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Reverse-Phase High Performance Liquid Chromatography and Linear Solvation Energy Relationship for Studies of Alkyl (1-Phenylsulfonyl) Cycloalkane-Carboxylates

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The unusual and diverse properties of sulphur atom have led to the development of a large variety of compounds containing sulphur atom in various oxidation states in recent years. These compounds are used more extensively as either synthesis intermediates in the manufacture of pesticides, herbicides and drug, or as floatation agents and extractant in the petrochemical and metallurgical industries(Han et al.1992; Pandeya et al. 1985). Accompanying these new chemicals being introduced into the environment, pollution effects by these kinds of compounds should be anticipated. It is widely recognized that knowledge on the environmental fate of pollutants is a basic need in the environmental risk assessment. In this paper, we report octanol/water partition coefficient and acute toxicity to Daphnia magna of 28 alkyl (1-phenylsulfonyl)cycloalkane-carboxylates and use two methods, RP-HPLC method(Carlson et al. 1975; Jinno 1984) and linear solvation energy relationship (LSER) method(Kamlet et al. 1986) to correlate and estimate these two properties of aromatic sulfone which are useful for understanding their environmental behavior. These two QSAR methods were evaluated for their accuracy and range of applicability.

MATERIALS AND METHODS

The liquid chromatograph was a Shimadzu LC-3A high performance liquid chromatography(HPLC), coupled with SPD-6AV UV-Vis spectrophotometric detector. Analytical grade solvents methanol and ethanol were redistilled before use. Analytical grade octanol was used. Water was doubly distilled in quartz. 28 alkyl (1-phenylsulfonyl) cycloalkane-carboxylates were synthesized in our laboratory. Their purities were monitored by HPLC to assure purity. The formulas and CAS No. (seventeen compounds don't have CAS No.) are given in Table 1.

The octanol/water partition coefficients were determined by shake-flask as described by OECD guideline for testing of chemicals(1981) at 25°C followed by centrifuging and were quantitatively measured with a UV-spectrophotometer against water blank. A Nucleosil C18 column, 15 cm x 4.6 mm (made by Dalian Institute of Chemical Physics, Academia Sinica, Dalian), was used with flow rate of 1.0 mL/min. at

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Table 1. Molecular formula for 28 alkyl (1-phenylsulfonyl) cycloalkane-carboxylates.

