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QSAR for Polychlorinated Organic Compounds (PCOCs). I. Prediction of Partition Properties for PCOCs Using Quantum Chemical Parameters

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Large quantities of polychlorinated organic compounds (PCOCs) including pesticides like chlordanes, DDT, HCH, and aldrin, industrial chemicals like polychlorinated biphenyls (PCBs), and others artificial chemicals like polychlorinated dibenzo-p-dioxins (PCDDs) and dibenzofurans (PCDFs), have been released to the global environment in the last 3-4 decades. Due to their persistence and bioaccumulative potential, PCOCs tend to magnify in the food chain and cause adverse effects including neuro, reproductional and immuno toxicities on human and wildlife situated on the top of the food chain (Ahlborg *et al.* 1992).

The octanol/water partition coefficient (Kow) and the soil sorption coefficient (Koc) are of critical importance for evaluating PCOCs fate and potential exposure to environment and, consequently, for the whole process of environmental risk assessment. Because the experimental determination of Kow and Koc values of PCOCs is often difficult and expensive, alternative methods of estimation are frequently employed. Quantitative structure-activity relationships (QSAR) are used increasingly to screen and predict fate and toxicity of chemicals released into the environment. The essential assumption for quantitative structure-activity relationship (QSAR) studies is that biological, chemical, and physical properties of compounds depend on their structures. The QSAR models are usually developed for a group of compounds with similar structure using two of the basic approaches including: (a) molecular connectivity and (b) quantum chemical descriptors, Molecular connectivity is a method describing molecular structure based solely on bonding and branching patterns rather than physical or chemical characteristics. For a given molecular structure, several types and orders of molecular connectivity indices (MCIs) can be calculated (Kier and Hall, 1976). A large number of studies have demonstrated that many physicochemical and biological properties, such as water solubility, n-octanol/water partition coefficient (Kow), soil sorption coefficient (Koc), and biological activity correlate with the connectivity index (Blum and Speece 1990). Quantum chemical parameters

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derived from molecular orbital calculations have the advantage of not being class dependent as is often the case with group theoretical, topological or topographical variables (where many correlations using these types of descriptors are usually limited to a single type of compound, such as aliphatic alcohols). MO derived descriptors are also readily computed, and can be selected in such a way as to assure (or nearly assure) orthogonality of the parameter space (Famini and Wilson 1997). Because of their advantages, they are widely used in the QSAR studies (Nevalainen 1994).

Several models based on molecular properties such as molecular volume, dipole moment, hydrogen bond acceptor basicity, hydrogen bond donor acidity (Hickey and Passino-reader 1990) have been reported to predict Kow and Koc of several chemical classes. Molecular connectivity models have been shown to outperform traditional empirical models based on physicochemical properties in predicting Kow and Koc (Meylan 1992). However, information on QSAR models based on quantum chemistry descriptors to predict Kow and Koc is limited (Reddy and Locke 1994). In this paper we describe and discuss QSAR modeling techniques to predict Kow and Koc values of 70 PCOCs based on quantum chemical descriptors.

MATERIALS AND METHODS

The logKow values are taken from literature (Sabljic 1995; Sangster 1993; Mackay 1992). We made sure to include in our study only partition coefficients that were measured by means of experimental methods: shake flask, slow stiring, and the generation column. The logKoc data were taken from the literature (Sabljic 1995; Mackay 1992; Meylan 1992). In general, the most recent compilation will contain the most reliable data presently available. In most instances, the median value is used when several measured Koc values are available for a given chemical. Molecular geometry was optimized and parameters were calculated using the semi-empirical orbital MOPAC6.0 procedures (Stewart 1990) according to methods AM1 (Dewar 1985). MOPAC was used to determine the individual structural parameters influencing Kow and Koc, including the dipole moment (μ), the energy of the highest occupied molecular orbital (E_{homo}), the energy of the lowest unoccupied molecular orbital (E_{lumo}), the most positive net atomic charges on hydrogen (qH^+), the largest negative atomic charge on an atom (q^-), and the total energy (TE) (Table 1). Units of the energy, charge, dipole and polarizability were electron volts (eV), atomic charge units(a.c.u.), and atomic units (a.u.), respectively. Molecular connectivity index was calculated using program developed by our laboratory (designed with

FORTRAN language) according to the method described by Kier and Hall (1976). Values of the first-order molecular connectivity index were then calculated (Table 1).

