and Pb^{2+}), provided extra cares are taken to minimize the effects of sorption and chemical equilibrium shift. This work has shown that, although fulvic acid cannot be defined clearly in structural terms, it can be investigated and described in terms of its group properties.

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Estimation of Bioconcentration Factors in Fish for Organic Nonelectrolytes Using the Linear Solvation Energy Relationship

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Bioconcentration factors (BCF) in fish of organic nonelectrolytes are well correlated by a linear solvation energy relationship (LSER) of the form:

$$\log \text{BCF} = -0.95 + 4.74\, V_I/100 - 4.39\, \beta + 0.88\, \alpha$$

where V_I is the intrinsic solute molecular volume and β and α are the solvatochromic parameters that measure hydrogen bond acceptor basicity and donor acidity of the compound. The LSER model can not only correlate the property with an accuracy comparable to molecular connectivity model but also provide a quantitative information on the nature and relative strength of solute-target system interactions affecting the property of interest. Such an information can hardly be obtained from molecular connectivity model.

Introduction

Over the past decades the chemical contamination of our environment has aroused increasing concern. A proper assessment of the risk to men and environment by exposure to these chemicals generally includes attempts to measure or predict the concentration in various environmental compartments in conjunction with toxicological data. However, the concentration data or the toxicological data are often not adequate for realistic assessments, and basic physical

and chemical data are often not available. Since an estimated 70,000 chemicals are currently in common use and their number grows by about 1,000 each year, it is obvious that our human and material resources are insufficient to experimentally obtain the necessary data. It is thus necessary to develop quantitative models that will accurately and rapidly predict environmental distribution coefficients and toxicity of organic pollutants.

Bioconcentration factor (BCF) is the concentration of a chemical in an organism divided by the concentration in water and it is one of the most important indicators for the fate of chemicals in the environment. A number of linear correlations between chemical properties such as water solubility (S_W) and octanol-water partition coefficient (K_{OW}) and BCF have been published[1-5]. The precision of correlation between BCF and S_W is very low due to the lack of accuracy in S_W data. A higher precision has been more often observed in correlations between BCF and K_{OW}[3,5]. However, a loss of linear correlation was observed for chemicals with a relatively high log K_{OW} (>5) and the factors causing the observed deviation from linearity have been discussed in datail[6]. Furthermore, experimental determination of K_{OW} may be very costly and time consuming. Recently, a quantitative model which uses nonempirical parameters such as molecular connectivity indices has been developed and demonstrated to be a fast and accurate predictive tool for BCF[7-9]. Although the model correlates very well connectivity indices with BCF, the model is not able to provide a quantitative information on chemical-target system interactions affecting the property of interest.

In this paper we report the use of the Kamlet-Taft solvatochromic parameters[10] in the linear solvation energy relationship (LSER)[11,12] to correlate and predict BCF. It has been demonstrated that many disparate physicochemical, biochemical, toxicological, pharmacological properties of organic nonelectrolytes that depend on solute/solvent interactions and aqueous solubilities in a variety of media can be correlated, rationalized, and predicted by the application of this methodology. Examples include octanol-water[13-15] and triolein-water partition coefficents[16], gas-blood partition coefficients[17], aqueous solubilities[18], inhibition of bioluminescence in *Photobacterium phosphoreum* (the Microtox test)[19], toxicities to the Golden Orfe Fish[20] and binding to bovine serum albumin[16], and retention behavior of solutes in gas and liquid chromatography[21-27].

The LSER for a property of solutes (SP) that depends on solute-solvent interactions in given by Eq. (1), which specifically identifies and evaluates the individual solute-solvent interactions that contribute to the SP.

$$SP = SP_0 + mV_I/100 + s\pi^* + d\delta + b\beta_m + a\alpha_m \quad (1)$$

The $mV_I/100$ term measures the endoergic process of separating the solvent molecules to provide a suitably sized cavity for the solute. V_I is computercalculated intrinsic molecular volume of the solute[28]. V_I is scaled by 1/100 so that it should cover roughly the same range as the other independent variables. The $s\pi^*$ and $d\delta$ term together measure exoergic solute-solvent dipole-dipole and dipole-induced dipole interactions; π^* is the solvatochromic parameter which measures the ability of a molecule to stabilize a neighboring charge or dipole, and to induce a dipole in a neighboring nondipolar molecule. The δ term in Eq. (1) is a polarizability correction parameter, equal to 0.0 for nonpolyhalogenated aliphatic compounds, 0.5 for polyhalogenated aliphatics, and 1.0 for single-ring aromatic compounds. For some multiple-ring aromatic compounds δ has values of 2.0[15]. Exoergic effects of hydrogen bonding interactions are measured by $b\beta_m$ and $a\alpha_m$ terms; β and α are the solvatochromic parameters that measure hydrogen bond acceptor (HBA) basicity and hydrogen bond donor (HBD) acidity, respectively. The subscript m indicates that for compounds capable of self-association, the parameter applies to the non-self-associated "monomer" solute, rater than the self-associated "oligomer" solvent. For non-self-associating compounds, $\alpha_m = \alpha$, $\beta_m = \beta$. The solvatochromic parameters of over 500 compounds available at present were either measured[10] or estimated by parameter estimation rules[14,15]. Any one or combination of terms in Eq. (1) may drop out if not applicable to the property studied. We use Eq. (1) to correlate BCF with the solute properties and to obtain an insight into the nature of chemical-target system interactions influencing these properties.