No.	compound	CAS No.	mp(°C)
1.	$4\text{-}NO_2\text{-ph-}SO_2\text{-}C(CH_2)_2\text{-}CO_2\text{-}CH_3$	145348-26-1	127.0
2.	$4\text{-}NO_2\text{-ph-}SO_2\text{-}C(CH_2)_2\text{-}CO_2\text{-}CH(CH_3)_2$	145348-27-2	122.7
3.	$4\text{-}NO_2\text{-ph-}SO_2\text{-}C(CH_2)_3\text{-}CO_2\text{-}CH(CH_3)_2$		65.5
4.	$4\text{-}NO_2\text{-ph-}SO_2\text{-}C(CH_2)_5\text{-}CO_2\text{-}CH(CH_3)_2$		110.5
5.	$4\text{-}NO_2\text{-ph-}SO_2\text{-}C(CH_2)_6\text{-}CO_2\text{-}CH(CH_3)_2$		83.5
6.	$4\text{-Br-ph-}SO_2\text{-}C(CH_2)_2\text{-}CO_2\text{-}CH_3$	145348-25-0	123.5
7.	$4\text{-Br-ph-}SO_2\text{-}C(CH_2)_3\text{-}CO_2\text{-}CH_3$		95.0
8.	$4\text{-Br-ph-}SO_2\text{-}C(CH_2)_4\text{-}CO_2\text{-}CH_3$		103.5
9.	$4\text{-Br-ph-}SO_2\text{-}C(CH_2)_5\text{-}CO_2\text{-}CH_3$		111.5
10.	$4\text{-Cl-ph-}SO_2\text{-}C(CH_2)_2\text{-}CO_2\text{-}CH_3$	145348-22-7	115.5
11.	$4\text{-Cl-ph-}SO_2\text{-}C(CH_2)_3\text{-}CO_2\text{-}CH_3$		76.2
12.	$4\text{-Cl-ph-}SO_2\text{-}C(CH_2)_2\text{-}CO_2\text{-}CH(CH_3)_2$	145348-23-8	89.8
13.	$4\text{-Cl-ph-}SO_2\text{-}C(CH_2)_2\text{-}CO_2\text{-}C(CH_3)_3$	145348-24-9	110.5
14.	$4\text{-Cl-ph-}SO_2\text{-}C(CH_2)_4\text{-}CO_2\text{-}CH(CH_3)_2$		92.5
15.	$4\text{-Cl-ph-}SO_2\text{-}C(CH_2)_5\text{-}CO_2\text{-}CH(CH_3)_2$		117.5
16.	$4\text{-Cl-ph-}SO_2\text{-}C(CH_2)_6\text{-}CO_2\text{-}CH(CH_3)_2$		106.5
17.	$4\text{-}CH_3\text{-ph-}SO_2\text{-}C(CH_2)_2\text{-}CO_2\text{-}CH(CH_3)_2$	145348-21-6	65.5
18.	$4\text{-}CH_3\text{-ph-}SO_2\text{-}C(CH_2)_3\text{-}CO_2\text{-}CH(CH_3)_2$		50.8
19.	$4\text{-}CH_3\text{-ph-}SO_2\text{-}C(CH_2)_2\text{-}CO_2\text{-}CH_3$	145348-19-2	97.2
20.	$4\text{-}CH_3\text{-ph-}SO_2\text{-}C(CH_2)_2\text{-}CO_2\text{-}CH_2CH_3$	145348-20-5	75.5
21.	$4\text{-}CH_3\text{-ph-}SO_2\text{-}C(CH_3)_3\text{-}CO_2\text{-}CH_2CH_3$		53.5
22.	$4\text{-}CH_3\text{-ph-}SO_2\text{-}C(CH_2)_4\text{-}CO_2\text{-}CH(CH_3)_2$		72.5
23.	$4\text{-}CH_3\text{-ph-}SO_2\text{-}C(CH_2)_5\text{-}CO_2\text{-}CH(CH_3)_2$		106.5
24.	$4\text{-}CH_3\text{-ph-}SO_2\text{-}C(CH_2)_5\text{-}CO_2\text{-}CH_3$		145.5
25.	$\text{ph-}SO_2\text{-}C(CH_2)_2\text{-}CO_2\text{-}CH_3$	97383-42-1	74.5
26.	$\text{ph-}SO_2\text{-}C(CH_2)_3\text{-}CO_2\text{-}CH_3$		107.5
27.	$\text{ph-}SO_2\text{-}C(CH_2)_4\text{-}CO_2\text{-}CH_3$		56.5
28.	$\text{ph-}SO_2\text{-}C(CH_2)_5\text{-}CO_2\text{-}CH_3$		114.5

ambient temperature(20°C±2). The detector was set at 254 nm (NO_2 alkyl (1-phenylsulfonyl) cycloalkane-carboxylates) and 230 nm (others compounds). The mobile phase consisted of different volume fractions of methanol in water(100:0, 95:5, 90:10, 85:15, 80:20, 75:25, 70:30), respectively. The column dead time (t_0) was determined by the injection of $NaNO_3$ dissolved in methanol, and the relative capacity factor k'[$k'=(t_R-t_0)/t_0$] of these compounds were measured. t_R is relative retention time. Table 2 collects the data from regression analysis of the relation between logk' and the volume fraction of methanol ($\phi_{CH_3OH}=0$) in the mobile phase.