The regression analysis was performed using the "Statgraphics" program (STSC Inc 1985).

All multiple linear regressions reported in this paper adhere to two conditions. First, this cross correlation of descriptors is minimized, as determined by the variance inflation factor (VIF). The VIF is defined as $1/(1-r^2)$, where r is the correlation coefficient of the subject independent variable against all other independent variables in the regression. A value of 1.0 indicates no correlation, with values under 5.0 being acceptable. Values over 10.0 indicate an unstable regression that should be reexamined. Second, all independent variables in the regressions have a significance of at least 95% (Based on Student's 2-tail t-score).

Table 1. Partition properties and molecular structure descriptors for 70 PCOCs.

compounds	μ	$-E_{homo}$	qH^+	$-q^-$	TE	χ^1	Koc			Kow		
							exp.	cal.[1]	diff.	exp.	cal.[2]	diff.
chlordane	1.266	9.912	0.136	0.171	3.991	8.114	5.15	5.13	0.02	5.80	6.20	-0.40
aldrin	0.988	9.883	0.154	0.177	3.871	8.276	4.69	5.03	-0.34	6.50	6.06	0.44
α-endosulfan	0.930	9.941	0.156	0.809	4.633	7.686	4.13	4.27	-0.14	3.83	3.45	0.38
heptachlor	0.765	9.952	0.163	0.185	3.962	7.703	*	5.13	*	6.10	6.14	-0.04
α-BHC	0.842	11.278	0.159	0.090	3.095	5.464	3.25	3.27	-0.02	3.80	4.01	-0.21
β-BHC	0.842	11.278	0.159	0.090	3.095	5.464	3.36	3.27	0.09	3.78	4.01	-0.23
γ-BHC	0.842	11.278	0.159	0.090	3.095	5.464	3.00	3.27	-0.27	3.76	4.01	-0.25
p.p'-DDT	0.423	9.585	0.151	0.127	3.785	8.874	5.31	5.50	-0.19	6.91	6.84	0.07
p.p'-DDE	0.027	9.285	0.151	0.127	3.396	8.575	4.82	5.38	-0.56	6.96	6.78	0.18
hexachlorobenzene	0.000	9.911	0.000	0.052	3.010	5.464	4.45	5.11	-0.66	6.18	6.77	-0.59
simazine	1.155	9.621	0.229	0.306	2.469	6.258	2.10	2.76	-0.66	2.18	3.06	-0.88
atrazine	1.204	9.564	0.230	0.309	2.625	6.613	2.24	2.98	-0.74	2.63	3.30	-0.67
cyanazine	2.074	9.625	0.248	0.316	2.945	7.465	2.28	2.93	-0.65	2.22	3.14	-0.92
dicamba	1.043	10.154	0.243	0.338	2.564	6.075	2.20	2.40	-0.20	2.21	2.44	-0.23
alachlor	1.051	9.580	0.137	0.357	3.290	8.855	3.09	4.05	-0.96	3.59	4.53	-0.94
benzhydrol	0.743	9.717	0.221	0.308	4.105	9.248	*	4.98	*	5.02	5.60	-0.58
PCB												
2,2'-	0.590	9.520	0.148	0.132	2.399	6.788	3.92	3.70	0.22	4.97	4.77	0.20
2,4'-	0.825	9.221	0.148	0.130	2.393	6.771	4.14	3.83	0.31	5.10	4.97	0.13
2,4,4'-	0.410	9.292	0.153	0.127	2.753	7.165	4.62	4.39	0.23	5.62	5.63	-0.01
2,2',5-	0.515	9.478	0.158	0.132	2.753	7.182	4.23	4.18	0.05	5.55	5.32	0.23
2,2',4-	0.771	9.575	0.162	0.131	2.753	7.182	4.84	4.00	0.84	5.60	5.08	0.52
2,2',6,6'-	0.002	9.597	0.152	0.130	3.113	7.609	5.01	4.79	0.22	5.94	6.03	-0.09
2,5,3',4'-	0.707	9.423	0.160	0.120	3.113	7.575	4.84	4.64	0.20	6.23	5.88	0.35

