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QSAR Models for Water Solubility of Organohalogen Compounds

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ABSTRACT

A multivariate calibration QSAR model to predict the water solubility (log W^{-1}) of polychlorinated biphenyls (PCBs) has been suggested. In the study, optimization of a tri-parametric model consisting topological parameters VDA (Vertex distance degree), MATS4m (Moran autocorrelation of lag4 weighted by mass) and ATS4m (Broto-Moreau autocorrelation of a topological structure – log 4/ weight by atomic masses) suggests that the PCB compounds having higher value of VDA, and MATS4m have higher molar solubility. While, the PCBs having lower value of ATS4m have higher molar solubility. Model expresses above than 95 ± 0.5 % predictive power for log W^{-1} value of the compounds. Moreover, the model is an appropriate model for modelling the water solubility of the PCBs. The degree of importance of each descriptor was evaluated by sensitivity analysis approach for the nonlinear model. A good result (Q^2 = 0.95 PRESS = 8.54 and PRESS/SSY=0.051) is obtained by applying cross-validation test that indicating the validation of descriptors in the obtained model in prediction of water solubility for these compounds.

Keywords: ATS4m, log W^{-1}, MATS4m, VDA.

INTRODUCTION

Organ halogen compounds, such as polychlorinated biphenyls (PCBs), polybrominated biphenyls (PBBs), polychlorinated benzenes, polybrominated benzenes and polychlorinated naphthalene's (PCNs) and so on, have some extent negative impact in the environment. Thus, the assessment of the environmental risk of these compounds is essential, and same can be done by studying their water solubility (log W^{-1}).

Among these organ halogens, polychlorinated biphenyls (PCB) are a group of 209 different congeners that have attracted much attention as environmental pollutants (Anonymous, 2023). On May 22, 2001, 127 governments adopted the Stockholm Convention on Persistent Organic Pollutants. PCBs were among the chemicals initially selected for elimination from production and use (UNEP, 2021). Production of PCB has been banned in the industrialized world since many years, but large quantities still remain in the environment (Öberg Tomas, 1996). Even, polychlorinated biphenyls (PCBs) are among the most widespread pollutants in the global ecosystem. Because of the lipophilic nature of molecules, PCBs bioaccumulate in the food chain and residues have been detected in fish and wildlife, in human adipose tissue, milk and serum. Therefore, still of utmost importance to estimate and monitor their fate in the environment and the biological food chains. The physical properties of the PCBs can also be used as input in calculating relationships to biological activity (Andersson *et al.,* 2000), or to other physical properties (Abramowitz *et al*., 1990). Measured physical properties have been reported for 20-60% of the PCB congeners (PCBs, 2023).

Since experimental determination of water solubility for contaminants is expensive, time consuming and needs very specific facilities, therefore developing theoretical models for prediction of water solubility from structural parameters of molecules are very interesting and necessary. One of these theoretical methods is quantitative structure activity relationship (QSAR) approaches. In QSAR, the structural features of molecules were encoded as molecular descriptors and related to interested molecular activity. There are many reports about the QSAR prediction of activity of organochlorine contaminants (Klasson *et al.*, 2002; Dearden, 2004; Wang *et al.*, 2006; Ruiz *et al.*, 2008).

EXPERIMENTAL

The data set

A data set of 134 PCBs is used as a training set. Experimental solubilities (-log W) of the training set of the PCBs are listed in (Table 1).

Descriptor generation and screening

Calculation of the molecular descriptors is the first step to model the water solubilities of the PCBs. Moreover, to obtaining a QSAR model, wherein the QSAR model is a numerical representation of the structural features of PCB molecules, the molecular descriptors of the PCBs are calculated by Dragon program 5.4. After calculation of the molecular descriptors, those that are constant for all molecules were eliminated and pairs of variables with a correlation coefficient greater than 0.90 were classified as inter-correlated, and one of them in each correlated pair was deleted. Then, stepwise multiple linear regression and genetic algorithm variable subset selection method was used for the selection of the most relevant descriptors from the pool of remaining 26 descriptors, which includes 9 physicochemical parameters and 17 topological parameters.

