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COMPARISON OF SCREENING METHODS FOR THE ESTIMATION OF ADSORPTION COEFFICIENTS ON SOIL

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ABSTRACT

The HPLC screening method for estimating soil sorption coefficients was compared to other QSAR approaches based on log P_{OW}, connectivity indices, molar refraction and molecular fragment approaches. For the data set under consideration (66 compounds from different chemical classes) only the HPLC screening method and, to a lesser extend, the log P_{OW} method proved to be suitable for predicting soil sorption coefficients with acceptable accuracy. The HPLC method and the regression with log P_{OW} were then cross-validated. Copyright © 1996 Elsevier Science Ltd

INTRODUCTION

The fate of an organic chemical in soil is mainly determined by sorption and degradation processes. Soil sorption coefficients depend on the chemical's properties as well as on soil properties. The soil sorption coefficient K_D of a chemical is defined as:

$$K_D = C_{Soil} / C_{Water}$$

where C_{Soil} and C_{Water} are the equilibrium concentrations of the substance in the soil and the aqueous phase, respectively. The adsorption coefficient related to the organic carbon content (OC) is defined as

$$K_{OC} = K_D / OC.$$

If no experimental data on the sorption behaviour of a substance are available, estimation methods to determine the K_{OC} are used for screening purposes. Commonly used screening methods are QSAR models based on several descriptors (log P_{OW}, aqueous solubility, connectivity indices according to Kier and Hall (1976) and other descriptors) which allow to estimate the K_{OC} either directly from the molecular structure or from experimental data (like solubilities). The applicability of most QSAR models described in the literature (see e.g. Lyman, 1982, von Oepen, 1990) is however limited since they are not sufficiently accurate or restricted to well defined compound classes (Sabljic et al., 1995).

The HPLC screening method, which regresses capacity factors (k') to the K_{OC}, was introduced by Hodson and Williams (1988). The method seems to be more accurate and applicable for a wider range of chemical compounds than QSAR models based on other descriptors. In this paper the HPLC method is therefore compared to QSAR models based on several descriptors. To ensure that the best available model for the respective descriptor is used for comparison, novel regression equations were developed based on the investigated data set instead of using existing regression equations. Additionally, two molecular fragment approaches and one compound class dependent model were considered: these are the method of Meylan et al. (1992), which is based on one topological descriptor and 27 molecular fragments (PCKOC), the method of Lohninger (1994), based on two topological descriptors and 9 molecular fragments (called „FRAG2" in the following) and the method of Sabljic (1987), based on one connectivity index and correction factors for 17 compound classes („FRAG3" in the following). The equation of Lohninger was derived from a set of 120 pesticides. An additional equation given by Lohninger is based on the above mentioned descriptors and on solubility in water. This equation has not been considered due to missing solubility data. The equation of Sabljic was derived from 72 non-polar compounds for the connectivity index equation and 143 polar compounds for the correction factors.

METHODS

Compounds. A data set of 66 compounds was used to compare the methods. This data set comprises 5 compound classes (Table 1).

Table 1: Compound classes investigated

Set	No. of compounds	Compound class
A	26	pesticides except B
B	5	triazines
C	8	benzamides
D	17	polar chemicals
E	10	nonpolar chemicals

HPLC screening method. The HPLC screening method is described by Kördel et al. (1993). Capacity factors as well as K_{OC} values used for the analysis were taken from Kördel et al. (1993) and Kördel (1993). Capacity factors were measured with a cyanopropyl column and methanol/water (55/45 % v/v) as the mobile phase. The K_{OC} data

are mean values from several results either measured in our institute according to the OECD guideline or kindly supplied by the producers of the pesticides (Hoechst AG and Bayer AG)

log P_{OW} data. Experimental data for the log P_{OW} were taken from the Pomona-database (MedChem software package). The available data included experimental log P_{OW} values for only 50 out of the 66 investigated compounds. Since all other descriptors were available for the whole data set, it was decided to make two regression analyses: one analysis based on the 50 experimental data solely and a second one based on 50 experimental and 16 calculated log P_{OW}s.

