

DFT-Based Prediction of Bioconcentration Factors of Polychlorinated Biphenyls in Fish Species Using Molecular Descriptors

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Abstract

Experimental determination of BCFs is expensive and demanding if performed correctly. Because of this, measuring the BCFs of many thousands of chemical substances that are potential regulatory interest is simply not possible. Hence, prediction of BCFs of the PCBs based on QSAR were made time to time to increase the probability of success and reduce the time and cost in exploring the toxicological and ecological characteristics of molecules. DFT methods are, in general, capable of generating a variety of isolated molecular descriptors as well as local reactivity descriptors quite accurately. In this work, prediction of BCFs of the fifty seven PCBs based on quantum chemical descriptors derived from DFT method using the B88-PW91 GGA energy function with the DZVP basis set have been made. The study concluded that dipole moment and ionization potential are reliable descriptors for correlation of bioconcentration factors of polychlorinated biphenyls with their electronic structures. The resulted QSAR model ($r^2 = 0.9139$, $r_{CV}^2 = 0.8986$, $k = 2$, $SE = 0.2668$) can be useful for predicting the BCFs of compounds prior to their synthesis.

Keywords

PCBs, QSAR, DFT, Quantum Chemical Descriptors

1. Introduction

In our recent communication [1], we have employed atomic descriptors derived from density functional theory (DFT) based methods to predict the bioconcentration factor (BCF) of polychlorinated biphenyls (PCBs) in fish. PCBs belong to

important group of environmental pollutants, which were industrially used as dielectric fluids in transformers and capacitors, as hydraulic and heat transfer fluids, and as plasticizers [2]. These chemicals were either washed down into the soil or into the water bodies [3]. From the soil, these are absorbed by the plants along with water and minerals, and from the water bodies, these are taken up by aquatic plants and animals [4]. This is one of the ways in which they enter the food chain [5]. As these chemicals are not degradable, these get accumulated progressively at each trophic level [4] [6] [7] [8]. As human beings occupy the top level in any food chains, the maximum concentration of these chemicals gets accumulated in our bodies [9]-[14]. Fish are the principal target organisms of BCF assessment due to their relevance as food for many species including humans and the availability of standardized testing protocols [15] [16] [17]. In general, however, experimental determination of BCFs is expensive and demanding if performed correctly. Hence, a number of QSAR based study of BCFs of the PCBs were made time to time [1] [18]-[34] because QSAR technique [35] increases the probability of success and reduce the time and cost in exploring the toxicological and ecological characteristics of molecules. A number of quantum chemical descriptors [36] [37] [38] have been identified in the framework of QSAR. In the present work, we present the DFT based derived quantum chemical descriptor to correlate the BCF of PCBs.

2. Theory

In 1960s, Hohenberg and Khon put forward two basic theorems to which DFT is based on and its performance in the description of structure, energetic, and magnetic molecular properties has been quite substantially reviewed time to time [39]-[46]. DFT methods are, in general, capable of generating a variety of isolated molecular properties, such as dipole moment, ionization energy, electron affinity, electronegativity, hardness, softness, electrophilicity index, etc., quite accurately [47] [48] [49] [50]. Here, following seven quantum chemical descriptors based on DFT method [39] have been tested and the final QSAR model was constructed with the help of significant descriptors. A concise description of these descriptors is as below.

The dipole moment is used to describe the polarity of the molecule [47] The dipole moment, μ , of a molecule is the vector sum of the dipole moments of the bonds and is calculated according to the rule of vector addition. If two bonds with the dipole moments P and Q are at an angle θ the total dipole moment is given by

$$\mu^2 = P^2 + Q^2 + 2PQ \cos \theta \quad (1)$$

For instance, two identical bonds with the opposite directions ($\theta = 180^\circ$) have $\mu = 0$. For identical bonds ($P = Q$) Equation (1) yields

$$\mu^2 = 2P^2 (1 + \cos \theta) \quad (1a)$$

Ionization energy (IE), electron affinity (EA), electronegativity (χ), hardness

(η) and softness (S) are defined as [48] [49]

$$IE = E_{tot}(A^+) - E_{tot}(A) \quad (2)$$

$$EA = E_{tot}(A) - E_{tot}(A^-) \quad (3)$$

$$\chi = -\mu = -(\delta E / \delta N)_{v(r)} \quad (4)$$

$$\eta = 1/2(\delta\mu/\delta N)_{v(r)} = 1/2(\delta^2 E / \delta N^2)_{v(r)} \quad (5)$$

$$S = 1/2\eta \quad (6)$$

where μ is chemical potential, E is the total energy, N is number of electrons of the chemical species and $v(r)$ the external potential. The operation definition of electronegativity, hardness and global softness are defined as:

