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Quantitative structure-property relationship of aromatic sulfur-containing carboxylates

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Abstract: Based on quantum chemical calculations, TLSER model (theoretical linear solvation energy relationships) and atomic charge approach were applied to model the partition properties (water solubility and octanol/water partition coefficient) of 96 aromatic sulfur-containing carboxylates, including phenylthio, phenylsulfinyl and phenylsulfonyl carboxylates. In comparison with TLSER models, the atomic charge models are more accurate and reliable to predict the partition properties of the kind of compounds. For the atomic charge models, the molecular descriptors are molecular surface area (S), molecular shape (O), weight (M_W), net charges on carboxyl group (Q_{OC}), net charges of nitrogen atoms (Q_N), and the most negative atomic charge (q^-) of the solute molecule. For water solubility (log S_W) and octanol/water partition coefficient (log K_{OW}), the correction coefficients r^2_{adj} (adjusted for degrees of freedom) are 0.936 and 0.938, and the standard deviations are 0.364 and 0.223, respectively.

Keywords: octanol/water partition coefficient; water solubility; atomic charge model; TLSER; quantum chemical descriptor

Introduction

It is widely recognized that the physicochemical profile of organic chemicals largely determines their distribution between environmental media. For the environmental behaviors of organic contaminants, water solubility (S_W) and octanol/water partition coefficient (K_{OW}) are tremendously important. Octanol/water partition coefficient has been widely related to biochemical and/or biological activity in quantitative structure-activity relationships (QSARs) (Leo, 1971). Water solubility corresponds to the dispersion tendency and to the recalcitrance toward biotic and abiotic degradation.

In order to avoid expensive and time consuming measurements, theoretical methods to estimate compound properties have become an important tool for screening, evaluating, and generating relevant data. Leo (Leo, 1993) gave an extensive overview and discussion of different approaches to calculate K_{OW}.

The well-known methods such as Leo and Hansch's fragment approach (Hansch, 1979; 1995), CLOGP (Leo, 1990; 1991), and LSER (Kamlet, 1983; 1988) have been somewhat limited because of their empirical origin. It is generally more useful to use descriptors derived mathematically from either two-dimensional or three-dimensional molecular structure. Especially, the approaches based on the three-dimensional molecular structure are more significant since flexible compounds can adopt different conformations in solvents of different polarity. The TLSER method (theoretical linear solvation energy relationships) (Famini, 1989; Wilson, 1991) has been extensively used to predict partition coefficients of a wide range of organic compounds. The predictability and applicability of the model is good. Atomic charge (Bodor, 1989; 1992) has been proposed as the basis for calculating octanol/water partition coefficients. The predictive power of the model has been demonstrated by the accurate estimation of K_{OW} for complex molecules. Some groups (Brinch, 1993; Haeberlein, 1997; Eisfeld, 1999) used theoretical descriptors from the molecular surface area and the electrostatic potential to predict the partition property. The parameters with which these approaches correlate K_{OW} more or less resemble the LSER ones.

Estimation of water solubility (S_W) through octanol/water partition coefficient (K_{OW}) is one method of choice (Yalkowsky, 1993), and most methods used to estimate K_{OW} are suitable for estimation of S_W.

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Aromatic sulfur-containing compounds, used extensively as intermediates in the manufacture of pesticides, herbicides and anthelmintics (Han, 1992), are being introduced into the environment. Their environmental behaviors and ecological effects should be investigated. To explore better models to predict their potential behavior, TLSER and atomic charge method are utilized to correlate two properties of the aromatic sulfur-containing chemicals, consisted of phenylthio, phenylsulfinyl and phenylsulfonyl carboxylates. The results should be valuable in evaluating the potential behavior of the kind of chemicals.

1 Materials and methods

1.1 Samples

The test of 96 compounds is listed in Table 1 together with water solubility and octanol/water partition coefficients at 25℃. Experimental data of 96 compounds were taken from the literatures (Feng, 1996; He, 1995; Hong, 1995; Liu, 2001).