Calculation of descriptors. log P_{OW} and molar refraction (MR) were calculated with the MedChem program (MedChem 1989), the molecular fragments of Meylan were calculated with the PCKOC program (PCKOC 1994), and the calculation of the connectivity indices ($^0\chi$ .. $^2\chi^v$, as defined by Kier and Hall, 1976) was done with *PropertEst* (1995).

Statistics. For all considered descriptors linear regression analyses were performed using the statistic program *SAR-Stat* (1994). The regression equations were compared with respect to coefficient of determination (r^2), standard deviation (s), cross-validated variance Q^2 (Wold and Eriksson, 1995), and, in some cases, with respect to the slope (b) and intercept (a). Since the molecular fragment approaches yield direct K_{OC} values as output, it is meaningless to put them into a regression equation again. Theoretically such an regression equation should have a slope of 1 and an intercept of 0. Therefore for the three molecular fragment approaches additionally the root of the mean square error (r.m.s.) is given in tables 2 and 5. This is not possible for the models based on other descriptors, unless the data set is divided into a training and a test set. In this case r.m.s. can be calculated for the other models as well.

The HPLC screening method and the model based on calculated log P_{OW} were cross-validated: some compounds are randomly excluded from the data set, and a regression analysis is done for the reduced data set. The values for the compounds left out are then predicted with the resulting equation. The procedure is repeated leaving out other compounds until all compounds have been left out once, but not more than once. The resulting estimates are used to calculate the cross-validated variance Q^2. According to a recommendation by Eriksson (1995), 15 compounds (≈ 20 %) were left out in each step. (The Q^2, which is given in table 2, is based on the „leave-one-out" approach, i.e. only one compound is left out in each cycle. To differentiate between these two Q^2 values, we introduced a subscript for the number of compounds left out in each cycle, e.g. $Q^2_{(1)}$, and $Q^2_{(15)}$ resp.). Because random numbers are used for splitting the data, each run of the program will lead to slightly different results for Q^2 (except for the „leave-one-out" method). Therefore, the cross-validation was performed hundred times, and the mean values of $Q^2_{(15)}$ were calculated. Minimum and maximum $Q^2_{(15)}$ values are also given.

Additionally, the HPLC method and the log P_{OW}-regression results were validated by dividing the data set in two subsets: S1 and S2. To systematically create two chemically diverse data sets, the compounds were sorted

according to their molecular weight, classifying all compounds with odd numbers into set S1 and all compounds with even numbers into set S2. Regression analyses were performed for both data sets. The resulting regression equation for data set S1 was applied to S2 and vice versa. The mean square error (m.s.e) was calculated and compared to the variance (s^2) of the regression equations.

RESULTS AND DISCUSSIONS

Table 2 presents the results of the linear regression for 12 descriptors. Figures 1 - 3 show regression lines for log k' and log P_{OW} and calculated vs. experimental log K_{OC}s for the PCKOC-method. Considering the coefficient of determination as well as the standard deviation and $Q^2_{(1)}$ it is evident that the HPLC method is superior to all other methods for this data set. The other descriptors turned out to be not suitable with the exception of log P_{OW} and the PCKOC models, which may be used for a rough estimation of K_{OC}. The calculated log P_{OW} values are better predictors than the experimental data, which may be a random effect of the data set investigated. As expected, all models solely based on topological indices are not suitable for the prediction of K_{OC} when substances of diverse compound classes are investigated. The fragment approach of Lohninger (FRAG2) shows results comparable to the topological index method. The correction factors for molecular fragments do not improve the results for the compounds in the investigated data set.

