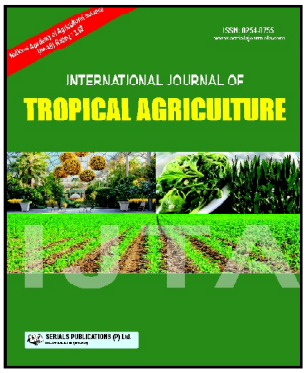


INTERNATIONAL JOURNAL OF TROPICAL AGRICULTURE

ISSN : 0254-8755

available at http: www.serialsjournal.com

Volume 35 • Number 1 • 2017

Quantitative Structure Property Relationship (QSPR) Studies of N-octanol / Water Partion Coeffcient for Polychlorinated Biphenyls (PCBS) Using Physiochemical and Topological Indices

Venkateshwar and Rajneesh Kumar

QSAR Chemical Laboratory, A.P.S. University, Rewa, M.P. and Mihir Bhoj P.G. College, Dadri, Ghaziabad, U.P.
E-mail: [1]vktvkt3@gmail.com

Abstract: The logarithmic n-octanol /water partition coefficient (log K_{ow}) is a very important property which is concerned with the water-solubility, bio concentration factor, toxicity and soil absorption coefficient of organic compounds. Quantitative structure–property relationship (QSPR) models for log K_{ow} of 133 polychlorinated biphenyls (PCBs) was examined using multiple linear regression analysis (MLR) followed by their statistical evaluation in the present study. In order to indicate the influence of different molecular descriptors on log K_{ow} values and understand the importance of structural features, affecting the experimental values, a set of physiochemical and topological parameters (especially Balaban and related index)were taken into consideration. After series of regression using mono, bi, tri tetra and penta parametric models, a penta parametric model was with R^2 0.9401 was chosen to be the best to model the log $K_{ow.}$ The obtained model was also judged through the cross validated parameters.

Keywords: Polychlorinated biphenyls; Quantitative structure–property relationship; n-octanol/water partition coefficient, cross validation.

INTRODUCTION

Polychlorinated biphenyls (PCBs) are persistent organic contaminants and widespread environmental pollutants; they were used in plasticizers formulation of coatings, inks, adhesives, flame retardants, pesticide extenders and in the micro-encapsulation of dyes for carbonless duplicating papers. Human exposure to PCBs occurs mainly from eating food that contains these chemicals (Schecter *et al.* [1], Juan *et al.* [2], Kiviranta *et al.* [3], Erdogrul *et al.* [4,5],

Coelhan *et al.* [6]). It has been reported that meat, dairy products, and fish, makes up more than 90% of the intake of PCBs for the general population (Schecter *et al.* [7], Llobet *et al.* [8], Bocio *et al.* [9], Huwe *et al.* [10]). PCBs are rapidly absorbed from the gastrointestinal tract, and are distributed and accumulated in the liver and adipose tissues. They also act as potent carcinogens.

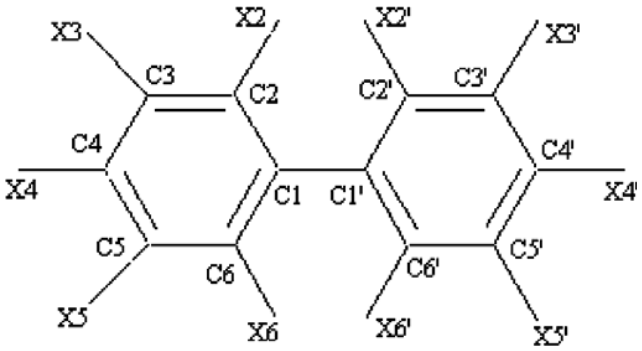
Thus, there is a need for prediction tools to study PCBs' properties including retention behavior, properties, and activity/toxicity for which analytical standards are currently difficult to obtain, but yet for which environmental data are needed. The logarithmic n-octanol /water partition coefficient (logKow) is an important property for pharmacology, toxicology and medicinal chemistry. In the past, a number of papers have been reported on the prediction of log Kow for PCBs, however most of the reported prediction methods were based on thermodynamically based theories (Kamlet *et al.*[11] Banerjee [12]), connectivity indexes (Randic *et al.* [13], Murray *et al.* [14], Hawker *et al.* [15], Patil *et al.*[16] , Sabljic *et al.* [17]) and characteristic root index (CRI) (Melek *et al.* [18]). Three-dimensional structure–property correlations for prediction of thermodynamic properties of PCBs have been recently made to predict the enthalpy of vapourization and enthalpy of sublimation (Puri *et al.* [19]).

