SUPPORTING INFORMATION TO ARTICLE:

Experimental determination of LSER parameters for a set of 76 diverse pesticides and pharmaceuticals

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Table S1: Calibration compounds and their solute descriptors used to determine the retention characteristics of the HPLC systems (1,2).

Name	S	A	B_0	E	V
Benzene	0.52	0	0.14	0.61	0.7164
Ethylbenzene	0.51	0	0.15	0.613	0.9982
Styrene	0.65	0	0.16	0.849	0.9552
Phenylethyne	0.58	0.12	0.24	0.679	0.912
Mesitylene	0.52	0	0.19	0.649	1.1391
Azulene	1.17	0	0.16	1.34	1.0854
Naphthalene	0.92	0	0.20	1.34	1.0854
Fluorobenzene	0.57	0	0.10	0.477	0.7341
Chlorobenzene	0.65	0	0.07	0.718	0.8388
1,3-Dichlorobenzene	0.73	0	0.02	0.847	0.9612
1,3,5-Trichlorobenzene	0.73	0	0	0.98	1.0836
Bromobenzene	0.73	0	0.09	0.882	0.8914
Iodobenzene	0.82	0	0.12	1.188	0.9746
Benzoic acid	0.90	0.59	0.40	0.73	0.932
Phenol	0.89	0.60	0.30	0.805	0.7751
Benzyl alcohol	0.87	0.33	0.56	0.803	0.916
2-Phenylethanol	0.91	0.30	0.64	0.811	1.0569
3-Phenylpropanol	0.90	0.30	0.67	0.821	1.1978
4-Methylphenol	0.87	0.57	0.31	0.82	0.916
4-Ethylphenol	0.90	0.55	0.36	0.80	1.0569
4-Propylphenol	0.88	0.55	0.37	0.793	1.1978
4-Hydroxybiphenyl	1.48	0.59	0.45	1.56	1.383
1-Naphthol	1.05	0.61	0.37	1.52	1.1441
Hydroquinone	1.27	1.16	0.60	1.00	0.8338
4-Fluorophenol	0.97	0.63	0.23	0.67	0.7928
4-Chlorophenol	1.08	0.67	0.20	0.915	0.8975
4-Bromophenol	1.17	0.67	0.20	1.08	0.9501
4-Iodophenol	1.22	0.68	0.20	1.38	1.0333
2-Butanone	0.70	0	0.51	0.166	0.6879
2-Pentanone	0.68	0	0.51	0.143	0.8288
2-Heptanone	0.68	0	0.51	0.123	1.1106
Cyclohexanone	0.86	0	0.56	0.403	0.8611
γ-Butyrolactone	1.74	0	0.45	0.366	0.638
Acetophenone	1.01	0	0.48	0.818	1.0139
Propiophenone	0.95	0	0.51	0.80	1.155
Pentanophenone	0.95	0	0.50	0.80	1.437
Methyl Formate	0.68	0	0.38	0.192	0.465
Propyl Formate	0.63	0	0.38	0.132	0.7466
Ethyl Acrylate	0.64	0	0.42	0.212	0.845
Butyl Acrylate	0.62	0	0.42	0.177	1.126
Anisole	0.75	0	0.29	0.708	0.916
Benzamide	1.50	0.49	0.67	0.99	0.9728
Acetanilide	1.40	0.50	0.67	0.87	1.113
Acetamidophenol	1.78	1.09	0.81	1.06	1.172
Methyl Benzoate	0.85	0	0.46	0.733	1.0726
Methylparaben	1.37	0.69	0.45	0.90	1.132
Ethyl Benzoate	0.85	0	0.46	0.689	1.2135
Propyl Benzoate	0.80	0	0.46	0.675	1.3544
Butylparaben	1.35	0.69	0.45	0.86	1.555
Methyl phenyl sulfoxide	1.80	0	0.75	1.104	1.080
Thiophenol	0.80	0.09	0.16	1.00	0.8799

Diethyl Sulfide	0.38	0	0.32	0.373	0.8357
Diphenyl Sulfide	1.20	0	0.30	1.628	1.488
Benzonitrile	1.11	0	0.33	0.742	0.8711
Nitrobenzene	1.11	0	0.28	0.871	0.8906
Aniline	0.96	0.26	0.50	0.955	0.8162
p-Toluidine	0.95	0.23	0.52	0.923	0.9571
2,6-Xylidine	0.89	0.20	0.59	0.972	1.098
4-Aminobiphenyl	1.48	0.26	0.58	1.565	1.424
1-Naphthylamine	1.26	0.20	0.57	1.67	1.1852
2-Chloroaniline	0.92	0.25	0.40	1.033	0.9386
3-Nitroaniline	1.71	0.40	0.35	1.20	0.9904
4-Nitroaniline	1.91	0.42	0.38	1.22	0.9904
4-Methylaminobenzoate	1.52	0.32	0.64	1.078	1.172
Benzocaine	1.52	0.32	0.64	1.04	1.313
Risocaine	1.50	0.32	0.64	1.03	1.454
Butamben	1.47	0.32	0.64	1.02	1.595
Pyrrole	0.73	0.41	0.29	0.613	0.5774
Indole	1.12	0.44	0.31	1.20	0.946
Oxazole	0.70	0	0.42	0.418	0.495
Benzothiazole	1.10	0	0.40	1.33	0.969
Thiophene	0.56	0	0.15	0.687	0.6411
Dibenzothiophene	1.31	0	0.18	1.959	1.3791
Dibenzofuran	1.02	0	0.17	1.407	1.2743
Quinoline	0.97	0	0.51	1.268	1.0443
Methylpyrazine	0.86	0	0.67	0.629	0.7751
2,5-Dimethylpyrazine	0.90	0	0.69	0.626	0.916
Quinoxaline	1.20	0	0.59	1.304	1.0032

Table S2: Results of the statistical tests for correlation and distribution of the solute descriptors of the calibration compounds.

	correlations (Pearson)						test of normality (Kolmogorov-Smirnov)	
	S	**A**	**B_0**	**E**	**V**		**significance**	**normally distributed**
S	1.00					**S**	0.001	no
A	0.47	1.00				**A**	0.000	no
B_0	0.47	0.23	1.00			**B_0**	0.179	yes
E	0.57	0.26	-0.03	1.00		**E**	0.180	yes
V	0.44	0.15	0.26	0.54	1.00	**V**	0.200	yes

Table S3: Specifications of HPLC systems.