These compounds were diluted with experiment water (dissolved oxygen concentration = 8.2±0.5 mg/L; pH = 7.5± 0.3; hardness = 115±8.0 mg/L expressed as $CaCO_3$). Acetone was used as dispersant-solvent for chemicals slightly soluble in water. The volume of acetone never exceeded 0.1 mL/L of experiment water. The Daphnia magna used in the experiments obtained from local waterbodies, about 3 years prior to the experiment, and cultured in 15 L glass carboy containing 10 L of

Table 2. Regression analysis of the relationship between logk' and the volume fraction of methanol in mobile phase: $\log k' = \log k_w - s\phi_{CH_3OH}$. ($\log k_w$ and s are regression coefficients)

compound	$\log k_w$	-s	r^2	sd	n
1	1.059(0.068)	1.636(0.079)	0.9884	0.021	7
2	1.746(0.044)	2.293(0.052)	0.9974	0.014	7
3	2.082(0.139)	2.614(0.162)	0.9813	0.043	7
4	3.167(0.194)	3.650(0.227)	0.9811	0.060	7
5	3.548(0.199)	3.597(0.232)	0.9831	0.061	7
6	1.548(0.089)	1.643(0.104)	0.9805	0.027	7
7	1.692(0.098)	1.786(0.114)	0.9799	0.030	7
8	2.121(0.117)	2.193(0.137)	0.9809	0.036	7
9	2.553(0.140)	2.600(0.170)	0.9803	0.044	7
10	1.228(0.070)	1.307(0.082)	0.9809	0.022	7
11	1.403(0.078)	1.486(0.091)	0.9817	0.024	7
12	1.860(0.095)	1.936(0.111)	0.9839	0.029	7
13	2.190(0.115)	2.264(0.134)	0.9829	0.035	7
14	2.613(0.121)	2.657(0.141)	0.9860	0.037	7
15	3.005(0.141)	3.014(0.165)	0.9853	0.043	7
16	3.549(0.130)	3.543(0.152)	0.9908	0.040	7
17	1.599(0.091)	1.693(0.107)	0.9805	0.028	7
18	1.808(0.099)	1.879(0.115)	0.9815	0.031	7
19	1.019(0.054)	1.114(0.063)	0.9845	0.017	7
20	1.309(0.073)	1.407(0.085)	0.9821	0.023	7
21	1.468(0.085)	1.557(0.099)	0.9801	0.026	7
22	2.240(0.095)	2.293(0.111)	0.9884	0.029	7
23	2.672(0.130)	2.700(0.152)	0.9845	0.040	7
24	1.903(0.087)	1.950(0.101)	0.9866	0.027	7
25	0.660(0.037)	0.779(0.043)	0.9849	0.011	7
26	0.849(0.051)	0.957(0.060)	0.9811	0.016	7
27	1.128(0.063)	1.207(0.073)	0.9819	0.019	7
28	1.524(0.079)	1.586(0.092)	0.9835	0.024	7

nutrient media. The green algae (Selenastrum capricornutum) was served as food source for Daphnia magna. Daphnia magna cultured at laboratory exposure chambers consisted of 250 mL glass beaker that contained 200 mL test solution. The concentration alkyl (1-phenylsulfonyl)cycloalkane-carboxylates range in which effects were likely to occur was determined from range-finding tests. Ten Daphnia magna (< 24 hr old) were randomly assigned to each of three replicates test vessels at each exposure level. Test chambers were loosely covered with glass plates to retard evaporation and renewed water each 24 hr(Francis 1986). There were also three replicates of the controls without chemical. Test were performed in darkness and at 22±1°C. Mortality was determined by probing for movement at the end of 48 hr. Toxicity values (LC_{50}) were determined by probit regression analysis(Exner 1988) and control mortality was less than 10% for all analysis. The level of statistical significance employed in all cases was $P < 0.05$. The results of Kow and LC_{50}(values are expressed in moles/L) are given in Table 3. All statistical analyses were performed using the STATGRAPHICS program.