The current paper is based on the octanol/ water partition coefficient of 133 polychlorinated biphenyl (PCBs) congeners, and their relationship with topological, particularly Balaban and related indices and physiochemical parameters.

2. MATERIALS AND METHODS

2.1. Data set

All data of the present investigation were obtained from the reference Lu *et al.*,[20]. The data set for this investigation consisted of 133 PCBs. The basic structure of the molecule is given below:



The list of PCB"s along with their log Kow values are reported in **Table 1.**

Table 1
List of compounds along with their experimental/ observed Log Kow

Compound No.	*Compound Name Log Kow*	*Experimental*
1	3-Chlorobiphenyl	4.66
2	4-Chlorobiphenyl	4.63
3	2,2'-DiChlorobiphenyl	4.72
4	2,3-DiChlorobiphenyl	4.99
5	2,3'-DiIChlorobiphenyl	4.84
6	2,4-DiChlorobiphenyl	5.15
7	2,4'-DiChlorobiphenyl	5.09
8	3,3'-DiChlorobiphenyl	5.27
9	3,4-DiChlorobiphenyl	5.23
10	3,4'-DiChlorobiphenyl	5.15
11	4,4'-DiChlorobiphenyl	5.23
12	2,2',3-TriChlorobiphenyl	5.12
13	2,2',4-TriChlorobiphenyl	5.39
14	2,2',5-TriChlorobiphenyl	5.33
15	2,2',6-TriChlorobiphenyl	5.04
16	2,3,3'-TriChlorobiphenyl	5.6
17	2,3,4-TriChlorobiphenyl	5.68
18	2,3.4'-TriChlorobiphenyl	5.29
19	2,3,6- TriChlorobiphenyl	5.44
20	2,3',4- TriChlorobiphenyl	5.54
21	2,3',5- TriChlorobiphenyl	5.65
22	2,4,4'- TriChlorobiphenyl	5.71
23	2,4',5- TriChlorobiphenyl	5.68