Name	Stationary phase	Particle size [µm]	Pore size [nm]	Mobile phase composition	Flow [ml/min]	Column dimensions [mm]	Supplier
C_{18}	Octadecyl	3	8	Methanol/Water 75/25	0.85	50 x 4.0	YMC CO., Ltd, Kyoto, Japan
Ph	Phenyl	3	12	Methanol/Water 64/36	0.85	50 x 4.0	YMC CO., Ltd, Kyoto, Japan
CN-RP	Cyano	3	12	Methanol/Water 45/55	0.50	150 x 4.0	YMC CO., Ltd, Kyoto, Japan
OH-RP	Diol	5	12	Methanol/Water 36/64	0.85	50 x 4.0	YMC CO., Ltd, Kyoto, Japan
HILIC	HILIC	5	20	Acetonitrile/Water 40/60	0.85	50 x 4.0	SeQuant AB, Umea, Sweden
CN-NP	Cyano	3	12	n-Hexane/Propan-2-ol/Acetonitrile 50/40/10	1.00	150 x 4.0	YMC CO., Ltd, Kyoto, Japan
OH-NP	Diol	5	12	n-Hexane/Propan-2-ol/Di-isopropyl ether 55/30/15	1.00	150 x 4.0	YMC CO., Ltd, Kyoto, Japan
NH_2-NP	Amine	5	10	n-Hexane/Propan-2-ol/ Di-isopropyl ether 55/30/15	1.00	150 x 3.0	SeQuant AB, Umea, Sweden

Table S4: Usage category, chemical class and acid dissociation constants of the target compounds ([a] B indicates the pK_a for the deprotonation of a protonated basic group; [b] est stands for estimated *pKa* values using (3)).

Name	Group	Class	pKa[a]	ref[b]
2,4,6-TNT	explosive agent	nitroaromatic	-	
2,4-Dinitrotoluene		nitroaromatic	-	
2-Nitroanisole		nitroaromatic	-	
3-Nitroanisole		nitroaromatic	-	
4-Nitroanisole		nitroaromatic	-	
Alachlor	herbizide	chloroacetanilide	-	
Amitrole	herbicide	triazole	4.2 B	(4)
Atrazine	herbizide	1,3,5-triazine	1.7 B	(4)
Azoxystrobin	fungicide	ß-methoxyacrylate	1.5 B	est
Bensulide	herbicide	organophosphorus	-	
Bromacil	herbicide	uracil	9.1	(4)
Carbamazepine	anticonvulsant	benzoazepine	-	
Carbaryl	insecticide	carbamate	-	
Carbendazim	fungicide	benzimidazole	4.2 B	(4)
Chlorobenzilate	insecticide	organochlorine	-	
Chlorothalonil	fungizide	chlorobenzonitrile	-	
Chlorpyrifos	insecticide	organophosphorus	-	
Clofentezine	insecticide	tetrazine	-	
Clothianidin	insecticide	nicotinoide	2.4 B	est
Cyanazine	herbizide	1,3,5-triazine	0.9 B	(4)
Cymoxanil	fungicide	acetamide	9.7	(4)
Cypermethrin	insecticide	synth. pyrethroid	-	

Cyproconazole	fungicide	triazole	2.3 B	est
Cyromazine	insecticide	1,3,5-triazine	5.2 B	(4)
Desethylatrazine	herbizide metabolite	1,3,5-triazine	4.6 B	est
Diazepam	anticonvulsant	benzoazepine	3.4 B	(4)
Diazinon	insecticide	organophosphorus	2.8 B	est
Dichlofluanid	fungicide	phenylsulfamide	-	
Diflufenican	herbizide	nicotinanilide	4.1 B	est
Dimethenamid	herbizide	acetamide	-	
Dinoseb	herbizide	dinitrophenol	4.6	(4)
Diuron	herbizide	phenylurea	-1.0 B	(5)
Endosulfan	insecticide	organochlorine	-	
Endrin	insecticide	organochlorine	-	
Ethofumesate	herbizide	benzofuranyl alkanesulfonate	-	
Famoxadone	fungicide	oxazolidinedione	-	
Fenthion	insecticide	organophosphorus	-	
Fluazinam	fungicide	2,6-dinitroaniline	6.3	(4)
Flucythrinate	insecticide	synth. pyrethroid	-	
Flumioxazin	herbicide	n-phenylphthalimide	-	
Fluorouracil	antineoplastic	uracil	8	(4)
Flusilazole	fungicide	triazole	2.5 B	(4)
Fosthiazate	nematicide	organophosphorus	-	
Imiprothrin	insecticide	synth. pyrethroid	-	
Irgarol	herbizide	1,3,5-triazine	-	
Isoproturon	herbizide	urea	-	
Metamitron	herbizide	1,2,4-triazinone	2.9 B	est
Metazachlor	herbizide	chloroacetanilide	1.6 B	est
Methidathion	insecticide	organophosphorus	2.3 B	est
Metolachlor	herbizide	chloroacetanilide	-	
Metoxuron	herbicide	phenylurea	-	
Metribuzin	herbicide	1,2,4-triazinone	1.0 B	(4)
Monuron	herbizide	phenylurea	-	
Napropamide	herbizide	alkanamide	-	
Nitrofen	herbicide	nitrophenyl ether	-	
Octhilinone	fungicide	isothiazolinone	-	
Orbencarb	herbizide	thiocarbamate	-	
Parathion	insecticide	organophosphorus	7.14	(5)
Phenmedipham	herbizide	bis-carbamate	0.1 B	(4)
Procymidone	fungicide	dicarboximid	-	
Propachlor	herbizide	chloroacetanilide	-	
Propaquizafop	herbicide	aryloxyphenoxy propionate	2.2 B	est
Propiconazole	fungizide	triazole	1.1 B	(4)
Propoxur	insecticide	carbamate	-	
Pymetrozine	insecticide	azomethine	3.8 B	est
Sulfentrazone	herbicide	aryl triazolinone	6.6	(4)
Tebutam	herbizide	amide	-	
Terbutryn	herbizide	1,3,5-triazine	4.3 B	(4)
Thiazopyr	herbicide	pyridine	4.4 B	est
Triallate	herbicide	thiocarbamate	-	
Triclabendazol	endectocide	benzamidazole	5.3 B	est
Triclosan	disinfectant	chlorophenoxyphenol	8.1	(6)
Triflumuron	insecticide	benzoyl phenylurea	7.6	est
Trifluralin	herbicide	2,6-dinitroaniline	-	
Vinclozolin	fungicide	dicarboximid	-	
Zearalenone	estrogen	resorcyclic acid lactone	7.6	(7)

Figure S1: Structural formulas of the target compounds (I).