(Table 1 Continued)

2,2',5,5'-	0.031	9.560	0.159	0.120	3.113	7.575	4.73	4.81	-0.08	6.09	6.07	0.02
3,3',4,4'-	0.692	9.291	0.157	0.117	3.114	7.575	4.41	4.76	-0.35	6.21	6.05	0.16
2,2',3,4,5'-	0.790	9.630	0.159	0.121	3.473	8.003	4.62	4.92	-0.30	6.37	6.15	0.22
2,2',4,5,5'-	0.434	9.612	0.168	0.120	3.473	7.986	4.63	5.05	-0.42	6.50	6.30	0.20
2,2',4,4',5-	0.429	9.648	0.167	0.127	3.473	7.486	5.68	5.00	0.68	6.41	6.23	0.18
2,2',3,3',4,4'-	0.902	9.846	0.158	0.120	3.833	8.430	5.05	5.18	-0.13	6.93	6.40	0.53
2,2',4,4',5,5'-	0.005	9.708	0.168	0.119	3.834	8.397	5.65	5.61	0.04	7.16	6.95	0.21
3,3',4,4',5,5'-	0.002	9.516	0.160	0.107	3.834	7.700	6.60	5.81	0.79	7.41	7.27	0.14
2,2',3,4,5,5',6-	0.440	9.677	0.156	0.120	4.193	8.841	5.95	5.96	-0.01	7.00	7.35	-0.35
PCDD												
1,2,3,4-	0.950	8.990	0.160	0.123	3.725	8.017	*	5.65	*	7.18	7.09	0.09
1,2,3,7-	0.435	9.007	0.177	0.125	3.725	8.559	5.98	5.78	0.20	6.91	7.23	-0.32
1,3,6,8-	0.077	9.073	0.176	0.122	3.725	8.541	5.98	5.88	0.10	7.20	7.37	-0.17
2,3,7,8-	0.045	9.008	0.176	0.124	3.725	8.541	6.30	5.94	0.36	7.02	7.44	-0.42
PCDF												
2,8-	0.255	9.230	0.160	0.121	2.685	7.237	*	4.41	*	5.44	5.67	-0.23
2,3,7,8-	0.049	9.288	0.174	0.118	3.405	8.059	5.20	5.34	-0.14	6.53	6.72	-0.19
chlorobenzene												
1,2-	0.774	9.601	0.151	0.122	1.571	3.805	2.44	2.88	-0.44	3.44	3.42	0.02
1,3-	0.775	9.601	0.151	0.121	1.571	3.788	2.50	2.52	-0.02	3.53	3.42	0.11
1,4-	0.005	9.522	0.153	0.117	1.571	3.788	2.48	2.52	-0.04	3.44	3.91	-0.47
1,2,3-	0.810	9.780	0.155	0.118	1.930	4.215	3.29	2.83	0.46	4.14	3.74	0.40
1,2,4-	0.405	9.620	0.165	0.117	1.931	4.198	3.15	3.08	0.07	4.05	4.07	-0.02
1,3,5-	0.001	9.919	0.166	0.122	1.931	4.182	2.85	3.00	-0.15	4.19	3.93	0.26
1,2,3,4-	0.636	9.733	0.160	0.111	2.291	4.626	3.48	3.40	0.08	4.60	4.43	0.17
1,2,3,5-	0.326	9.761	0.169	0.116	2.291	4.609	3.20	3.46	-0.26	4.66	4.47	0.19
1,2,4,5-	0.326	9.763	0.169	0.116	2.291	4.609	3.25	3.46	-0.21	4.70	4.47	0.23
Pentachlorobenzene	0.310	9.788	0.173	0.109	2.651	5.037	4.11	3.91	0.20	5.18	5.00	0.18
chloroaniline												
2,4-	0.989	8.661	0.207	0.336	1.792	4.198	2.72	2.66	0.06	2.91	3.09	-0.18
2,6-	0.433	8.718	0.212	0.338	1.792	4.215	3.25	2.81	0.44	2.82	3.27	-0.45
3,5-	1.002	8.93	0.195	0.333	1.792	4.182	2.49	2.50	-0.01	2.90	2.88	0.02
3,4-	1.274	8.735	0.194	0.333	1.791	4.198	2.29	2.54	-0.25	2.69	2.96	-0.27
2,3,4-	1.281	8.795	0.211	0.337	2.152	4.626	2.60	2.89	-0.29	3.68	3.31	0.37
2,3,4,5-	1.262	8.923	0.216	0.340	2.512	5.037	3.03	3.24	-0.21	4.27	3.67	0.60
2,3,5,6-	0.726	8.984	0.224	0.349	2.512	5.037	3.94	3.36	0.58	4.10	3.78	0.32
2,3,4,5,6-	1.072	8.956	0.228	0.350	2.871	5.464	4.62	3.69	0.93	4.82	4.14	0.68
chloronitrobenzene												
2,3,4,5-	1.358	10.367	0.187	0.339	3.121	5.947	4.23	3.01	1.22	3.93	3.15	0.78
2,3,5,6-	1.689	10.223	0.178	0.320	3.12	5.947	4.05	3.07	0.98	3.89	3.29	0.60
2,3,4,5,6-	1.425	10.337	0.000	0.318	3.481	6.375	4.36	4.13	0.23	4.64	4.75	-0.11
chlorophenol												
2,3-	0.329	9.428	0.231	0.242	1.891	4.215	2.65	2.65	0.00	2.84	3.19	-0.35