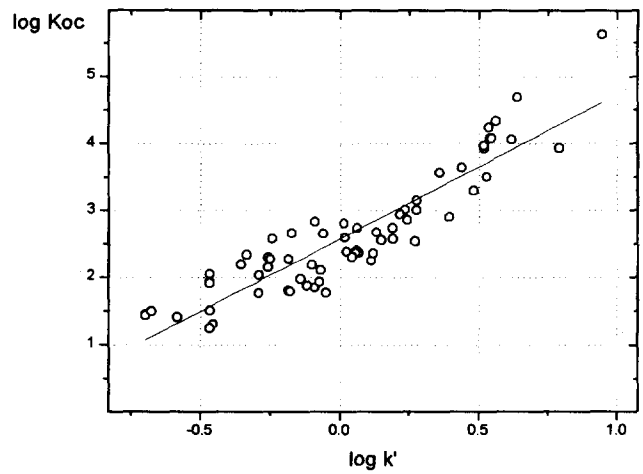
Table 2: Linear regression results for several descriptors

	r^2	s.d.	$Q^2_{(1)}$	r.m.s	n
log k'	0.829	0.379	0.812		66
log Pow (calc.)	0.712	0.489	0.692		66
log Pow (exp.)	0.696	0.514	0.658		50
log Pow (exp./calc.)	0.668	0.525	0.643		66
log PCKOC	0.569	0.598	0.537	0.69	66
FRAG3	0.436	0.684	0.401	1.06	66
$^2\chi^v$	0.395	0.709	0.356		66
molar refraction	0.400	0.705	0.365		66
$^0\chi^v$	0.381	0.717	0.345		66
$^1\chi^v$	0.374	0.721	0.338		66
$^2\chi$	0.354	0.732	0.319		66
FRAG2	0.344	0.738	0.308	0.75	66
$^1\chi$	0.324	0.749	0.290		66
$^0\chi$	0.317	0.753	0.281		66

In a next step the data were divided into compound classes according to the classification presented in Table 1. Considering the unsatisfactory results obtained for most of the descriptors the classification was restricted to the HPLC method, the calculated log P_{OW} and the two molecular fragment approaches PCKOC and FRAG2. (Although FRAG2 gave worse results than most of the other descriptors, this method was taken into account to check whether it is able to describe the K_{OC} of the pesticides).

The results are summarised in Tables 3 - 6. Figures 4 - 6 show the regression lines for the descriptors log k', log P_{OW} and log PCKOC. Similar slopes and intercepts were only obtained for the HPLC regressions, whereas the log P_{OW} regressions and the fragment approaches yielded clearly deviating slopes and intercepts for the different compound classes. This indicates that a model suitable for one compound class cannot be used to estimate compounds of other classes. This restriction is usual for QSAR models, however, not all compound classes are well defined on a chemical basis (e.g. set A: pesticides), and estimates for a compound may be necessary although no model is available for the respective compound class. It should be noticed that the fragment methods yield intercepts and slopes evidently deviating from the theoretical values of 0 resp. 1. This indicates that although regression results may be good in some cases, estimates may not be satisfying, since the results from fragment methods are K_{OC}-values directly and should not be entered into a regression equation again.

Figure 1: Regression of log K_{OC} vs. log k'



The results obtained for the four approaches were compared for each of the five compound classes. For all classes the HPLC method yielded the best results. For the mixed compound class of pesticides (set A) acceptable results were achieved with the log k', the log P_{OW}-regression, and with FRAG2, whereas PCKOC does not seem applicable for this set of substances. The training set of FRAG2 included 8 compounds out of the 26 compounds in the investigated data set. In general good estimates were obtained for the triazines (set B) with the exception of FRAG2. The log P_{OW} and the PCKOC-regression show intercepts and slopes evidently deviating from the equation for the complete data set, this does not apply for log k'. The intercept and slope from FRAG2 deviates dramatically from the theoretical values of 0 and 1 resp. A further examination of the data showed that the experimental data for triazines in Lohninger (1994) deviate significantly from the data used in our study. This is not the case for the other pesticides. According to this problem a comparison of the FRAG2 results of triazines to