These descriptors have been used as inputs for construction of QSAR models. QSAR modelling of the training set of 134 PCBs with the physicochemical parameters provides maximum value of $R^2 = 0.9274$, therefore to find better QSAR model topological parameters were used for modeling the water solubilities of the training set. Correlation matrix of the parameters suggested that topological parameters and autocorrelation type of indices have maximum inter-correlation with the - log W. Accordingly, VDA (Vertex distance degree), Weiner type indices. Connectivity

indices (χ0-3 and χ0v-3v) are highly correlated to -log W and MATS4m (Moreau autocorrelation of a topological structure – lag 4/ weight by atomic masses) also has good correlation with it. MATS4m is poorly correlated to solubility. Moreover, the topological parameters found to be more potential than physiochemical parameters for modeling the solubility. Calculated values of the topological parameters are given in (Table 1).

Wherein, the Vertex distance degree (VDA) is the sum of the distances of all the other atoms to a given atom:

$$VDA = \sum_{j=1}^{A} d_{ij}$$

where d_{ij} is the topological distance between atoms *i* and *j*.

Further, the Moran autocorrelation descriptor (MATSdw) is given as below:

$$MATSdw = \frac{\frac{1}{\Delta} \cdot \sum_{i=1}^{A} \sum_{j=1}^{A} \delta_{ij} \cdot (w_i - \overline{w}) \cdot (w_j - \overline{w})}{\frac{1}{A} \sum_{i=1}^{A} (w_i - \overline{w})^2}$$

Where $\overline{w}$ is the average value of the property for the molecule and Δ is the number of vertex pairs at distance equal to *d*.

Furthermore, Broto Moreau autocorrelation of a topological structure lag 4 / weighted by atomic masses (ATS4m), is given as below:

$$ATSdw = \ln\left(1 + \sum_{i=1}^{A} \sum_{j=1}^{A} \delta_{ij} \cdot w_i \cdot w_j\right)$$

RESULT AND DISCUSSION

Optimized parameters were tested for a significant mono parametric model, the best mono-parametric model was obtained with VDA, wherein VDA has a highest correlation with -log W, among all the calculated topological parameters. The model is given below:

-log W = 0.1236 (± 0.0026) VDA + 0.4832
N = 134, R^2 = 0.9434, R^2 A = 0.9429, Se = 0.2729, F = 2198.776, Q = 3.5778 ……. (1)

Other optimized topological parameters were tested for their synergic effect with VDA, as a result seven bi-parametric QSAR models were obtained. However, the bi-parametric QSAR model having topological parameters VDA and MATS4m was the most substantial model due to highest regression coefficient. The model is shown below:

-log W = 0.1230(± 0.0025) VDA – 0.6678(± 0.1624) MATS4m + 0.5510
N = 134, R^2 = 0.9498, R^2 A = 0.9491, Se = 0.2578, F = 1240.387, Q = 3.7803 …… (2)

Three parameters were tested together only one tri-parametric model was obtained. The model contains VDA, MATS4m and ATS4m with R^2 value 0.9508. The model is given below.

$-\log W = 0.1323(\pm 0.0064)\ VDA + 0.8149(\pm 0.1868)\ MATS4m - 0.2153(\pm 0.1374)\ ATS4m + 1.9695$

$N = 134,\ R^2 = 0.9508,\ R^2\ A = 0.9496,\ Se = 0.2564,\ F = 836.934,\ Q = 3.8030$ …… ...(3)

The observed and estimated molar solubility values of log W^{-1} for the PCB compounds using the best QSAR model of the present study *viz.* model of equation (3). The predictive power of model is obtained by plotting a graph between observed and estimated logW^{-1}. A combination of the physiochemical and the topological parameters was also tried but no significant model was obtained. Hence topological as well as physiochemical parameters are capable to model molar solubility of PCBs but topological parameters are more effective to model molar solubilities of the Polychlorinated biphenyls (PCBs).

Table 1: List of Organ halogen Compounds and their Water Solubility (log W).