1.2 Calculation of geometric and electronic descriptors

The molecule was drawn using the CS Chem3D 5.0 (CambridgeSoft Corp, 1999) software to generate the starting geometry. Then geometric optimization was performed; geometric and electronic properties were determined by the AM1 method of the MOPA 97 program. Using the optimum geometry, the molecular surface area (S in $Å^2$), volume (V in $Å^3$), and ovality (O) were calculated by Connolly method (Connolly, 1983; 1985). Molecular weight (M_W) was also included. The electronic descriptors such as dipole moment (μ in D), polarizability (α in au), energy of the highest occupied molecular orbital (E_{HOMO} in eV), energy of the lowest unoccupied molecular orbital (E_{LUMO} in eV), atomic net charge (in acu), were achieved. All possible sum of squared charges for each given element, and that of the absolute values of atomic charges on different functional groups were generated. Because of the expected nonlinearity of the model, all squared and square-rooted descriptors were generated. The most negative atomic charge (q^- in acu) and the most positive charge of a hydrogen atom (qH^+ in acu) in the solute molecule were obtained.

1.3 Data manipulation

The stepwise linear regression analysis with a confidence limit of 95% was performed by SPSS 8.0 software package (SPSS Inc., 1989—1997). To get the best fit of the K_{OW} values to the experimental data, the linear least-squares method is performed. Model adequacy was measured by the squared correction coefficient (r^2_{adj}) (adjusted for degrees of freedom), the standard deviation (SD), the F-test value (F), and the significance level of F-value (p).

2 Results and discussion

2.1 TLSER method

Based on TLSER model, six descriptors: V_{mc}; π^*; ε_a, ε_b, qH^+, q^-; which represent cavity, dipolarity/polarizability, and hydrogen bonding terms, are calculated by using AM1 procedure.

V_{mc} is $V_m/100$, where V_m is the molecular van der Waals volume calculated according to Connolly method. π^* is equal to α/V_m. The hydrogen-bonding effects are separated into donor and acceptor components. The covalent contribution to Lewis basicity, ε_b, is represented as the difference in energy between E_{LUMO} of water and E_{HOMO} of solute. The electrostatic basicity contribution, denoted as q^-, is simply the most negative atomic charge in the solute molecule. Analogously, the hydrogen-bonding donating ability is divided into two components: ε_a is the energy difference between E_{HOMO} of water and E_{LUMO} of solute, whereas qH^+ is the most positive charge of a hydrogen atom in the solute molecule.

Table 1 List of experimental and predicted log K_{OW} and log S_W values for sulfur-containing compounds