contd. table 1

Compound No.	*Compound Name Log Kow*	*Experimental*
24	2,4',6- TriChlorobiphenyl	5.24
25	2,3',4'- TriChlorobiphenyl	5.71
26	2,3',5'- TriChlorobiphenyl	5.71
27	2,2',3,3'- TetraChlorobiphenyl	5.67
28	2,2',3,4- TetraChlorobiphenyl	5.79
29	2,2',3,4'- TetraChlorobiphenyl	5.72
30	2,2',3,5'- TetraChlorobiphenyl	5.73
31	2,2',3,6- TetraChlorobiphenyl	4.84
32	2,2'3,6'- TetraChlorobiphenyl	4.84
33	2,2',4,4'- TetraChlorobiphenyl	5.94
34	2,2',4,5- TetraChlorobiphenyl	5.69
35	2,2',4,5'- TetraChlorobiphenyl	5.87
36	2,2',4,6- TetraChlorobiphenyl	5.75
37	2,2',4,6'- TetraChlorobiphenyl	5.51
38	2,2',5,5'- TetraChlorobiphenyl	5.79
39	2,2',5,6'- TetraChlorobiphenyl	5.55
40	2,2',6,6- TetraChlorobiphenyl	5.24
41	2,3,3',4- TetraChlorobiphenyl	6.1
42	2,3,4,4'- TetraChlorobiphenyl	6.24
43	2,3,4',5- TetraChlorobiphenyl	6.1
44	2,3,4',6- TetraChlorobiphenyl	5.76
45	2,3,5,6- TetraChlorobiphenyl	5.96
46	2,3',4,4'- TetraChlorobiphenyl	5.98
47	2,3',4,5- TetraChlorobiphenyl	6.32
48	2,3',4,6- TetraChlorobiphenyl	6.03
49	2,3',4,6- TetraChlorobiphenyl	5.76
50	2,4,4',5- TetraChlorobiphenyl	6.1
51	2,4,4',6- TetraChlorobiphenyl	6.03
52	2,3',4',5'- TetraChlorobiphenyl	5.98
53	2,2',3,3',6- PentaChlorobiphenyl	5.6
54	2,2',3,4,4'- PentaChlorobiphenyl	6.18
55	2,2',3,4,5- PentaChlorobiphenyl	6.38
56	2,2',3,4,5'- PentaChlorobiphenyl	6.23
57	2,2',3,4,6- PentaChlorobiphenyl	6.5
58	2,2',3,4,6'- PentaChlorobiphenyl	5.6
59	2,2',3,4',5- PentaChlorobiphenyl	6.32
60	2,2',3,4',6- PentaChlorobiphenyl	5.87
61	2,2',3,5,5'- PentaChlorobiphenyl	6.32
62	2,2',3,5,6- PentaChlorobiphenyl	6.06
63	2,2',3,5',6- PentaChlorobiphenyl	5.92
64	2,2',3,4',5'- PentaChlorobiphenyl	6.3
65	2,2',3,4',6'- PentaChlorobiphenyl	6.04
66	2,2',4,4',5- PentaChlorobiphenyl	6.41
67	2,2',4,4',6- PentaChlorobiphenyl	6.23
68	2,2',4,5',6- PentaChlorobiphenyl	6.11
69	2,3,3',4,4'- PentaChlorobiphenyl	6.79
70	2,3,3',4,5- PentaChlorobiphenyl	6.92
71	2,3,3',4',6- PentaChlorobiphenyl	6.2
72	2,3,3',5,6- PentaChlorobiphenyl	6.41
73	2,3,3',5',6- PentaChlorobiphenyl	6.45
74	2,3,4,4',5- PentaChlorobiphenyl	6.71
75	2,3,4,4',6- PentaChlorobiphenyl	6.44
76	2,3,4',5,6- PentaChlorobiphenyl	6.39
77	2,3',4,4',5- PentaChlorobiphenyl	6.57
78	2,3',4,4',6- PentaChlorobiphenyl	6.4
79	2,3',4,5,5'- PentaChlorobiphenyl	6.3
80	2,3',4,5',6- PentaChlorobiphenyl	6.42
81	2,3',4,4',5'- PentaChlorobiphenyl	6.64
82	2,2',3,3',4,5- HexaChlorobiphenyl	6.76
83	2,2',3,3',4,5'- HexaChlorobiphenyl	7.3
84	2,2',3,3',4,6- HexaChlorobiphenyl	6.78
85	2,2',3,3',4,6'- HexaChlorobiphenyl	6.2
86	2,2',3,3',5,6- HexaChlorobiphenyl	6.2
87	2,2',3,3',5,6'- HexaChlorobiphenyl	6.32
88	2,2',3,4,4',5- HexaChlorobiphenyl	6.82
89	2,2',3,4,4',5'- HexaChlorobiphenyl	6.73
90	2,2',3,4,4',6'- HexaChlorobiphenyl	6.58
91	2,2',3,4,5,5'- HexaChlorobiphenyl	6.75
92	2,2',3,4,5,6'- HexaChlorobiphenyl	6.56
93	2,2',3,4,5',6- HexaChlorobiphenyl	6.45
94	2,2',3,4',5,5'- HexaChlorobiphenyl	6.85
95	2,2',3,4',5',6- HexaChlorobiphenyl	6.41
96	2,2',3,5,5',6- HexaChlorobiphenyl	6.42
97	2,2',4,4',5,5'- HexaChlorobiphenyl	6.8
98	2,2',4,4',5,6'- HexaChlorobiphenyl	6.65