Results and Discussion

The BCF data, taken from a compilation of Sabljic[9], are assembled in Table 1 for the 51 (of 87) compounds whose solvatochromic parameters are known or could be estimated using the present parameter estimation rules[14,15]. The multiple linear regression equation for 51 compounds of Table 1 is given by Eq. (2).

$$\log BCF = -0.89(\pm 0.24) + 4.56(\pm 0.37)\, V_I/100 + 0.11(\pm 0.37)\pi^* - 0.05(\pm 0.25)\delta - 3.72(\pm 0.59)\beta + 0.73(\pm 0.42)\alpha \quad (2)$$
$$n = 51,\ r = 0.944,\ s.d. = 0.45$$

The coefficients for π^* and δ are statistically zero and not significant at the 0.95 confidence level. Thus log BCF values were regressed using a three-parameter equation which includes V_I, β and α. The resulting LSER equation is given as follows.

$$\log BCF = -0.95(\pm 0.23) + 4.74(\pm 0.25)\, V_I/100 - 4.39(\pm 0.62)\beta + 0.88(\pm 0.38)\alpha \quad (3)$$
$$n = 51,\ r = 0.947,\ s.d. = 0.42$$

Important requirements that need to be met for an LSER to correctly represent the property studied are a high correlation coefficient (r) and a low standard deviation ($s.d.$). An equally important and more rigorous test is that the equation be 'robust', *i.e.*, the intercept and the coefficients for the independent variables should be reasonably similar for different subsets of the data. To test robustness of Eq. (3) we performed a jackknife test with removal of 10% of randomly selected compounds in each run. In Table 2 are listed the correlation equations for different subsets of the data. It is seen that the equation is quite 'robust'. The intercepts and coefficients of the independent variables for the subsets agree quite we with the corresponding terms for the full data set. Since all chlorobenzenes and PCBs included in run no. 5 have α value of zero, $a\alpha$ term does not appear in the LSER equation.

The following information may be adduced from Eq. (3) regarding BCF: (a) Since water is a more cohesive solvent than the lipid or protein components of the bioorganism,