No.	Compounds	log K_{OW}			log S_W		
		Expt.	Pred.		Expt.	Pred.	
			Eq.(1)	Eq.(3)		Eq.(2)	Eq.(4)
1	$PhSCH_2CO_2Me$	1.50	1.74	1.86	−1.02	−1.01	−0.84
2	$PhSCH_2CO_2Et$	2.12	2.00	2.26	−1.57	−1.31	−1.44
3	$PhSCH_2CO_2$-*i*-Pr	2.53	2.27	2.60	−2.08	−1.60	−1.98
4	$PhSCH_2CO_2Pr$	2.69	2.25	2.64	−2.15	−1.60	−1.98
5	$PhSCH_2CO_2$-*i*-Bu	3.02	2.60	2.97	−2.56	−2.00	−2.49
6	$PhSCH_2CO_2$-*n*-Bu	3.26	2.52	2.98	−2.75	−1.90	−2.48
7	$PhSCH_2CH_2CO_2Et$	2.72	2.47	2.57	−2.12	−1.60	−1.88
8	$PhSCH_2CH_2CO_2Me$	2.04	2.21	2.18	−1.52	−1.30	−1.35
9	$PhSCH(Me)CH_2CO_2Me$	2.61	2.46	2.50	−2.00	−1.56	−1.86
10	$PhSCH_2CH(Me)CO_2Me$	2.63	2.45	2.48	−2.12	−1.57	−1.85
11	$PhSCH(CO_2Me)CH_2CO_2Me$	1.42	2.40	1.83	−0.85	−2.01	−1.20
12	$PhSCH(CO_2Et)CH_2CO_2Et$	2.60	2.96	2.62	−2.04	−2.64	−2.10
13	$PhSCH(CO_2$-*i*-Pr$)CH_2CO_2$-*i*-Pr	3.53	3.11	3.29	−3.10	−2.79	−2.97
14	$PhSCH_2CH(CO_2Me)CH_2CO_2Me$	1.96	3.05	2.24	−1.50	−2.35	−1.78
15	$PhSCH_2CH(CO_2Et)CH_2CO_2Et$	2.98	3.63	3.04	−2.52	−2.98	−2.62
16	$PhSCH_2CH(CO_2$-*i*-Pr$)CH_2CO_2$-*i*-Pr	3.95	4.29	3.64	−3.56	−3.69	−3.43
17	4-$NO_2PhSCH_2CO_2Me$	1.16	1.52	1.78	−0.70	−1.57	−1.46
18	4-$NO_2PhSCH_2CO_2$-*i*-Pr	2.79	2.76	2.51		−2.15	−2.55
19	2-Cl-4-$NO_2PhSCH_2CO_2Me$	2.26	2.39	2.21		−1.81	−2.07
20	2-Cl-4-$NO_2PhSCH_2CO_2$-*i*-Pr	3.20	2.90	2.94		−2.40	−3.11
21	2-$NO_2PhSCH_2CO_2Me$	1.88	1.43	1.80	−0.76	−1.46	−1.54
22	2-$NO_2PhSCH_2CO_2$-*i*-Pr	2.76	2.01	2.44		−2.15	−2.53
23	4-Cl-2-$NO_2PhSCH_2CO_2Me$	2.24	1.67	2.18	−1.70	−1.85	−2.04
24	4-Cl-2-$NO_2PhSCH_2CO_2$-*i*-Pr	3.00	2.19	2.90		−2.44	−3.12
25	2,4-di$NO_2PhSCH_2CO_2Me$	2.05	1.75	2.05		−2.10	−2.15
26	2,4-di$NO_2PhSCH_2CO_2$-*i*-Pr	2.81	2.24	2.77		−2.67	−3.20
27	4-$NO_2PhSOCH_2CO_2Me$	0.80	1.42	0.77		−2.53	−1.66
28	4-$NO_2PhSOCH_2CO_2$-*i*-Pr	1.64	1.93	1.53		−3.11	−2.70
29	2-Cl-4-$NO_2PhSOCH_2CO_2Me$	1.35	1.56	1.23		−2.74	−2.30
30	2-Cl-4-$NO_2PhSOCH_2CO_2$-*i*-Pr	2.01	2.09	1.96		−3.35	−3.28
31	2-$NO_2PhSOCH_2CO_2Me$	0.74	1.57	0.73		−2.47	−1.67
32	2-$NO_2PhSOCH_2CO_2$-*i*-Pr	1.59	2.00	1.54		−3.11	−2.75
33	4-Cl-2-$NO_2PhSOCH_2CO_2Me$	1.29	1.71	1.20		−2.75	−2.30
34	4-Cl-2-$NO_2PhSOCH_2CO_2$-*i*-Pr	2.22	2.15	1.96		−3.38	−3.36
35	2,4-di$NO_2PhSOCH_2CO_2Me$	0.63	1.59	1.09		−2.94	−2.41
36	2,4-di$NO_2PhSOCH_2CO_2$-*i*-Pr	1.61	2.12	1.83		−3.54	−3.38
37	4-$NO_2PhSO_2CH_2CO_2Me$	0.78	1.20	0.80		−2.66	−1.99
38	4-$NO_2PhSO_2CH_2CO_2$-*i*-Pr	1.80	1.71	1.51		−3.26	−2.99
39	2-Cl-4-$NO_2PhSO_2CH_2CO_2Me$	1.45	1.36	1.24		−2.89	−2.57
40	2-Cl-4-$NO_2PhSO_2CH_2CO_2$-*i*-Pr	2.40	1.86	1.91		−3.53	−3.58
41	2-$NO_2PhSO_2CH_2CO_2Me$	0.78	1.05	1.36		−2.43	−2.36
42	2-$NO_2PhSO_2CH_2CO_2$-*i*-Pr	1.72	1.75	2.06		−3.08	−3.32
43	4-Cl-2-$NO_2PhSO_2CH_2CO_2Me$	1.30	1.44	1.18		−2.90	−2.56
44	4-Cl-2-$NO_2PhSO_2CH_2CO_2$-*i*-Pr	2.45	1.86	2.51		−3.37	−3.89
45	$PhSO_2CH_2CO_2Me$	0.93	1.08	0.84	−1.14	−2.18	−1.38
46	4-$ClPhSO_2CH_2CO_2$-*i*-Pr	2.04	1.77	2.06	−2.41	−3.10	−3.08
47	4-$ClPhSO_2CH_2CO_2Me$	1.31	1.28	1.32	−2.38	−2.46	−2.03
48	4-$BrPhSO_2CH_2CO_2Me$	1.52	1.36	1.71	−2.48	−2.57	−2.55