Table 3. The experimental and estimated logKow and log $1/LC_{50}$ for compounds of this class.

compound	logKow			log $1/LC_{50}$		
	exptl.	calcd.	diff.	exptl.	calcd.	diff.
1	1.33	1.41	-0.08		3.16	
2	2.05	1.94	0.11	3.60	3.48	0.12
3	2.36	2.21	0.15	3.70	3.64	0.06
4	2.84	3.06	-0.22	3.97	4.14	-0.17
5	3.41	3.42	-0.01		4.34	
6	2.32	2.30	0.02	3.54	3.59	-0.05
7	2.45	2.40	0.05	3.70	3.66	0.04
8	2.73	2.74	-0.01	3.83	3.86	-0.03
9	2.94	3.09	-0.15		4.06	
10	2.03	2.08	-0.05	3.43	3.46	-0.03
11	2.28	2.20	0.08	3.59	3.54	0.05
12	2.64	2.55	0.09	3.67	3.74	-0.07
13	2.68	2.79	-0.11	3.78	3.89	-0.11
14	3.16	3.13	0.03	3.97	4.09	-0.12
15	3.49	3.46	0.03	4.16	4.28	-0.12
16	3.83	3.87	-0.04		4.53	
17	2.52	2.33	0.19	3.72	3.62	0.10
18	2.78	2.51	0.27	3.96	3.72	0.24
19	1.77	1.91	-0.14	3.21	3.36	-0.15
20	2.23	2.12	0.11	3.49	3.49	0.00
21	2.31	2.24	0.07	3.75	3.56	0.19
22	2.88	2.85	0.03	4.11	3.92	0.19
23	3.21	3.19	0.02	4.25	4.12	0.13
24	2.54	2.61	-0.07		3.77	
25	1.43	1.62	-0.19	3.03	3.19	-0.16
26	1.63	1.77	-0.14	3.18	3.28	-0.10
27	1.98	2.01	-0.03	3.39	3.41	-0.02
28	2.30	2.31	-0.01		3.60	

RESULTS AND DISCUSSION

In RP-HPLC, the mobile phase effects can be separated from stationary phase effects by using the linear relationship between the retention values and the composition of the mobile phase. The linear approximation of the relationship between the logarithm of the capacity factors(logk') and the composition of the mobile phase(φ) can be described by(Snyder et al. 1979),

$$\log k' = \log k_w - s\varphi_{CH_3OH} \qquad (1)$$

where k' is the capacity factor, φ_{CH_3OH} is the volume fraction of methanol in binary mobile phase, k_w represents the k' value for a compound if pure water is used as eluent($\varphi_{CH_3OH}=0$), and s is slope of the regression curve. Table 2 collects the data from regression analysis of the relation between logk' and φ_{CH_3OH}.
Table 2 shows that the above-stated relationship has produced good linear regression lines for all substances.

The relation between lok' and logKow, log $1/LC_{50}$ can be expressed as (Carlson et al. 1975; Jinno 1984),

$$\log P = a + b\log k' \tag{2}$$

where logP represents logKow or log $1/LC_{50}$, k' is the capacity factor, a and b are regression coefficients. To perform the liquid chromatographic determination of Kow, the HPLC capacity factors of all investigated substances were correlated with the corresponding octanol/water coefficients which were determined by shake-flask method. As can be seen from eq.3, good linear relationship between logKow and logk' was obtained at the methanol-water eluent of composition 60:40(v/v) (extrapolated).

$$\log K_{ow} = 1.265(0.051) + 1.843(0.069)\log k'(60\%) \tag{3}$$

$n=28 \quad r^2=0.964 \quad sd=0.116$

in this and all the regression equations that follow, n is the number of data points in the regression, r is the correlation coefficient and sd is the standard deviation. As described above, we obtain eq.4 for log $1/LC_{50}$-logk'.

$$\log 1/LC_{50} = 2.949(0.073) + 0.887(0.083)\log k'(50\%) \tag{4}$$

$n=22 \quad r^2=0.852 \quad sd=0.126$

The above equations can be used to calculate logKow and log $1/LC_{50}$ for compounds of this class. Table 3 lists the estimated logKow and log $1/LC_{50}$ values which were derived from RP-HPLC method. The estimated values of these compounds studied in this paper are in good agreement with our experimental values. Thus, these relationships provided a rapid and simple way to predict these two properties of compounds of this class.

