QSAR Study on Photoinduced Toxicity of Polycyclic Aromatic Hydrocarbons

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Abstract
The paper describes Quantitative Structure Activity Relationship (QSAR) study for photoinduced toxicity of polycyclic aromatic hydrocarbons (PAHs). These compounds are extremely toxic in the presence of sunlight. Connectivity type topological indices yielded excellent models. Higher parametric models were found to be statistically more significant. The results are critically discussed on the basis of variety of statistical parameters.

Keywords: QSAR, Connectivity Type Indices, Photoinduced Toxicity, Homo-Lumo gap, Topological descriptors

Introduction:
Polycyclic aromatic hydrocarbons are ubiquitous contaminants of aquatic eco systems. Although some PAHs occur as a result of natural process such as forest fibers, the predominant sources of PAHs are linked to human activities such as oil spills and burning fossil as a consequence they may be found in different environment[1, 2]. Interactive research is carried out in modeling and prediction of toxicity of this class of compounds [3, 4]. Many of the PAHs are reported to be carcinogenic to humans and are toxic to aquatic organisms when activated by ultra-violet (UV) light [2]. It is worth mentioning that PAHs are generally not acutely toxic in conventional laboratory tests, many are extremely toxic in the presence of sunlight [1].

According to the mechanism of PAHs toxicity these compounds absorb UV radiation producing excited triplet state which then transfers the energy to molecular oxygen producing singlet molecular oxygen or other free radicals. These radicals can react with cellular compounds and macromolecules thus producing damages. Newsted and Giesy [5] attempted to relate their photo toxicity results to a variety of spectroscopic data including energies of lowest singlet and triplet excited state, singlet triplet splitting energy and phosphorescence lifetime obtained from fluorescence and phosphorescence emission spectra. They reported a parabolic relationship between toxicity of PAHs and energy of triplet state of a large variety of PAHs.
In this paper we describe QSARs for photoinduced toxicity of a set of 28 polycyclic aromatic hydrocarbons (PAHs). The structural details for these 28 PAHs are presented in Table1. They exhibit Photoinduced toxicity. Since photoinduced toxicity is the result of stability and light absorbance, a multiple relationship between photoinduced toxicity and structure is obvious. This was indeed found to be the case by Mekenyan and coworker[1]. Based on HOMO- LUMO gap they provided an explanation as to why Phenanthrene and Tetracene are non toxic while. Anthracene is highly phototoxic. Also, that the PAHs exhibiting photoinduced toxicity were consistently within HOMO-LUMO gap. Based on such relationship PAHs were classified as: (i) stable and (ii) unstable PAHs. For the stable PAHs the following model was proposed;

$$\log(1/ALT5O) = 2.473 - 0.687(\pm 0.132)\Delta E^{PM3}_{HOMO-LUMO}$$

$R^2 = 0.68$, $S^2 = 0.04$, $F = 27.08$

$$\log(1/ALT50) = 2.369 - 0.674(\pm 0.126)\Delta^{AM_1}_{HOMO-LUMO}$$

$R^2 = 0.68$, $S^2 = 0.04$, $F = 27.54$

Where the correlation HOMO-LUMO gap was calculated using PM_3 and AM_1 methods respectively. For the unstable PAHs the following relationships between photoinduced toxicity and HOMO-LUMO gap were proposed:

$$\log(1/ALT50) = -11.4 + 1.306(\pm 0.084)\Delta^{PM_3}_{HOMO-LUMO}$$

$R^2 = 0.99$, $S^2 = 0.003$, $F = 242.9$

$$\log(1/ALT50) = -10.18 + 1.128(\pm 0.070)\Delta^{AM_1}_{HUMO-LUMO}$$

$R^2 = 0.99$, $S^2 = 0.003$, $F = 220.9$

The aforementioned models for photoinduced toxicity of PAHs were developed using the basic principles of molecular spectroscopy and quantum-theoretical chemistry. Photoinduced toxicity was considered as an over all effect of two factors: (1) molecular structure factor involving capacity of PAHs to absorb light and (2) its stability. In addition, the energy and intensity of light irradiation were also responsible for the exhibition of photoinduced toxicity of PAHs. In such studies the HOMO-LUMO gap for PAHs was considered as the most suitable ground state index.

In view of the above, particularly dividing PAHs into two groups on the basis of stability, we thought it necessary to reinvestigate the study consisting of photoinduced toxicity of 28 PAHs. This reinvestigation is made by us particularly for the purpose of obtaining a better model that too without splitting 28 PAHs into two groups.

Modeling Methods

The structural details of 28 PAHs, are given in Table 1.The observed toxicity (adjustable Lethal Time log 1/LT 50), energy of singlet and triplet states and HOMO-LUMO gap calculated from PM3 and AM1 methods are shown in Table 2. Tables 3-6 record the different types of topological indices for the used set of 28 PAHs.

Experimental

Adjustable Lethal Time(log1/LT50)

The experimental values of the adjustable
Lethal time of PAHs (log 1/LT 50) were taken from earlier study [1].

HOHO-LUMO Gap, AM_1, PM_3.

The values of HOHO-LUMO Gap, AM_1 and PM_3 were also taken from earlier study[1].

Topological indices

All the distance and connectivity based topological indices (W, J, Jhetv, Jhetz, Jhetm,
Jhete, Jhetp, (χ_0, χ_1, χ_2, χ_{0V}, χ_{1V} χ_{2v},) were calculated using DRAGON software [6]. The optimization of the structures was made using Hyperchem[7] or ACD Labs software[8].

Regression analysis All the regression analysis [9] was performed using Regress-1 program provided by I. Lukovits.

Results and discussion:

Polycyclic aromatic hydrocarbons (PAHs) are major products of combustion processes, as a consequence they may be found in different environmental scenarios. Consequently, modeling and predicting of PAHs toxicity to different species has attracted a lot of attention. Due to complex nature of photo-induced toxicity, a multi-linear relationship between toxicity of PAHs and their chemical structures is obvious. Consequent to above, we have followed simple as well as multi-parametric regression analyses for obtaining statistically excellent models for modeling toxicity vis-à-vis adjusted lethal time (log 1/LT50) of PAHs.

To start with initially we have used 47 molecular descriptors(25 distance based, 12 connectivity based, 5 information and 5 geometric topological indices), for arriving at most appropriate model for modeling the toxicity of PAHs. In doing so we had also taken care of the rule of thumb[10,11].

The structural details of 28 PAHs, are given in Table 1.The observed toxicity (adjustable Lethal Time log 1/LT 50), energy of singlet and triplet states and HOMO-LUMO gap calculated from PM3 and AM1 methods are shown in Table 2. Table 3-6 records the different types of topological indices for the used set of 28 PAHs.

Using variable selection for multiple regression analysis of 27 different types we have examined the models obtained in each of these selections. The results obtained are summarized in Table 7. From these results we have analysed statistically significant models. The regression parameters and quality of statistically significant models are summarized in Table 8.