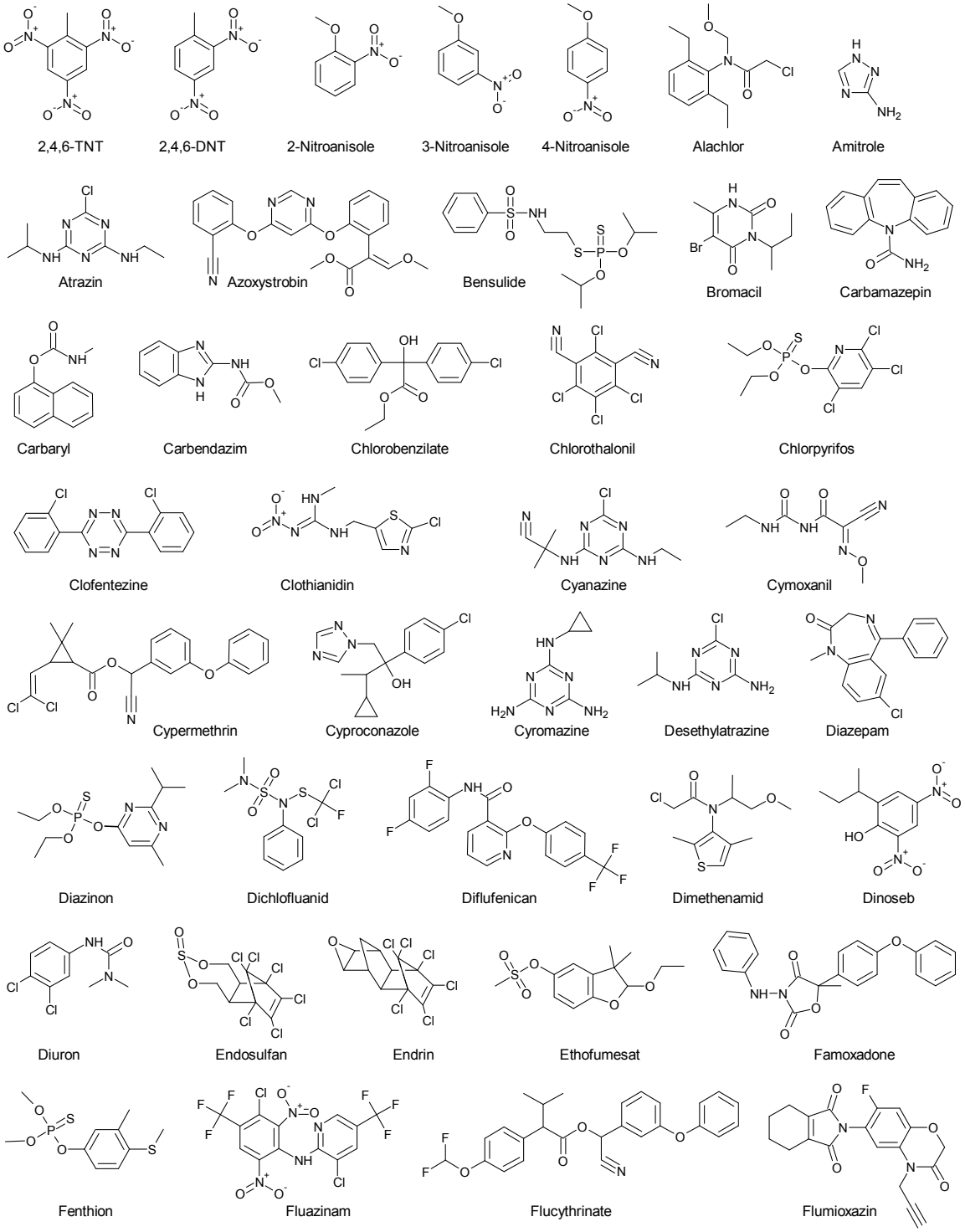


Figure S2: Structural formulas of the target compounds (II).

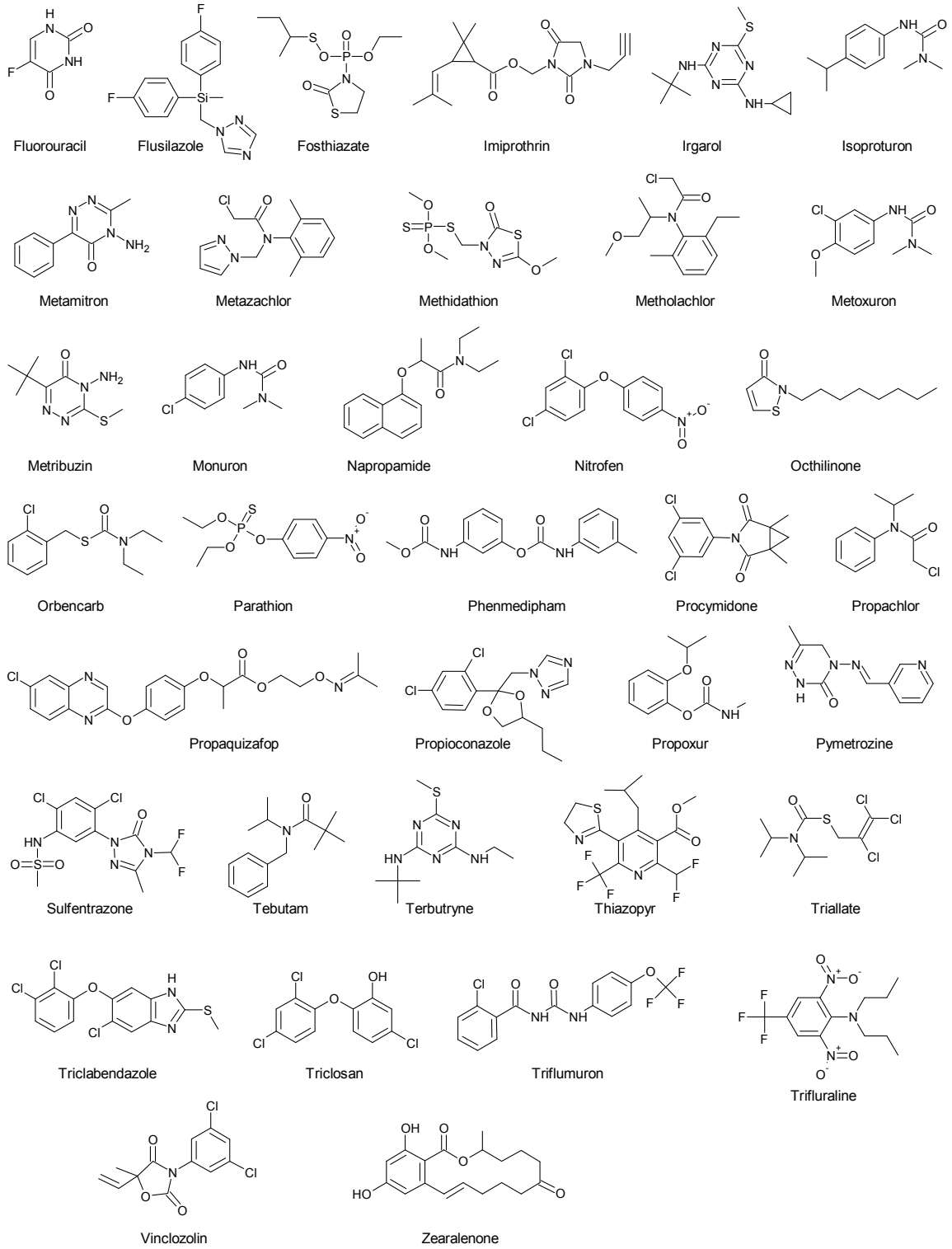


Table S5: Phase descriptors, standard errors and statistics of the partition systems used for validation.

phase descriptor	log K_{hm}	log K_{ow}	log K_{aw}
c	-0.056 ± 0.061	0.088 ± 0.015	0.994 ± 0.031
e	0.164 ± 0.045	0.562 ± 0.014	-0.577 ± 0.032
s	-0.62 ± 0.067	-1.054 ± 0.021	-2.549 ± 0.037
a	-1.337 ± 0.045	0.034 ± 0.021	-3.813 ± 0.04
b	-0.957 ± 0.093	-3.46 ± 0.026	-4.841 ± 0.04
v	0.507 ± 0.047	3.814 ± 0.015	0.869 ± 0.031
r^2	0.986	0.997	0.998
SE	0.086	0.116	0.151
n	65	613	408
F	413	23 162	16 810
ref	(8)	(2)	Recalculated from equation for L_w in ref. (9)