Figure 2: Regression of log K_{OC} vs. log P_{OW}

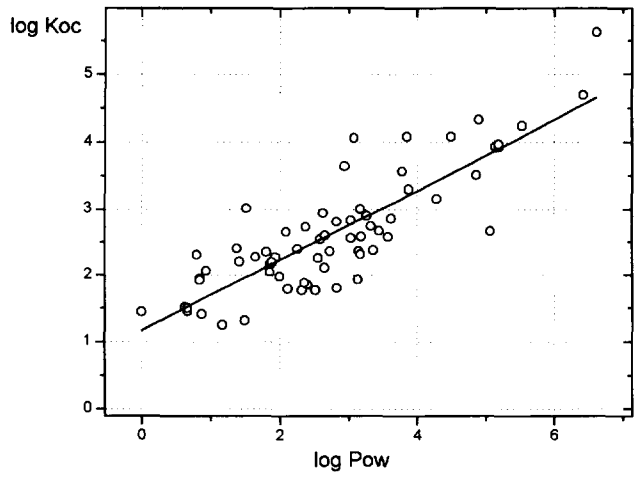
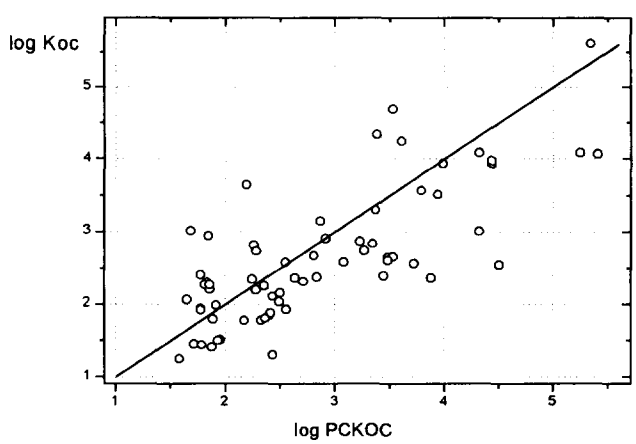


Figure 3: log K_{OC} vs. calculated log (PCKOC)



the other methods is not possible at the moment. Modelling the K_{OC}s for benzamides (set C) was possible only for log k' and for FRAG2 which includes a correction factor for the amide function. The polar compounds (set D), for which estimates generally are generally difficult, are best, but not well, described by the HPLC method. Except FRAG2 all models were able to model the non-polar compounds (set E), as could be expected corresponding to the inherent assumptions of the defining equations for K_{OC}. However, all methods show deviations from the regression line for the complete data set. This may be due to the large amount of polar compounds in the data set.

At this point it should be noted that regression equations for the log K_{OC} based on log P_{OW} (see e.g. Lyman, 1982, Sabljic et al. 1995) show very deviating intercepts and slopes depending on the compound classes.

Table 3: Regression results of log k' with log K_{OC}

Set	n	a	b	r^2	Q^2	s.d.	F
A	26	2.42	2.42	0.763	0.704	0.389	77.0
B	5	2.27	2.14	0.891	0.609	0.151	24.5
C	8	2.70	1.87	0.766	0.613	0.172	19.6
D	17	2.55	1.73	0.555	0.431	0.322	18.7
E	10	2.28	3.50	0.985	0.976	0.155	524.6
all	66	2.58	2.15	0.827	0.812	0.379	305.5

Table 4: Regression results of log Pow with log K_{OC}

Set	n	a	b	r^2	Q^2	s.d.	F
A	26	1.27	0.54	0.635	0.579	0.482	41.8
B	5	-0.64	0.91	0.777	0.188	0.215	10.5
C	8	1.36	0.50	0.191	-1.17	0.319	1.41
D	17	1.66	0.26	0.351	0.124	0.389	8.12
E	10	0.36	0.74	0.900	0.821	0.401	71.8
all	66	1.18	0.53	0.712	0.692	0.489	158.3

Table 5: Regression results of log PCKOC with log K_{OC}

Set	n	a	b	r^2	Q^2	s.d.	F	r.m.s.
A	26	1.68	0.41	0.319	0.217	0.659	11.2	0.912
B	5	-1.04	1.24	0.800	0.393	0.204	12.0	0.460
C	8	3.05	-0.74	0.035	-0.551	0.348	0.22	0.357
D	17	1.26	0.40	0.342	0.200	0.391	7.80	0.582
E	10	-0.50	1.14	0.840	0.794	0.507	42.0	0.472
all	66	0.68	0.69	0.569	0.537	0.598	84.5	0.693