$$\chi = -\mu = (IP + EA)/2 \quad (4a)$$

$$\eta = 1/2(IP - EA) \quad (5a)$$

$$S = 1/(IP - EA) \quad (6a)$$

Parr *et al.* introduced the global electrophilicity index [50], in terms of chemical potential and hardness. The electrophilicity index, ω , is a reliable property of a chemical system and its operation definition is

$$\omega = \mu^2 / 2\eta \quad (7)$$

3. Materials and Methods

Fifty seven PCB congeners listed in **Figure 1** are the study materials for the present study. These congeners were taken from the literature with their experimental logarithmic BCF values ($\text{LogBCF}_{\text{exp}}$) for several fish species (guppies, fathead minnow, rainbow trout, and bluegill sunfish) [23]. For BCF prediction, the 3D modeling [51] and geometry optimization of all the compounds have been performed on workspace program of CAChe pro software of Fujitsu [52] using the B88-PW91 GGA energy function with the DZVP basis set. The values of various descriptors, such as dipole moment (μ), ionization energy (IE) and electron affinity (EA) have been directly obtained from DFT calculation results and have been tabulated in **Table 1**. However, the values of electronegativity (χ), hardness (η), softness (S) and electrophilicity index (ω) have been calculated by solving equations given in theory and the necessary values taken from DFT calculation results and have also been tabulated in **Table 1**. The Project Leader program associated with CAChe has been used for multiple linear regression (MLR) analysis [53] using leave-out method and various regression equations have been developed for prediction of BCF ($\text{LogBCF}_{\text{pre}}$).

4. Results and Discussion

The assessment of BCF of a hypothetical compound is of prime interest. The QSAR method saves time and cost in determining the BCF of a series of compounds with the help of BCF of previously known compounds. The biphenyl