Table S6: Literature data for the octanol-water partition coefficient, K_{ow}, and the air-water partition coefficient, K_{aw}, used for validation of the substance descriptors of the target compounds. The column labeled as "origin" indicates whether K_{aw} was obtained from measured Henry's law constants, *H'*, or calculated from water solubility (S_w) and saturated vapor pressure (P^0).

substance	log K_{ow}	n	ref	log K_{aw} average	log K_{aw} min; max	origin	ref
2,4,6-TNT	2.06	1	(10)	- 5.98		S_w/P^0	(4)
2,4-Dinitrotoluene	2.00 ± 0.02	3	(5)	- 5.40	- 5.66; - 5.14	H' & S_w/P^0	(4)
2-Nitroanisole	1.73	1	(10)	- 4.76		S_w/P^0	(4)
3-Nitroanisole	2.16	1	(10)	n.a.			
4-Nitroanisole	2.03	1	(10)	- 4.29		H'	(4)
Alachlor	2.77 ± 0.42	3	(5)	- 6.17	- 6.47; - 5.60	H' & S_w/P^0	(5)
Amitrole	-0.16 ± 0.68	3	(5)	- 11.37	- 13.18; - 9.92	H' & S_w/P^0	(5)
Atrazine	2.59 ± 0.21	4	(5)	- 6.71	- 6.93; -6.60	H' & S_w/P^0	(5)
Azoxystrobin	2.50	1	(5)	- 11.53		S_w/P^0	(4)
Bensulide	4.10	1	(11)	- 6.16		S_w/P^0	(4)
Bromacil	1.87	1	(5)	- 8.28	- 8.43; - 8.19	H' & S_w/P^0	(5)
Carbamazepine	2.63 ± 0.49	3	(5,12)	n.a.			
Carbaryl	2.34 ± 0.04	2	(5)	- 6.70	- 6.75; - 6.65	H' & S_w/P^0	(5)
Carbendazim	1.51 ± 0.16	5	(5)	- 9.20		S_w/P^0	(5)
Chlorobenzilate	4.58	1	(11)	- 5.53		S_w/P^0	(4)
Chlorothalonil	2.97 ± 0.12	2	(5)	- 4.48	- 4.87; - 4.09	H' & S_w/P^0	(4)
Chlorpyrifos	5.07 ± 0.23	3	(5)	- 3.68	- 3.88; - 3.39	H' & S_w/P^0	(5)
Clofentezine	3.10	1	(11)	- 6.35	- 7.50; - 5.20	H' & S_w/P^0	(4)
Clothianidin	0.60 ± 0.14	2	(11)	- 13.40		S_w/P^0	(13)
Cyanazine	2.15 ± 0.10	3	(5)	- 9.92		S_w/P^0	(5)
Cymoxanil	0.67	1	(11)	- 7.84		S_w/P^0	(4)
Cypermethrin	5.66 ± 1.09	3	(5)	- 5.48	- 5.85; - 5.10	H' & S_w/P^0	(5)
Cyproconazole	2.91	1	(11)	- 7.76	- 8.15; - 7.54	H' & S_w/P^0	(4)

Cyromazine	-0.16	1	(11)	- 11.61		S_w/P^0	(4)
Desethylatrazine	1.70 ± 0.26	2	(5)	n.a.			
Diazepam	3.04 ± 0.31	2	(5)	n.a.			
Diazinon	3.35 ± 0.40	3	(5)	- 5.14	- 5.34; - 4.94	H' & S_w/P^0	(5)
Dichlofluanid	3.70	1	(11)	- 5.81		S_w/P^0	(4)
Diflufenican	4.90	1	(5)	- 4.87	- 4.88; - 4.87	H' & S_w/P^0	(4)
Dimethenamid	2.15	1	(5)	- 5.47		S_w/P^0	(4)
Dinoseb	3.47 ± 0.22	4	(5)	- 4.90		S_w/P^0	(5)
Diuron	2.67 ± 0.02	2	(5)	- 7.36	- 7.60; - 7.25	H' & S_w/P^0	(5)
Endosulfan	3.67 ± 0.15	3	(5)	- 4.24	- 4.92; - 3.36	H' & S_w/P^0	(5)
Endrin	4.88 ± 0.45	2	(5)	- 4.81	- 4.88; - 4.77	H' & S_w/P^0	(5)
Ethofumesate	2.69	1	(5)	- 6.16		S_w/P^0	(4)
Famoxadone	4.73 ± 0.11	2	(11)	- 5.71		S_w/P^0	(4)
Fenthion	4.13 ± 0.06	2	(5)	- 5.46	- 5.88; - 5.05	H' & S_w/P^0	(5)
Fluazinam	3.56	1	(14)	n.a.			
Flucythrinate	5.92 ± 0.52	2	(5)	- 6.36	- 6.36; - 6.35	H' & S_w/P^0	(5)
Flumioxazin	2.55	1	(15)	n.a.			
Fluorouracil	-0.89	1	(10)	n.a.			
Flusilazole	3.75 ± 0.01	2	(16)	- 7.04		S_w/P^0	(4)
Fosthiazate	1.75	1	(17)	- 8.25	- 8.36; - 8.15	H' & S_w/P^0	(4)
Imiprothrin	2.90	1	(18)	- 8.61		S_w/P^0	(4)
Irgarol	3.95	1	(19)	n.a.			
Isoproturon	2.38 ± 0.18	2	(5)	- 8.34	-8.37; - 8.30	H' & S_w/P^0	(5)
Metamitron	0.69 ± 0.20	2	(5)	- 10.41		S_w/P^0	(4)
Metazachlor	2.13	1	(5)	- 7.63		S_w/P^0	(4)
Methidathion	2.39 ± 0.26	2	(11)	- 6.59		S_w/P^0	(4)
Metolachlor	3.21 ± 0.11	2	(5)	- 6.43		S_w/P^0	(5)
Metoxuron	1.64	1	(16)	- 6.23		S_w/P^0	(4)
Metribuzin	1.65 ± 0.07	2	(5)	- 8.32		S_w/P^0	(4)
Monuron	1.82 ± 0.26	5	(5)	- 7.64		S_w/P^0	(5)
Napropamide	3.36	1	(5)	- 7.60		S_w/P^0	(4)
Nitrofen	4.64	1	(4)	n.a.			
Octhilinone	2.45	1	(20)	- 6.07		S_w/P^0	(4)
Orbencarb	3.50 ± 0.09	2	(5)	- 6.39		S_w/P^0	(5)
Parathion	3.83 ± 0.09	3	(5,21)	- 5.34	- 5.45; - 5.26	H' & S_w/P^0	(5)
Phenmedipham	3.59	1	(5)	- 10.46		S_w/P^0	(4)
Procymidone	3.07 ± 0.10	2	(5)	- 3.55		S_w/P^0	(5)
Propachlor	2.19 ± 0.59	5	(5)	- 5.37	- 5.38; - 5.35	H' & S_w/P^0	(4)
Propaquizafop	4.69 ± 0.13	2	(4,16)	- 9.90		S_w/P^0	(4)
Propiconazole	3.61 ± 0.16	2	(5)	- 7.15		S_w/P^0	(5)
Propoxur	1.55	1	(5)	- 7.25		S_w/P^0	(4)
Pymetrozine	-0.18	1	(22)	n.a.			
Sulfentrazone	0.99	1	(23)	- 10.58		S_w/P^0	(4)
Tebutam	3.50 ± 0.71	2	(5)	- 4.97		S_w/P^0	(4)
Terbutryn	3.61 ± 0.20	3	(5)	- 5.96		S_w/P^0	(4)
Thiazopyr	3.89	1	(24)	- 4.72		S_w/P^0	(4)
Triallate	4.66 ± 0.51	4	(5)	- 3.31		S_w/P^0	(5)
Triclabendazol	n.a.			n.a.			
Triclosan	4.92 ± 0.42	3	(5)	n.a.			
Triflumuron	4.91	1	(4)	- 6.64		S_w/P^0	(4)