Table 1(Cont'd)

No.	Compounds	log K_{OW}			log S_W		
		Expt.	Pred.		Expt.	Pred.	
			Eq.(1)	Eq.(3)		Eq.(2)	Eq.(4)
49	4-$NO_2PhSO_2C(CH_2)_2CO_2Me$	1.33	1.61	1.20	-3.38	-3.12	-2.75
50	4-$NO_2PhSO_2C(CH_2)_2CO_2$-*i*-Pr	2.05	2.20	2.05	-4.26	-3.76	-3.69
51	4-$NO_2PhSO_2C(CH_2)_3CO_2$-*i*-Pr	2.36	2.48	2.35	-3.76	-4.10	-4.15
52	4-$NO_2PhSO_2C(CH_2)_5CO_2$-*i*-Pr	2.84	3.06	2.90	-4.88	-4.76	-4.90
53	4-$NO_2PhSO_2C(CH_2)_6CO_2$-*i*-Pr	3.41	3.32	3.14	-5.07	-5.05	-5.21
54	4-$BrPhSO_2C(CH_2)_2CO_2Me$	2.32	1.96	2.21	-3.67	-3.05	-3.31
55	4-$BrPhSO_2C(CH_2)_3CO_2Me$	2.45	2.06	2.52	-3.55	-3.35	-3.78
56	4-$BrPhSO_2C(CH_2)_4CO_2Me$	2.73	2.28	2.80	-4.01	-3.65	-4.20
57	4-$BrPhSO_2C(CH_2)_5CO_2Me$	2.94	2.53	3.16	-4.48	-4.02	-4.68
58	4-$ClPhSO_2C(CH_2)_2CO_2Me$	2.03	1.89	1.82	-3.31	-2.94	-2.80
59	4-$ClPhSO_2C(CH_2)_3CO_2Me$	2.28	1.98	2.17	-3.00	-3.25	-3.33
60	4-$ClPhSO_2C(CH_2)_2CO_2$-*i*-Pr	2.64	1.61	2.57	-3.54	-3.59	-3.75
61	4-$ClPhSO_2C(CH_2)_2CO_2$-*t*-Bu	2.68	2.68	2.86	-4.12	-3.91	-4.18
62	4-$ClPhSO_2C(CH_2)_4CO_2$-*i*-Pr	3.16	2.81	3.12	-4.65	-4.21	-4.58
63	4-$ClPhSO_2C(CH_2)_5CO_2$-*i*-Pr	3.49	3.11	3.42	-5.54	-4.59	-5.00
64	4-$ClPhSO_2C(CH_2)_6CO_2$-*i*-Pr	3.83	3.36	3.64	-5.52	-4.87	-5.30
65	4-$MePhSO_2C(CH_2)_2CO_2$-*i*-Pr	2.52	2.49	2.46	-3.23	-3.63	-3.61
66	4-$MePhSO_2C(CH_2)_3CO_2$-*i*-Pr	2.78	2.66	2.81	-3.34	-3.99	-4.14
67	4-$MePhSO_2C(CH_2)_2CO_2Me$	1.77	2.01	1.73	-2.88	-3.01	-2.69
68	4-$MePhSO_2C(CH_2)_2CO_2Et$	2.23	2.20	2.12	-3.01	-3.12	-3.15
69	4-$MePhSO_2C(CH_2)_3CO_2Et$	2.31	2.45	2.38	-2.96	-3.65	-3.65
70	4-$MePhSO_2C(CH_2)_4CO_2$-*i*-Pr	2.88	2.94	3.03	-3.91	-4.27	-4.45
71	4-$MePhSO_2C(CH_2)_5CO_2$-*i*-Pr	3.21	3.23	3.33	-4.62	-4.65	-4.87