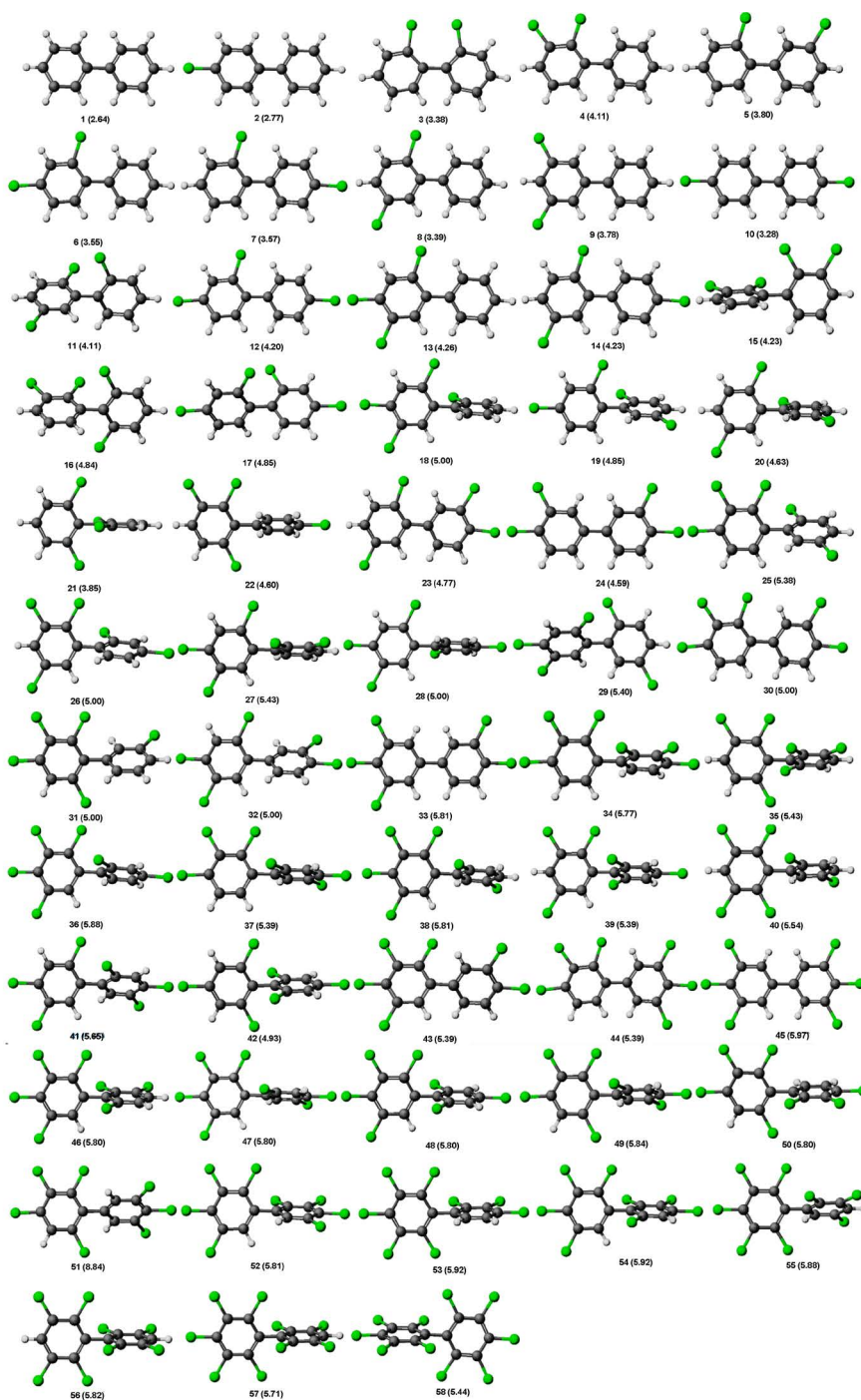


Figure 1. Biphenyl, its chloro-derivatives and their congeners with their experimental logarithmic BCF [23].

and its fifty seven chloro-derivatives (mono-, di-, tri-, tetra-, penta-, hexa-, hepta-, nona- and decachlorobiphenyl are one, eight, four, ten, nine, twelve, six, five and one in number, respectively) and their experimental logarithmic BCF values have been taken from the literature. A number of quantum chemical descriptors have been identified which are capable of successfully correlating the activity with the structure of a chemical system. The present study is based on seven

Table 1. Values of quantum chemical descriptors, experimental BCF and predicted BCF.