Trifluralin	4.73 ± 0.62	5	(5)	- 3.35	- 4.08; - 2.62	H' & S_w/P^0	(5)
Vinclozolin	2.74 ± 0.37	2	(5)	- 6.27		S_w/P^0	(5)
Zearalenone	4.12 ± 0.86	3	(7,25)	n.a.			

Experimental procedure for the determination of n-heptane-methanol partition coefficients (K_{hm})

A 2 mL crimp cap vial was filled with 0.75 mL of each, methanol and n-heptane. The vials had been oven-dried for one hour at 105°C just before filling. The target compound was added as a saturated solution in methanol at a volume of 50 µL. The vials were shaken for 10 min in an overhead shaker and then allowed to stand for at least 1 h but no longer than 24 h prior to injection into the HPLC system. The chromatographic set up was a C_{18} (50 × 4 mm) stationary phase with methanol as mobile phase at a flow rate of 1 mL/min. The injection volume was 10 µL. The target solutes were detected at a wavelength of 230, 254 and 270 nm respectively, with the wavelengths closest to maximum UV absorbance selected for the analysis of each solute. The partition coefficients of the solutes were determined as the ratio of the solute peak areas in the heptane and the methanol phases. Before and after every run the partition coefficient of toluene was determined by the same procedure to check the accuracy of the injection volumes. The K_{hm} of toluene varied within 5% for the whole series of K_{hm} measurements.

Table S7: Measured and calculated n-heptane-methanol partition coefficients of the target substances and their detection wavelengths.

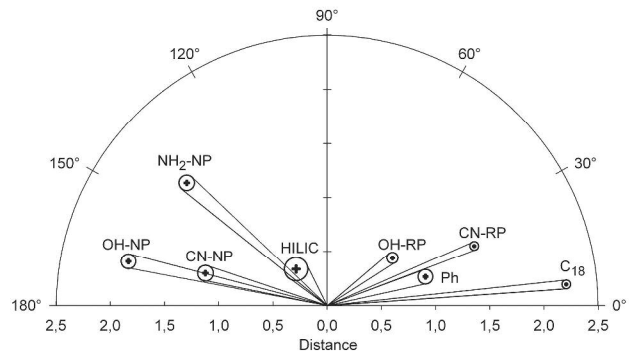
Substance	**Measured**	**Calculated**	**λ [nm]**
2,4,6-TNT	-0.802 ± 0.122	-0.942 ± 0.732	230
2,4-DNT	-0.649 ± 0.066	-0.850 ± 0.631	230
2-Nitroanisole	n.d.		
3-Nitroanisole	-0.478 ± 0.026	-0.652 ± 0.568	230
4-Nitroanisole	-0.737 ± 0.013	-0.795 ± 0.569	230
Alachlor	-0.496 ± 0.028	-0.632 ± 0.216	230
Amitrole	n.d.		
Atrazine	-0.912 ± 0.006	-0.739 ± 0.200	230
Azoxystrobin	-1.294 ± 0.103	-1.364 ± 0.332	254
Bensulide	-1.566 ± 0.075	-1.388 ± 0.297	254
Bromacil	-1.522 ± 0.029	-1.723 ± 0.256	254
Carbamazepine	-1.387 ± 0.051	-1.487 ± 0.257	230
Carbaryl	-1.139 ± 0.091	-1.144 ± 0.181	254
Carbendazim	n.d.		
Chlorobenzilate	-0.356 ± 0.039	-0.528 ± 0.374	254
Chlorothalonil	-0.709 ± 0.017	-0.570 ± 0.280	254
Chlorpyrifos	0.022 ± 0.015	0.046 ± 0.455	254
Clofentezine	-0.515 ± 0.014	-0.601 ± 0.285	230
Chlothianidin	-2.351 ± 0.315	-2.194 ± 0.265	230
Cyanazine	-1.299 ± 0.244	-1.207 ± 0.230	254

Cymoxanil	-1.769 ± 0.111	-1.809 ± 0.202	270
Cypermethrin	-0.169 ± 0.062	-0.157 ± 0.683	254
Cyproconazole	-1.124 ± 0.316	-1.074 ± 0.266	254
Cyromazine	-2.052 ± 0.020	-1.899 ± 0.484	230
Desethylatrazine	-1.295 ± 0.164	-1.164 ± 0.179	254
Diazepam	n.d.		
Diazinon	-0.343 ± 0.037	-0.386 ± 0.215	230
Dichlofluanid	-0.716 ± 0.035	-0.619 ± 0.294	254
Diflufenican	-0.596 ± 0.074	-0.476 ± 0.249	254
Dimethenamid	-0.720 ± 0.343	-0.752 ± 0.227	230
Dinoseb	n.d.		
Diuron	-1.226 ± 0.098	-1.323 ± 0.188	254
Endosulfan	-0.496 ± 0.088	-0.527 ± 0.318	230
Endrin	-0.125 ± 0.132	-0.103 ± 0.228	230
Ethofumesate	-1.041 ± 0.102	-1.018 ± 0.225	254
Famoxadone	-1.435 ± 0.036	-1.043 ± 0.298	254
Fenthion	-0.485 ± 0.063	-0.553 ± 0.227	230
Fluazinam	-0.930 ± 0.154	-1.130 ± 0.302	230
Flucythrinate	-0.869 ± 0.044	-1.050 ± 0.459	270
Flumioxazin	-1.610 ± 0.119	-1.105 ± 0.335	254
Fluoruracil	n.d.		
Flusilazole	-1.078 ± 0.015	-1.183 ± 0.235	230
Fosthiazate	-1.390 ± 0.119	-1.220 ± 0.278	254
Imiprothrin	-1.093 ± 0.083	-1.143 ± 0.258	254
Irgarol	-0.524 ± 0.058	-0.469 ± 0.239	230
Isoproturon	-1.342 ± 0.017	-1.349 ± 0.192	254
Metamitron	-1.739 ± 0.062	-1.535 ± 0.223	254
Metazachlor	-0.992 ± 0.040	-0.940 ± 0.243	254
Methidathion	-0.811 ± 0.071	-0.861 ± 0.295	270
Metolachlor	-0.556 ± 0.041	-0.712 ± 0.219	230
Metoxuron	-1.448 ± 0.088	-1.639 ± 0.205	230
Metribuzin	-0.952 ± 0.148	-0.970 ± 0.219	254
Monuron	-1.357 ± 0.192	-1.416 ± 0.180	254
Napropamide	-0.742 ± 0.073	-0.718 ± 0.228	230
Nitrofen	n.d.		
Octhilinone	-0.993 ± 0.109	-1.090 ± 0.190	254
Orbencarb	-0.194 ± 0.015	-0.327 ± 0.196	230
Parathion	-0.535 ± 0.095	-0.632 ± 0.226	270
Phenmedipham	-1.753 ± 0.076	-1.496 ± 0.239	254
Procymidone	-0.529 ± 0.036	-0.407 ± 0.326	254
Propachlor	-0.760 ± 0.041	-0.752 ± 0.194	230
Propaquizafop	-0.565 ± 0.124	-0.482 ± 0.516	230
Propiconazole	-0.777 ± 0.100	-0.683 ± 0.258	254
Propoxur	-1.326 ± 0.063	-1.134 ± 0.186	270
Pymetrozine	n.d.		
Sulfentrazone	-1.643 ± 0.092	-1.597 ± 0.361	270
Tebutam	-0.554 ± 0.030	-0.661 ± 0.199	254
Terbutryn	-0.612 ± 0.016	-0.537 ± 0.203	230
Thiazopyr	-0.714 ± 0.045	-0.727 ± 0.247	254
Triallate	0.020 ± 0.054	-0.767 ± 0.253	254
Triclabendazole	-1.099 ± 0.157	-0.868 ± 0.262	254
Triclosan	-0.949 ± 0.044	-1.361 ± 0.256	230
Triflumuron	-1.077 ± 0.018	-1.043 ± 0.257	270
Trifluraline	-0.043 ± 0.022	-0.020 ± 0.490	230
Vinclozolin	-0.508 ± 0.014	-0.440 ± 0.332	254
Zearalenone	n.d.		