Table 6: Regression results of log Koc (FRAG2) with log K_{OC}

Set	n	a	b	r^2	Q^2	s.d.	F	r.m.s.
A	26	0.164	1.01	0.672	0.626	0.457	49.2	0.473
B	5	-6.42	2.93	0.661	0.131	0.265	5.9	0.847
C	8	-0.204	1.07	0.738	0.538	0.182	16.9	0.175
D	17	2.29	-0.025	0.000	-0.675	0.482	0.0	0.558
E	10	-0.701	1.87	0.415	-0.013	0.965	5.7	1.483
all	66	0.506	0.860	0.344	0.308	0.738	33.5	0.748

Cross-validation. The cross-validation procedure was performed 100 times, and mean values for $Q^2_{(15)}$ as well as maximum and minimum values were obtained as described in the methods section. The results are summarised in Table 7.

Figure 4: Regression lines for log k'

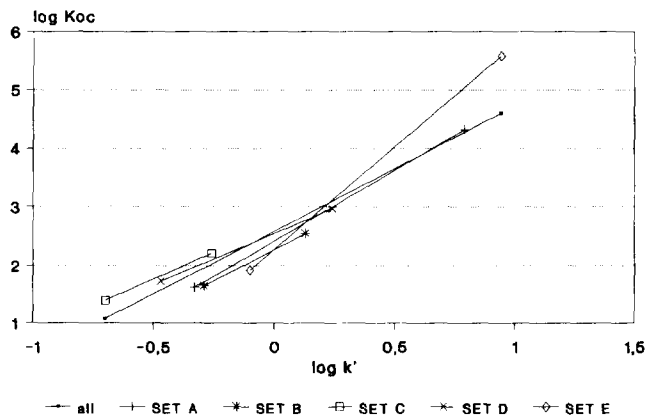


Figure 5: Regression lines for log P_{OW}

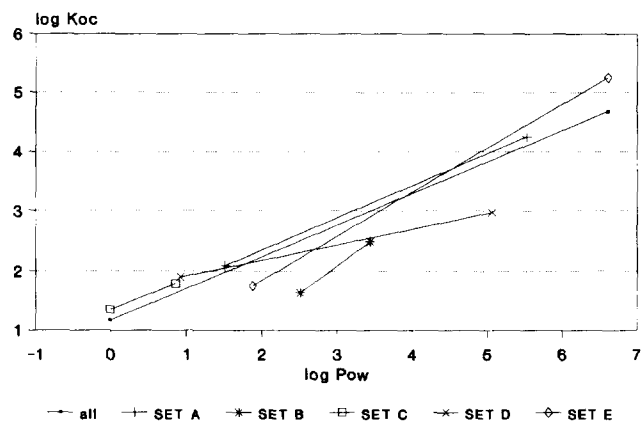


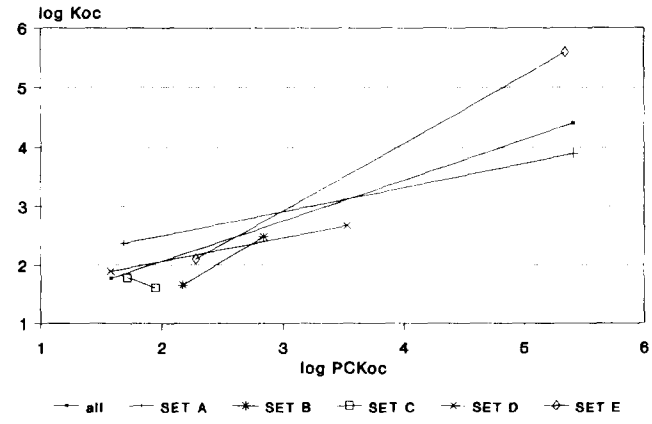
Table 7: $Q^2_{(15)}$ for log k' and log P_{OW} regressions

	log k'	log P_{OW}
$Q^2_{(15)}$ (mean value)	0.809	0.689
$Q^2_{(15)}$ (maximum value)	0.824	0.710
$Q^2_{(15)}$ (minimum value)	0.772	0.645

Evidently, the results for log k' are better than the results for log P_{OW}. The minimum Q^2 for log k' is even higher than the maximum Q^2 for log P_{OW}. It is also higher than the r^2 of the log P_{OW} regression. The log k'-method

therefore seems to be a stable regression model, independent of the compounds taken into account.

