Supporting Information

Developing predictive models for carrying ability of micro-plastics towards organic pollutants

Xiaoxuan Wei, Miao Li, Yifei Wang, Lingmin Jin, Guangcai Ma and Haiying Yu *

College of Geography and Environmental Sciences, Zhejiang Normal University, Yingbin Avenue 688, 321004, Jinhua, P.R. China

* Correspondence: yhy@zjnu.cn; Tel.: 0086 579 8228 2273

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The redeveloped models of the training sets are listed as following:

$$\log K_d = (-3.822 \pm 0.000) \times B + (3.054 \pm 0.000) \times V + (1.293 \pm 0.000) \times E + (-1.411 \pm 0.000) \quad \text{(S1)}$$

$$\log K_d = (-3.328 \pm 0.321) \times B + (6.046 \pm 1.299) \times V + (-4.807 \pm 2.482) \quad \text{(S2)}$$

$$\log K_d = (-2.517 \pm 0.122) \times B + (2.804 \pm 0.164) \times V + (1.085 \pm 0.259) \quad \text{(S3)}$$

$$\log K_d = (-3.248 \pm 0.242) \times B + (1.244 \pm 0.155) \times E + (3.225 \pm 0.353) \quad \text{(S4)}$$

$$\log K_d = (0.470 \pm 0.082) \times \log K_{OW} + (4.217 \pm 0.422) \times \pi + (-3.242 \pm 0.661) \quad \text{(S5)}$$

The regression models of the test sets are listed as following:

$$\log K_d = (-6.241 \pm 0.365) \times B + (2.901 \pm 0.356) \times V + (1.164 \pm 0.130) \times E + (-0.273 \pm 0.502) \quad \text{(S6)}$$

$$\log K_d = (-4.000 \pm 0.432) \times B + (2.729 \pm 1.419) \times V + (1.560 \pm 2.736) \quad \text{(S7)}$$

$$\log K_d = (-3.646 \pm 0.291) \times B + (3.088 \pm 0.083) \times V + (0.762 \pm 0.172) \quad \text{(S8)}$$

$$\log K_d = (-4.411 \pm 0.564) \times B + (1.399 \pm 0.200) \times E + (3.077 \pm 0.465) \quad \text{(S9)}$$

$$\log K_d = (0.392 \pm 0.164) \times \log K_{OW} + (4.006 \pm 0.872) \times \pi + (-2.838 \pm 1.415) \quad \text{(S10)}$$

Text S1. The computational formulations of the squared correlation coefficient R^2, predictive squared correlation coefficient Q^2, root-mean-square error (*RMSE*) and variance inflating factor (VIF) are shown here. The two statistics are used to quantify the validation and prediction performance of the developed QSPR models.

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i^{fit} - y_i^{exp})^2}{\sum_{i=1}^{n}(y_i^{exp} - \bar{y}^{exp})^2} \tag{S11}$$

$$Q^2 = 1 - \frac{\sum_{i=1}^{n}(y_i^{pred} - y_i^{exp})^2}{\sum_{i=1}^{n}(y_i^{exp} - \bar{y}^{exp})^2} \tag{S12}$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(y_i^{pred} - y_i^{exp})^2}{n}} \tag{S13}$$

$$VIF = \frac{1}{1 - R_i^2} \tag{S14}$$

where, y_i^{fit}, y_i^{exp}, $\bar{y}^{exp}$, and y_i^{pred} is the regression-fitted, experimental, average experimental, and predictive value of logK_d, respectively. R_i^2 is the determination coefficient for the regression of one parameter on all other independent variables in the dataset.

In statistics, the mean absolute error (*MAE*) is a quantity used to measure how close the predictive values are to the experimental values. The mean absolute error can be calculated by:

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|E_i| \quad , \quad |E_i| = |y_i^{\,a} - y_i^{\,b}| \tag{S15}$$

where, the y_i^a is the predictive value and the y_i^b is the experimental values.

A systematic error is an error that will occur consistently in only direction each time the experiment is performed and the values of the measurement will always be greater or lesser than the real values. Systematic errors most commonly arise from defects in the instrumentation or from using improper measuring techniques. The systematic error can be calculated by:

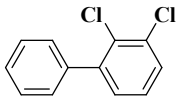
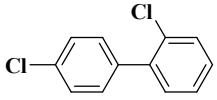
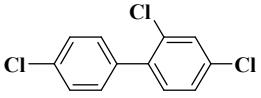
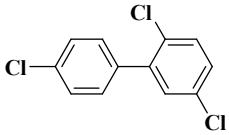
$$BIAS = \frac{1}{n}\sum_{i=1}^{n}E_i \quad , \quad E_i = y_i^{\,a} - y_i^{\,b} \tag{S15}$$