Detailed analysis of diversity of HPLC systems

The diversity of the HPLC systems was examined with an angle analysis according to Ishihama and Asakawa (26) (Figure S1). An angle of 90° between two systems indicates maximal difference of retention characteristics, whereas an angle of 180° implies that the retention characteristics between mobile and stationary phases are perfectly opposite in the two systems, resulting in a reversed elution order. Hence there is no new information in a system that lies at an 180° angle from another system.

Figure S3: Angle plot of eight HPLC systems. Each HPLC system is shown as endpoint of a vector whose length and orientation is determined by the phase descriptors of that system. The diameter of the circles represents the uncertainty of the phase descriptors for each system.



The systems can be grouped in two classes: The RP systems in the first and the NP systems in the second quadrant. Whereas the typical RP systems (C18, Ph, CN-RP) and the typical NP systems (OH-NP, CN-NP) span angles close to 180°, the HILIC, NH_2-NP and OH-RP systems occupy an intermediate position, thereby ensuring that the set of systems shows diverse retention behavior.

The retention of solutes in the RP systems is primarily governed by the molecular volume *V* and the ability of the solutes to form hydrogen bonds with the mobile phase components water or methanol (27,28), resulting in marked and negative *b* descriptors for such systems. The dominant phase descriptors in the NP systems are *s*, *a* and *b* with positive values. In this case the functional groups of the stationary phase provide a higher potential for polar interactions than the only weakly polar mobile phase. Further system diversity is introduced by the fact that the OH-NP and the NH_2-NP system are complementary regarding their *a* and *b* descriptors. The hydroxy groups of the OH-phase act predominantly as H-donors and can form H-bonds with H-bond accepting solutes, resulting in a large *b* descriptor. The contrary is the case for the NH_2 phase. The amino groups predominantly act as H-acceptors, hence yielding a large *a* descriptor. The NH_2-

NP and also the HILIC system thus play an important role in that they strongly respond to the H-donor capability of solutes and are therefore essential in determining the *A* solute descriptor.

Table S8: Regression coefficients for eqs 4a-c for target compounds that were not measured in all eight HPLC systems.

for alachlor, carbamazepine, diazepam, metamitron, methidathion, triclosan and zearalenone

System	**S**	**A**	**B**
const.	0.176 ± 0.048	-0.028 ± 0.022	-0.041 ± 0.015
C_{18}	-0.525 ± 0.263	0.460 ± 0.122	-0.237 ± 0.085
Ph	2.369 ± 0.637	-1.828 ± 0.295	-0.503 ± 0.205
CN-RP	0.211 ± 0.226	0.423 ± 0.105	-0.264 ± 0.073
OH-RP	-0.267 ± 0.290	0.125 ± 0.134	-0.109 ± 0.093
CN-NP	1.204 ± 0.293	-0.161 ± 0.136	-0.363 ± 0.094
OH-NP	0.146 ± 0.214	-0.158 ± 0.099	0.071 ± 0.069
NH_2-NP	0.224 ± 0.119	0.352 ± 0.055	-0.157 ± 0.038
r^2	0.859	0.947	0.956
SE	0.135	0.060	0.042
F	51	149	182
n	67	67	67

for amitrole

System	**S**	**A**	**B**
const.	0.140 ± 0.050	-0.009 ± 0.022	-0.030 ± 0.016
C_{18}	-1.219 ± 0.193	0.594 ± 0.084	-0.093 ± 0.060
Ph	0.818 ± 0.581	-1.450 ± 0.254	-0.135 ± 0.181
CN-RP	0.929 ± 0.197	0.287 ± 0.086	-0.499 ± 0.061
OH-RP	-0.314 ± 0.281	0.156 ± 0.123	-0.025 ± 0.088
HILIC	-1.405 ± 0.284	0.481 ± 0.124	0.396 ± 0.089
NH_2-NP	0.235 ± 0.112	0.301 ± 0.049	-0.145 ± 0.035
r^2	0.859	0.952	0.958
SE	0.130	0.057	0.041
F	60	197	226
n	65	65	65

for dinoseb

System	**S**	**A**	**B**
const.	0.136 ± 0.048	0.000 ± 0.027	-0.030 ± 0.017
C_{18}	-0.684 ± 0.256	0.438 ± 0.146	-0.165 ± 0.093
Ph	0.886 ± 0.480	-2.548 ± 0.274	0.279 ± 0.175
CN-RP	0.942 ± 0.182	0.656 ± 0.104	-0.610 ± 0.066
OH-RP	-0.438 ± 0.287	0.361 ± 0.164	-0.109 ± 0.105
HILIC	-0.822 ± 0.284	0.645 ± 0.162	0.222 ± 0.103
CN-NP	0.602 ± 0.280	-0.276 ± 0.160	-0.094 ± 0.102
OH-NP	0.294 ± 0.196	0.045 ± 0.112	-0.020 ± 0.071
r^2	0.869	0.952	0.948
SE	0.125	0.072	0.046
F	56	104	153
n	67	67	67

for famoxadone and fluazinam

System	S	A	B
const.	0.177 ± 0.055	-0.017 ± 0.025	-0.045 ± 0.022
C_{18}	0.140 ± 0.207	0.370 ± 0.094	-0.670 ± 0.081
HILIC	-0.868 ± 0.294	0.623 ± 0.133	0.265 ± 0.115
CN-NP	-0.207 ± 0.187	-0.066 ± 0.085	0.213 ± 0.073
OH-NP	-0.207 ± 0.187	-0.066 ± 0.085	0.213 ± 0.073
NH_2-NP	0.296 ± 0.091	0.486 ± 0.041	-0.255 ± 0.036
r^2	0.810	0.931	0.913
SE	0.148	0.067	0.058
F	54	169	133
n	69	69	69

Table S9: Experimentally determined substance descriptors *S*, *A*, and *B*. The *E* descriptor was calculated with the SPARC online calculator.