A perusal of Table 8 shows that generally higher parametric models are statistically more significant and that the one variable models were of similar quality. Also the models 3, 4, 5, 24, 41 and 85 were of similar quality. In comparison to these models the models 25-29, 43, 44, 61, 62, 77-79, 83 and 84 exhibits better quality statistics. Finally, the models 46-48, 65, 80-82 and 85-88 were found more appropriate for modeling photoinduced toxicity of PAHs used. It becomes obvious to discuss the most appropriate models in detail. A close examination of these models we observed that they contain connectivity type indices. This indicates that connectivity is the main parameter for the exhibition of photoinduced toxicity of PAHs used. Further examination has indicated that the model 88 is the best model for modeling photoinduced toxicity of PAHs. This model happened to be 8 parametric model containing D_{DI}, χ_{5V}, χ_4, χ_5, χ_{3V}, χ_{2V} ,W_{3D}, as the correlation parameters.

From the Table 8 we observed that there are two models of similar quality which can be considered as the second best models for modeling photoinduced toxicity of PAHs. These models are 82 and 87. Both these modes are also 8- parametric models. The model 82 contains $\chi_{0,}\chi_{1,}\chi_{2,}\chi_{3},\chi_{4},\chi_{5,}$, DDL and RCI as the correlating parameters. On the other hand the model 87 contains χ_{2}, χ_{3}, χ_{5}, χ_{3V}, χ_{4V}, W_{3D} and DDI as the correlating parameters.

In view of the above we have carried out detail regression analysis for the models 82, 87 and 88 and the same are presented in Table 9-11 respectively. Based on these results we propose the following models for modeling photoinduced toxicity of PAHs used.

Model-82

$$\log(1/LT50) = 730.071 - 415.323(\pm 69.857)\chi_2 + 325.052(\pm 83.024)\chi_3$$
$$785.00(\pm 138.00)DDI - 20.402(\pm 8.102)RCI + 78.640(\pm 28.565)\chi_1$$
$$-130.117(\pm 45.436)\chi_4 + 56.258(\pm 26.941)\chi_5 + 1.495\times 10^{-3}(\pm 1\times 10^{-3})^0\chi$$

$R^2 = 0.874$, $S^2 = 0.874$, $F = 13.035$

Model – 87

$$\log(1/LT50) = 818.102 - 758.430(\pm 88.666)\chi_2 + 603.454(\pm 90.249)\chi_3$$
$$-764.481(\pm 185.066)\chi_{4V} + 3.718(\pm 0.818)DDI - 319.00(\pm 0.117)W_{3D}$$
$$+67.254(35.095)\chi_5 + 456.351(\pm 169.704)\chi_{3V}$$

$R^2 = 0.875$, $S^2 = 0.875$, $F = 16.00$

Model-88

$$\log(1/LT50) = 801.192 - 110.155(\pm 44.176)\chi_1 - 638.406(\pm 91.705)\chi_4$$
$$+870.699(\pm 134.302)\chi_5 - 1452.107(\pm 138.441)\chi_{2V}$$
$$+2523.183(\pm 303.987)\chi_{3V} - 2041.425(\pm 341.790)\chi_{5V}$$
$$-0.514(\pm 0.122)W_{3D} + 5.140(\pm 0.887)DDI$$

$R^2 = 0.925$, $S^2 = 13.7485$, $F = 23.285$

A comparison of the above models indicates that models 82 and 87 both accounts for 87.50% variation in photoinduced toxicity of PAHs used. On the other hand the model 88 accounts for 92.50% variation in the photoinduced toxicity of PAHs used. It is clear therefore, that the model 88 is the best model for modeling photoinduced toxicity.

The results also show that one variable models proposed by us are inferior to the earlier models based on HOMO-LUMO gap. This is probably due to the fact that in the methodology used by us we have not splitted 28 PAHs into two groups. Also, that higher variable model proposed by us that too without splitting, are better models than those based on HOMO-LUMO gap.

Acknowledgement
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Table1. Structural Details of PAHs

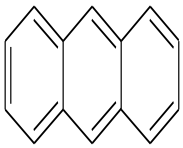
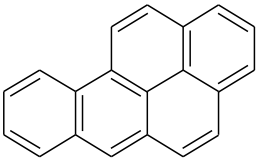
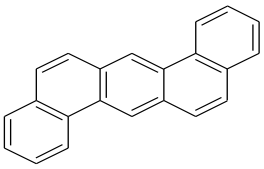
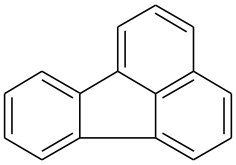
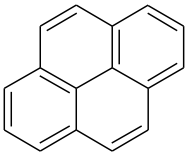
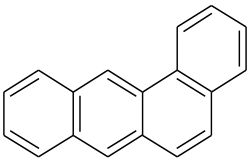
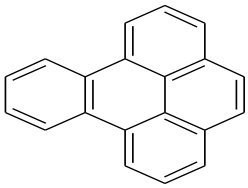
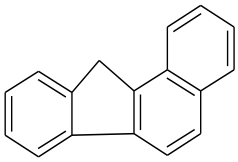
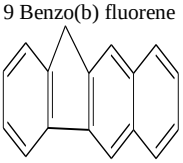
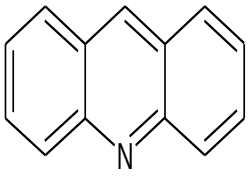
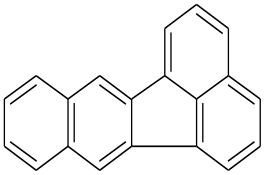
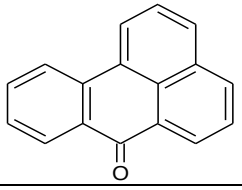
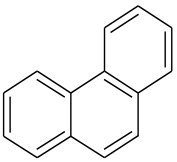
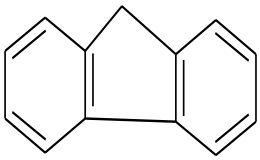
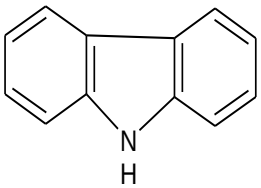
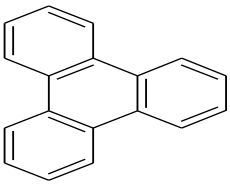
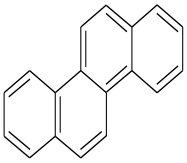
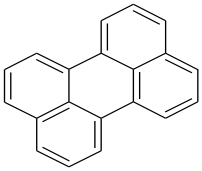
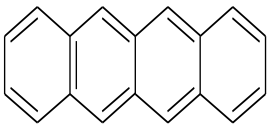
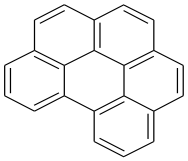
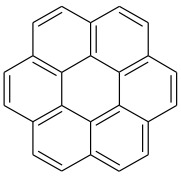
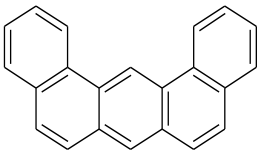
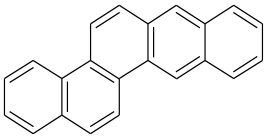
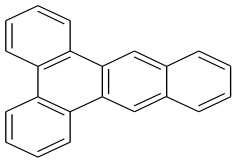
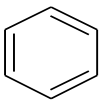
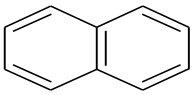
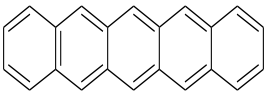
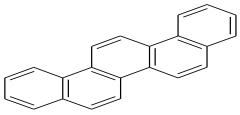
1 Anthracene 	2 Benzo(a)pyrene 	3Dibenzo (a, h) antharacee 	4 Fluoranthene 
5 Pyrene 	6 Benzo(a)anthracene 	7 Benzo(e)pyrene 	8 Benzo(a)fluorene 
9 Benzo(b) fluorene 	10 Acridine 	11 Benzo(k)fluoranthene 	12 Benzanthrone 
13 Phenanthrene 	14 Fluorene 	15 Carbazole 	16 Triphenylene 
17 Chrysene 	18 Perylene 	19 Benzo(b)anthracene 	20 Benzo(g,h,i)perylene 
21 Coronene 	22 Dibenzo(a,j) anthracene 	23 Benzo(b)chrysene 	24 Benzo(b)triphenylene 
25 Benzene 	26 Napthalene 	27 Dibenzo(b,i) anthracene 	28 Benzo(a)chrysene 