S.N.	CAS NO	Descriptors							$LogBCF_{exp}$	$LogBCF_{pre}$						
		μ	IP	EA	χ	η	S	ω		Equation (8)	Equation (9)	Equation (10)	Equation (11)	Equation (12)	Equation (13)	Equation (14)
1	92-52-4	0	5.557	1.982	3.770	1.788	0.280	3.975	2.64	2.77	2.74	2.42	2.47	2.48	2.55	2.37
2	2051-62-9	2.005	5.618	2.184	3.901	1.717	0.291	4.432	2.77	3.00	3.03	2.80	2.80	2.82	2.79	2.71
3	13029-08-8	3.141	5.809	2.427	4.118	1.691	0.296	5.014	3.38	3.72	3.77	3.77	3.74	3.74	3.65	3.69
4	16605-91-7	2.667	5.863	2.361	4.112	1.751	0.286	4.828	4.11	3.92	3.95	3.89	3.86	3.87	3.86	3.86
5	25569-80-6	3.442	5.893	2.395	4.144	1.749	0.286	4.909	3.80	4.04	4.09	4.03	3.99	4.00	4.04	4.08
6	33284-50-3	2.076	5.793	2.363	4.078	1.715	0.292	4.848	3.55	3.66	3.67	3.64	3.63	3.64	3.55	3.52
7	34883-43-7	2.713	5.774	2.367	4.071	1.704	0.294	4.863	3.57	3.59	3.62	3.65	3.62	3.62	3.53	3.57
8	34883-39-1	0.789	5.892	2.407	4.150	1.743	0.287	4.941	3.89	4.03	4.00	4.12	4.14	4.14	4.12	4.08
9	34883-41-5	2.414	5.951	2.428	4.190	1.762	0.284	4.982	3.78	4.26	4.27	4.35	4.33	4.34	4.37	4.41
10	2050-68-2	0	5.677	2.369	4.023	1.654	0.302	4.893	3.28	3.22	3.18	3.23	3.28	3.28	3.06	2.95
11	37680-65-2	1.770	6.048	1.907	3.978	2.071	0.241	3.820	4.11	4.62	4.60	4.08	4.08	4.07	4.15	4.10
12	7012-37-5	1.295	5.828	2.537	4.183	1.646	0.304	5.315	4.20	3.79	3.78	4.04	4.05	4.04	3.84	3.87
13	15862-07-4	2.200	5.92	2.535	4.228	1.693	0.295	5.279	4.26	4.14	4.15	4.37	4.35	4.35	4.34	4.40
14	16606-02-3	1.168	5.927	2.581	4.254	1.673	0.299	5.409	4.23	4.17	4.14	4.37	4.39	4.39	4.26	4.27
15	38444-93-8	3.668	6.233	1.998	4.116	2.118	0.236	3.999	4.23	5.33 ^a	5.35 ^a	4.84	4.79	4.77	4.69	4.76 ^a
16	41464-39-5	2.875	6.174	1.960	4.067	2.107	0.237	3.925	4.84	5.10	5.10	4.52	4.49	4.48	4.44	4.43
17	2437-79-8	2.024	6.138	2.203	4.171	1.968	0.254	4.420	4.85	4.97	4.94	4.75	4.74	4.74	4.80	4.79
18	70362-47-9	2.845	6.121	2.192	4.157	1.965	0.255	4.397	5.00	4.90	4.91	4.68	4.64	4.65	4.68	4.70
19	41464-40-8	1.376	6.12	2.189	4.155	1.966	0.254	4.391	4.84	4.90	4.86	4.67	4.68	4.68	4.76	4.72
20	35693-99-3	0.409	6.122	2.265	4.194	1.929	0.259	4.559	4.63	4.91	4.83	4.77	4.80	4.81	4.86	4.79
21	15968-05-5	0.011	6.194	1.812	4.003	2.191	0.228	3.657	3.85	5.18 ^a	5.08 ^a	4.41	4.46	4.42	4.19	4.08
22	52663-58-8	2.050	6.072	2.295	4.184	1.889	0.265	4.634	4.60	4.72	4.70	4.62	4.61	4.62	4.69	4.69
23	32598-11-1	2.204	6.039	2.727	4.383	1.656	0.302	5.800	4.77	4.59	4.58	4.95	4.93	4.93	4.86	4.97
24	32598-13-1	2.542	5.937	2.687	4.312	1.625	0.308	5.721	4.59	4.20	4.22	4.54	4.51	4.50	4.32	4.43
25	38380-02-8	2.311	6.164	2.363	4.264	1.901	0.263	4.782	5.38	5.06	5.05	5.03	5.01	5.02	5.10	5.13
26	68194-07-0	1.611	6.266	2.266	4.266	2.000	0.250	4.550	5.00	5.45	5.40	5.21	5.21	5.22	5.17	5.14
27	41464-51-1	2.648	6.216	2.334	4.275	1.941	0.258	4.708	5.43	5.26	5.25	5.11	5.09	5.10	5.10	5.12
28	38380-01-7	1.309	6.194	2.350	4.272	1.922	0.260	4.748	5.00	5.18	5.13	5.05	5.06	5.08	5.11	5.07
29	37680-73-2	1.437	5.971	2.084	4.028	1.944	0.257	4.173	5.40	4.33	4.31 ^a	4.01 ^a	4.02 ^a	4.03 ^a	4.16 ^a	4.10 ^a
30	32598-14-4	3.152	6.025	2.801	4.413	1.612	0.310	6.041	5.00	4.54 ^a	4.56	4.98	4.95	4.93	4.84	5.02
31	74472-35-8	1.993	6.222	2.395	4.309	1.914	0.261	4.850	5.00	5.28	5.25	5.28	5.27	5.28	5.35	5.38
32	31508-00-6	1.282	6.148	2.504	4.326	1.822	0.274	5.136	5.00	5.00	4.96	5.07	5.08	5.10	5.19	5.17
33	57465-28-8	1.412	6.062	2.826	4.444	1.618	0.309	6.103	5.81	4.68 ^a	4.64 ^a	5.15	5.15	5.13	5.02 ^a	5.14 ^a
34	38380-07-3	3.269	6.309	2.429	4.369	1.940	0.258	4.920	5.77	5.61	5.61	5.55	5.51	5.52	5.54	5.60
35	38411-22-2	1.453	6.222	2.130	4.176	2.046	0.244	4.262	5.43	5.28	5.23	4.89	4.90	4.90	4.86	4.80
36	35694-06-5	1.928	6.331	2.360	4.346	1.986	0.252	4.755	5.88	5.70	5.65	5.62	5.61	5.61	5.56	5.59
37	35065-28-2	1.997	6.325	2.260	4.293	2.033	0.246	4.533	5.39	5.67	5.63	5.48	5.47	5.46	5.38	5.40
38	52712-04-6	2.049	6.256	2.455	4.356	1.901	0.263	4.991	5.81	5.41	5.38	5.47	5.46	5.46	5.53	5.57