S. No	Compounds	Observed Solubility (-log Wo)	Estimated Solubility (-log We)	VDA	ATS4m	MATS4m
1	3- Chlorobiphenyl	5.39	5.04	37.85	7.86	-0.01
2	4-Chlorobiphenyl	5.33	5.04	38.77	7.7	-0.16
3	2,2'- Di Chlorobiphenyl	5.72	5.79	41	8.38	-0.15
4	2,3- Di Chlorobiphenyl	5.35	5.30	41.57	8.27	-0.08
5	2,3'- Di Chlorobiphenyl	5.26	5.79	42	8.27	-0.08
6	2,4- Di Chlorobiphenyl	5.56	5.79	42.57	8.46	0.14
7	2,4'-Di Chlorobiphenyl	5.46	5.79	43	8.16	-0.19
8	3,3'-Di Chlorobiphenyl	6.45	5.79	43	8.14	-0.01
9	3,4- Di Chlorobiphenyl	6.39	5.79	43.29	8.03	-0.11
10	3,4'- Di Chlorobiphenyl	6.40	6.10	44	8.03	-0.11
11	4,4'- Di Chlorobiphenyl	6.37	5.79	45	7.9	-0.22
12	2,2',3-Tri Chlorobiphenyl	6.10	6.33	45.87	8.56	-0.2
13	2,2',4- Tri Chlorobiphenyl	6.49	5.79	46.93	8.7	-0.02
14	2,2',5- Tri Chlorobiphenyl	6.17	6.33	46.13	8.56	-0.2
15	2,2',6- Tri Chlorobiphenyl	5.90	6.33	45.07	8.83	-0.02
16	2,3,4-Tri Chlorobiphenyl	6.18	6.33	46.93	8.62	0.06
17	2,3,4'-Tri Chlorobiphenyl	5.80	6.33	48	8.38	-0.21
18	2,3,6- Tri Chlorobiphenyl	6.49	6.33	45.6	8.76	0.06
19	2,3',4- Tri Chlorobiphenyl	6.11	6.33	48	8.62	0.06
20	2,3',5- Tri Chlorobiphenyl	6.14	6.33	47.2	8.47	-0.12
21	2,4,4'- Tri Chlorobiphenyl	6.22	6.33	49.07	8.55	-0.03
22	2,4',5- Tri Chlorobiphenyl	6.18	6.33	48.27	8.38	-0.21
23	2,4',6- Tri Chlorobiphenyl	6.16	6.33	47.2	8.7	-0.02
24	2,3',4'- Tri Chlorobiphenyl	6.21	6.33	47.73	8.38	-0.21
25	2,3',5'- Tri Chlorobiphenyl	6.30	6.33	46.93	8.69	0.14
26	2,2',3,3'- Tetra Chlorobiphenyl	6.83	6.88	51	8.71	-0.27
27	2,2',3,4- Tetra Chlorobiphenyl	7.00	6.88	51.5	8.84	-0.12
28	2,2',3,4'- Tetra Chlorobiphenyl	6.96	6.88	52.13	8.84	-0.12
29	2,2',3,5'-Tetra Chlorobiphenyl	6.91	6.88	51.25	8.71	-0.27
30	2,2',3,6- Tetra Chlorobiphenyl	6.30	6.88	50	8.95	-0.13
31	2,2',3,6'-Tetra Chlorobiphenyl	6.30	6.88	50.13	8.95	-0.13
32	2,2',4,4'- Tetra Chlorobiphenyl	7.23	6.88	53.25	8.95	0.04
33	2,2',4,5- Tetra Chlorobiphenyl	6.86	6.88	51.75	8.84	-0.12
34	2,2',4,5'- Tetra Chlorobiphenyl	7.12	6.88	52.38	8.84	-0.12
35	2,2',4,6- Tetra Chlorobiphenyl	6.94	6.88	50.88	9.18	0.25
36	2,2',4,6'- Tetra Chlorobiphenyl	6.65	6.88	51.25	9.05	0.02
37	2,2',5,5'- Tetra Chlorobiphenyl	7.00	6.88	51.5	8.71	-0.27
38	2,2',5,6'- Tetra Chlorobiphenyl	6.65	6.88	50.38	8.95	-0.13
39	2,2',6,6'- Tetra Chlorobiphenyl	6.20	6.88	49.25	9.14	0.01