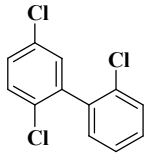
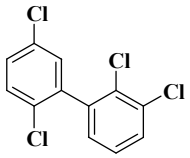
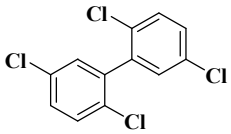
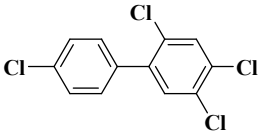
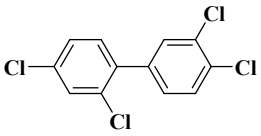
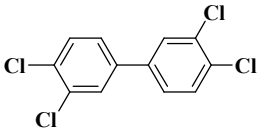
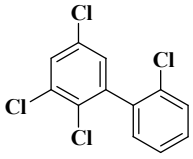
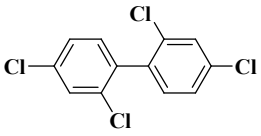
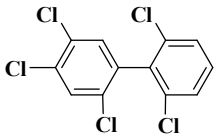
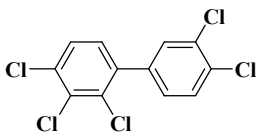
where, the y_i^a is the predictive value and the y_i^b is the experimental values.

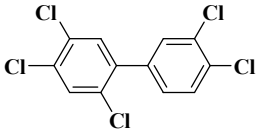
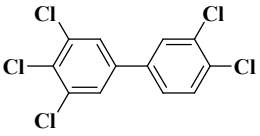
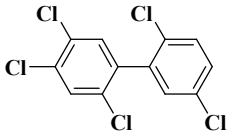
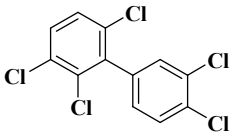
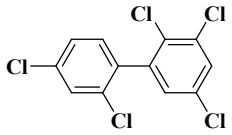
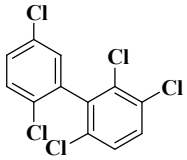
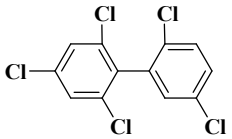
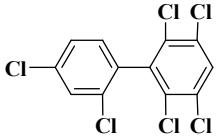
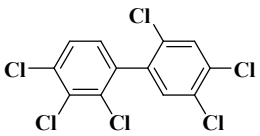
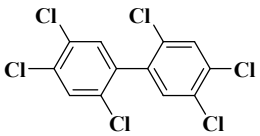
Table S1. Coefficients, *t* value of the *t* test, significance level (*p* value) and variance inflation factor (*VIF*) of the molecular structural descriptors involved in log K_d models.

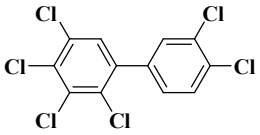
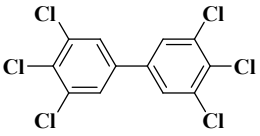
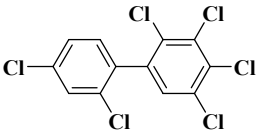
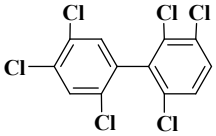
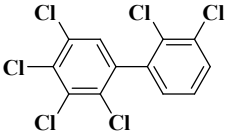
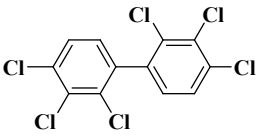
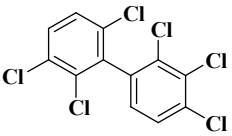
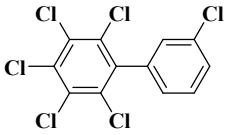
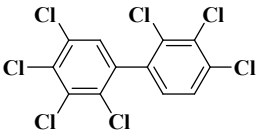
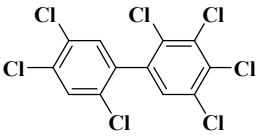
Models	Parameters	Coefficients	*t* value	*p* value	*VIF*
Model (1)	*B*	−3.822	−17.240	<0.001	1.471
	V	3.054	8.776	<0.001	1.464
	E	1.293	7.482	<0.001	1.065
Model (2)	*B*	−3.302	−14.168	<0.001	1.211
	V	5.594	6.307	<0.001	1.211
Model (4)	*B*	−2.594	−25.788	<0.001	1.395
	V	2.940	24.364	<0.001	1.395
Model (5)	*B*	−3.357	−15.342	<0.001	1.001
	E	1.299	10.229	<0.001	1.001
Model (6)	*A*	−14.645	−6.945	<0.001	1.000
Model (7)	π	4.141	11.173	<0.001	1.007
	logK_{ow}	0.435	6.173	<0.001	1.007