Table 2. Observed adjustable Lethal Time, log1/LT 50, energy of singlet and triplet states, and HOMO-LUMO gap calculated using PM_3 and AM_1 methods.

Comp. No	Compound	Adjusted Lethal Time, log(1/ LT50)	Energy (kj/mol)		HOMO-LUMO Gap	
		Obsvd.	Singlet	Triplet	PM_3 (e V)	AM_1 (e V)
1	Anthracene	-2.46	319	178	7.279	7.284
2	Benzo(a)pyrene	-2.43	297	177	6.817	6.812
3	Dibenzo(a,h)antharacene	-2.44	303	218	7.458	7.452
4	Fluoranthene	-2.81	295	221	7.68	7.7.1
5	Pyrene	-2.31	322	203	7.239	7.239
6	Benzo(a)anthracene	-2.52	310	200	7.395	7.392
7	Benzo(e)pyrene	-2.95	327	221	7.365	7.362
8	Benzo(a)fluorene	-3.17	326	241	7.845	7.804
9	Benzo(b)fluorene	-3.16	326	240	7.974	7.986
10	Acridine	-1.73	315	190	7.402	7.531

11	Benzo(k)fluoranthene	-2.89	299	211	7.382	7.389
12	Benzanthrone	-2.52	303	192	7.455	7.427
13	Phenanthrene	-3.2	346	259	8.202	8.207
14	Fluorene	-3.2	397	284	8.507	8.493
15	Carbazole	-3.2	355	293	8.191	8.309
16	Triphenylene	-3.2	352	282	8.215	8.204
17	Chrysene	-2.54	332	239	7.713	7.693
18	Perylene	-2.67	275	148	6.712	6.7
19	Benzo(b)anthracene	-2.89	254	123	6.517	6.517
20	Benzo(g,h,i)perylene	-2.36	294	193	6.971	6.957
21	Coronene		279	232	6.907	6.967
22	Dibenzo(a,j)anthracene		303	221	7.035	7.119
23	Benzo(b)chrysene		305	190	6.519	6.606
24	Benzo(b)triphenylene		320	213	7.088	7.163
25	Benzene				7.958	8.052
26	Napthalene				10.06	10.164
27	Dibenzo(b,i)anthracene				5.328	5.386
28	Benzo(a)chrysene				7.097	7.203

Table 3. Topological indices for the 28 PAHs.

ZM_1	ZM_2	Q_{INDEX}	Xt	Pol	SMTI	GMTI	Xu	SPI	W	Har	Q_W	RHyDp
76	90	13	0.297	21	1324	1392	13.815	0	279	25.316	163.848	29.257
120	151	23	0.242	40	3302	3712	18.891	0	680	41.347	358.672	49.069
128	158	23	0.233	41	4620	8786	21.079	0	971	44.593	550.41	53.02
94	118	18	0.272	29	1772	1926	15.264	0	364	31.449	205.06	36.786
94	117	18	0.272	30	1770	1933	15.237	0	362	31.525	191.242	36.893
102	124	18	0.259	31	2624	2869	17.513	0	553	34.852	319.74	40.955
120	152	23	0.242	41	3160	3532	18.672	0	652	41.677	348.287	49.574
98	121	18	0.265	29	2211	2414	16.495	0	461	33.009	268.87	38.66
98	120	18	0.265	28	2262	2479	16.589	0	471	32.837	273.569	38.405
76	90	13	0.297	21	1324	1392	13.815	0	279	25.316	163.848	29.257
120	151	23	0.242	38	3384	3805	19.013	0	698	41.021	389.157	48.586
104	130	19	0.262	35	2374	2551	17.045	4.576	503	35.795	289.033	42.317
76	91	13	0.297	22	1284	1342	13.696	0	271	25.476	160.784	29.493
72	87	13	0.307	19	1056	1101	12.695	0	219	23.537	130.869	27.076
72	87	13	0.307	19	1056	1101	12.695	0	219	23.537	130.869	27.076
102	126	18	0.259	33	2424	2619	17.16	0	513	35.396	299.727	41.779
102	125	18	0.259	32	2584	2819	17.451	0	545	35.012	314.778	41.19
120	152	23	0.242	41	3172	3550	18.682	0	654	41.657	350.11	49.543
102	123	18	0.259	30	2704	2969	17.642	0	569	34.64	325.754	40.635
138	178	28	0.228	49	4032	4637	20.173	0	851	48.074	402.137	57.567
156	204	33	0.216	57	5040	5934	21.651	0	1002	54.587	462.029	65.757
128	158	23	0.233	41	4540	5086	20.98	0	955	44.65	550.049	53.117
128	158	23	0.233	41	4620	5186	21.085	0	971	44.493	549.447	53.02
128	159	23	0.233	42	4300	4786	20.73	0	907	45.121	83.284	53.845
24	24	3	0.49	3	132	108	5.382	0	27	7.833	17.5	8.5
50	57	8	0.359	12	520	505	9.751	0	109	16.288	66.429	18.4
128	156	23	0.233	39	4820	5436	21.279	0	1011	44.146	568.145	52.341
128	159	23	0.233	42	4580	5136	21.048	0	963	44.753	542.373	53.756

Table 4. Balaban and Balaban type topological indices for the PAHs used in the present study.