contd. table 1

Compound No.	Compound Name Log Kow	Experimental
99	2,2',4,4',6,6'- HexaChlorobiphenyl	6.54
100	2,3,3',4,4',5- HexaChlorobiphenyl	7.44
101	2,3,3'4,4',6- HexaChlorobiphenyl	6.78
102	2,3,3',4',5,6- HexaChlorobiphenyl	6.78
103	2,3,3',4',5',6- HexaChlorobiphenyl	6.63
104	2,3,3',5,5',6- HexaChlorobiphenyl	7
105	2,3',4,4',5,5'- HexaChlorobiphenyl	7.29
106	3,3',4,4',5,5'- HexaChlorobiphenyl	7.55
107	2,2',3,3',4,4',5- Hepta Chlorobiphenyl	7.08
108	2,2',3,3',4,5,5'- Hepta Chlorobiphenyl	7.21
109	2,2',3,3',4,5,6'- Hepta Chlorobiphenyl	6.85
110	2,2',3,3',4,5',6- Hepta Chlorobiphenyl	6.92
111	2,2',3,3',4,6,6'- Hepta Chlorobiphenyl	6.55
112	2,2',3,3',4,5',6'- Hepta Chlorobiphenyl	6.73
113	2,2',3,3',5,5',6- Hepta Chlorobiphenyl	6.85
114	2,2',3,3',5,6,6'- Hepta Chlorobiphenyl	6.41
115	2,2',3,4,4',5,5'- Hepta Chlorobiphenyl	7.21
116	2,2',3,4,4',5,6- Hepta Chlorobiphenyl	7.13
117	2,2',3,4,4',5,6'- Hepta Chlorobiphenyl	6.92
118	2,2',3,4,4',5',6- Hepta Chlorobiphenyl	7.04
119	2,2',3,4,5,5',6- Hepta Chlorobiphenyl	6.99
120	2,2',3,4',5,6,6'- Hepta Chlorobiphenyl	6.78
121	2,3,3',4,4',5,5'- Hepta Chlorobiphenyl	7.72
122	2,3,3',4,4',5,6- Hepta Chlorobiphenyl	7.08
123	2,3,3',4,4',5',6- Hepta Chlorobiphenyl	7.21
124	2,3,3',4,5,5',6- Hepta Chlorobiphenyl	7.21
125	2,3,3',4',5,5',6- Hepta Chlorobiphenyl	7.21
126	2,2',3,3',4,4',5,5'- Octa Chlorobiphenyl	7.62
127	2,2',3,3',4,4',5,6- Octa Chlorobiphenyl	7.35
128	2,2',3,3',4,4',5,6'- Octa Chlorobiphenyl	7.43
129	2,2',3,4,4',5,5',6- Octa Chlorobiphenyl	7.49
130	2,2',3,4,4',5,6,6'- Octa Chlorobiphenyl	7.48
131	2,3,3',4,4',5,5',6- Octa Chlorobiphenyl	7.62
132	2,2',3,3',4,4',5,5',6- Nona Chlorobiphenyl	7.94
133	2,2',3,3',4,4',5,6,6'- Nona Chlorobiphenyl	7.88

contd. table 1

2.2. Molecular descriptor generation

To obtain a suitable QSPR model, compounds are often represented by the molecular descriptors. The calculation process of the molecular descriptors is described as below: The two-dimensional molecular structures of 133 PCBs were drawn by Chem sketch 11.0 and were geometrically optimized, followed by formation of mole files which include hydrogen suppressed graphs. These mole files were exported to DRAGON software for calculation of topological and connectivity indices. Topological descriptors include valence and non-valence molecular connectivity indices calculated from the hydrogen-suppressed formula of the molecule, encoding information about the size, composition and the degree of branching of a molecule. The topological descriptors describe the atomic connectivity in the molecule. The topological parameters used in the

current study were; Weiner index (W), Balaban index (J) and Balaban type indices. The entire data comprising of physiochemical and topological parameters were than statistically evaluated using SPSS software, to obtain relevant QSAR models.