Nr.	substance	S	A	B	E	V
1	2,4,6-TNT	1.70 ± 0.19	0.13 ± 0.09	0.59 ± 0.06	1.40	1.380
2	2,4-Dinitrotoluene	1.27 ± 0.18	0.07 ± 0.08	0.51 ± 0.06	1.18	1.206
3	2-Nitroanisole	1.47 ± 0.07	0.21 ± 0.03	0.31 ± 0.02	0.96	1.090
4	3-Nitroanisole	1.20 ± 0.08	0.14 ± 0.04	0.27 ± 0.03	0.96	1.090
5	4-Nitroanisole	1.32 ± 0.10	0.19 ± 0.05	0.25 ± 0.03	0.91	1.090
6	Alachlor	1.15 ± 0.13	0.06 ± 0.06	1.23 ± 0.04	1.38	2.140
7	Amitrole	0.86 ± 0.20	1.11 ± 0.09	0.35 ± 0.06	0.44	0.595
8	Atrazine	1.20 ± 0.08	0.01 ± 0.04	0.94 ± 0.03	0.94	1.620
9	Azoxystrobin	2.08 ± 0.20	0.15 ± 0.09	1.88 ± 0.07	2.24	2.917
10	Bensulide	1.72 ± 0.16	0.51 ± 0.08	1.55 ± 0.05	2.09	2.873
11	Bromacil	1.02 ± 0.14	0.86 ± 0.07	0.92 ± 0.05	1.26	1.631
12	Carbamazepine	1.52 ± 0.29	0.44 ± 0.13	1.45 ± 0.09	3.42	1.811
13	Carbaryl	1.34 ± 0.13	0.40 ± 0.06	0.83 ± 0.04	1.71	1.541
14	Carbendazim	1.69 ± 0.15	0.58 ± 0.07	0.68 ± 0.05	1.87	1.361
15	Chlorobenzilate	0.36 ± 0.28	0.06 ± 0.13	1.44 ± 0.09	1.65	2.266
16	Chlorothalonil	2.08 ± 0.20	-0.26 ± 0.09	0.43 ± 0.06	1.35	1.515
17	Chlorpyrifos	0.34 ± 0.40	-0.37 ± 0.19	1.11 ± 0.13	1.29	2.150
18	Clofentezine	0.93 ± 0.21	0.09 ± 0.10	1.06 ± 0.07	2.08	2.012
19	Clothianidin	2.07 ± 0.16	0.92 ± 0.08	0.84 ± 0.05	1.38	1.576
20	Cyanazine	1.64 ± 0.09	0.27 ± 0.04	1.08 ± 0.03	1.15	1.774
21	Cymoxanil	1.80 ± 0.18	0.56 ± 0.09	0.77 ± 0.06	0.46	1.455
22	Cypermethrin	0.24 ± 0.60	0.02 ± 0.28	1.55 ± 0.19	1.72	2.973
23	Cyproconazole	1.07 ± 0.16	0.35 ± 0.08	1.36 ± 0.05	1.70	2.162
24	Cyromazine	0.03 ± 0.28	1.36 ± 0.13	1.17 ± 0.09	1.24	1.207
25	Desethylatrazine	1.03 ± 0.09	0.40 ± 0.04	0.96 ± 0.03	1.06	1.338
26	Diazepam	1.46 ± 0.21	0.10 ± 0.10	1.36 ± 0.07	2.49	2.074
27	Diazinon	1.00 ± 0.12	0.02 ± 0.06	1.16 ± 0.04	0.89	2.306
28	Dichlofluanid	1.17 ± 0.18	-0.03 ± 0.09	1.18 ± 0.06	1.64	2.046
29	Diflufenican	1.00 ± 0.20	0.36 ± 0.09	1.11 ± 0.06	1.39	2.435
30	Dimethenamid	1.28 ± 0.13	-0.02 ± 0.06	1.25 ± 0.04	1.26	2.065
31	Dinoseb	1.77 ± 0.24	0.13 ± 0.14	0.53 ± 0.09	1.28	1.687
32	Diuron	1.59 ± 0.08	0.50 ± 0.04	0.74 ± 0.03	1.54	1.599
33	Endosulfan	0.88 ± 0.12	0.47 ± 0.06	0.98 ± 0.04	1.26	2.082
34	Endrin	1.28 ± 0.25	-0.01 ± 0.12	0.38 ± 0.08	0.54	2.007