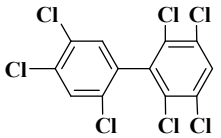
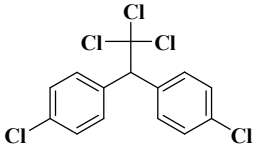
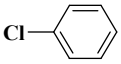
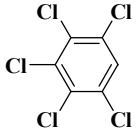
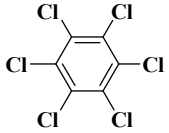
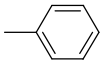
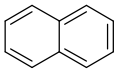
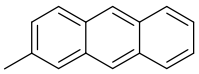
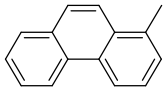
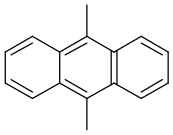
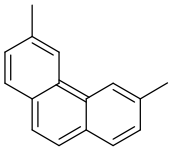
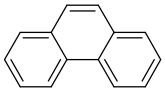
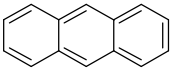
Table S2. Molecular structures and CAS number of all the studied organic compounds

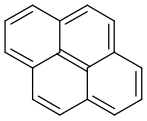
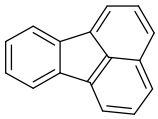
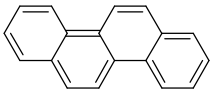
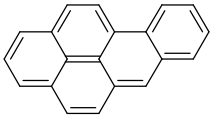
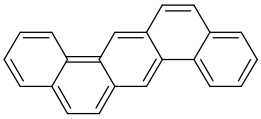
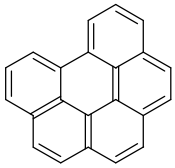
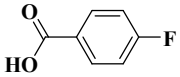
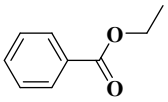
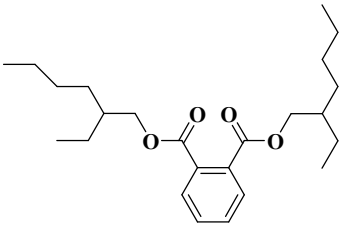
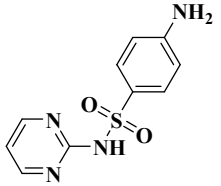
No.	Organic pollutants	CAS	Structures
1	2,3-dichlorobiphenyl	16605-91-7	
2	2,4'-dichlorobiphenyl	34883-43-7	
3	2,4,4'-trichlorobiphenyl	7012-37-5	
4	2,4',5-trichlorobiphenyl	16606-02-3	

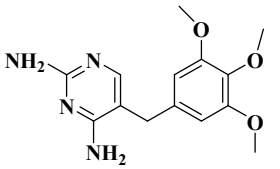
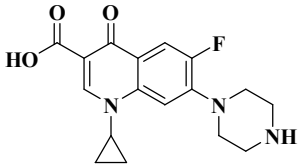
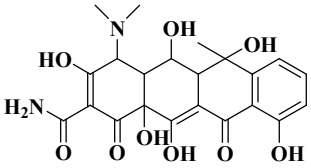
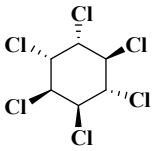
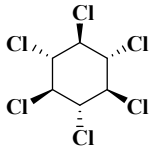
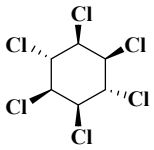
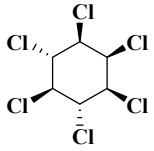
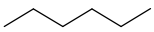
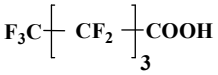
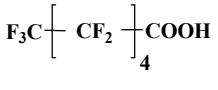
No.	Organic pollutants	CAS	Structures
5	2,2',5-trichlorobiphenyl	37680-65-2	
6	2,2',3,5'-tetrachlorobiphenyl	41464-39-5	
7	2,2',5,5'-tetrachlorobiphenyl	35693-99-3	
8	2,4,4',5-tetrachlorobiphenyl	32690-93-0	
9	2,3',4,4'-tetrachlorobiphenyl	32598-10-0	
10	3,3',4,4'-tetrachlorobiphenyl	32598-13-3	
11	2,2',3,5-tetrachlorobiphenyl	70362-46-8	
12	2,2',4,4'-tetrachlorobiphenyl	2437-79-8	
13	2,2',4,5,6'-pentachlorobiphenyl	68194-06-9	
14	2,3,3',4,4'-pentachlorobiphenyl	32598-14-4	

No.	Organic pollutants	CAS	Structures
15	2,3',4,4',5-pentachlorobiphenyl	31508-00-6	
16	3,3',4,4',5-pentachlorobiphenyl	57465-28-8	
17	2,2',4,5,5'-pentachlorobiphenyl	37680-73-2	
18	2,3,3',4',6-pentachlorobiphenyl	38380-03-9	
19	2,2',3,4',5-pentachlorobiphenyl	68194-07-0	
20	2,2',3,5',6-pentachlorobiphenyl	38379-99-6	
21	2,2',4,5',6-pentachlorobiphenyl	60145-21-3	
22	2,2',3,4',5,6-hexachlorobiphenyl	68194-13-8	
23	2,2',3,4,4',5'-hexachlorobiphenyl	35065-28-2	
24	2,2',4,4',5,5'-hexachlorobiphenyl	35065-27-1	