2.3. Methodology used

The entire exercise is based on the generation of statistically superior models using multiple linear regression (MLR) method, followed by cross validation, which is an important feature to choose the best among the finally selected models. The essential feature of the multiple regression analysis is cross validation which assesses the predictivity of the computed model. Cross validation provides the values of PRESS, SSY, S_{PRESS}, R^2_{CV} and PSE (the details of all these parameters can be obtained in standard statistical books) from which we can investigate the predictive power of the proposed model.

It is argued that PRESS is a good estimate of the real prediction error of the model and if it is smaller than SSY the model predicts better than chance and can be considered "statistically" significant. Furthermore the ratio of PRESS/SSY can be used to calculate the approximate confidence intervals of prediction of new compound. To be a reasonable QSAR model, PRESS/SSY should be smaller than 0.4 and the value of this ratio smaller than 0.1 indicates an excellent model. R^2_{CV} is the complement of the traces of unexplained variance over the total variance.

3. RESULTS AND DISCUSSION

By carrying out the MLR analysis, between observed or experimental log K_{ow} values and physiochemical and topological indices, a large number of regression models were developed for a set of 133 PCBs reported by **Lu** *et al.* The MLR analysis performed for the whole set provided the optimal equations for different numbers of descriptors in the range of two to five. No, single parameter was found to be significant; hence it has been omitted from the analysis. Given below are two to five descriptors containing models. As the number of parameters or descriptors are increasing, the value of R^2 is also increasing with simultaneous decrease in the value of Se and increase in the value of F ratio. A steady increase in the value of R^2A shows that the added descriptor at each step in every equation is significantly contributing towards the activity.

The two to five parameter models are listed as follows:

Two-parameter model:

$LogK_{ow}$ = -4.3940(±0.3983)J + 0.0537(±0.0020)MV +3.7964

N=133, Se=0.0351, R^2=0.9172, R^2A=0.9159, F-Ratio = 719.7780

Three-parameter model:

$LogK_{ow}$ = -22.5880(±3.7216)J + 12.2788 (±2.4994) Jhetz + 0.1619 (±0.0361)POL +10.8623

N=133, Se=0.0323, R^2=0.9301, R^2A=0.9285, F-Ratio = 572.5100

Four-parameter model:

$LogK_{ow}$ = -30.1901 (±2.7908) J + 17.4635 (±3.0513) Jhetz + 0.0473 (±0.0093)MV - 0.2482(±0.0873)ST +17.0350

N=133, Se=0.0315, R^2=0.9343, R^2A=0.9322, F-Ratio = 454.8980

Five-parameter model:

$LogK_{ow}$ = -41.4273(±5.7337)J + 29.5005(±4.4399) + Jhetz -21.1025 (±4.5788)Jhetm

20.3258(±4.9566)Jhetp + 0.0289(±0.0055)MV +3.5328

N=133, Se=0.0302, R^2=0.9401, R^2A= 0.9378, F-Ratio=398.9350

(Here, MV is molecular volume, POL is polarazability, J is Balaban index, Jhetz is Balaban"s

electronegativity index, Jhetp is Balaban"s polarizability index, and Jhetm is Balaban"s mean weighted index).

4. CONCLUSION

A close look of all the models reveals that the pentaparametric model is well suited to establish a relation between Log K_{ow} and the physiochemical and topological descriptors. Here, Balaban index (J) has a negatve coeffcientwhich signifies that the aromatic content should be kept low moreover Jhetm is also negative hence this parameter must also be kept low.Also, a close look of **Table 2** reveals that compound number; 7,39,57,58,70,83, 104,105 and

Table 2
Comparison between observed and calculated activity for the compounds using penta parametric model