Table 1. Data Used for Correlation of Bioconcentration Factors

No.	Compound	$V_I/100^a$	π^{*a}	δ^a	β^a	α^a	log BCF		
							Exptl.	Eq. (3)	Diff.[b]
1	toluene	0.592	0.55	1	0.11	0	0.92	1.37	0.45
2	ethylbenzene	0.687	0.53	1	0.12	0	1.19	1.78	0.59
3	1,2-dimethylbenzene	0.671	0.51	1	0.12	0	1.15	1.71	0.56
4	1,3-dimethylbenzene	0.671	0.51	1	0.12	0	1.17	1.71	0.54
5	1,4-dimethylbenzene	0.671	0.51	1	0.12	0	1.17	1.71	0.54
6	isopropylbenzene	0.775	0.51	1	0.12	0	1.55	2.20	0.65
7	1,2,4-trimethylbenzene	0.769	0.47	1	0.13	0	2.12	2.13	0.01
8	naphthalene	0.753	0.70	1	0.15	0	2.20	1.96	−0.24
9	2-methylnaphthalene	0.851	0.66	1	0.16	0	2.61	2.38	−0.23
10	phenanthrene	1.015	0.80	1	0.20	0	3.42	2.98	−0.44
11	2-methylphenanthrene	1.113	0.76	1	0.21	0	3.48	3.40	−0.08
12	anthracene	1.015	0.80	1	0.20	0	3.13	2.98	−0.15
13	9-methylanthracene	1.113	0.76	1	0.21	0	3.66	3.40	−0.26
14	benz[a]anthracene	1.277	0.90	1	0.25	0	4.00	4.01	0.01
15	acenaphthene	0.896	0.62	1	0.17	0	2.60	2.55	−0.05
16	pyrene	1.156	0.91	1	0.25	0	3.43	3.43	0.00
17	benzo[a]pyrene	1.418	1.00	1	0.30	0	3.70	4.45	0.75
18	fluorene	0.960	0.66	2	0.21	0	3.11	2.68	−0.43
19	chlorobenzene	0.581	0.71	1	0.07	0	1.08	1.50	0.42
20	1,2-dichlorobenzene	0.671	0.80	1	0.03	0	1.95	2.10	0.15
21	1,3-dichlorobenzene	0.671	0.75	1	0.03	0	1.82	2.10	0.28
22	1,4-dichlorobenzene	0.671	0.70	1	0.03	0	2.10	2.10	0.00
23	1,2,3-trichlorobenzene	0.761	0.85	1	0	0	2.69	2.66	0.01
24	1,2,4-trichlorobenzene	0.761	0.75	1	0	0	3.23	2.66	−0.57
25	1,3,5-trichlorobenzene	0.761	0.70	1	0	0	3.24	2.66	−0.58
26	1,2,3,5-tetrachlorobenzene	0.851	0.80	1	0	0	3.50	3.09	−0.41
27	1,2,3,4-tetrachlorobenzene	0.851	0.80	1	0	0	3.58	3.09	−0.49
28	1,2,4,5-tetrachlorobenzene	0.851	0.70	1	0	0	3.65	3.09	−0.56
29	pentachlorobenzene	0.941	0.75	1	0	0	3.74	3.51	−0.23
30	hexachlorobenzene	1.031	0.70	1	0	0	4.23	3.94	−0.29
31	2-chlorophenanthrene	1.105	0.91	1	0.16	0	3.63	3.59	−0.04
32	1,2-dichloroethane	0.442	0.81	0.5	0.10	0	0.30	0.71	0.41
33	1,1,2-trichloroethylene	0.492	0.53	0.5	0.05	0	1.20	1.17	−0.03
34	tetrachloroethylene	0.578	0.28	0.5	0.05	0	1.70	1.57	−0.13
35	biphenyl	0.920	1.18	2	0.20	0	2.42	2.53	0.11
36	4-chlorobiphenyl	1.010	1.20	2	0.17	0	2.77	3.09	0.32
37	4,4′-PCB	1.100	1.40	2	0.14	0	4.10	3.65	−0.45
38	2,4,4′-PCB	1.190	1.46	2	0.10	0	4.66	4.25	−0.41
39	2,2′,5-PCB	1.190	1.45	2	0.10	0	4.69	4.25	−0.44
40	2,2′,4,4′-PCB	1.280	1.50	2	0.06	0	4.85	4.86	0.01
41	2,2′,5,5′-PCB	1.280	1.35	2	0.06	0	4.86	4.86	0.00
42	2,2′,4,5,5′-PCB	1.370	1.40	2	0.03	0	4.83	5.41	0.58
43	2,2′,4,4′,5,5′-PCB	1.460	1.50	2	0	0	4.98	5.97	0.99
44	3-chlorophenol	0.626	0.77	1	0.23	0.69	1.25	1.62	0.37
45	4-bromopheonl	0.669	0.79	1	0.23	0.69	1.56	1.82	0.26
46	4-nitrophenol	0.676	1.15	1	0.32	0.82	2.10	1.57	−0.53
47	aniline	0.562	0.73	1	0.50	0.16	0.78	−0.04	−0.82
48	N,N-diethylaniline	0.948	0.75	1	0.44	0	2.08	1.61	−0.47
49	nitrobenzene	0.631	1.01	1	0.30	0	1.18	0.73	−0.45
50	chloronitrobenzene	0.721	1.01	1	0.26	0	1.00	1.33	0.33
51	cyclohexane	0.598	0	0	0	0	2.22	1.89	−0.33

[a] Solute parameters are either from refs. 14 and 15 or estimated by parameter estimation rules [15]. [b] Calculated minus experimental.

Table 2. Comparison of Correlation Equations for Different Subsets of the Data log BCF=$SP_O+mV_I/100+b\beta+a\alpha$

Run	Data set[a]	SP_O[b]	m[b]	b[b]	a[b]	n	r	s.d.
1	all solutes	−0.94(0.22)	4.74(0.24)	−4.39(0.62)	0.88(0.37)	51	0.947	0.42
2	1,8,20,32,37	−0.79(0.25)	4.58(0.27)	−4.41(0.64)	0.82(0.38)	46	0.943	0.42
3	6,13,26,31,43	−1.07(0.22)	4.95(0.25)	−4.75(0.62)	0.98(0.35)	46	0.953	0.39
4	4,10,24,34,36	−0.95(0.24)	4.72(0.25)	−4.26(0.64)	0.86(0.37)	46	0.951	0.42
5	chlorobenzenes and PCBs only	−0.51(0.51)	4.31(0.47)	−4.95(1.62)		21	0.953	0.43

[a]The numbers in runs 2-4 indicate the compound numbers, which were removed from the data set. For compound numbers, see Table 1. [b]The numbers in parentheses are standard deviations in the coefficient estimates.