35	Ethofumesate	1.69 ± 0.08	0.13 ± 0.04	1.01 ± 0.03	0.85	2.051
36	Famoxadone	2.21 ± 0.15	0.26 ± 0.07	1.21 ± 0.06	2.63	2.735
37	Fenthion	1.75 ± 0.09	-0.04 ± 0.04	0.67 ± 0.03	1.42	1.988
38	Fluazinam	1.70 ± 0.17	0.24 ± 0.08	1.23 ± 0.07	1.13	2.364
39	Flucythrinate	-0.09 ± 0.44	0.71 ± 0.21	2.57 ± 0.14	1.69	3.300
40	Flumioxazin	2.17 ± 0.15	0.12 ± 0.07	1.10 ± 0.05	0.42	2.416
41	Fluoruracil	0.67 ± 0.23	1.05 ± 0.11	0.77 ± 0.07	1.08	0.769
42	Flusilazole	n.a.	n.a.	n.a.	n.a.	n.a.
43	Fosthiazate	1.37 ± 0.10	0.34 ± 0.05	1.21 ± 0.03	0.86	2.091
44	Imiprothrin	1.33 ± 0.17	0.23 ± 0.08	1.40 ± 0.06	0.92	2.463
45	Irgarol	1.51 ± 0.12	-0.24 ± 0.06	0.95 ± 0.04	1.32	1.975
46	Isoproturon	1.53 ± 0.09	0.39 ± 0.04	0.97 ± 0.03	1.24	1.777
47	Metamitron	1.72 ± 0.11	0.35 ± 0.05	0.86 ± 0.04	0.84	1.500
48	Metazachlor	1.50 ± 0.19	0.09 ± 0.09	1.41 ± 0.06	1.85	2.087
49	Methidathion	1.77 ± 0.12	0.03 ± 0.06	0.91 ± 0.04	1.28	1.889
50	Metolachlor	1.03 ± 0.13	0.04 ± 0.06	1.44 ± 0.04	1.44	2.281
51	Metoxuron	1.79 ± 0.10	0.48 ± 0.05	0.92 ± 0.03	1.51	1.676
52	Metribuzin	1.09 ± 0.10	0.45 ± 0.05	0.78 ± 0.03	0.29	1.620
53	Monuron	1.51 ± 0.08	0.46 ± 0.04	0.82 ± 0.03	1.40	1.477
54	Napropamide	1.43 ± 0.09	0.04 ± 0.04	1.21 ± 0.03	1.43	2.246
55	Nitrofen	0.82 ± 0.31	-0.29 ± 0.15	0.87 ± 0.10	1.83	1.802
56	Octhilinone	1.68 ± 0.18	0.15 ± 0.08	0.59 ± 0.06	0.72	1.786
57	Orbencarb	1.17 ± 0.08	-0.07 ± 0.04	0.83 ± 0.03	1.22	1.963
58	Parathion	1.75 ± 0.08	0.07 ± 0.04	0.68 ± 0.03	1.14	1.998
59	Phenmedipham	1.64 ± 0.18	0.58 ± 0.09	1.38 ± 0.06	2.15	2.236
60	Procymidone	0.51 ± 0.19	-0.01 ± 0.09	1.25 ± 0.06	1.45	1.862
61	Propachlor	1.41 ± 0.11	-0.08 ± 0.05	0.96 ± 0.03	1.11	1.659
62	Propaquizafop	1.42 ± 0.46	-1.05 ± 0.22	2.52 ± 0.15	1.80	3.168
63	Propiconazole	1.41 ± 0.08	0.12 ± 0.04	1.18 ± 0.03	1.24	2.343
64	Propoxur	1.21 ± 0.10	0.36 ± 0.05	0.95 ± 0.03	0.95	1.654
65	Pymetrozine	2.52 ± 0.30	0.56 ± 0.14	0.73 ± 0.10	0.94	1.600
66	Sulfentrazone	1.28 ± 0.21	0.75 ± 0.10	1.55 ± 0.07	1.74	2.245
67	Tebutam	1.11 ± 0.08	0.03 ± 0.04	1.11 ± 0.03	0.75	2.100
68	Terbutryn	1.33 ± 0.09	-0.12 ± 0.04	0.95 ± 0.03	1.21	1.943
69	Thiazopyr	1.07 ± 0.19	0.06 ± 0.09	1.32 ± 0.06	0.80	2.499
70	Triallate	0.90 ± 0.27	0.22 ± 0.13	0.71 ± 0.09	0.86	2.121
71	Triclabendazole	1.67 ± 0.11	0.39 ± 0.05	1.03 ± 0.03	2.84	2.243
72	Triclosan	1.66 ± 0.19	0.74 ± 0.09	0.33 ± 0.06	2.00	1.809
73	Triflumuron	1.14 ± 0.15	0.64 ± 0.07	0.94 ± 0.05	1.62	2.212
74	Trifluraline	0.39 ± 0.32	-0.07 ± 0.15	1.29 ± 0.10	0.77	2.204
75	Vinclozolin	1.24 ± 0.20	-0.29 ± 0.10	1.24 ± 0.07	1.35	1.845
76	Zearalenone	1.57 ± 0.13	0.84 ± 0.06	1.25 ± 0.04	1.75	2.463

Figure S4: Boxplot comparing the range of values of solute descriptors of the calibration and the target compounds.

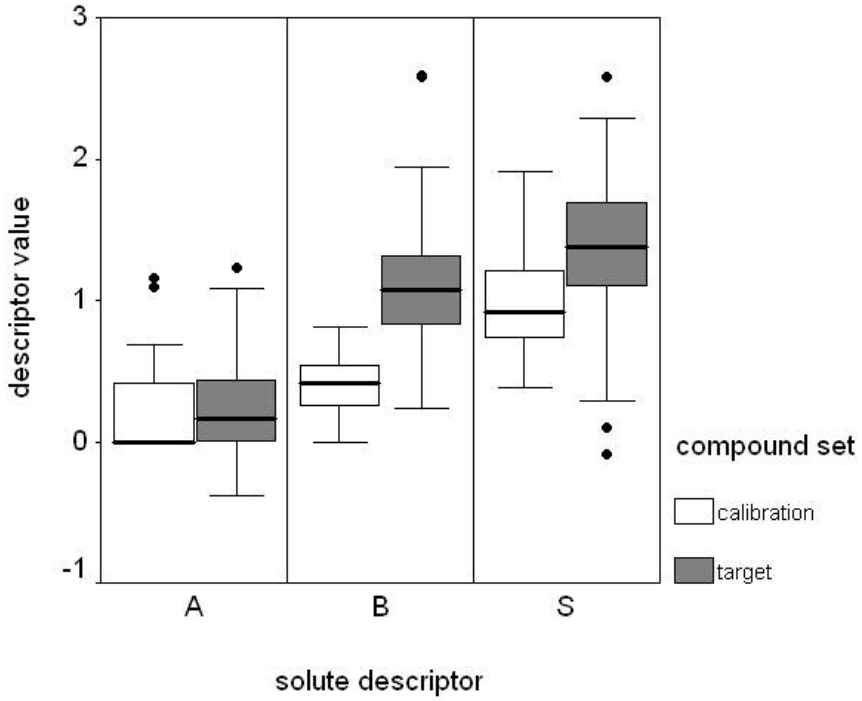
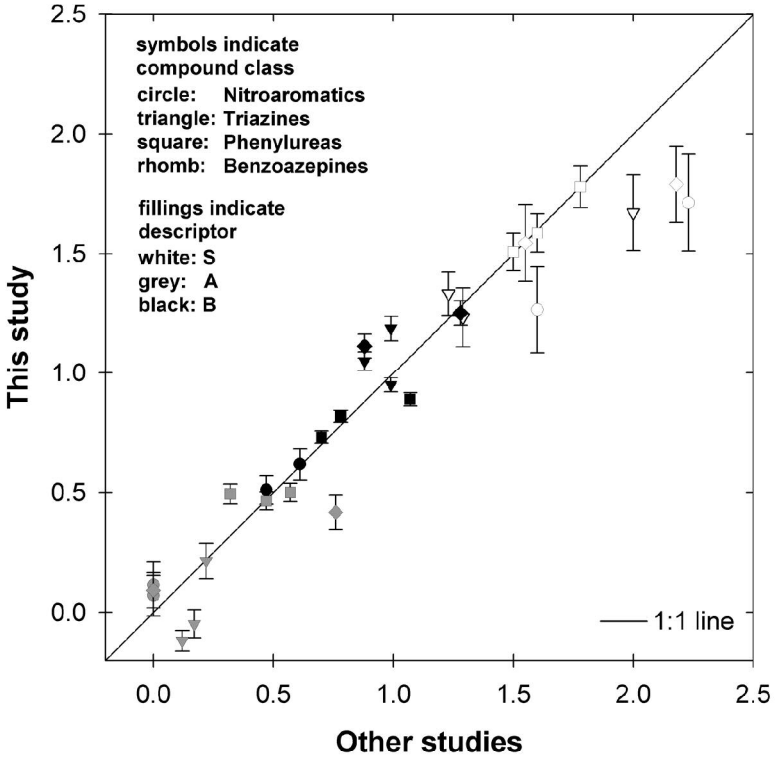


Figure S5: Comparison of experimentally determined solute descriptors *S*, *A* and *B* from this study and from various other workers for two nitroaromatics (TNT and 2,4-DNT) (29), three triazines (atrazin, cyanazin and terbutryn) (30), three phenylureas (diuron, monuron and metoxuron) (31) and two benzoazepines (carbamazepine and diazepam) (32,33). Error bars indicate one standard error.



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