72	4-$MePhSO_2C(CH_2)_5CO_2Me$	2.54	2.57	2.68	-4.61	-3.97	-4.06
73	$PhSO_2C(CH_2)_2CO_2Me$	1.43	1.70	1.35	-2.26	-2.66	-2.19
74	$PhSO_2C(CH_2)_3CO_2Me$	1.63	1.78	1.66	-3.00	-2.96	-2.69
75	$PhSO_2C(CH_2)_4CO_2Me$	1.98	2.00	1.94	-2.55	-3.25	-3.13
76	$PhSO_2C(CH_2)_5CO_2Me$	2.30	2.24	2.30	-3.85	-3.61	-3.63
77	4-$NO_2PhSO_2CH(Me)CO_2Me$	1.06	1.43	1.17	-2.96	-2.98	-2.64
78	4-$NO_2PhSO_2C(Me)_2CO_2Me$	1.38	1.70	1.45	-3.39	-3.26	-3.05
79	4-$NO_2PhSO_2C(Et)_2CO_2Me$	2.24	2.23	2.18	-4.18	-3.79	-3.90
80	4-NO_2PhSO_2C(*n*-Bu)$_2CO_2Me$	3.38	3.42	3.93	-5.55	-5.32	-5.33
81	4-$NO_2PhSO_2C(CH_2Ph)_2CO_2Me$	4.46	4.23	4.78	-6.24	-5.97	-6.42
82	4-NO_2PhSO_2C(*n*-Bu)$_2CO_2Et$	3.81	3.73	3.69	-5.76	-5.54	-5.70
83	4-$NO_2PhSO_2C(Me)(CH_2Ph)CO_2Et$	3.40	3.31	3.32	-5.44	-5.10	-5.28
84	4-$NO_2PhSO_2C(Me)(CH_2CH=CH_2)CO_2Et$	2.30	2.51	2.36	-4.56	-4.17	-4.20
85	4-$NO_2PhSO_2C(Me)(CH_2$-α-Naph)CO_2Et	4.40	4.13	4.33	-5.83	-6.00	-6.14
86	4-NO_2PhSO_2C(*n*-Bu)$_2CO_2$-*i*-Pr	4.06	4.09	3.95	-5.85	-5.93	-5.97
87	4-$NO_2PhSO_2CH(Me)CO_2CH(CH_2)_5$	2.82	2.61	3.27	-4.61	-4.28	-4.84
88	4-$NO_2PhSO_2CH(CH_2CO_2Et)CO_2Me$	1.40	2.40	1.20	-3.04	-4.05	-2.68
89	4-$NO_2PhSO_2CH(CH_2CO_2$-*i*-Pr)CO_2-*i*-Pr	2.18	3.24	2.86	-4.29	-4.89	-4.21
90	4-$NO_2PhSO_2C(CH_2CO_2Et)_2CO_2$-*i*-Pr	3.56	4.62	3.35	-4.81	-6.54	-4.83
91	4-$NO_2PhSO_2C(=CHPh)CO_2Me$	2.90	2.84	2.63	-4.57	-4.42	-4.26
92	4-$NO_2PhSO_2C(=CHPh)CO_2Et$	3.20	3.12	2.95	-4.6	-4.77	-4.66
93	4-$NO_2PhSO_2C(=CHPh)CO_2$-*i*-Pr	3.62	3.34	3.74	-5.07	-4.88	-5.23
94	4-$NO_2PhSO_2C(=CHPh)CO_2$-*i*-Bu	3.68	3.60	3.86	-5.28	-5.37	-5.55
95	4-$MePhSO_2C(=CHPh)CO_2$-*i*-Pr	3.92	3.67	3.73	-5.50	-4.93	-4.98
96	4-$ClPhSO_2C(=CHPh)CO_2$-*i*-Pr	4.18	3.59	4.05	-5.65	-4.70	-5.12

