	Houser et al.[27]
progesterone	2.62	12.47	1.97	1.51	0.00	this work
	2.62	11.67	2.21	1.39	0.00	Karunasekara and Poole[20]
ametryn	1.80	8.36	1.02	1.16	0.33	this work
	1.80	8.61	1.26	1.02	0.17	Abraham et al.[28]
atrazine	1.62	7.60	0.97	1.05	0.49	this work
	1.62	7.78	1.29	1.01	0.17	Abraham et al.[28]
diphenylamine	1.42	6.89	0.96	0.20	0.61	this work
	1.42	6.80	1.28	0.53	0.15	Karunasekara and Poole[20]
	1.42	6.92	1.05	0.28	0.39	Atapattu et al.[21]
	1.42	6.89	1.08	0.55	0.34	Poole et al.[26]
	1.42	7.40	1.32	0.28	0.30	Abraham et al.[25]
prometryn	1.94	8.36	1.11	0.87	0.33	this work

compound	V^a	L	S	B	A	ref
	1.94	8.96	1.23	1.01	0.17	Abraham et al.[28]
terbutryn	1.94	8.41	1.20	0.83	0.30	this work
	1.94	8.98	1.23	0.99	0.12	Abraham et al.[28]
carbazole	1.32	7.33	1.91	0.15	0.44	this work
	1.32	7.53	1.55	0.23	0.39	Karunasekara and Poole[20]
	1.32	8.00	2.12	0.10	0.09	Abraham et al.[19]
	1.32	7.64	1.37	0.26	0.64	Atapattu et al.[21]
indole	0.95	5.08	1.26	0.32	0.40	this work
	0.95	5.14	1.24	0.22	0.42	Poole et al.[26]

[a]molar volume in $(cm^3/mol)/100$

Table S9. Comparison of HCH substance descriptors from this work and the literature.

compound	V^a	L	S	B	A
from this work					
α-HCH	1.58	7.35	1.31	0.50	0.15
β-HCH	1.58	7.47	1.52	0.51	0.40
γ-HCH (lindane)	1.58	7.59	1.35	0.47	0.17
δ-HCH	1.58	7.56	1.61	0.44	0.27
from Goss et al.[29]					
α-HCH	1.58	7.34	1.20	0.47	0.00
β-HCH	1.58	7.63	1.18	0.58	0.12
γ-HCH (lindane)	1.58	7.57	1.28	0.50	0.00
from Abraham et al.[28]					
α-HCH	1.58	7.32	0.73	0.71	0.00
β-HCH	1.58	7.49	0.88	0.69	0.00
γ-HCH (lindane)	1.58	7.47	0.91	0.68	0.00
δ-HCH	1.58	7.63	0.94	0.63	0.00

[a]molar volume in $(cm^3/mol)/100$

Table S10. Comparison of PCB substance descriptors from this work and the literature (*A* is always zero).

compound	V^a	L	S	B
from this work				
PCB 1	1.45	6.43	1.07	0.23
PCB 2	1.45	6.81	1.10	0.15
PCB 3	1.45	6.87	1.08	0.33
PCB 4	1.57	6.90	1.19	0.12
PCB 15	1.57	7.75	1.24	0.13
PCB 28	1.69	8.14	1.17	0.09
PCB 29	1.69	8.07	1.08	0.13
PCB 52	1.81	8.38	1.23	0.13
PCB 101	1.94	9.21	1.19	0.15
PCB 153	2.06	10.11	1.17	0.24
from this work, using van Noort et al. V, recalculation of L, S and B				
PCB 1	1.36	6.38	1.08	0.17
PCB 2	1.45	6.81	1.10	0.15