Continued

39	74472-41-6	1.073	6.284	2.243	4.264	2.021	0.247	4.498	5.39	5.52	5.45	5.32	5.33	5.33	5.29	5.27
40	52663-63-5	0.472	6.221	2.302	4.262	1.960	0.255	4.634	5.54	5.28	5.20	5.16	5.19	5.20	5.19	5.14
41	35065-27-1	0.156	6.257	2.493	4.375	1.882	0.266	5.085	5.65	5.42	5.32	5.44	5.49	5.50	5.47	5.42
42	33979-03-2	0.004	6.535	2.153	4.344	2.191	0.228	4.306	4.93	6.47 ^a	6.34 ^a	6.03 ^a	6.08 ^a	6.03 ^a	5.54	5.48
43	38380-08-4	1.712	6.221	2.629	4.425	1.796	0.278	5.451	5.39	5.28	5.24	5.48	5.48	5.49	5.60	5.64
44	69782-90-7	2.096	6.158	2.940	4.549	1.609	0.311	6.430	5.39	5.04	5.02	5.62	5.61	5.59	5.53	5.73
45	32774-16-6	0.002	6.178	2.960	4.569	1.609	0.311	6.487	5.97	5.12	5.03 ^a	5.72	5.76	5.73	5.65	5.76
46	38411-25-5	2.751	6.351	2.291	4.321	2.030	0.246	4.599	5.80	5.77	5.75	5.54	5.51	5.51	5.46	5.49
47	35065-29-3	0.839	6.340	2.558	4.449	1.891	0.264	5.234	5.80	5.73	5.65	5.82	5.84	5.86	5.91	5.90
48	60145-23-5	1.823	6.376	2.319	4.348	2.029	0.246	4.659	5.80	5.87	5.81	5.73	5.73	5.72	5.67	5.69
49	52663-69-1	0.933	6.329	2.388	4.359	1.971	0.254	4.820	5.84	5.69	5.61	5.65	5.67	5.66	5.60	5.59
50	52663-68-0	2.193	6.441	2.327	4.384	2.057	0.243	4.672	5.80	6.11	6.06	5.90	5.89	5.88	5.72	5.74
51	74472-50-7	1.833	6.373	2.620	4.497	1.877	0.266	5.387	5.84	5.86	5.80	6.08	6.07	6.08	6.19	6.27
52	35694-08-7	1.101	6.419	2.675	4.547	1.872	0.267	5.522	5.81	6.03	5.95	6.24	6.25	6.27	6.32	6.36
53	52663-78-2	1.956	6.46	2.465	4.463	1.998	0.250	4.984	5.92	6.18	6.13	6.21	6.20	6.19	6.14	6.20
54	42740-50-1	1.529	6.421	2.460	4.441	1.981	0.252	4.978	5.92	6.04	5.97	6.06	6.06	6.06	6.05	6.08
55	68194-17-2	0.875	6.369	2.587	4.478	1.891	0.264	5.302	5.88	5.84	5.76	5.95	5.98	5.99	6.05	6.05
56	2136-99-4	0.002	6.34	2.403	4.372	1.969	0.254	4.854	5.82	5.73	5.62	5.71	5.75	5.75	5.68	5.64
57	52663-77-1	0.915	6.387	2.521	4.454	1.933	0.259	5.131	5.71	5.91	5.82	5.94	5.96	5.97	5.91	5.90
58	2051-24-3	0.006	6.486	2.695	4.591	1.896	0.264	5.558	5.44	6.28 ^a	6.16	6.57 ^a	6.61 ^a	6.61 ^a	6.61 ^a	6.64 ^a

^adata point not used in the model, μ is the dipole moment in debye, IP is the ionization energy in eV, EA is the electron affinity in eV, χ is the electronegativity in eV, η is the absolute hardness in eV, S is the global softness and ω is the electrophilicity of the molecule.

quantum chemical reactivity descriptors: dipole moment, ionization potential, electron affinity, electronegativity, hardness, softness and electrophilicity index. Dipole moment (μ) gives valuable information regarding the symmetry of molecule. It also helps in explaining the solubility of substances. The computational result of dipole moment of the compounds (**Table 1**) show that all the compounds have definite dipole moment, except compound no. 1 and 10. Thus, both of these compounds are symmetrical. The range of dipole moment is 0.002 - 0.011D (5), 0.156 - 0.933D (8), 1.073 - 1.997D (20), 2.005 - 2.875D (18) and 3.141 - 3.668D (5). Ionization potential (IP) of a molecule is the minimal energy needed for the detachment of an electron for a molecule. According to Koopman's theorem the IE is simply the eigenvalue of HOMO with change in sign and characterizes the susceptibility of the molecule toward attack by electrophiles. IP value as included in **Table 1** shows that fifteen compounds have their IP in the range of 5.557 - 5.971 eV and the rest forty five in the range of 6.028 - 6.535 eV. Electron affinity (EA) is the energy difference between an uncharged species and its negative ion. It is an important property of atoms and molecules. According to Koopman's theorem [54] the EA is simply the eigenvalue of LUMO with change in sign and characterizes the susceptibility of the molecule toward attack by nucleophiles. The experimental and/or theoretical determina-