Comp. No.	*Observed log kow*	*Calculated log kow*	*Residual*
1	4.6600	4.6020	0.0580
2	4.6300	4.8610	-0.2310
3	4.7200	4.5680	0.1520
4	4.9900	4.9530	0.0370
5	4.8400	4.8570	-0.0170
6	5.1500	5.1700	-0.0200
7	5.0900	4.7520	0.3380
8	5.2700	5.1590	0.1110
9	5.2300	5.3930	-0.1630
10	5.1500	5.3420	-0.1920
11	5.2300	5.5420	-0.3120
12	5.1200	5.1010	0.0190
13	5.3900	5.3480	0.0420
14	5.3300	5.1730	0.1570
15	5.0400	4.8720	0.1680
16	5.6000	5.3800	0.2200
17	5.6800	5.6960	-0.0160
18	5.2900	5.5800	-0.2900
19	5.4400	5.3400	0.1000
20	5.5400	5.6010	-0.0610
21	5.6500	5.3950	0.2550
22	5.7100	5.7750	-0.0650
23	5.6800	5.6240	0.0560
24	5.2400	5.3980	-0.1580
25	5.7100	5.5440	0.1660
26	5.7100	5.3640	0.3460
27	5.6700	5.5940	0.0760
28	5.7900	5.8260	-0.0360
29	5.7200	5.7980	-0.0780
30	5.7300	5.6460	0.0840
31	4.8400	5.4960	-0.6560
32	4.8400	5.3490	-0.5090
33	5.9400	5.9760	-0.0360
34	5.6900	5.8710	-0.1810
35	5.8700	5.8170	0.0530
36	5.7500	5.6550	0.0950
37	5.5100	5.5990	-0.0890
38	5.7900	5.6860	0.1040
39	5.5500	5.1290	0.4210
40	5.2400	5.1290	0.1110
41	6.1000	6.0730	0.0270
42	6.2400	6.2470	-0.0070
43	6.1000	6.1200	-0.0200
44	5.7600	5.9250	-0.1650
45	5.9600	6.1490	-0.1890
46	5.9800	6.1620	-0.1820
47	6.3200	6.1180	0.2020
48	6.0300	5.9060	0.1240
49	5.7600	5.8170	-0.0570
50	6.1000	6.2790	-0.1790
51	6.0300	6.0850	-0.0550
52	5.9800	6.0210	-0.0410
53	5.6000	5.9050	-0.3050
54	6.1800	6.4150	-0.2350
55	6.3800	6.3670	0.0130
56	6.2300	6.2430	-0.0130
57	6.5000	6.1790	0.3210
58	5.6000	6.0170	-0.4170
59	6.3200	6.2900	0.0300
60	5.8700	6.0590	-0.1890
61	6.3200	6.1270	0.1930
62	6.0600	6.0460	0.0140
63	5.9200	5.9110	0.0090
64	6.3000	6.2470	0.0530