40	2,3,3’,4- Tetra Chlorobiphenyl	6.77	6.88	52.63	8.77	-0.03
41	2,3,4,4’- Tetra Chlorobiphenyl	6.86	6.88	53.75	8.71	-0.1
42	2,3,4’,5- Tetra Chlorobiphenyl	6.77	6.88	53.13	8.77	-0.03
43	2,3,4’,6- Tetra Chlorobiphenyl	7.02	6.88	52.25	8.84	-0.12
44	2,3,5,6- Tetra Chlorobiphenyl	7.25	6.88	50.25	9.04	0.18
45	2,3’,4,4’- Tetra Chlorobiphenyl	6.63	6.88	54.13	8.71	-0.1
46	2,3’,4,6-Tetra Chlorobiphenyl	7.26	6.88	52	9.13	0.34
47	2,3’,4’,5- Tetra Chlorobiphenyl	6.69	6.88	53.25	8.56	-0.25
48	2,3’,4’,6- Tetra Chlorobiphenyl	7.02	6.88	52.13	8.84	-0.12
49	2,4,4’,5- Tetra Chlorobiphenyl	6.77	6.88	54	8.71	-0.1
50	2,4,4’,6- Tetra Chlorobiphenyl	7.26	6.88	53.13	9.09	0.27
51	2,3’,4’,5’-Tetra Chlorobiphenyl	6.71	6.88	52.38	8.77	-0.03
52	2,2’,3,3’,6- Penta Chlorobiphenyl	6.78	7.61	55.29	9.06	-0.25
53	2,2’,3,4,4’- Penta Chlorobiphenyl	7.62	7.61	58.12	9.05	-0.07
54	2,2’,3,4,5- Penta Chlorobiphenyl	7.87	7.61	56.24	9.1	-0.01
55	2,2’,3,4,5’- Penta Chlorobiphenyl	7.66	7.61	57.18	8.95	-0.21
56	2,2’,3,4,6- Penta Chlorobiphenyl	7.92	7.61	55.53	9.26	0.1
57	2,2’,3,4,6’- Penta Chlorobiphenyl	6.78	7.61	56	9.15	-0.11
58	2,2’,3,4’,5- Penta Chlorobiphenyl	7.82	7.61	57.41	9.1	-0.01
59	2,2’,3,4’,6- Penta Chlorobiphenyl	7.17	7.61	56.47	9.15	-0.11
60	2,2’,3,5,5’- Penta Chlorobiphenyl	7.82	7.61	56.47	9	-0.15
61	2,2’,3,5,6- Penta Chlorobiphenyl	7.40	7.61	54.82	9.19	-0.04
62	2,2’,3,5’,6-Penta Chlorobiphenyl	7.19	7.61	55.53	9.06	-0.25
63	2,2’,3,4’,5’- Penta Chlorobiphenyl	7.76	7.61	57.18	8.95	-0.21
64	2,2’,3,4’,6’- Penta Chlorobiphenyl	7.40	7.61	56.24	9.26	0.1
65	2,2’,4,4’,5- Penta Chlorobiphenyl	7.95	7.61	58.35	9.05	-0.07
66	2,2’,4,4’,6- Penta Chlorobiphenyl	7.66	7.61	57.41	9.34	0.24
67	2,2’,4,5’,6-Penta Chlorobiphenyl	7.47	7.61	56.47	9.26	0.1
68	2,3,3’,4,4’- Penta Chlorobiphenyl	7.52	7.61	59.06	8.84	-0.18