(Table 1 continued)

2,4-	0.159	9.270	0.231	0.241	1.891	4.198	2.75	2.84	-0.09	3.06	3.45	-0.39
2,4,6-	0.422	9.390	0.235	0.226	2.251	4.609	3.02	3.14	-0.12	3.69	3.78	-0.09
2,4,5-	0.512	9.388	0.233	0.237	2.251	4.609	3.36	3.08	0.28	3.72	3.68	0.04
3,4,5-	0.810	9.423	0.226	0.240	2.251	4.609	3.56	2.95	0.61	4.01	3.52	0.49
2,3,5-	0.166	9.594	0.234	0.238	2.251	4.069	3.36	3.06	0.30	4.21	3.64	0.57
2,3,6-	0.314	9.458	0.235	0.227	2.251	4.626	*	3.13	*	3.77	3.76	0.01
2,3,4,6-	0.187	9.451	0.237	0.224	2.611	5.037	3.35	3.65	-0.30	4.45	4.37	0.08
pentachlorophenol	0.488	9.575	0.238	0.222	2.971	5.464	3.73	3.90	-0.17	5.12	4.62	0.50
4,5,6-trichloroguaiacol	0.730	9.304	0.233	0.236	2.727	5.575	3.11	3.67	-0.56	3.83	4.37	-0.54
tetrachloroguaiacol	0.836	9.469	0.235	0.230	3.087	6.002	3.15	3.98	-0.83	4.42	4.70	-0.28

[1] using equation (2), [2] using equation (1)

* The data was not available.

RESULTS AND DISCUSSION

In order to describe the relationships among Kow, Koc, and calculated structural parameters, a multiparameter regression analysis was performed. The obtained QSAR equations are presented as follows:

$$\begin{aligned}\log Kow &= 13.07(\pm 1.06) - 0.50\mu(\pm 0.13) - 1.05E_{homo}(\pm 0.11) - 5.08qH^{+}(\pm 1.23)\\ &\quad - 5.84q^{-}(\pm 0.53) + 1.47TE(\pm 0.07)\end{aligned}$$

$$n=70,\ r(\text{adj})=0.962,\ r=0.965,\ SE=0.40,\ F=171.15,\ p=0.0000 \qquad (1)$$