As in linear solvation energy relationships (LSERs) (Kamlet 1986), solvent-dependent properties, represented by the term XYZ, depend on linear combination of energy contributions of three types of terms: cavity term, dipolar-polarizability term and hydrogen bonding terms, characterized by $mV_I/100$, π^*, α_m, β_m. We obtain,

$$XYZ = XYZ_0 + mV_I/100 + s\pi^* + a\alpha_m + b\beta_m \tag{5}$$

The $mV_1/100$ term measures the endoergic process of separating the solvent molecules to provide a suitably sized cavity for the solute. V_1 is intrinsic molecular volume of the solute. V_1 is scaled by 1/100 so that it should be comparable to other three variables. The $s\pi^*$ term measures the (usually) exoergic effects of solute-solvent dipole-dipole, dipole-induced dipole and dispersion interactions. $a\alpha_m$ and $b\beta_m$ terms measure exoergic effects of hydrogen bonding interactions; α_m and β_m are the solvatochromic parameters that measure hydrogen bond donor(HBD) acidity and hydrogen bond acceptor(HBA) basicity, respectively. For non-self-associating compounds, $\alpha_m=\alpha$, $\beta_m=\beta$. The term in α_m drops out of eq.6 for alkyl (1-phenylsulfonyl)cycloalkane-carboxylates are not hydrogen bond donors(Kamlet et al. 1986). The alkyl (1-phenylsulfonyl)cycloalkane-carboxylates follow nonreactive toxicity mechanism because of their hydrolyzing very slowly at pH = 7 and 25°C(Han et al. 1992; Kamlet et al. 1987). Recently, Hickey and Passino-Reader(1991) developed a method to estimate LSER variable values quickly for vast array of possible organic compounds such as those found in the environment. The calculated LSER variable values of 28 alkyl (1-phenylsulfonyl)cycloalkane-carboxylates are shown in Table 4.

We applied the LSER of eq.5 in order to correlate logKow, $\log k_w$ and log $1/LC_{50}$ and to obtain quantitative information on the factors affecting them. The multiple linear regression equations for 28 alkyl (1-phenylsulfonyl)cycloalkane-carboxylates are given by eq.6, eq.7 and eq.8,

$$\log K_{ow} = 2.576(1.229)+3.206(0.126)V_I/100-1.064(0.510)\pi^*-2.584(0.252)\beta \tag{6}$$

$n=28 \quad r^2=0.960 \quad sd=0.119$

$$\log k_w = 4.564(1.330)+4.084(0.136)V_I/100-3.443(0.553)\pi^*-1.531(0.273)\beta \tag{7}$$

$n=28 \quad r^2=0.972 \quad sd=0.129$

$$\log 1/LC_{50}=1.177(1.048)+1.880(0.127)V_I/100+0.299(0.443)\pi^*-0.893(0.242)\beta \tag{8}$$

$n=22 \quad r^2=0.912 \quad sd=0.094$

In eq.8, the coefficient for π^* is statistically zero and not significant at the 0.95 confidence level. Thus, log $1/LC_{50}$ values were regressed using a two-parameters equation which includes V_1 and β. The resulting LSER equation is given as follows.

$$\log 1/LC_{50} = 1.866(0.240)+1.883(0.125)V_I/100-0.954(0.222)\beta \tag{9}$$

$n=22 \quad r^2=0.916 \quad sd=0.093$

It can be seen in eqs. 6, 7, 8 and 9 that logKow, $\log k_w$ and log $1/LC_{50}$ are correlated well with the solvatochromic parameters. The following information may be deduced from eqs.6, 7, 8 and 9: (a) since water is a more cohesive solvent than 1-octanol, alkane and lipid or protein components of the bioorganism, increasing V_I leads to increasing logKow, $\log k_w$ and log $1/LC_{50}$(a positive sign of the coefficient). (b) Because water is a stronger HBD acid than 1-octanol, alkane and any components of the organism, increasing chemical β should, and does lead to decreasing these three properties. (c) Increasing dipolarity and polarizability(π^*) leads to increasing water solubility, which in turn decrease logKow and $\log k_w$. However, as polarity increases, aqueous solubility and log $1/LC_{50}$ increases. This is true for the correlations determined here as well as other toxicity correlations with solvatochromic parameters(Blum et al. 1991). Dipolarity/ polarizability term plays not very important role in eq.8 and is dropped out of in eq.9.