J	JhetZ	Jhetm	Jhetv	Jhete	Jhetp	TIE	PW_2	PW_3	PW_4	PW_5	BAC
1.682	2.524	2.524	2.524	2.524	2.524	10.441	0.573	0.34	0.195	0.114	0
1.487	2.231	2.231	2.231	2.231	2.231	16.649	0.592	0.37	0.227	0.136	0
1.346	2.019	2.019	2.019	2.019	2.019	19.299	0.587	0.361	0.213	0.124	0
1.677	2.816	2.816	2.816	2.816	2.816	12.38	0.584	0.37	0.234	0.135	0
1.671	2.506	2.506	2.506	2.506	2.506	12.347	0.589	0.368	0.224	0.132	0
1.512	2.268	2.268	2.268	2.268	2.268	14.825	0.582	0.353	0.206	0.121	0
1.553	2.329	2.329	2.329	2.329	2.329	16.721	0.589	0.373	0.236	0.144	0
1.56	2.108	2.108	2.108	2.108	2.108	13.869	0.583	0.361	0.217	0.123	0
1.522	2.074	2.074	2.074	2.074	2.074	13.819	0.584	0.354	0.209	0.12	0
1.682	2.62	2.62	2.401	2.617	2.361	10.649	0.573	0.34	0.195	0.114	0
1.453	2.18	2.18	2.18	2.18	2.18	16.612	0.591	0.368	0.225	0.133	0
1.672	2.291	2.291	2.291	2.291	2.291	20.848	0.588	0.375	0.23	0.133	2
1.74	2.61	2.61	2.61	2.61	2.61	10.528	0.571	0.349	0.206	0.116	0

1.762	2.321	2.321	2.321	2.321	2.321	9.617	0.574	0.35	0.212	0.116	0
1.762	2.698	2.698	2.492	2.696	2.443	9.281	0.574	0.35	0.212	0.116	0
1.642	2.463	2.463	2.463	2.463	2.463	14.976	0.575	0.361	0.229	0.136	0
1.538	2.308	2.308	2.308	2.308	2.308	14.927	0.58	0.36	0.214	0.121	0
1.545	2.318	2.318	2.318	2.318	2.318	16.737	0.589	0.375	0.238	0.141	0
1.465	2.197	2.197	2.197	2.197	2.197	14.728	0.583	0.347	0.199	0.118	0
1.475	2.212	2.212	2.212	2.212	2.212	18.459	0.6	0.382	0.24	0.15	0
1.409	2.113	2.113	2.113	2.113	2.113	20.185	0.61	0.387	0.241	0.155	0
1.367	2.051	2.051	2.051	2.051	2.051	19.299	0.587	0.361	0.213	0.124	0
1.348	2.022	2.022	2.022	2.022	2.022	19.303	0.587	0.361	0.212	0.124	0
1.119	2.174	2.174	2.174	2.174	2.174	19.355	0.583	0.361	0.221	0.134	0
2	3	3	3	3	3	2.414	0.5	0.25	0.125	0.063	0
1.925	2.88	2.88	2.88	2.88	2.88	6.284	0.554	0.326	0.182	0.095	0
1.288	1.932	1.932	1.932	1.932	1.932	19.087	0.59	0.352	0.201	0.121	0
1.361	2.041	2.041	2.041	2.041	2.041	19.417	0.586	0.366	0.218	0.124	0

Table 5. Connectivity type indices for the PAHs used in the present study.

χ_0	χ_1	χ_2	χ_3	χ_4	χ_5	χ_{0V}	χ_{1V}	χ_{2V}	χ_{3V}	χ_{4V}	χ_{5V}
8.77	6.933	6.081	5.344	4.588	4.052	7.774	4.809	3.547	2.614	1.883	1.388
13.104	9.916	9.128	8.624	8.139	7.586	10.928	6.97	5.454	4.371	3.489	2.74
14.518	10.899	9.891	9.213	8.319	7.579	12.083	7.631	5.868	4.609	3.51	2.687
10.535	7.949	7.139	6.733	6.413	5.727	8.774	5.565	4.255	3.412	2.743	2.048
10.535	7.933	7.212	6.738	6.285	5.752	8.774	5.559	4.29	3.393	2.67	2.051
11.949	8.916	7.986	7.278	6.454	5.813	9.928	6.22	4.707	3.611	2.696	2.037
13704	9.933	9.054	8.63	8.252	7.767	10.928	6.976	5.419	4.393	3.557	2.823
11.242	8.433	7.558	7.031	6.42	5.561	9.481	6.022	4.647	3.715	2.906	2.12
11.242	8.416	7.644	6.976	6.288	5.507	9.481	6.017	4.69	3.66	2.827	2.087
9.38	6.933	6.081	5.344	4.588	4.052	7.643	4.679	3.374	2.425	1.72	1.244
13.104	9.916	9.131	8.624	8.1	7.404	10.928	6.97	5.454	4.371	3.476	2.673
12.113	8.86	7.998	7.533	6.965	6.251	9.682	6.02	4.584	3.611	2.816	2.116
9.38	6.949	5.994	5.394	4.745	4.108	7.774	4.815	3.508	2.654	1.955	1.409
8.673	6.449	5.652	5.091	4.574	3.821	7.326	4.612	3.491	2.706	2.08	1.45
8.673	6.449	5.652	5.091	4.574	3.821	7.119	4.405	3.216	2.414	1.799	1.238
11.949	8.949	7.837	7.274	6.754	6.15	9.928	6.232	4.637	3.652	2.859	2.179
11.949	8.933	7.899	7.327	6.621	5.848	9.928	6.226	4.669	3.651	2.771	2.051
13.104	9.933	9.054	8.616	8.323	7.728	10.928	6.976	5.419	4.39	3.58	2.8
11.949	8.899	8.072	7.222	6.328	5.758	9.928	6.214	4.746	3.569	2.634	2.01
14.259	10.916	10.271	9.999	9.686	9.401	11.928	7.72	6.2	5.138	4.235	3.481
15.413	11.899	11.489	11.382	11.055	11.049	12.928	8.464	6.982	5.887	4.893	4.155
14.518	10.899	9.891	9.213	8.323	7.56	12.083	7.631	5.868	4.609	3.511	2.681
14.518	10.899	9.891	9.212	8.33	7.555	12.083	7.631	5.868	4.608	3.512	2.68
14.518	10.916	9.828	9.166	8.441	7.822	12.083	7.637	5.836	4.611	3.592	2.803
40.243	3	2.121	1.5	1.061	0.75	3.464	2	1.155	0.667	0.385	0.222
6.812	4.966	4.089	3.466	2.858	2.316	5.619	3.405	2.347	1.659	1.133	0.757
14.518	10.865	10.064	9.099	8.068	7.463	12.083	7.619	5.945	4.525	3.386	2.632
14.518	10.916	9.804	9.26	8.497	7.592	12.083	7.637	5.829	4.648	3.587	2.694

Table 6. Information and Geometric indices for the PAHs used in the present study.