Figure 6: Regression lines for log PCKOC



Division of data set into two subsets. The data set was divided into the subsets S1 and S2 as described in the methods section. The following regression equations were obtained:

Table 8: log k' regression equations for subsets S1 and S2

Set	a	b	r^2	s
S1	2.58	2.17	0.804	0.395
S2	2.58	2.14	0.847	0.377

For these two regressions, both based on diverse data sets, nearly the same results were obtained. Intercept and slope are very similar to each other and to the regression results obtained from the complete data set (Table 3). The coefficients of determination are high compared to the regressions with all other descriptors (see Table 1). The regression equations were used to estimate log K_{OC} from log k' for the other data set (i.e. the equation obtained from S1 was applied to S2 and vice versa). The root of the mean square error (r.m.s.) was 0.373. This value is comparable to the standard deviation of the regression equation of the complete data set (s = 0.379) and is much lower than the r.m.s. of the fragment approaches.

Table 9: log P_{OW} regression equations for subsets S1 and S2

Set	a	b	r^2	s
S1	1.14	0.534	0.796	0.404
S2	1.22	0.518	0.640	0.574

For the regressions based on log P_{OW} similar results were obtained comparing subsets S1 and S2, the results were also similar compared to the complete data set. The results for set S2 are not satisfactory. The log K_{OC} for set S1 correlates much better with the parameter log P_{OW} than the log K_{OC} for the compounds in subset S2. This indicates that for log P_{OW} a much larger training set than for log k' is required to obtain a stable regression equation. In analogy to log k' the regressions were used to estimate log K_{OC} for the other data set. The root of the mean square error was 0.482, the standard deviation of the regression equation for the total data set was 0.489. Again, this r.m.s is much lower than the r.m.s. from the fragment approaches.

CONCLUSION

The HPLC method is a suitable tool for estimating K_{OC} values with higher accuracy than QSAR models based on calculated descriptors. The method however requires measurement of the capacity factor k'. If this is not possible or inappropriate (e.g. screening of compounds in databases), regressions with calculated log P_{OW} as independent variable may be useful. These regression analyses should be based on a data set including compounds similar to the compound under consideration. Based on our data set, it can be concluded that the fragment models are less useful than the log P_{OW} regressions. Prediction ability of PCKOC seems to be restricted to nonpolar compounds, whereas FRAG2 was designed explicitly for pesticides.

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APPENDIX

Table 10: List of compounds, experimental K_{OC} and descriptors

No.	compound	SET	log K_{OC}	log k'	log P_{OW} (calc.)	log PCKOC
1.	Monuron	A	1.99	-0.143	1.99	1.92
2.	Quintozen	A	4.34	0.561	4.89	3.38
3.	Endosulfan alcohol	A	3.02	0.233	1.51	1.68
4.	Endosulfan sulfat	A	4.07	0.618	3.07	5.41
5.	Endosulfan	A	4.09	0.538	3.84	5.24
6.	Trifluralin	A	3.94	0.791	5.13	3.99
7.	Monolinuron	A	1.78	-0.0506	2.31	2.33
8.	Fenoxaprop-p-ethyl	A	3.94	0.519	5.18	4.43
9.	Fenoxaprop-ethyl	A	3.98	0.517	5.18	4.43
10.	Triazophos	A	2.55	0.270	2.58	4.50
11.	Linuron	A	2.59	0.190	3.18	2.54
12.	Pyrazophos	A	3.65	0.436	2.93	2.19
13.	Diclofop-methyl	A	4.25	0.535	5.52	3.61
14.	Isoproturon	A	1.86	-0.0915	2.40	2.40
15.	Carbendazim	A	2.35	-0.337	1.80	2.25
16.	Azinophos-methyl	A	2.95	0.215	2.62	1.84
17.	Disulfoton	A	2.91	0.393	3.26	2.91
18.	Fenthion	A	3.31	0.481	3.86	3.37
19.	Fenamiphos	A	2.26	0.111	2.55	2.35