69	2,3,3’,4,5-Penta Chlorobiphenyl	7.68	7.61	57.41	9.04	0.09
70	2,3,3’,4’,6- Penta Chlorobiphenyl	7.65	7.61	57.41	8.95	-0.21
71	2,3,3’,5,6- Penta Chlorobiphenyl	7.95	7.61	56	9.14	0.06
72	2,3,3’,5’,6- Penta Chlorobiphenyl	7.76	7.61	56.47	9.14	0.06
73	2,3,4,4’,5- Penta Chlorobiphenyl	7.50	7.61	58.59	8.99	0.03
74	2,3,4,4’,6- Penta Chlorobiphenyl	7.96	7.61	57.88	9.18	0.13
75	2,3,4’,5,6- Penta Chlorobiphenyl	7.88	7.61	57.18	9.1	-0.01
76	2,3’,4,4’,5- Penta Chlorobiphenyl	7.33	7.61	59.29	8.84	-0.18
77	2,3’,4,4’,6- Penta Chlorobiphenyl	7.91	7.61	58.35	9.18	0.13
78	2,3’,4,5’,6- Penta Chlorobiphenyl	7.92	7.61	57.41	9.33	0.4
79	2,3’,4,4’,5’- Penta Chlorobiphenyl	7.42	7.61	59.06	8.99	0.03
80	2,2’,3,3’,4,5-Hexa Chlorobiphenyl	8.42	8.17	61.89	9.19	-0.13
81	2,2’,3,3’,4,6- Hexa Chlorobiphenyl	8.48	8.17	61.11	9.34	-0.05
82	2,2’,3,3’,4,6’- Hexa Chlorobiphenyl	7.65	8.17	61.44	9.23	-0.24
83	2,2’,3,3’,5,6- Hexa Chlorobiphenyl	7.65	8.17	60.33	9.27	-0.18
84	2,2’,3,3’,5,6’-Hexa Chlorobiphenyl	7.82	8.17	60.67	9.27	-0.18
85	2,2’,3,4,4’,5-Hexa Chlorobiphenyl	8.52	8.17	63.11	9.27	0
86	2,2’,3,4,4’,5’- Hexa Chlorobiphenyl	8.38	8.17	63.44	9.15	-0.19
87	2,2’,3,4,4’,6’-Hexa Chlorobiphenyl	8.24	8.17	62.44	9.41	0.09
88	2,2’,3,4,5,5’- Hexa Chlorobiphenyl	8.42	8.17	62.11	9.19	-0.13
89	2,2’,3,4,5,6’- Hexa Chlorobiphenyl	8.13	8.17	60.89	9.34	-0.05
90	2,2’,3,4,5’,6- Hexa Chlorobiphenyl	8.01	8.17	61.33	9.34	-0.05
91	2,2’,3,4’,5,5’-Hexa Chlorobiphenyl	8.58	8.17	62.67	9.19	-0.13
92	2,2’,3,4’,5’,6-Hexa Chlorobiphenyl	7.94	8.17	61.67	9.23	-0.24
93	2,2’,3,5,5’,6- Hexa Chlorobiphenyl	7.93	8.17	60.56	9.27	-0.18
94	2,2’,4,4’,5,5’- Hexa Chlorobiphenyl	8.49	8.17	63.67	9.15	-0.19
95	2,2’,4,4’,5,6’- Hexa Chlorobiphenyl	8.12	8.17	62.67	9.41	0.09
96	2,2’,4,4’,6,6’-Hexa Chlorobiphenyl	8.12	8.17	61.67	9.62	0.36