65	6.0400	6.0940	-0.0540	106	7.5500	7.1280	0.4220
66	6.4100	6.4330	-0.0230	107	7.0800	6.8770	0.2030
67	6.2300	6.2440	-0.0140	108	7.2100	7.1170	0.0930
68	6.1100	6.0790	0.0310	109	6.8500	6.9480	-0.0980
69	6.7900	6.6120	0.1780	110	6.9200	6.9670	-0.0470
70	6.9200	6.5420	0.3780	111	6.5500	6.7940	-0.2440
71	6.2000	6.2740	-0.0740	112	6.7300	6.9380	-0.2080
72	6.4100	6.2590	0.1510	113	6.8500	6.8300	0.0200
73	6.4500	6.1390	0.3110	114	6.4100	6.6320	-0.2220
74	6.7100	6.7660	-0.0560	115	7.2100	7.2310	-0.0210
75	6.4400	6.5660	-0.1260	116	7.1300	7.1680	-0.0380
76	6.3900	6.4920	-0.1020	117	6.9200	7.0620	-0.1420
77	6.5700	6.6400	-0.0700	118	7.0400	7.0840	-0.0440
78	6.4000	6.4460	-0.0460	119	6.9900	7.0820	-0.0920
79	6.3000	6.4800	-0.1800	120	6.7800	6.7830	-0.0030
80	6.4200	6.2820	0.1380	121	7.7200	7.3980	0.3220
81	6.6400	6.5830	0.0570	122	7.0800	7.3610	-0.2810
82	6.7600	6.7350	0.0250	123	7.2100	7.2440	-0.0340
83	7.3000	6.7080	0.5920	124	7.2100	7.2140	-0.0040
84	6.7800	6.5550	0.2250	125	7.2100	7.1320	0.0780
85	6.2000	6.4850	-0.2850	126	7.6200	7.6060	0.0140
86	6.2000	6.3970	-0.1970	127	7.3500	7.5130	-0.1630
87	6.3200	6.3400	-0.0200	128	7.4300	7.4970	-0.0670
88	6.8200	6.8790	-0.0590	129	7.4900	7.5320	-0.0420
89	6.7300	6.8510	-0.1210	130	7.4800	7.3590	0.1210
90	6.5800	6.6410	-0.0610	131	7.6200	7.6740	-0.0540
91	6.7500	6.7370	0.0130	132	7.9400	7.8720	0.0680
92	6.5600	6.5330	0.0270	133	7.8800	7.7370	0.1430
93	6.4500	6.5570	-0.1070				
94	6.8500	6.7220	0.1280				
95	6.4100	6.5120	-0.1020				
96	6.4200	6.4320	-0.0120				
97	6.8000	6.8860	-0.0860				
98	6.6500	6.6760	-0.0260				
99	6.5400	6.5030	0.0370				
100	7.4400	7.0570	0.3830				
101	6.7800	6.9150	-0.1350				
102	6.7800	6.7860	-0.0060				
103	6.6300	6.6620	-0.0320				
104	7.0000	6.6600	0.3400				
105	7.2900	6.9780	0.3120				

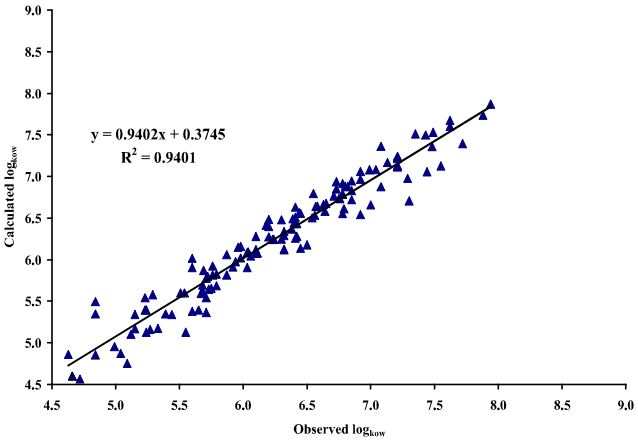


Figure 2: Correlation between Observed and Calculated activity using penta parametric model

Table 3
Cross validated values for the model containing five parameters

Parameters used	*PRESS*	*SSY*	*PRESS/SSY*	R^2cv	*PSE*	S_{PRESS}
MV, J, Jhet z,Jhet m, Jhet p	4.5319	71.1785	0.0636	0.9364	0.1845	0.1889

106 have large residual values than the rest. This highlights the position of chloine atom is crucial in determining the activity, and the position like 2,3 and 4 on both the rings if substituted by halogen atoms, create steric hindrance which ultimately effects the activity. The other parameters in the model have positive coeffcients, hence these parameters would be helpful in determining the activity.

As can be seen from above discussion, the log K_{ow} values of PCBs depended on the molecular inherent electronic properties, the positions of Cl-atom and the conjugate bonds in benzene rings system. From the obtained results, it was showed that the selected descriptors could account for these features. The above model is not only stastically best than earlier predicted models, but is also superior in terms of cross validated parametrs, with very high R^2cv value reported in **Table 3.**

The current work not only presents an effective method for the prediction of the log K_{ow} values of PCBs but also the effective use of QSPR (quantitative structure property relationship) models for the prediction of log K_{ow} values of unknown compounds.

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