INFORMATION INDICES					**GEOMETRIC INDICES**				
IAC	U_{INDEX}	V_{INDEX}	X_{INDEX}	Y_{INDEX}	W_{3D}	J_{3D}	H_{3D}	DDI	RCI
23.577	18.117	0.328	0.476	1.009	1153.02	10899	85.243	299.181	1.33
30.542	23.506	0.257	0.364	0.792	2328.09	1.596	138.288	530.253	1.33
34.707	26.864	0.214	0.321	0.63	3285.05	1.562	163.992	658.681	1.33
24.992	19.162	0.316	0.445	1.042	1428.27	1.65	96.148	368.658	2.304
24.992	19.179	0.314	0.444	1.029	1347.4	1.754	99.324	353.447	0
29.129	22.568	0.262	0.387	0.795	2033.23	1.725	122.833	461.568	1.33
30.542	23.384	0.265	0.378	0.863	2256.94	1.646	140.265	528.242	1.33
28.375	20.884	0.28	0.407	0.87	1876.33	1.699	117.093	446.554	1.33
28.375	20.935	0.271	0.398	0.826	2078.02	1.534	106.811	484.002	1.486
27.407	18.117	0.328	0.476	1.009	1060.65	1.826	78.554	275.729	1.33
30.542	23.543	0.244	0.356	0.759	2516.07	1.47	132.386	556.205	1.33
31.9	22.37	0.298	0.424	0.965	1636.72	1.11	112.417	403.546	1.33
23.517	18.038	0.343	0.49	1.09	1118.05	1.958	86.661	296.375	1.33
22.717	16.365	0.363	0.512	1.172	1108.29	1.742	76.541	301.85	1.33

26.559	16.365	0.363	0.512	1.172	1014.48	1.677	69.389	277.542	1.33
29.129	22.358	0.291	0.416	0.938	1927.15	1.823	126.152	458.344	1.33
29.129	22.544	0.268	0.393	0.822	2009.1	1.747	123.959	460.225	1.33
30.542	23.401	0.263	0.377	0.853	2261.99	1.642	140.192	528.618	1.33
29.129	22.644	0.252	0.376	0.746	2110.96	1.662	120.701	467.339	1.33
31.847	24.506	0.243	0.347	0.797	2619.34	1.515	154.874	602.212	1.33
33.059	25.675	0.226	0.321	0.742	3014.24	1.414	169.987	680.22	1.33
34.707	26.795	0.218	0.325	0.649	3209.52	1.595	165.348	654.206	1.33
34.707	26.858	0.214	0.321	0.632	3314.98	1.55	163.497	662.043	1.33
34.707	26.642	0.234	0.343	0.726	3143.84	1.635	166.864	658.085	1.33
12	8.192	0.684	0.91	2.056	191.142	2.483	26.999	74.84	1.33
17.839	13.302	0.457	0.634	1.477	539.362	2.184	53.611	168.536	1.33
34.707	26.949	0.202	0.308	0.581	3493.63	1.47	159.244	673.509	1.33
34.707	26.857	0.216	0.324	0.643	3268.44	1.571	164.697	658.434	1.33

Table 7. Model summary using multiple variable selections

Variable selection	Model	Parameters	R	R Square	Adjusted R Square	Std. Error of the Estimate	F
1	1	GMT_1	0.225	0.051	-0.002	0.4014	0.9694
	2	GMT_1 SPI,	0.262	0.069	-0.041	0.4092	0.628
	3	X_t X_U, Qw	0.415	.172	0.017	0.3976	1.10
	4	X_t GMT_1,X_U, Qw	0.658	0.433	0.282	0.3398	2.866
	5	X_t GMT_1,X_U, Qw RHyDp	0.693	0.480	0.294	0.3371	2.580
	6	Pol, SMT_1, Xu ,SPI, Qw, RHyDp	0.725	0.526	0.307	0.3339	2.403
	7	Pol, SMT_1, GMT_1, Xu ,SPI, Har, Qw,	0.735	0.540	0.271	0.3424	2.009
2	1	X_t	0.621	0.386	0.358	23.6411	13.807
	2	Xu, W,	0.647	0.419	0.364	23.5255	7.580
	3	SMT_1,Xu, W,	0.663	0.439	0.355	23.6916	5.218
	4	SMT_1,Xu, W, Qw	0.671	0.450	0.335	24.0618	3.891
	5	SMT_1,Xu, SPI, W, Qw	0.674	0.454	0.302	24.6361	2.995
	6	ZM_1,ZM_2 , Qim, X_t, Pol, SPI,	0.812	0.659	0.538	20.0406	5.471
	7	ZM_1,ZM_2 , Qim, X_t, Pol, SPI, Qw	0.812	0.659	0.510	20.6423	4.424
	8	ZM_1,ZM_2, Qim Pol, SMT_1 W, Qw, RHyDp	0.813	0.662	0.481	21.2447	3.668
3	1	X_t	0.353	0.124	0.085	38.8740	3.124
	2	X_t Har	0.436	0.190	0.113	38.2606	2.468
	3	X_t,SPI, RHyDp	0.458	0.210	0.91	38.7296	1.771
	4	ZM_2, Qim,X_t,RHyDp	0.625	0.391	0.262	34.8920	3.047
	5	ZM_2, Qim,X_t, SPI, RHyDp	0.746	0.557	0.434	30.5648	4.528
	6	ZM_2, Qim,, X_t, SPI , W, RHyDp	0.750	0.562	0.408	31.2604	3.642
	7	ZM_1,ZM_2 ,X_t, Pol, SMT_1, Har, Qw	0.483	0.233	-0.037	41.3788	0.862
	8	ZM_1,ZM_2 ,X_t, Pol, SMT_1, W, Har, Qw	0.486	0.236	-0.098	42.5709	0.707
4	1	χ_2	0.209	0.044	-0.010	0.4030	0.820
	2	χ_4, χ_5	0.477	0.228	0.137	0.3726	2.506
	3	χ_3, χ_4, χ_5	0.578	0.334	0.209	0.3567	2.763
	4	χ_0 χ_3, χ_4, χ_5	0.620	0.384	0.220	0.3542	2.339
	5	χ_0 χ_1 χ_3, χ_4, χ_5	0.635	0.403	0.190	0.3610	1.890
	6	χ_0 χ_1, χ_2, χ_3, χ_4, χ_5	0.650	0.422	0.156	0.3686	1.583
5	1	χ_2	0.605	0.367	0.338	24.0035	12.734
	2	χ_1, χ_2	0.635	0.404	0.347	23.8407	7.105
	3	χ_1, χ_2, χ_3	0.720	0.518	0.445	21.9684	7.156
	4	χ_1, χ_2, χ_3, χ_4	0.746	0.557	0.463	21.6091	5.964
	5	χ_0 χ_1, χ_2, χ_3, χ_4	0.758	0.575	0.456	21.7491	4.862
	6	χ_0 χ_1, χ_2, χ_3, χ_4, χ_5	0.761	0.579	0.431	22.2570	3.900
6	1	χ_2,	0.325	0.105	0.065	39.2905	2.595
	2	χ_2, χ_3	0.464	0.215	0.141	37.6615	2.884
	3	χ_2, χ_3, χ_5	0.637	0.406	0.317	33.5748	4.560
	4	χ_1, χ_2, χ_3, χ_4	0.688	0.473	0.362	32.4489	4.265
	5	χ_1, χ_2, χ_3, χ_4, χ_5	0.700	0.490	0.349	32.7922	3.462
	6	χ_0 χ_1, χ_2, χ_3, χ_4, χ_5	0.704	0.495	0.317	33.5783	2.779
7	1	χ_{0V}	0.172	0.030	-0.024	0.4059	0.552
	2	χ_{0V}, χ_{1V}	0.327	0.107	0.002	0.4006	1.021
	3	χ_{0V}, χ_{1V} ,χ_{2V}	0.407	0.166	0.009	0.3992	1.059
	4	, χ_{2V}, χ_{3V}, χ_{4V}, χ_{5V}	0.593	0.352	0.179	0.3634	2.035
	5	χ_{0V} χ_{1V}, χ_{2V}, χ_{4V}, χ_{5V}	0.645	0.416	0.207	0.3572	1.991
	6	χ_{0V} , χ_{1V}, χ_{2V}, χ_{3V}, χ_{4V}, χ_{5V}	0.646	0.417	0.148	0.3703	1.549
8	1	χ_{2V}	0.578	0.334	0.304	24.6136	11.033
	2	χ_{2V}, χ_{3V}	0.613	0.376	0.316	24.3921	6.318
	3	χ_{2V}, χ_{3V}, χ_{5V}	0.708	0.501	0.426	22.3397	6.700