No.	Organic pollutants	CAS	Structures
25	2,3,3',4,4',5-hexachlorobiphenyl	38380-08-4	
26	3,3',4,4',5,5'-hexachlorobiphenyl	32774-16-6	
27	2,2',3,4,4',5-hexachlorobiphenyl	35694-06-5	
28	2,2',3,4',5',6-hexachlorobiphenyl	38380-04-0	
29	2,2',3,3',4,5-hexachlorobiphenyl	55215-18-4	
30	2,2',3,3',4,4'-hexachlorobiphenyl	38380-07-3	
31	2,2',3,3',4,6'-hexachlorobiphenyl	38380-05-1	
32	2,3,3',4,5,6-hexachlorobiphenyl	41411-62-5	
33	2,2',3,3',4,4',5-heptachlorobiphenyl	35065-30-6	
34	2,2',3,4,4',5,5'-heptachlorobiphenyl	35065-29-3	

No.	Organic pollutants	CAS	Structures
35	2,2',3,4',5,5',6-heptachlorobiphenyl	52663-68-0	
36	Dichlorodiphenyltrichloroethane	3547-04-4	
37	Chlorobenzene	108-90-7	
38	Pentachlorobenzene	608-93-5	
39	Hexachlorobenzene	118-74-1	
40	Benzene	71-43-2	
41	Toluene	108-88-3	
42	Naphthalene	91-20-3	
43	2-Methylanthracene	613-12-7	
44	1-methylphenanthrene	832-69-9	
45	9,10-Dimethylanthracene	781-43-1	
46	3,6-dimethylphenanthrene	1576-67-6	
47	Phenanthrene	85-01-8	
48	Anthracene	120-12-7	

No.	Organic pollutants	CAS	Structures
49	Pyrene	129-00-0	
50	Fluoranthene	206-44-0	
51	Chrysene	218-01-9	
52	Benzoapyrene	50-32-8	
53	Dibenzanthracene	53-70-3	
54	Benzo[g,h,i]perylene	191-24-2	
55	4-Fluorobenzoic acid	456-22-4	
56	Ethyl benzoate	93-89-0	
57	Dioctyl phthalate	117-81-7	
58	Sulfadiazine	68-35-9	

No.	Organic pollutants	CAS	Structures
59	Trimethoprim	738-70-5	
60	Ciprofloxacin	85721-33-1	
61	Oxytetracycline	79-57-2	
62	Cyclohexane	110-82-7	
63	α-Hexachlorocyclohexane	319-84-6	
64	β-Hexachlorocyclohexane	319-85-7	
65	γ-Hexachlorocyclohexane	58-89-9	
66	δ-Hexachlorocyclohexane	319-86-8	
67	Hexane	110-54-3	
68	Perfluoropentanoic acid	2706-90-3	
69	Perfluorohexanoic acid	307-24-4	

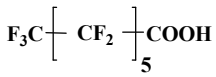
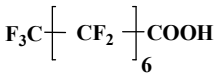
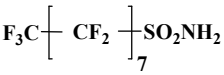
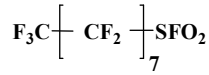
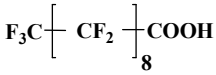
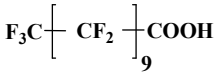
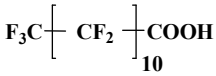
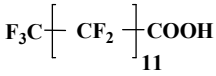
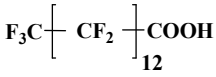
No.	Organic pollutants	CAS	Structures
70	Perfluoroheptanoic acid	375-85-9	
71	Pentadecafluorooctanoic acid	335-67-1	
72	Heptadecafluorooctanesulfonamide	754-91-6	
73	Perfluoro-1-octanesulfonyl fluoride	307-35-7	
74	Perfluorodecanoic acid	335-76-2	
75	Perfluoroundecanoic acid	2058-94-8	
76	Perfluorododecanoic acid	307-55-1	
77	Pentacosafluorotridecanoic acid	72629-94-8	
78	Perfluorotetradecanoic acid	376-06-7	

Table S3. Experimental conditions of log K_d values and size of microplastics

Microplastic	Water type	Temperature range (°C)	Particle size range (μm)	Ref
PE	Seawater	18~25	10-440	[1-5]
PE	Freshwater	18~25	10-180	[1,5,6]
PE	Pure water	25	20-250	[2,7-9]
PP	Seawater	12~25	75-180, 320-440, 1000-5000	[1] [3,10] [10]
PS	Seawater	25	320-440	[1,3,11]