Notes: Expt. is the experimental value; Pred. is the predictive value, S_W is in mol/L

With the six parameters, the models for S_W and K_{OW} of the compounds were founded through stepwise regression analysis as follows:

$$\log K_{OW} = -12.576 + 1.808 V_{mc} + 76.995 \varepsilon_a + 3.501 \pi^* , \quad (1)$$

$$(n = 96,\ r^2_{adj} = 0.766,\ SD = 0.433,\ F = 104.94,\ p < 0.001)$$

$$\log S_W = 5.194 - 2.012 V_{mc} - 1.874 q^- - 3.560 \pi^* , \quad (2)$$

$$(n = 71,\ r^2_{adj} = 0.855,\ SD = 0.545,\ F = 139.13,\ p < 0.001)$$

where n represents the number of compounds. As can be seen, V_{mc}, ε_a, π^*, q^- of six parameters are significant. From the equations, the lower correction coefficients of 0.766 and 0.855, together with the greater standard errors of 0.433 and 0.545 are obtained. Fig.1 and Fig.2 show that the fit is not good. It suggests that the models are not more successful. The structures of compounds are significantly different, and result in the different solvation mechanics.

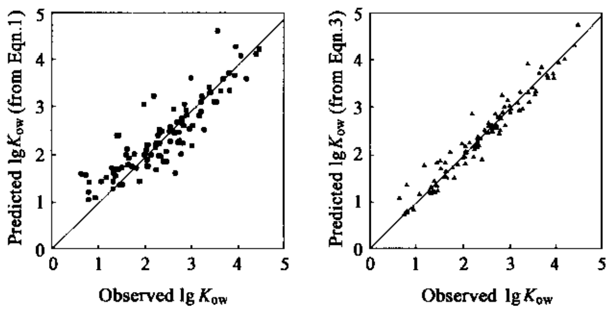

Fig.1 Plot of predicted log K_{OW} vs. observed log K_{OW}

2.2 Atomic charge model

All possible geometric and electronic descriptors (Table 2) were used to correlate the partition properties of 96 sulfur-containing carboxylates. By the stepwise linear regression, the following regression equations were found the best:

$$\log K_{OW} = 0.412 + 0.015 S + 0.007 M_W - 1.340 Q_{OC} - 1.135 Q_X - 2.309 q^- , \quad (3)$$

$$(n = 96,\ r^2_{adj} = 0.938,\ SD = 0.223,\ F = 289.24,\ p < 0.001)$$

$$\log S_W = 1.943 - 0.047 S + 0.475 S^2 - 0.009 M_W + 1.468 Q_{OC} + 0.410 Q_N + 3.076 O , \quad (4)$$