97	2,3,3',4,4',5- Hexa Chlorobiphenyl	8.31	8.17	64.11	9.1	-0.08
98	2,3,3',4,4',6- Hexa Chlorobiphenyl	8.48	8.17	63.33	9.27	0
99	2,3,3',4',5,6- Hexa Chlorobiphenyl	8.48	8.17	62.56	9.19	-0.13
100	2,3,3',4',5',6-Hexa Chlorobiphenyl	8.27	8.17	62.44	9.19	-0.13
101	2,3',4,4',5,5'- Hexa Chlorobiphenyl	8.21	8.17	64.44	9.1	-0.08
102	3,3',4,4',5,5'- Hexa Chlorobiphenyl	8.85	8.17	65.22	9.05	0.03
103	2,2',3,3',4,4',5- Hepta Chlorobiphenyl	8.90	8.72	68.42	9.35	-0.14
104	2,2',3,3',4,5,5'- Hepta Chlorobiphenyl	9.10	8.72	67.58	9.38	-0.08
105	2,2',3,3',4,5,6'- Hepta Chlorobiphenyl	8.59	8.72	66.53	9.42	-0.2
106	2,2',3,3',4,5',6- Hepta Chlorobiphenyl	8.68	8.72	66.74	9.51	-0.01
107	2,2',3,3',4,6,6'- Hepta Chlorobiphenyl	8.15	8.72	65.68	9.54	-0.14
108	2,2',3,3',4,5',6' Hepta Chlorobiphenyl	8.42	8.72	66.74	9.42	-0.2
109	2,2',3,3',5,5',6- Hepta Chlorobiphenyl	8.59	8.72	65.9	9.45	-0.14
110	2,2',3,3',5,6,6'- Hepta Chlorobiphenyl	7.94	8.72	64.84	9.48	-0.27
111	2,2',3,4,4',5,5'- Hepta Chlorobiphenyl	9.10	8.72	68.63	9.35	-0.14
112	2,2',3,4,4',5,6- Hepta Chlorobiphenyl	8.97	8.72	67.16	9.57	0.12
113	2,2',3,4,4',5,6'- Hepta Chlorobiphenyl	8.68	8.72	67.58	9.57	0.12
114	2,2',3,4,4',5',6- Hepta Chlorobiphenyl	8.85	8.72	67.79	9.48	-0.07
115	2,2',3,4,5,5',6- Hepta Chlorobiphenyl	8.75	8.72	66.11	9.51	-0.01
116	2,2',3,4',5,6,6'- Hepta Chlorobiphenyl	8.49	8.72	65.9	9.62	0.05
117	2,3,3',4,4',5,5'- Hepta Chlorobiphenyl	8.72	8.72	69.47	9.31	-0.01
118	2,3,3',4,4',5,6- Hepta Chlorobiphenyl	8.91	8.72	68.21	9.44	0.05
119	2,3,3',4,4',5',6- Hepta Chlorobiphenyl	9.10	8.72	68.63	9.44	0.05
120	2,3,3',4,5,5',6- Hepta Chlorobiphenyl	9.10	8.72	67.16	9.56	0.3
121	2,3,3',4',5,5',6- Hepta Chlorobiphenyl	9.10	8.72	67.79	9.38	-0.08
122	2,2',3,3',4,4',5,5'- Octa Chlorobiphenyl	9.70	9.45	73.8	9.51	-0.11
123	2,2',3,3',4,4',5,6- Octa Chlorobiphenyl	9.29	9.45	72.6	9.63	-0.06
124	2,2',3,3',4,4',5,6'- Octa Chlorobiphenyl	9.42	9.45	72.9	9.63	-0.06
125	2,2',3,3',4,4',6,6'- Octa Chlorobiphenyl	9.10	9.45	72	9.73	-0.02
126	2,2',3,3',4,5,5',6- Octa Chlorobiphenyl	9.42	9.45	71.7	9.65	0
127	2,2',3,3',4,5,5',6'-Octa Chlorobiphenyl	9.10	9.45	72	9.57	-0.19
128	2,2',3,3',4,5,6,6'-Octa Chlorobiphenyl	9.20	9.45	70.6	9.68	-0.15
129	2,2',3,3',4,5',6,6'- Octa Chlorobiphenyl	9.29	9.45	71.1	9.68	-0.15
130	2,2',3,4,4',5,5',6- Octa Chlorobiphenyl	9.50	9.45	72.8	9.63	-0.15
131	2,2',3,4,4',5,6,6'- Octa Chlorobiphenyl	9.48	9.45	71.7	9.8	0.18
132	2,3,3',4,4',5,5',6- Octa Chlorobiphenyl	9.70	9.45	73.7	9.6	0.08
133	2,2',3,3',4,4',5,5',6-Nona Chlorobiphenyl	10.18	10.01	78.1	9.75	-0.08
134	2,2',3,3',4,4',5,6,6'- Nona Chlorobiphenyl	10.07	10.01	77.14	9.84	-0.05