Table S4. Parameter values for pp-LFERs

No.	Organic compounds	*E*	*S*	*A*	*B*	*V*
1	2,3-dichlorobiphenyl	1.628	1.198	0.000	0.163	1.547
2	2,4'-dichlorobiphenyl	1.620	1.198	0.000	0.166	1.552
3	2,4,4'-trichlorobiphenyl	1.758	1.310	0.000	0.129	1.670
4	2,4',5-trichlorobiphenyl	1.766	1.334	0.000	0.132	1.674
5	2,2',5-trichlorobiphenyl	1.758	1.310	0.000	0.145	1.648
6	2,2',3,5'-tetrachlorobiphenyl	1.905	1.443	0.000	0.150	1.770
7	2,2',5,5'-tetrachlorobiphenyl	1.903	1.423	0.000	0.147	1.770
8	2,4,4',5-tetrachlorobiphenyl	1.903	1.473	0.000	0.130	1.792
9	2,3',4,4'-tetrachlorobiphenyl	1.903	1.473	0.000	0.130	1.792
10	3,3',4,4'-tetrachlorobiphenyl	1.915	1.503	0.000	0.110	1.814
11	2,2',3,5-tetrachlorobiphenyl	1.905	1.443	0.000	0.150	1.770
12	2,2',4,4'-tetrachlorobiphenyl	1.890	1.443	0.000	0.150	1.770
13	2,2',3,4',5-pentachlorobiphenyl	2.045	1.575	0.000	0.130	1.893
14	2,2',3,5',6-pentachlorobiphenyl	2.045	1.545	0.000	0.130	1.871
15	2,2',4,5',6-pentachlorobiphenyl	2.038	1.545	0.000	0.130	1.871
16	2,2',4,5,6'-pentachlorobiphenyl	2.038	1.545	0.000	0.130	1.871
17	2,3,3',4,4'-pentachlorobiphenyl	2.035	1.603	0.000	0.110	1.922
18	2,3',4,4',5-pentachlorobiphenyl	2.050	1.606	0.000	0.110	1.919
19	3,3',4,4',5-pentachlorobiphenyl	2.075	1.643	0.000	0.090	1.936
20	2,2',4,5,5'-pentachlorobiphenyl	2.043	1.530	0.000	0.133	1.893
21	2,3,3',4',6-pentachlorobiphenyl	2.045	1.575	0.000	0.130	1.893
22	2,2',3,4',5,6-hexachlorobiphenyl	2.188	1.675	0.000	0.110	1.993

No.	Organic compounds	*E*	*S*	*A*	*B*	*V*
23	2,2',4,4',5,5'-hexachlorobiphenyl	2.183	1.473	0.000	0.113	2.015
24	2,3,3',4,4',5-hexachlorobiphenyl	2.196	1.742	0.000	0.090	2.041
25	3,3',4,4',5,5'-hexachlorobiphenyl	2.183	1.783	0.000	0.070	2.059
26	2,2',3,4,4',5-hexachlorobiphenyl	2.185	1.708	0.000	0.110	2.015
27	2,2',3,3',4,5-hexachlorobiphenyl	2.193	1.708	0.000	0.110	2.015
28	2,2',3,4,4',5'-hexachlorobiphenyl	2.183	1.718	0.000	0.110	2.009
29	2,2',3,4',5',6-hexachlorobiphenyl	2.188	1.675	0.000	0.110	1.993
30	2,2',3,3',4,4'-hexachlorobiphenyl	2.185	1.708	0.000	0.110	2.015
31	2,2',3,3',4,6'-hexachlorobiphenyl	2.188	1.675	0.000	0.110	1.993
32	2,3,3',4,5,6-hexachlorobiphenyl	2.193	1.708	0.000	0.110	2.015
33	2,2',3,3',4,4',5-heptachlorobiphenyl	2.333	1.840	0.000	0.090	2.138
34	2,2',3,4,4',5,5'-heptachlorobiphenyl	2.298	1.850	0.000	0.090	2.131
35	2,2',3,4',5,5',6-heptachlorobiphenyl	2.338	1.805	0.000	0.090	2.116
36	Dichlorodiphenyltrichloroethane	1.810	1.765	0.000	0.180	2.218
37	Chlorobenzene	0.720	0.650	0.000	0.070	0.839
38	Pentachlorobenzene	1.330	0.944	0.060	0.000	1.328
39	Hexachlorobenzene	1.475	0.939	0.000	0.130	1.451
40	Benzene	0.610	0.510	0.000	0.140	0.716
41	Toluene	0.600	0.520	0.000	0.140	0.857
42	Naphthalene	1.340	0.919	0.000	0.199	1.085
43	2-Methylanthracene	2.290	1.300	0.000	0.310	1.595
44	1-methylphenanthrene	2.060	1.250	0.000	0.275	1.595
45	9,10-Dimethylanthracene	2.236	1.270	0.000	0.300	1.736