	4	$\chi_{1V}, \chi_{2V}, \chi_{3V}, \chi_{4V}$	0.750	0.562	0.470	21.4802	6.093
	5	χ_{0V} , $\chi_{1V}, \chi_{2V}, \chi_{3V}, \chi_{4V}$	0.780	0.608	0.499	20.8741	5.589
	6	χ_{0V} , $\chi_{1V}, \chi_{2V}, \chi_{3V}, \chi_{4V}, \chi_{5V}$	0.786	0.618	0.483	21.2031	4.586
9	1	χ_{0V}	0.313	0.098	0.057	39.4492	2.397
	2	χ_{0V} , χ_{1V}	0.374	0.140	0.058	39.4346	1.708
	3	$\chi_{2V}, \chi_{3V}, \chi_{4V}$	0.688	0.473	0.394	31.6159	5.995
	4	$\chi_{1V}, \chi_{2V}, \chi_{3V}, \chi_{4V}$	0.739	0.546	0.450	30.1287	5.707
	5	χ_{0V} , $\chi_{1V}, \chi_{2V}, \chi_{3V}, \chi_{4V}$	0.772	0.596	0.484	29.1874	5.314
	6	χ_{0V} , $\chi_{1V}, \chi_{2V}, \chi_{3V}, \chi_{4V}, \chi_{5V}$	0.777	0.603	0.463	29.7597	4.312
10	1	Y_{index}	0.227	0.052	-0.001	0.4013	0.979
	2	V_{index} Y_{index}	0.247	0.061	-0.050	0.4109	0.551
	3	I_{AC} V_{index} Y_{index}	0.304	0.092	-0.078	0.4164	0.542
	4	I_{AC} V_{index} X_{index} Y_{index}	0.308	0.095	-0.146	0.4294	0.393
	5	I_{AC} U_{index} V_{index} X_{index} Y_{index}	0.308	0.095	-0.228	0.4445	0.294
11	1	U_{index}	0.562	0.316	0.284	24.9517	10.144
	2	U_{index} X_{index}	0.686	0.471	0.420	22.4576	9.340
	3	I_{AC} U_{index} X_{index}	0.688	0.473	0.394	22.9598	5.988
	4	I_{AC} U_{index} V_{index} Y_{index}	0.691	0.478	0.368	23.4539	4.345
	5	I_{AC} U_{index} $V_{index}$$X_{index}$ Y_{index}	0.691	0.478	0.333	24.0942	3.295
12	1	Y_{index}	0.438	0.191	0.155	37.3552	5.209
	2	I_{AC} Y_{index}	0.483	0.234	0.161	37.2213	3.202
	3	I_{AC} U_{index} Y_{index}	0.485	0.236	0.121	38.0916	2.056
	4	I_{AC},$U_{index,}$ $X_{index}$$Y_{index}$	0.487	0.237	0.076	39.0531	1.474
	5	I_{AC} U_{index} V_{index} X_{index} Y_{index}	0.487	0.237	0.025	40.1224	1.117
13	1	RCI	0.243	0.059	0.007	0.3997	1.133
	2	$H_{3D,}$ DDL	0.377	0.142	0.042	0.3926	1.412
	3	W_{3D} , $H_{3D,}$ DDL	0.453	0.205	0.056	0.3897	1.376
	4	W_{3D} , H_{3D} DDL RCI	0.481	0.231	0.026	0.3958	1.128
	5	W_{3D} ,J_{3D} H_{3D} DDL RCI	0.496	0.246	-0.024	0.4058	0.913
14	1	H_{3D}	0.524	0.275	0.242	25.6878	8.328
	2	H_{3D} RCI	0.535	0.287	0.219	26.0728	4.220
	3	J_{3D} H_{3D} RCI	0.546	0.298	0.193	26.5006	2.832
	4	W_{3D} ,J_{3D} H_{3D} RCI	0.554	0.307	0.162	27.0105	2.108
	5	W_{3D} ,J_{3D} H_{3D} DDL RCI	0.555	0.308	0.116	27.7361	1.603
15	1	H_{3D}	0.209	0.084	0.043	39.7514	2.028
	2	J_{3D} H_{3D}	4.04	0.163	0.083	38.9016	2.044
	3	$J_{3D,}$ H_{3D} DDL	0.440	0.193	0.072	39.1354	1.597
	4	W_{3D} ,J_{3D} H_{3D} DDL	0.445	0.198	0.029	40.0290	1.174
	5	W_{3D} ,J_{3D} H_{3D} DDL RCI	0.447	0.200	-0.022	41.0804	0.900
16	1	Y_{index}	0.227	0.052	-0.001	0.4013	0.979
	2	X_{index} DDL	0.530	0.281	0.197	0.3594	3.328
	3	I_{AC} X_{index} DDL	0.589	0.347	0.225	0.3531	2.840
	4	I_{AC} X_{index} $J_{3D,}$ DDL	0.625	0.391	0.228	0.3523	2.405
	5	I_{AC} X_{index} $J_{3D,}$,RCI DDL	0.656	0.430	0.226	0.3528	2.110
	6	I_{AC} V_{index} X_{index} $W_{3D,}$ $J_{3D,}$ DDL	0.682	0.465	0.218	0.3546	1.885
	7	I_{AC} V_{index} X_{index} $W_{3D,}$ $J_{3D,}$ DDL, RCI	0.704	0.495	0.200	0.3587	1.680
	8	I_{AC} U_{index} X_{index} Y_{index} $W_{3D,}$ $J_{3D,}$ H_{3D} DDL	0.726	0.527	0.182	0.3626	1.530
17	1	X_{index}	0.636	0.405	0.378	23.2626	14.952
	2	X_{index} DDL	0.800	0.640	0.606	18.5143	18.692
	3	X_{index} Y_{index} DDL	0.818	0.669	0.620	18.1920	13.490
	4	X_{index} Y_{index} DDL ,RCI	0.835	0.697	0.633	17.8710	10.916
	5	X_{index} Y_{index} $J_{3D,}$ DDL ,RCI	0.847	0.718	0.640	17.7022	9.173
	6	I_{AC} X_{index} Y_{index} $J_{3D,}$ DDL ,RCI	0.852	0.726	0.629	17.9709	7.495
	7	I_{AC} U_{index} X_{index} Y_{index} , $J_{3D,}$ DDL ,RCI	0.861	0.741	0.628	17.9997	6.538
	8	I_{AC} U_{index} X_{index} Y_{index} $W_{3D,}$ $J_{3D,}$ DDL ,RCI	0.869	0.755	0.624	18.0855	5.773
18	1	Y_{index}	0.438	0.191	0.155	37.2552	5.209
	2	V_{index} W_{3D}	0.678	0.459	0.408	31.2648	8.921
	3	V_{index} W_{3D} J_{3D}	0.718	0.515	0.442	30.3379	7.084
	4	U_{index} V_{index} W_{3D} J_{3D}	0.729	0.532	0.434	30.5763	5.403
	5	X_{index} Y_{index} W_{3D} J_{3D} DDL	0.771	0.594	0.481	29.2574	5.271
	6	I_{AC} X_{index} Y_{index} W_{3D} J_{3D} DDL	0.774	0.599	0.457	29.9390	4.226
	7	I_{AC} V_{index} X_{index} Y_{index} W_{3D} J_{3D} DDL	0.774	0.599	0.424	30.8381	3.418
	8	I_{AC} V_{index} X_{index} Y_{index} W_{3D} J_{3D} DDL ,RCI	0.774	0.600	0.386	31.8352	2.808
19	1	Y_{index}	0.227	0.052	-0.001	0.4013	0.979
	2	X_{index} DDL,	0.530	0.281	0.197	0.3594	3.328
	3	χ_{2V}, χ_{3V} , DDL	0.705	0.497	0.403	0.3099	5.277
	4	χ_{2V}, χ_{3V} , W_{3D} DDL	0.774	0.600	0.493	0.2855	5.621
	5	χ_{2V}, χ_{3V} , U_{index} W_{3D} DDL	0.775	0.600	0.475	0.2954	4.205
	6	χ_{2V}, χ_{3V} , U_{index} I_{AC} W_{3D} DDL,	0.799	0.638	0.471	0.2917	3.820
	7	χ_{0V}, χ_{1V} χ_{2V}, χ_{3V} , I_{AC} W_{3D} DDL	0.829	0.688	0.506	0.2819	3.778
	8	χ_{0V}, χ_{1V} χ_{2V}, χ_{3V} , I_{AC} U_{index} W_{3D} DDL	0.822	0.676	0.488	0.2871	3.583
20	1	X_{index}	0.636	0.405	0.378	23.2626	14.982
	2	X_{index} DDL,	0.800	0.640	0.606	18.5143	18.692
	3	χ_{2V} , V_{index} DDL,	0.836	0.698	0.653	17.3747	15.431