tion of this quantity is an important task. A close look at **Table 1**, shows all the compounds have definite value of electron affinity (1.812 to 1.998 eV (5) and 2.084 - 2.960 eV (53). Electronegativity (χ) measures the ability to attract electron itself. Large χ values characterize acids and small χ values are found for bases. If two molecules are brought together, electrons will flow from the one of lower χ to that of higher χ . All the compounds have definite value of χ ranging from 4.003 to 4.591 eV, except three compounds (1, 2 and 11) have χ value lower than 4.0 eV. The parameter hardness (η) is interpreted as the resistance of the chemical potential to change in the number of electrons or resistance to deformation or change. All the compounds have definite value of η in the range 1.609 - 1.998 eV (46) and 2.0 - 2.191 eV (12). The minimum value of hardness is zero and it corresponds to the maximum softness (S). The ranges of softness values are 0.228 - 0.299 (50) and 0.302 - 0.311 (8). Electrophilicity index (ω) measures the stabilization in energy when the system acquires an additional electronic charge from the environment. The electrophilicity index is positive, definite quantity and the direction of the charge is completely determined by the electronic chemical potential ($\mu = -\chi$) of the molecule because an electrophile is a chemical species capable of accepting electrons from the environment and its energy must decrease upon accepting electronic charge. All the compounds have definite value of ω included in **Table 1**. The range of ω is 3.657 - 3.999 (5), 4.179 - 4.991 (34), 5.014 - 5.8 (15) and 6.041 - 6.487 (4).

Multiple linear regression analyses were employed to developed reliable models for the prediction of BCF. For MLR analysis, above descriptors (**Table 1**) were used as independent variables and the experimental logarithmic BCF values as dependent variable. MLR analysis has been made by Project Leader software associated with CAChe, using the descriptors in various combinations. The best seven models (for $k = 1, 2, 3, 4, 5, 6$ and 7) are presented here.

When, $k = 1$, single descriptor has been used as independent variable, then with respect to each descriptor seven equations were made and the best-fitted equation of this class is Equation (8), where IP is the ionization potential of the molecule and, it has a positive descriptor coefficient magnitude that shows that its direct relationship with the BCF.

$$\begin{aligned} \text{LogBCF}_{pre} &= 3.7854 \times IP - 18.2697 \\ r^2 &= 0.9118, r_{cv}^2 = 0.8953, SE = 0.2698 \end{aligned} \quad (8)$$

The predicted logarithmic BCF values from Equation (8) are also given in **Table 1**. The statistical quality of the equation is good as is evident from its correlation coefficient r^2 value = 0.9118 and a cross-validated coefficient $r_{cv}^2 = 0.8953$. The predicted BCF is reliable as is evident from its standard error (SE) value. The trend of the experimental and predicted BCFs is shown in **Figure 2(a)** which shows that there is little difference between experimental and predicted BCFs.

For $k = 2$, the best-fitted equation is Equation (9), where μ and IP is the dipole moment and ionization potential of the molecule, respectively. Both, μ and