$$\begin{aligned}\log Koc &= 8.74(\pm 1.26) - 0.39\mu(\pm 0.15) - 0.74E_{homo}(\pm 0.13) - 3.18qH^{+}(\pm 1.44)\\ &\quad - 2.72q^{-}(\pm 0.62) + 1.29TE(\pm 0.09)\end{aligned}$$

$$n=65,\ r(\text{adj})=0.917,\ r=0.924,\ SE=0.459,\ F=68.70,\ p=0.0000 \qquad (2)$$

$$\log Koc = 0.456(\pm 0.183) + 0.722\log Kow\ (\pm 0.037)$$

$$n=65,\ r=0.927,\ SE=0.435,\ F=385.70,\ p=0.0000 \qquad (3)$$

$$\log Koc = 0.641(\pm 0.376) + 0.526\chi^{1}(\pm 0.057)$$

$$n=65,\ r=0.756,\ SE=0.759,\ F=84.07,\ p=0.0000 \qquad (4)$$

$$\log Kow = 0.855(\pm 0.478) + 0.632\chi^{1}(\pm 0.074)$$

$$n=70,\ r=0.720,\ SE=1.026,\ F=73.17,\ p=0.0000 \qquad (5)$$

Where *n* represents the number of samples, *r* is the regression coefficient, *SE* is the standard deviation, *F* denotes the *F*-test value, *p* is the significance level of the whole equation. The number in parentheses is the standard deviation associated with each coefficient.

Considering the wide range of physicochemical properties for these compounds, equations (1) and (2) were quite good with large correlation coefficients and small SE values. This indicated that Kow and Koc can be predicted by models based on quantum chemical descriptors. Equations (4) and (5) predicted Kow and Koc based on molecular connectivity, but, the correlation was weak with large SE compared with the quantum chemical method. This indicated that the quantum chemical method is more effective than molecular connectivity methods for predicting Kow and Koc for studied compounds. The predicted values and the residuals for the studies of compounds are shown in Table 1. The predicted Kow (using equation 1) and Koc (using equation 2) were well fitted with observed Kow and Koc (Figures 1 and 2).

According to principle of statistics, a regression equation is of no relevance when the explanatory variables applied were mutually interrelated by simple or multiple correlations. However, as it was shown by the correlation coefficients of the independent variables and the VIF values (Table 2), the two obtained equations are of significance.

Table 2. Correlation coefficient matrix for significant independent variables and the variance inflation factors (VIF) for equations 1 and 2.

	Correlation matrix					(VIF)
	μ	E_{homo}	qH^+	q^-	TE	
μ	1.000					1.377
E_{homo}	-0.28	1.000				1.178
qH^+	0.018	0.202	1.000			1.256
q^-	-0.53	0.217	-0.299	1.000		1.530
TE	0.06	-0.198	0.264	-0.144	1.000	1.090

Student *t*-values for partial correlation coefficients in equation 1 are -3.863, -10.016, –4.114, –11.114, 21.006 for μ, E_{homo}, qH^+, q^-, and TE, respectively. This indicates that the total molecular energy (TE) descriptor is the most significant factor for Kow. Since the TE provides information about the bulkiness of the solute, this size-related descriptor may be related to the interaction between the solute molecule and the water phase. The most positive net atomic charges on hydrogen (qH^+) and the largest negative atomic charge on an atom (q^-) descriptor are related to the ability of the solutes to participate in hydrogen-bonding interactions with solvent molecules. E_{homo} descriptor is related to the ability of solutes to participate in electron pair donor-acceptor interactions with solvent molecules. As may be concluded from the partial correlation coefficients, this kind of interaction is less important than the q^- for Kow. The parameters μ and qH^+, are not important for Kow. The student *t*-values for partial correlation