Table 4. The solvatochromic parameters and estimated logKow, $\log k_w$ and log $1/LC_{50}$ for 28 alkyl (1-phenylsulfonyl)cycloalkane-carboxylates.

No.	$V_I/100$	π^*	β	logKow		$\log k_w$		log $1/LC_{50}$	
				calcd.	diff.	calcd.	diff.	calcd.	diff.
1	1.326	2.02	1.26	1.42	-0.09	1.095	-0.036	3.16	
2	1.526	2.02	1.26	2.06	-0.01	1.912	-0.166	3.54	0.06
3	1.610	2.03	1.26	2.32	0.04	2.221	-0.139	3.70	0.00
4	1.806	2.04	1.26	2.94	-0.10	2.987	0.180	4.06	-0.09
5	1.904	2.04	1.26	3.25	0.16	3.387	0.161	4.25	
6	1.317	2.08	0.97	2.08	0.24	1.296	0.252	3.42	0.12
7	1.415	2.09	0.97	2.38	0.07	1.662	0.030	3.60	0.10
8	1.513	2.10	0.97	2.68	0.05	2.028	0.093	3.79	0.04
9	1.611	2.10	0.97	3.00	-0.06	2.428	0.125	3.97	
10	1.276	2.07	0.96	1.98	0.05	1.178	0.050	3.35	0.08
11	1.374	2.08	0.96	2.29	-0.01	1.544	-0.141	3.54	0.05
12	1.462	2.07	0.96	2.58	0.06	1.938	-0.078	3.70	-0.03
13	1.560	2.07	0.96	2.89	-0.21	2.338	-0.148	3.89	-0.11
14	1.658	2.09	0.96	3.19	-0.03	2.669	-0.056	4.07	-0.10
15	1.756	2.09	0.96	3.50	-0.01	3.070	-0.065	4.26	-0.10
16	1.854	2.09	0.96	3.81	0.02	3.470	0.079	4.40	
17	1.470	2.16	1.03	2.33	0.19	1.554	0.045	3.65	0.07
18	1.568	2.17	1.03	2.63	0.15	1.919	-0.111	3.84	0.12
19	1.284	2.16	1.03	1.73	0.04	0.794	0.225	3.30	-0.09
20	1.382	2.16	1.03	2.05	0.18	1.194	0.115	3.49	0.00
21	1.480	2.17	1.03	2.35	-0.04	1.560	-0.092	3.67	0.08
22	1.666	2.18	1.03	2.93	-0.05	2.285	-0.045	4.02	0.09
23	1.764	2.18	1.03	3.25	-0.04	2.685	-0.013	4.20	0.05
24	1.578	2.18	1.03	2.65	-0.11	1.926	-0.023	3.85	
25	1.186	2.12	1.01	1.51	-0.08	0.562	0.098	3.14	-0.11
26	1.281	2.13	1.01	1.81	-0.18	0.916	-0.067	3.31	-0.13
27	1.376	2.14	1.01	2.10	-0.12	1.269	-0.141	3.49	-0.10
28	1.471	2.14	1.01	2.40	-0.10	1.657	-0.133	3.67	

The RP-HPLC equations have simple, logical interpretations. As capacity factor increases, logKow and log $1/LC_{50}$ increase. The LSER equations can not only correlate and predict but also provide quantitative analysis of the factors determining the properties studied; As the intrinsic molar volume increases, logKow, logk_w and log $1/LC_{50}$ increase; As the hydrogen bond acceptor basicity increases, logKow, logk_w and log $1/LC_{50}$ decrease; As polarity increases, Kow and k_w decrease and log $1/LC_{50}$ increases. The accuracy of predicted values for logKow and log $1/LC_{50}$ by RP-HPLC models are comparable to those by the LSER while range of applicability is less broad than LSER models since capacity factors determined by RP-HPLC are not as easily obtained as solvatochromic parameters.

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