$$(n = 71,\ r^2_{adj} = 0.936,\ SD = 0.364,\ F = 170.31,\ p < 0.001)$$

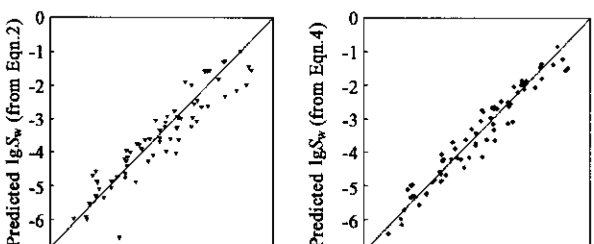

Fig.2 Plot of predicted log S_W vs. observed log S_W

Q_{OC} is the sum of absolute values of atomic charges on carbon and oxygen atoms of carboxyl group, Q_N is the square root of sum of squared charges on nitrogen atoms. Of all variables, only six were found statistically significant, and others were omitted.

For log K_{OW} and log S_W, the equations give correction coefficients (r^2_{adj}) of 0.938 and 0.936, standard deviations (SD) of 0.223 and 0.364, and F-test values (F) of 289.24 and 170.31, respectively. In comparison with TLSER models, the models of the atomic charge method have better predictive capability. Fig. 1 and Fig. 2 illustrate better fit between the predicted and observed values. These results reveal the value of the equations. The function of geometric and electronic parameters can be seen to fit well with the experimental data for the compounds.

It is clear that for the partition properties of compounds, molecular size, molecular shape, carboxyl, nitrogen and the most negative charge play dominant roles. The contribution of q^-, representing the hydrogen-bonding accepting capability of solute molecule, is great. The signs with S and M_W agree with theoretical expectation: K_{OW} increases and S_W decreases with increasing cavity formation energy in water

(Pearlman, 1986) or increasing preference for solute-solvent dispersion interactions (Hermann, 1972; Schüürmann, 1995). M_W picks up some of the significance of the surface area. The negative effect (for K_{OW}) and the positive effect (for S_W) of the electronic descriptors show that K_{OW} increases and S_W decreases with decreasing electrostatic interactions among the solvent and solute molecules, involving polarizability and the capability of hydrogen-bonding formation. The predicting models are well suited to predict the partition properties of the compounds because they more completely illustrate the solvation mechanism.

Table 2 The calculated geometric and electronic descriptors

Symbol	Defination
S	The molecular surface area
S^2	Equal to $S \times S \times 10^{-4}$
M_W	The molecular weight
O	The molecular ovality
O^2	The square of the ovality
μ	The dipole moment
α	The polarizability
Q_O	The square root of sum of the squared net charges on oxygen atoms
Q_O2	The square of Q_O
Q_O4	The square of Q_O2
Q_N	The square root of sum of the squared net charges on nitrogen atoms
Q_N2	The square of Q_N
Q_N4	The square of Q_N2
Q_S	The square root of sum of the squared net charges on sulfur atoms
Q_S2	The square of Q_S
Q_S4	The square of Q_S2
Q_{OC}	The sum of absolute values of atomic net charges on carbon and oxygen atoms of carboxyl
Q_{ON}	The sum of absolute values of atomic net charges on nitrogen and oxygen atoms of nitro
Q_{OS}	The sum of absolute values of atomic net charges on sulfur and oxygen atoms of sulfonyl
q^-	The absolute value of the most negative atomic net charge
qH^+	The most positive net charge of hydrogen atom
E_{HOMO}	Energy of the highest occupied molecular orbital
E_{LUMO}	Energy of the lowest unoccupied molecular orbital

3 Conclusions

For the partition properties of aromatic sulfur-containing compounds, the atomic charge approach is more successful because of its inclusion of more complete factors influencing solvation effect. The geometric and electronic descriptors account for cavity effects, electrostatic interactions, and hydrogen-bonding effect. The obtained models can reveal the solvation mechanism for the structural dependence of compound properties. The theoretical predictive models for partition properties based on semiempirical MO calculations performed on the whole molecule have better predictive capability and general applicability and are easy to use.

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