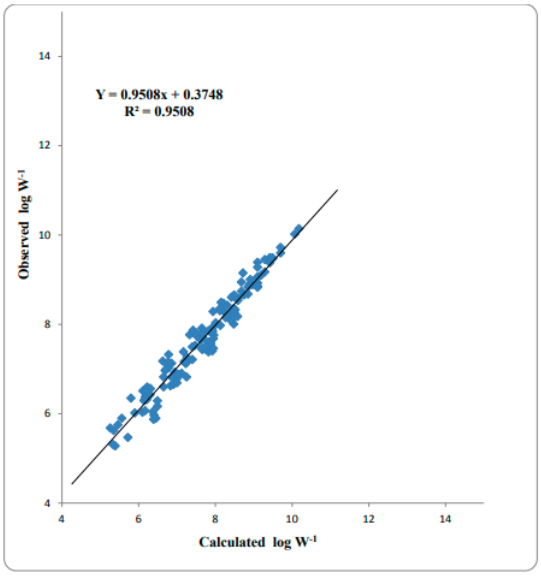

Fig. 1: Correlation between Observed and Estimated log W^{-1} using Model no.3.

CONCLUSIONS

The tri-parametric model obtained using topological parameters indicates that the compounds having high value of VDA and MATS4m have higher molar solubility. The compounds having low value of ATS4m have higher molar solubility. As the best tri-parametric equation have positive coefficient of VDA, MATS4m and negative coefficient of ATS4m. Further confirmation in favour of tri-parametric model is obtained by calculating the cross-validation parameters for the given model *i.e.* PRESS/ SSY for the entire model have been found to be more than zero, which shows that the models are free from the defect of chance. R^2cv is highest for the present tri-parametric model which suggests that this model is most appropriate model for modeling log W^{-1} values of the compounds under present investigation.

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العلاقات الكمية بين التركيب والفعالية لذوبان مركبات الهالوجين العضوية في الماء

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الملخص

تم اقتراح نموذج للعلاقة الكمية بين التركيب والفعالية (QSAR) متعدد المتغيرات للتنبؤ بالذوبان في الماء (log W-1) لثنائي الفينيل متعدد الكلور (PCBs). في هذه الدراسة، تم تحسين نموذج ثلاثي الواصفات يتكون من خواص طوبولوجية VDA (درجة مسافة قمة الرأس)، و MATS4m (ارتباط موران التلقائي لـ lag4 مرجح بالكتلة) و ATS4m (ارتباط بروتو–مورو التلقائي للبنية الطوبولوجية – 4 log/ الوزن بالكتل الذرية). حيث يشير إلى أن مركبات ثنائي الفينيل متعدد الكلور ذات القيمة الأعلى لـ VDA، و MATS4m لها قابلية ذوبان مولاري أعلى. في حين أن مركبات ثنائي الفينيل متعدد الكلور التي لها قيمة أقل من ATS4m لها قابلية ذوبان مولاري أعلى. يعبر النموذج عن قوة تنبؤية تزيد عن 95 ± 0.5٪ لقيمة (log W-1) للمركبات. علاوة على ذلك، يعد هذا النموذج نموذجًا مناسبًا لنمذجة قابلية ذوبان مركبات ثنائي الفينيل متعدد الكلور في الماء. تم تقييم درجة أهمية كل واصف من خلال منهج تحليل الحساسية للنموذج غير الخطي. تم الحصول على نتيجة جيدة (Q^2 = 0.95 PRESS = 8.54 و PRESS/SSY = 0.051) من خلال تطبيق اختبار التحقق المتبادل الذي يشير إلى التحقق من صحة الواصفات في النموذج الذي تم الحصول عليه في التنبؤ بالذوبان في الماء لهذه المركبات.

الكلمات الدالة: ATS4m, log W^{-1}, MATS4m, VDA.