Table 3. Comparison of Estimated Log BCF Values to Experimental values for Compounds Not Used in Developing the LSER Equation

Compound	$V_I/100$	β	α	Eq. 3	Exptl.	diff.	Lit.
Acenaphthene	0.896	0.17	0	2.55	2.59	−0.04	29
Benzene	0.491	0.10	0	0.94	1.10	−0.16	29
Perylene	1.415	0.30	0	4.44	3.86	0.58	35
Tetrachloromethane	0.514	0.10	0.	1.05	1.36	−0.31	29
Chloroform	0.427	0.10	0.35	0.95	0.78	0.17	29
Pentachloroethane	0.700	0.10	0	1.93	1.83	0.10	29
1,1,2,2,-tetrachloroethane	0.617	0.10	0	1.54	1.25	0.29	29
1,1,1-trichloroethane	0.519	0.10	0	1.07	0.95	0.12	29

increasing V_I leads to increasing solubility in the organism over water. This should, and does lead to increased bioconcentration (a positive sign of the coefficient m). (b) Because water is a stronger HBD acid than any components of the organism, increasing chemical β should, and does lead to decreasing bioconcentration (a negative sign of the coefficient b). (c) Because the lipid and protein component of the organism are stronger HBA bases than water (β values; water 0.2-0.4, lipid R-CO-O-R 0.5, protein R-CO-NH-R 0.8)[19], increasing α should, and does lead to increasing bioconcentration (a positivie sign of the coefficient a). The size of each coefficient in Eq. (3) tells us that the leading term influencing bioconcentration of organic chemicals in fish is endoergic effect of cavity formation, which is followed by the exoergic hydrogen bonding between the solute as the acceptor and water as the donor. Hydrogen bonding between the solute as donor lipid and protein in fish as the acceptor reflect only secondary dependence on these interactions.

Accuracy of applicability of the LSER (Eq. (3)) is only slightly lower than those of correlations with molecular connectivity indices[9]. However, in view of large scatters in measured BCF values due to a number of significant variables affecting the accuracy of measurements of BCF[29-34], an average error of 0.42 log units associated with the LSER correlation represents a reasonable level of accuracy. The LSER correlation can provide quantitative analysis of factors that cause to increase or decrease BCF in the organism. Although correlations with molecular connectivity indices are simple and slightly more precise than the LSER, they are hardly useful in providing a quantitative information on solute-target system interactions affecting the property of interest.

Performance of the LSER model (Eq. (3)) was tested by choosing different subsets of organic chemical compounds and their corresponding log BCF values from the literature. Estimated log BCF values are compared with the experimental values in Table 3. The differences between experimental and estimated BCF values for compounds except perylene are smaller than the standard error of estimate (0.42) obtained from the LSER model. Although the body of data used in the test is not large, this result demonstrates the applicability of Eq. (3) to prediction of BCF values for various classes of organic compounds used to develop the model.

Conclusion

Bioconcentration factors in fish of organic nonelectrolytes are well correlated by linear solvation energy relatioships. The accuracy of predicted values for BCF by the LSER model is comparable to that by molecular connectivity model. As shown above the LSER can not only correlate and predict but also provid quantitative analysis of the factors determining BCF. Such an information can hardly be obtained from molecular connectivity model. The LSER equation for BCF suggested in this paper will be useful in estimating BCF for many other organic compounds whose solvatochromic parameters can be estimated by the parameter estimation rules.

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Viologen-mediated Reductive Transformations of *gem*-Bromonitro Compounds and α-Nitro Ketones by Sodium Dithionite

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Reductive transformations of *gem*-bromonitro compounds and α-nitro ketones were carried out conveniently with sodium dithionite by using dioctyl viologen as an electron-transfer catalyst in dichloromethane-water two-phase system: the bromine atom in *gem*-bromonitro compounds and the nitro group in α-nitro ketones are replaced by hydrogen.

Introduction

Viologens (1,1'-dialkyl-4,4'-bipyridiniums, V^{2+}) undergo two consecutive one-electron reduction processes to the respective cationic radical ($V^{+\cdot}$) and quinoid (V) forms. The reduced forms are readily reoxidized to V^{2+}. They have at-