compound	V^a	L	S	B
PCB 3	1.45	6.87	1.08	0.33
PCB 4	1.40	6.82	1.21	0.00
PCB 15	1.57	7.75	1.24	0.13
PCB 28	1.60	8.09	1.18	0.02
PCB 29	1.60	8.02	1.10	0.06
PCB 52	1.64	8.28	1.25	0.00
PCB 101	1.76	9.11	1.22	0.02
PCB 153	1.88	9.96	1.19	0.11
from van Noort et al.[30]				
PCB 1	1.36	6.34	1.03	0.17
PCB 2	1.45	6.67	1.18	0.17
PCB 3	1.45	6.72	1.18	0.17
PCB 4	1.40	6.82	1.05	0.11
PCB 15	1.57	7.58	1.35	0.11
PCB 28	1.60	7.90	1.35	0.06
PCB 29	1.60	7.72	1.35	0.06
PCB 52	1.64	8.14	1.33	0.00
PCB 101	1.76	8.87	1.47	0.00
PCB 153	1.88	9.59	1.61	0.00
from Abraham and Hussaini[31]				
PCB 1	1.45	6.34	1.07	0.20
PCB 2	1.45	6.67	1.05	0.18
PCB 3	1.45	6.72	1.05	0.18
PCB 4	1.57	6.82	1.22	0.20
PCB 15	1.57	7.58	1.18	0.16
PCB 28	1.69	7.90	1.33	0.15
PCB 29	1.69	7.72	1.33	0.15
PCB 52	1.81	8.14	1.48	0.15
PCB 101	1.94	8.87	1.61	0.13
PCB 153	2.06	9.59	1.74	0.11

[a]molar volume in $(cm^3/mol)/100$

Table S11. Recalculated pp-LFER substance descriptors and rmse values for 30 target compounds using retention times from Tülp et al.[11] and Bronner et al.[17] in addition to the data measured in this work.

compound	S	A^a	B	V^b	L	rmse
alachlor	1.56	0.00	1.02	2.14	8.07	0.16
chlorothalonil	2.02	0.00	0.33	1.52	7.40	0.17
chlorpyrifos-ethyl	1.20	0.00	0.71	2.15	8.61	0.38
dichlofluanid	1.92	0.00	0.76	2.07	8.25	0.24
dimethenamid	1.33	0.00	1.21	2.06	7.96	0.17
endosulfan	1.35	0.00	0.80	2.08	9.39	0.20
endrin	1.51	0.00	0.48	2.01	9.49	0.08
fenthion	1.75	0.00	0.63	1.99	8.37	0.16
flusilazole	2.23	0.00	0.90	2.31	9.34	0.12
metazachlor	1.70	0.00	1.20	2.09	8.60	0.15
metolachlor	1.42	0.00	1.23	2.28	8.62	0.16

compound	S	A[a]	B	V[b]	L	rmse
napropamide	1.70	0.00	1.12	2.25	9.23	0.12
nitrofen	1.60	0.00	0.68	1.80	9.12	0.33
octhilinone	1.58	0.00	0.93	1.79	7.79	0.20
orbencarb	1.28	0.00	0.80	1.96	8.29	0.11
parathion-ethyl	1.52	0.00	0.80	2.00	8.35	0.15
procymidone	1.54	0.00	0.93	1.86	8.56	0.31
vinclozolin	1.64	0.00	0.83	1.84	7.53	0.32
2,4-dinitrotoluene	1.77	0.00	0.48	1.21	5.82	0.23
2-nitroanisole	1.61	0.00	0.49	1.09	5.24	0.18
3-nitroanisole	1.23	0.00	0.40	1.09	5.38	0.14
4-nitroanisole	1.48	0.00	0.38	1.09	5.51	0.15
progesterone	1.96	0.00	1.50	2.62	12.30	0.13
atrazine	0.92	0.50	0.98	1.62	7.25	0.17
bromacil	1.31	0.47	0.92	1.63	8.08	0.21
carbaryl	1.55	0.00	0.86	1.54	7.76	0.22
chlorobenzilate	1.01	0.48	1.02	2.27	9.79	0.33
metribuzin	0.60	0.74	1.18	1.62	7.63	0.27
terbutryn	1.21	0.25	0.86	1.94	8.28	0.09
triclosan	1.06	0.57	0.56	1.81	9.23	0.35

[a]Due to the non-existence of any H-bond donor functional group, A has been set to zero for the first half of the chemicals ranging from alachlor up to progesterone.
[b]molar volume in $(cm^3/mol)/100$

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