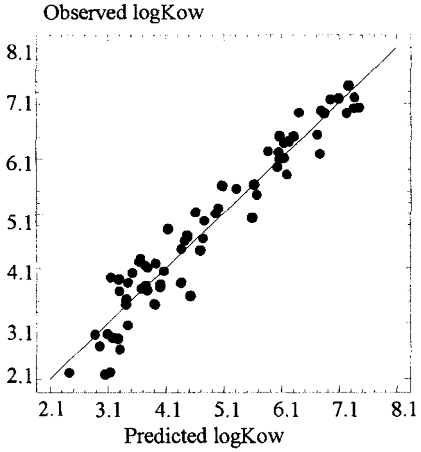

Figure 1. Plot of observed 1ogKow vs. calculated 1ogKow using equation 1

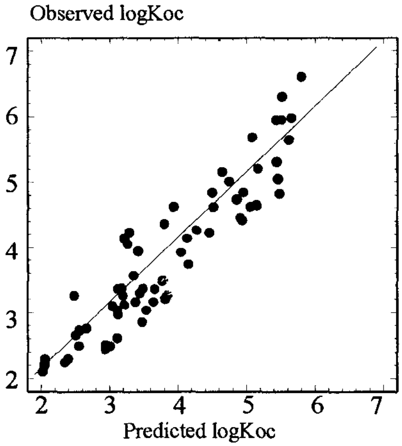

Figure 2. Plot of observed 1ogKoc vs calculated 1ogKoc using equation 2

coefficients in equation 2 are -2.543, -5.963, -2.205, -4.41, and 15.094 for μ, E_{homo}, qH^+, q^-, and TE, respectively. This indicated that the total molecular energy (TE) descriptor is the most significant factor for Koc. The TE provides information about the bulkiness of the solute. As the soil is primarily organic, it can be expected that the TE is both significant and positive, indicating larger molecules adsorb into the soil better (Famini and Wilson 1997). E_{homo} descriptor is related to the ability of solutes to participate in electron pair donor-acceptor interactions with organic in soil. As may be concluded from the partial correlation coefficients, this kind of interaction is less important for Koc. In addition, the q^- determines Koc for test compounds, and is related to the ability of the solutes to participate in hydrogen-bonding interactions with the organic molecules. Its participation in the correlation is less than the E_{homo}. The parameters μ and qH^+, are not important for Koc. The parameters μ, E_{homo}, qH^+, and q^-, had a negative sign, which means that the larger μ, E_{homo}, qH^+, and q, the smaller is the Koc value.

The results of this study indicate that the regression equations based on quantum chemical descriptors are successful in predicting 1ogKow and 1ogKoc for PCOCs. To test the robustness of equations 1 and 2, a modified form of the "jackknife test" as suggested by Dietrich *et al*, was applied to this data set where a random number of observations were deleted at a time, and the regression was rerun for the remaining observations, a randomly selected number of regression runs were done with different members deleted every time. All of the regression statistics were averaged. To maintain stability, the number of deletions was kept below 10% of the total number of observations. The overall results of the deletion study are summarized in Table 3. It indicates that the models are quite “robust” and that it is not due to a chance correlation. None of the regression parameters for the diminished data sets is significantly different from those for the full data set. These average *r* values do not any unduly high variation, suggesting that the data set is fairly consistent and the models are not biased by any particular data point. This aspect of the study tests the predictive quality of the models, and these results demonstrate that the equations 1 and 2 have high predictive ability.

Table 3. Summary of results of random deletion test.

			Kow			Koc	
no. of cases deleted (<10% of N)[a]	no. of regression runs	av. *r*	av. adjusted *r*	av. SE	av. *r*	av. adjusted r	av. SE
2	31	0.965	0.962	0.402	0.924	0.917	0.460
4	14	0.965	0.962	0.401	0.925	0.917	0.460
6	11	0.965	0.962	0.404	0.925	0.918	0.459
		0.965[b]	0.962[b]	0.402[b]	0.925[b]	0.917[b]	0.460[b]

[a]N= total number of cases=70, [b]Overall average.

In summary, the information presented in this study shows that these models based on quantum chemistry descriptors can accurately predict not only Kow but also Koc. Compared with empirical descriptors, the quantum chemistry descriptors have following advantages: (a) the structure descriptors can be easily and precisely obtained by computation instead of experimentation. (b) The quantum parameters have clear “chemical sense”. These models can provide a useful starting point for predicting the potential environmental contaminant of new compounds.

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