No.	Organic compounds	*E*	*S*	*A*	*B*	*V*
46	3,6-dimethylphenanthrene	2.053	1.290	0.000	0.290	1.736
47	Phenanthrene	2.033	1.292	0.000	0.276	1.454
48	Anthracene	2.077	1.329	0.000	0.272	1.454
49	Pyrene	2.698	1.669	0.000	0.282	1.585
50	Fluoranthene	2.354	1.527	0.000	0.247	1.585
51	Chrysene	2.897	1.709	0.000	0.325	1.823
52	Benzoapyrene	3.554	1.960	0.000	0.417	1.954
53	Dibenzanthracene	3.972	2.058	0.000	0.462	2.192
54	Benzo[g,h,i]perylene	4.004	1.930	0.000	0.455	2.084
55	Ethyl benzoate	0.690	0.853	0.000	0.459	1.214
56	Dioctyl phthalate	0.650	1.277	0.000	1.088	3.401
57	Sulfadiazine	2.080	2.550	0.650	1.370	1.723
58	Trimethoprim	1.962	2.382	0.207	1.832	2.181
59	Ciprofloxacin	2.200	2.340	0.700	2.520	2.305
60	Oxytetracycline	3.600	3.050	1.650	3.500	3.158
61	Cyclohexane	0.310	0.113	0.000	0.000	
62	α-Hexachlorocyclohexane	1.450	0.940	0.150	0.620	1.580
63	β-Hexachlorocyclohexane	1.450	1.068	0.260	0.632	1.580
64	γ-Hexachlorocyclohexane	1.450	1.026	0.170	0.624	1.580
65	δ-Hexachlorocyclohexane	1.450	1.108	0.270	0.583	1.580
66	Hexane	0.000	0.025	0.000	0.000	0.954

Table S5. Log K_{OW} values and quantum chemical descriptors

No	Organic compounds	log K_{ow}	M_w a.u.	ε_α eV	ε_β eV	qH^+ acu	q^- acu	v' cm^3/mol	π
1	Pentachlorobenzene	5.220	247.852	0.246	0.339	0.168	-0.081	133.966	1.138
2	Hexachlorobenzene	5.860	281.813	0.234	0.344	-	-0.067	141.531	1.204
3	Phenanthrene	4.350	178.078	0.254	0.294	0.105	-0.157	136.263	1.518
4	Anthracene	4.350	178.078	0.230	0.276	0.105	-0.221	137.049	1.616
5	Perylene	4.930	202.078	0.236	0.279	0.106	-0.174	141.302	1.794
6	Fluoranthene	4.930	202.078	0.226	0.296	0.111	-0.168	156.458	1.553
7	Chrysene	5.520	228.094	0.243	0.287	0.106	-0.160	171.341	1.661
8	Benzoapyrene	6.110	252.094	0.226	0.271	0.107	-0.253	180.919	1.924
9	Dibenzanthracene	6.700	278.110	0.235	0.283	0.108	-0.238	194.648	1.847
10	Benzo[g,h,i]perylene	6.700	230.110	0.230	0.246	0.135	-0.275	182.472	1.388
11	4-Fluorobenzoic acid	2.070	140.027	0.245	0.339	0.350	-0.504	88.566	1.074
12	Sulfadiazine	-0.340	250.052	0.249	0.297	0.322	-0.684	169.805	1.174
13	Trimethoprim	0.730	290.138	0.281	0.291	0.286	-0.651	209.410	1.165
14	α-Hexachlorocyclohexane	4.260	287.860	0.254	0.386	0.225	-0.043	152.922	1.024
15	β-Hexachlorocyclohexane	4.260	287.860	0.237	0.382	0.216	-0.182	145.969	1.082
16	γ-Hexachlorocyclohexane	4.260	287.860	0.257	0.378	0.225	-0.202	147.124	1.056
17	δ-Hexachlorocyclohexane	4.260	287.860	0.244	0.386	0.223	-0.197	155.934	1.004
18	Perfluoropentanoic acid	2.810	263.983	0.252	0.387	0.371	-0.467	100.143	0.701
19	Perfluorohexanoic acid	3.480	313.980	0.251	0.387	0.371	-0.467	119.440	0.698
20	Perfluoroheptanoic acid	4.150	363.977	0.251	0.387	0.371	-0.467	136.286	0.708
21	Pentadecafluorooctanoic acid	4.810	413.974	0.250	0.388	0.371	-0.455	151.904	0.723
22	Heptadecafluorooctanesulfonamide	5.800	498.953	0.277	0.397	0.341	-0.694	180.121	0.789