20.	Methiocarb	A	2.82	0.0128	2.82	2.26
21.	Pencycuron	A	3.52	0.528	4.85	3.94
22.	Tebuconazol	A	3.01	0.274	3.17	4.32
23.	Triadimefon	A	2.57	0.149	3.03	3.72
24.	Triadimenol	A	2.40	0.0212	2.25	3.45
25.	Fuberidazol	A	2.84	-0.0915	3.03	3.34
26.	Triapenthenol	A	2.37	0.117	2.72	3.88
27.	Simazine	B	1.78	-0.292	2.51	2.17
28.	Atrazine	B	1.81	-0.187	2.82	2.36
29.	Propazine	B	1.94	-0.0757	3.13	2.55
30.	Prometryn	B	2.38	0.0645	3.35	2.84
31.	Terbutryn	B	2.68	0.130	3.44	2.80
32.	Benzamide	C	1.46	-0.699	0.65	1.71
33.	N,N-Dimethylbenzamide	C	1.52	-0.469	0.61	1.95
34.	3,5-Dinitrobenzamide	C	2.31	-0.260	0.79	1.84
35.	N-Methylbenzamide	C	1.42	-0.585	0.86	1.87
36.	2-Nitrobenzamide	C	1.45	-0.699	-0.01	1.78
37.	3-Nitrobenzamide	C	1.95	-0.469	0.83	1.77
38.	4-Nitrobenzamide	C	1.93	-0.469	0.83	1.77
39.	2-Chlorbenzamide	C	1.51	-0.678	0.65	1.93
40.	Benzoic acid methyl ester	D	1.80	-0.181	2.11	1.89
41.	Benzoic acid phenyl ester	D	2.87	0.241	3.62	3.23
42.	3,5-Dinitro benzoic acid	D	2.74	0.0607	2.37	2.28
43.	Phenyl acetic acid ethyl ester	D	1.89	-0.119	2.35	2.41
44.	1-Naphthylamine	D	2.66	-0.0605	2.09	3.48
45.	Aniline	D	2.07	-0.469	0.92	1.65
46.	3,5-Dinitro aniline	D	2.41	0.0569	1.37	1.78
47.	N-Methyl aniline	D	2.28	-0.252	1.64	1.81
48.	4-Methyl aniline	D	2.21	-0.357	1.41	1.86
49.	4-Chloro aniline	D	2.28	-0.187	1.93	1.86
50.	Phenol	D	1.32	-0.456	1.48	2.43
51.	Pentachlorophenol	D	2.67	-0.174	5.06	3.53
52.	2-Nitrophenol	D	2.17	-0.260	1.85	2.50
53.	4-Nitrophenol	D	2.05	-0.292	1.85	2.49
54.	2,4,6-Trichlorophenol	D	2.59	-0.244	3.57	3.08
55.	1-Naphthol	D	2.61	0.0170	2.65	3.48
56.	Acetanilide	D	1.26	-0.469	1.16	1.58
57.	Naphthaline	E	2.75	0.188	3.32	3.26
58.	Acenaphthene	E	3.58	0.358	3.77	3.79
59.	Phenanthrene	E	4.09	0.545	4.49	4.32
60.	Toluene	E	2.12	-0.0706	2.64	2.43
61.	p-Xylene	E	2.37	0.0531	3.14	2.64
62.	Ethylbenzene	E	2.32	0.0414	3.17	2.71
63.	Nitrobenzene	E	2.20	-0.102	1.88	2.28
64.	Hexachlorobenzene	E	4.70	0.640	6.42	3.53
65.	1,2,3-Trichlorobenzene	E	3.16	0.274	4.28	2.87
66.	DDT	E	5.63	0.944	6.61	5.34