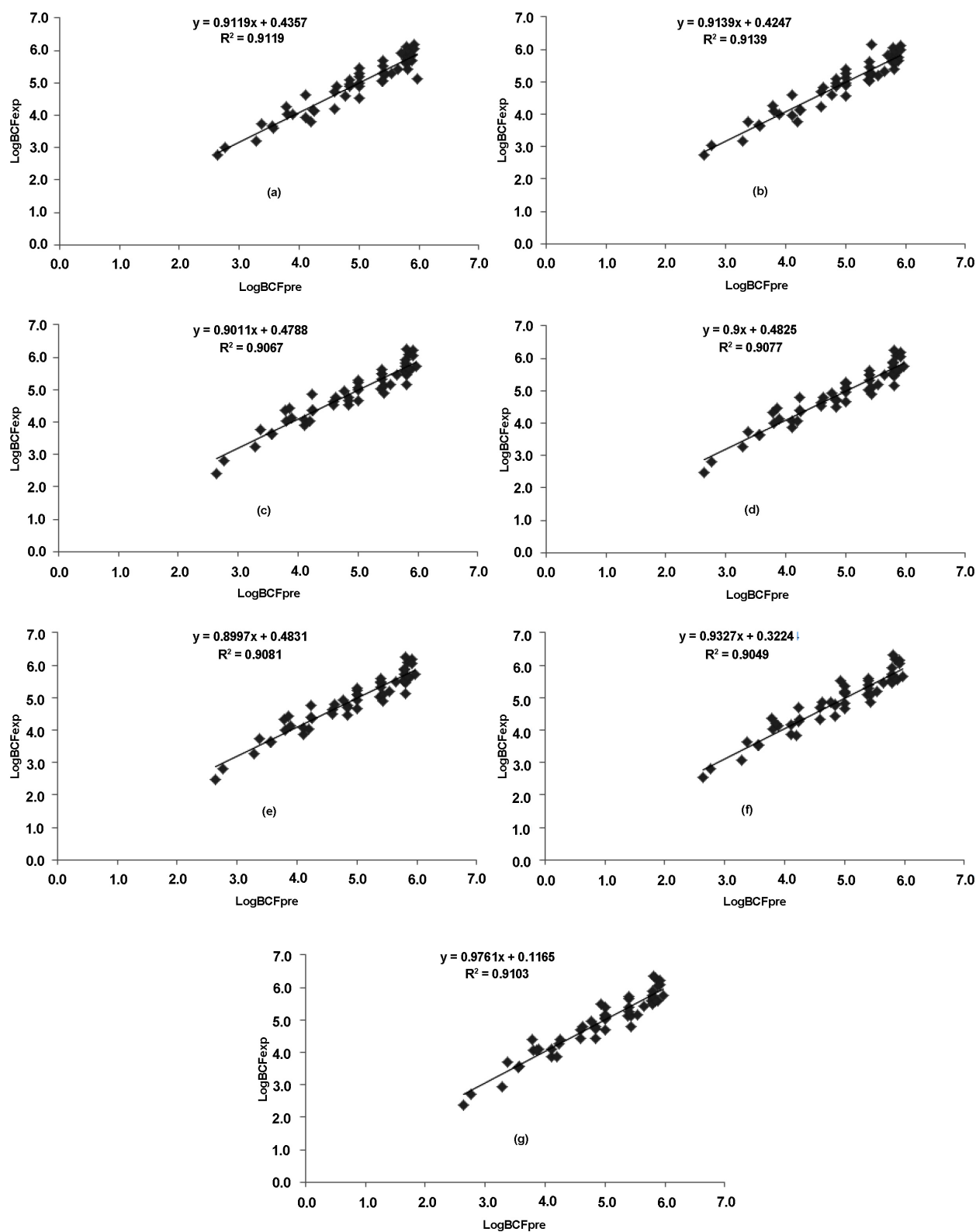


Figure 2. Trend of experimental BCF and predicted BCF.

IP have positive descriptor coefficient magnitudes that show direct relationships with the BCF.

$$\begin{aligned} \text{LogBCF}_{pre} &= 0.0319265 \times \mu + 3.68314 \times IP - 17.7294 \\ r^2 &= 0.9139, r_{CV}^2 = 0.8986, SE = 0.2668 \end{aligned} \quad (9)$$

The predicted logarithmic BCF values from Equation (9) are also given in **Table 1**. The statistical quality of the equation is more reliable than Equation (8) as is evident from its correlation coefficient r^2 value = 0.91389 and a cross-validated coefficient $r_{CV}^2 = 0.8986$. The predicted BCF is reliable as is evident from its standard error (SE) value. The trend of the experimental and predicted BCFs is shown in **Figure 2(b)**.

For $k = 3$, the best-fitted equation is Equation (10), where IP , EA and χ is the ionization potential, electron affinity and of the molecule, respectively.

$$\begin{aligned} \text{LogBCF}_{pre} &= -68.2118 \times IP - 70.5862 \times EA + 143.542 \times \chi - 19.7812 \\ r^2 &= 0.9102, r_{CV}^2 = 0.8946, SE = 0.2775 \end{aligned} \quad (10)$$

Both, IP and EA have negative descriptor coefficient magnitudes that show indirect relationships with the BCF, while the third descriptor, χ , has a positive magnitude *i.e.*, direct relationship. The statistical quality of the equation is $r^2 = 0.9102$, $r_{CV}^2 = 0.8946$ and $SE = 0.2775$. The predicted logarithmic BCF values as obtained from this model are also given in **Table 1**. The trend of the experimental and predicted BCFs is shown in **Figure 2(c)**.

For $k = 4$, the best-fitted equation is Equation (11). The variables of this model are dipole moment, ionization potential, electron affinity and electronegativity, all with negative descriptor coefficient magnitudes except the electronegativity.

$$\begin{aligned} \text{LogBCF}_{pre} &= -0.0271479 \times \mu - 65.5176 \times IP - 67.889 \times EA + 138.139 \times \chi - 19.6776 \\ r^2 &= 0.9110, r_{CV}^2 = 0.8887, SE = 0.2779 \end{aligned} \quad (11)$$

The predicted logarithmic BCF values as obtained from this model are also given in **Table 1**. The trend of the experimental and predicted BCFs is shown in **Figure 2(d)**.