No	Organic compounds	log K_{ow}	M_w a.u.	ε_α eV	ε_β eV	qH^+ acu	q^- acu	v' cm^3/mol	π
23	Perfluoro-1-octanesulfonyl fluoride	7.840	501.933	0.255	0.417	-	-0.457	186.953	0.721
24	Perfluorodecanoic acid	6.150	513.967	0.250	0.388	0.371	-0.456	180.358	0.755
25	Perfluoroundecanoic acid	6.820	563.964	0.251	0.388	0.371	-0.467	199.076	0.748
26	Perfluorododecanoic acid	7.490	613.961	0.251	0.388	0.371	-0.462	226.064	0.720
27	Pentacosafluorotridecanoic acid	8.160	663.958	0.251	0.388	0.371	-0.455	236.926	0.741
28	Perfluorotetradecanoic acid	8.830	713.955	0.251	0.388	0.371	-0.455	246.230	0.766

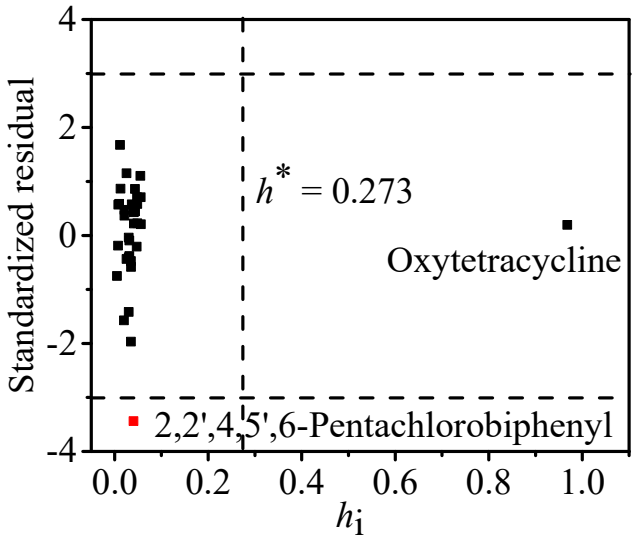


Figure S1. Williams plot for model (3)

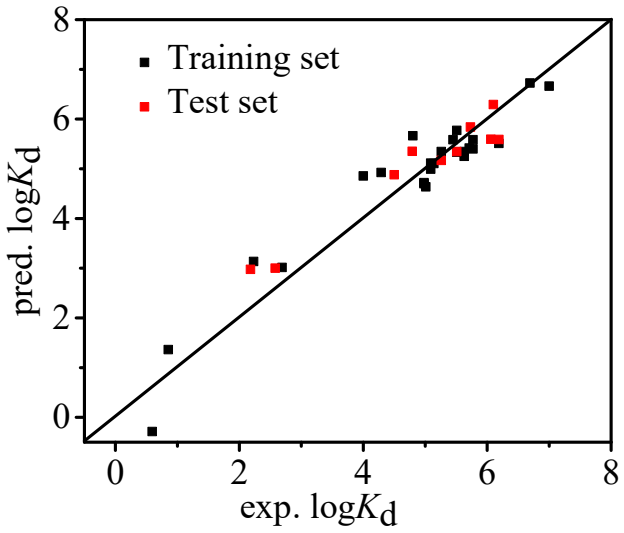


Figure S2. Fitting plots of experimental and predicted log K_d values by model (5).

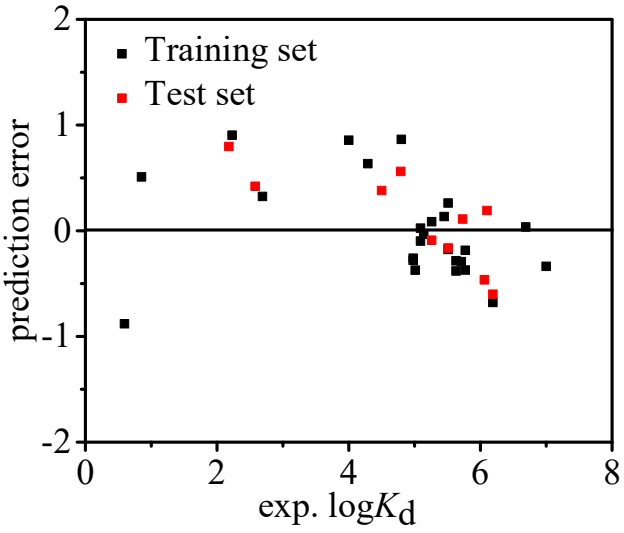


Figure S3. Distributions of prediction errors of log K_d calculated by model (5).