	4	$\chi_{2V}, \chi_{3V},$ DDL, RCI	0.878	0.772	0.723	15.5138	16.038
	5	$\chi_{2V}, \chi_{3V},$ X_{index} DDL, RCI	0.895	0.801	0.746	14.8693	14.503
	6	$\chi_{2V}, \chi_{3V}, \chi_{4V},$ V_{index} W_{3D}, DDL, RCI	0.908	0.825	0.763	14.3720	13.315
	7	$\chi_{2V}, \chi_{3V}, \chi_{4V},$ X_{4V}, V_{index} DDL, RCI	0.927	0.859	0.798	13.2666	13.958
	8	$\chi_{1V}, \chi_{2V}, \chi_{3V}, \chi_{4V},$ $V_{index,}$ DDL, RCI	0.932	0.869	0.799	13.2324	12.412
21	1	Y_{index}	0.438	0.191	0.155	37.3552	5.209
	2	V_{index} W_{3D}	0.678	0.459	0.408	31.2648	8.921
	3	V_{index} W_{3D} J_{3D}	0.718	0.515	0.442	30.3379	7.084
	4	U_{index} ,V_{index} W_{3D} J_{3D}	0.729	0.532	0.434	30.5763	5.403
	5	$\chi_{2V}, \chi_{3V}, \chi_{4V}, \chi_{5V}$ DDL	0.903	0.816	0.765	19.7167	15.933
	6	$\chi_{2V}, \chi_{3V}, \chi_{4V}, \chi_{5V}$, J_{3D} DDL	0.928	0.860	0.811	17.6570	17.464
	7	$\chi_{2V}, \chi_{3V}, \chi_{4V}, \chi_{5V}$, W_{3D} J_{3D} DDL	0.936	0.876	0.822	17.1630	16.127
	8	$\chi_{2V}, \chi_{3V}, \chi_{4V}, \chi_{5V}$, I_{AC} W_{3D} J_{3D} DDL	0.943	0.890	0.831	16.7030	15.136
22	1	Y_{index}	0.227	0.052	-0.001	0.4013	0.979
	2	χ_{5}, χ_{4V}	0.670	0.448	0.384	0.3149	6.911
	3	χ_{5}, χ_{3V} , Y_{index}	0.700	0.490	0.394	0.3122	5.115
	4	$\chi_{5}, \chi_{1V}, \chi_{4V}$ Y_{index}	0.750	0.563	0.446	0.2985	4.825
	5	$\chi_{5}, \chi_{1V}, \chi_{3V}, \chi_{4V}$, Y_{index}	0.764	0.584	0.435	0.3015	3.925
	6	$\chi_{0}, \chi_{5}, \chi_{1V}, \chi_{3V}, \chi_{4V}$,Y_{index}	0.778	0.605	0.422	0.3048	3.316
	7	$\chi_{4}, \chi_{5}, \chi_{1V}, \chi_{3V}, \chi_{4V},$ Y_{index}	0.790	0.625	0.452	0.2970	3.608
	8	$\chi_{1}, \chi_{4}, \chi_{5}, \chi_{2V}, \chi_{3V}, \chi_{4V}$,$\chi_{5V},$ V_{index} Y_{index}	0.800	0.639	0.429	0.3031	3.038
23	1	X_{index}	0.636	0.405	0.378	23.2626	14.982
	2	$U_{index,}$ X_{index}	0.686	0.471	0.420	22.4576	9.340
	3	χ_{0} $U_{index,}$ X_{index}	0.699	0.488	0.412	22.6280	6.362
	4	$\chi_{5}, \chi_{0V}, \chi_{1V}$, X_{index}	0.875	0.766	0.717	15.7028	15.540
	5	χ_{0} $\chi_{5,}$, χ_{1V} , χ_{3V} , X_{index}	0.888	0.789	0.731	15.3058	13.485
	6	χ_{0} $\chi_{5,}$, χ_{1V} , χ_{2V} χ_{3V} , X_{index}	0.891	0.794	0.721	15.5739	10.918
	7	χ_{0} $\chi_{5,}$, χ_{1V} , χ_{2V} χ_{3V} χ_{4V} ,X_{index}	0.898	0.807	0.722	15.5436	9.547
	8	χ_{0} $\chi_{5,}$, χ_{0V}, χ_{1V} , χ_{2V} χ_{3V} χ_{4V} , V_{index}	0.905	0.819	0.722	15.5422	8.481
24	1	Y_{index}	0.438	0.191	0.155	37.3552	5.209
	2	I_{AC} Y_{index}	0.483	0.234	0.161	37.2213	3.202
	3	χ_{3V}, χ_{5V} , X_{index}	0.729	0.531	0.461	29.8374	7.549
	4	, $\chi_{2V}, \chi_{3V}, \chi_{5V},$ X_{index}	0.739	0.545	0.450	30.1373	5.701
	5	$\chi_{2V}, \chi_{3V}, \chi_{4V}$,$\chi_{5V},$ X_{index}	0.769	0.591	0.478	29.3565	5.211
	6	$\chi_{5,}$, χ_{1V} , χ_{2V} χ_{3V} χ_{4V} , V_{index}	0.807	0.651	0.528	27.9070	5.292
	7	χ_{1}, χ_{2}, χ_{0V}, χ_{1V} , χ_{2V} χ_{3V} ,I_{AC}	0.712	0.507	0.370	32.2415	3.705
	8	χ_{1}, χ_{2}, χ_{0V}, χ_{2V} , χ_{4V} ,$I_{AC,}$ $U_{index,}$ Y_{index}	0.755	0.570	0.382	31.9465	3.029
25	1	RCI	0.243	0.059	0.007	0.3997	1.133
	2	X_3 $X_{3V,}$	0.624	0.389	0.317	0.3314	5.411
	3	χ_{3}, χ_{3V} , RCI	0.660	0.435	0.330	0.3284	4.113
	4	χ_{3}, χ_{3V} , J_{3D} RCI	0.692	0.479	0.340	0.3258	3.446
	5	χ_{0}, χ_{3}, χ_{3V} , J_{3D} RCI	0.709	0.503	0.326	0.3293	2.838
	6	χ_{0V} , χ_{2V} χ_{3V} χ_{4V} , W_{3D} ,DDL	0.785	0.616	0.439	0.3003	3.483
	7	$\chi_{1}, \chi_{3}, \chi_{1V}$, $\chi_{2V}, \chi_{3V}, \chi_{4V}$,$\chi_{5V},$ W_{3D}	0.796	0.634	0.465	0.2934	3.751
	8	$\chi_{0}, \chi_{1}, \chi_{3}, \chi_{1V}$, χ_{2V}, χ_{3V} W_{3D} ,DDL	0.801	0.641	0.432	0.3023	3.064
26	1	X_2	0.605	0.367	0.338	24.0035	12.734
	2	X_2,X_{1v}	0.704	0.495	0.447	21.9339	10.299
	3	X_2,X_3 DDL	0.831	0.691	0.644	17.5925	14.887
	4	X_2,X_3,DDL,RCI	0.866	0.750	0.697	16.2309	14.241
	5	X_1,X_2,X_3,DDL,RCI	0.889	0.791	0.732	15.2613	13.585
	6	X_1,X_2,X_3,X_4 DDL,RCI	0.901	0.812	0.746	14.8609	12.269
	7	X_1,X_2,X_3,X_4,X_5, DDL,RCI	0.926	0.857	0.795	13.3708	13.706
	8	Xo,X_1,X_2,X_3,X_4,X_5, DDL,RCI	0.935	0.874	0.807	12.9529	13.035
27	1	χ_2	0.325	0.105	0.065	39.2905	2.595
	2	χ_2, χ_{3V}	0.513	0.263	0.193	36.5016	3.748
	3	χ_2, χ_{3V} ,W_{3D}	0.821	0.674	0.626	24.8590	13.813
	4	χ_2, χ_{3V} , χ_{4V} ,DDL	0.881	0.776	0.729	21.1657	16.438
	5	χ_2, χ_{3V} , χ_{4V} , W_{3D} ,DDL	0.902	0.814	0.762	19.8046	15.760
	6	χ_2, χ_4, χ_{3V} , χ_{4V} , W_{3D} ,DDL	0.922	0.851	0.798	18.2652	16.134
	7	χ_2, χ_3, χ_5 χ_{3V}, χ_{4V}, W_{3D},X_3 DDL	0.935	0.875	0.820	17.2227	16.000
	8	χ_1, χ_4, χ_5 χ_{2V}, χ_{3V} χ_{5V} DDI, W_{3D},	0.962	0.925	0.885	13.7485	23.233