For $k = 5$, the best-fitted equation is the Equation (12). The variables of this model are dipole moment, ionization potential, electron affinity, electronegativity and softness all with negative descriptor coefficient magnitudes except the electronegativity.

$$\begin{aligned} \text{LogBCF}_{pre} &= -0.0261386 \times \mu - 58.9446 \times IP - 60.2176 \times EA \\ &\quad + 123.883 \times \chi - 7.45897 \times S - 15.5638 \\ r^2 &= 0.9112, r_{CV}^2 = 0.8630, SE = 0.2815 \end{aligned} \quad (12)$$

The predicted logarithmic BCF values as obtained from this model are also given in **Table 1**. The trend of the experimental and predicted BCFs is shown in **Figure 2(e)**.

For $k = 6$, the best-fitted equation is the Equation (13). The variables of this model are ionization potential, electron affinity, electronegativity, hardness, softness and electronegativity index.

$$\begin{aligned} \text{LogBCF}_{pre} = & -77.8689 \times IP - 5.08309 \times EA + 83.4781 \times \chi \\ & + 65.3488 \times \eta - 99.3578 \times S + 1.79358 \times \omega + 34.4746 \quad (13) \\ r^2 = & 0.9077, r_{CV}^2 = 0.6856, SE = 0.2874 \end{aligned}$$

The predicted logarithmic BCF values as obtained from this model are also given in **Table 1**. The trend of the experimental and predicted BCFs is shown in **Figure 2(f)**.

For $k = 7$, seven descriptors have been used as independent variables and the resulted equation is Equation (14).

$$\begin{aligned} \text{LogBCF}_{pre} = & 0.0413017 \times \mu - 106.417 \times IP + 97.0787 \times EA + 9.55439 \times \chi \\ & + 197.236 \times \eta - 94.8928 \times S + 2.04835 \times \omega + 31.0716 \quad (14) \\ r^2 = & 0.9071, r_{CV}^2 = 0.8007, SE = 0.2928 \end{aligned}$$

The predicted logarithmic BCF values as obtained from this model are also given in **Table 1**. The trend of the experimental and predicted BCFs is shown in **Figure 2(g)**.

For comparative study and selection of the reliable model among the above seven models, the regression summary is presented as below.

Regression summary of the above models

S. N.	k	n	r^2	r_{CV}^2	SE	Variables
Equation (8)	1	52	0.9118	0.8953	0.2698	IP
Equation (9)	2	52	0.9139	0.8986	0.2668	μ, IP
Equation (10)	3	55	0.9102	0.8946	0.2775	IP, EA, χ
Equation (11)	4	55	0.9110	0.8887	0.2779	μ, IP, EA, χ
Equation (12)	5	55	0.9112	0.8630	0.2815	μ, IP, EA, χ, S
Equation (13)	6	55	0.9077	0.6856	0.2874	$IP, EA, \chi, \eta, S, \omega$
Equation (14)	7	54	0.9071	0.8007	0.2928	$\mu, IP, EA, \chi, \eta, G, \omega$

From the above summary, the reliable model is the Equation (9) as it has higher value of r^2 and r_{CV}^2 , lower values of “ k ” and SE than other models. The current study accounts for previous findings in most easier and convenient way. Ivanciuc *et al.*, for the first time made QSAR study on these compounds aggregated from various literature reports. Predictive ability of their models was “ r ” between 0.903 and 0.935 for splinoid QSSAR and “ r ” between 0.745 and 0.887 for cluster-expansion [23]. In continuation to this Katritzky *et al.*, reported QSAR results of the same data sets based on 486 constitutional, topological, geometrical, electrostatic, quantum chemical and thermodynamic descriptors derived solely from molecular structure using CODESSA Pro software and proposed that two-parameter model satisfactorily describes the relationship between observed and calculated values in terms of statistical parameters [18]. E.B. de Melo reported QSAR results based on E-state and topological descriptors using SMILE software and the best model present five descriptors (one E-state index

and four topological descriptors) [55]. Liu *et al.* made QSAR studies of BCFs of PCBs using DFT, PCS and CoMFA, and their result show that the electrostatic descriptors ($R^2 = 0.926$; $Q^2 = 0.821$; $RMSE = 0.235$) play a more significant role in BCFs of PCBs [56]. Using deep belief network QSPR models for predicting the physicochemical properties of PCBs were also made by Safder *et al.* [57].

5. Conclusions

On the basis of present study, it has been concluded that DFT-based quantum chemical descriptors have sufficient reliability to relate the bioconcentration factors of polychlorinated biphenyls with their electronic structures. The QSAR model, " $\text{LogBCF}_{pre} = 0.0319265 \times \mu + 3.68314 \times IP - 17.7294$ ", can be useful for predicting the BCF of compounds prior to their synthesis and dipole moment and ionization potential are reliable descriptors for predicting BCF, and Both dipole moment and ionization potential have direct relationship with log BCF.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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