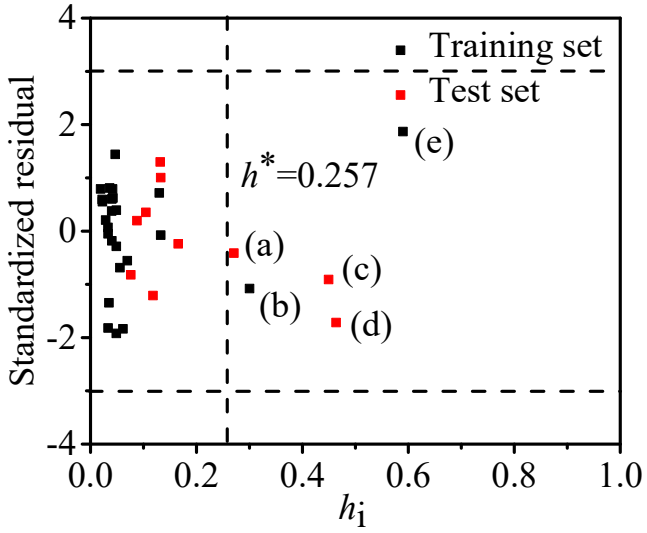


Figure S4. Williams plot for the applicability domain of model (5). The h_i refers to the verse leverage value. (a): benzoapyrene, (b): sulfadiazine, (c): γ-hexachlorocyclohexane, (d): β-hexachlorocyclohexane, (e): trimethoprim.

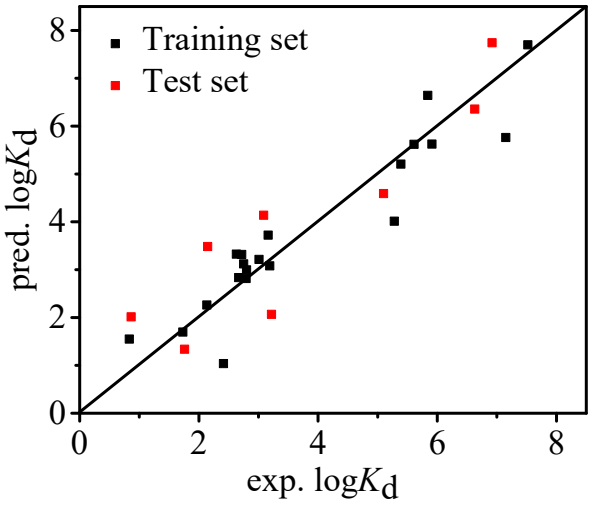


Figure S5. Fitting plots of experimental and predicted log K_d values by model (7).

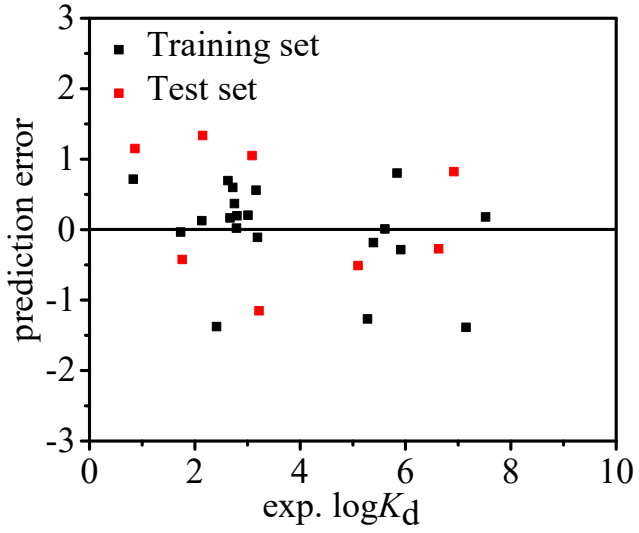


Figure S6. Distributions of prediction errors of log K_d calculated by model (7).

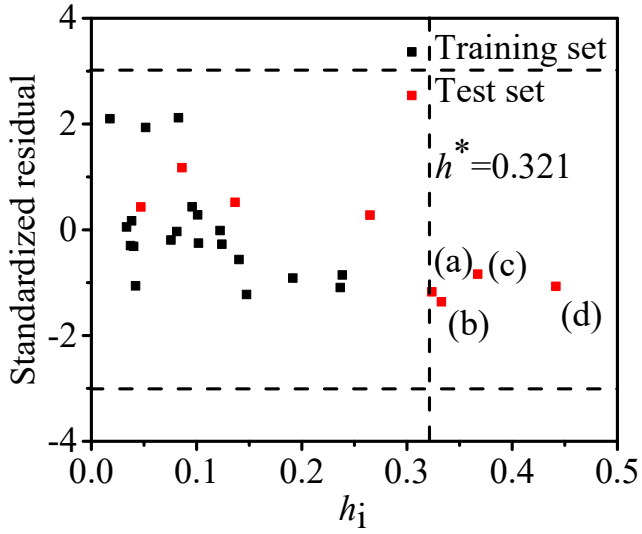


Figure S7. Williams plot for the applicability domain by model (7). Williams plot for the applicability domain of model (5). The h_i refers to the verse leverage value. (a): trimethoprim, (b): perfluoro-1-octanesulfonyl fluoride, (c): benzoapyrene, (d): perfluorotetradecanoic acid.

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