Table 8: Statistically significant models

Reg. model	Dependent	Parameters	R	R Square	Adjusted R Square	Std. Error of the Estimate	F
1	Obsd.	Pol, SMT_1, Xu ,SPI, $Qw_{,}$ RHyDp	0.725	0.526	0.307	0.3339	2.403
2	Obsd	Pol, SMT_1, GMT_1, Xu ,SPI, Har, Qw	0.735	0.540	0.271	0.3424	2.009
3	Singlet	ZM_1,ZM_2 , Qim, X_t, Pol, $SPI_{,}$	0.812	0.659	0.538	20.0406	5.471
4	Singlet	ZM_1,ZM_2 , Qim, X_t, Pol, SPI, Qw	0.812	0.659	0.510	20.6423	4.424
5	Singlet	ZM_1,ZM_2, Qim Pol, SMT_1 W, $Qw_{,,}$ RHyDp	0.813	0.662	0.481	21.2447	3.668
6	Triplet	ZM_2, Qim,X_t, SPI, RHyDp	0.746	0.557	0.434	30.5648	4.528
7	Triplet	ZM_2, Qim,, X_t, SPI , W, RHyDp	0.750	0.562	0.408	31.2604	3.642
8	Singlet	χ_1, χ_2, χ_3	0.720	0.518	0.445	21.9684	7.156

Reg. model	Dependent	Parameters	R	R Square	Adjusted R Square	Std. Error of the Estimate	F
9	Singlet	$\chi_1, \chi_2, \chi_3, \chi_4$	0.746	0.557	0.463	21.6091	5.964
10	Singlet	$\chi_0 \chi_1, \chi_2, \chi_3, \chi_4$	0.758	0.575	0.456	21.7491	4.862
11	Singlet	$\chi_0 \chi_1, \chi_2, \chi_3, \chi_4, \chi_5$	0.761	0.579	0.431	22.2570	3.900
12	Triplet	$\chi_1, \chi_2, \chi_3, \chi_4, \chi_5$	0.700	0.490	0.349	32.7922	3.462
13	Triplet	$\chi_0 \chi_1, \chi_2, \chi_3, \chi_4, \chi_5$	0.704	0.495	0.317	33.5783	2.779
14	Singlet	$\chi_{2V}, \chi_{3V}, \chi_{5V}$	0.708	0.501	0.426	22.3397	6.700
15	Singlet	$\chi_{1V}, \chi_{2V}, \chi_{3V}, \chi_{4V}$	0.750	0.562	0.470	21.4802	6.093
16	Singlet	$\chi_{0V}, \chi_{1V}, \chi_{2V}, \chi_{3V}, \chi_{4V}$	0.780	0.608	0.499	20.8741	5.589
17	Singlet	$\chi_{0V}, \chi_{1V}, \chi_{2V}, \chi_{3V}, \chi_{4V}, \chi_{5V}$	0.786	0.618	0.483	21.2031	4.586
18	Triplet	$\chi_{1V}, \chi_{2V}, \chi_{3V}, \chi_{4V}$	0.739	0.546	0.450	30.1287	5.707
19	Triplet	$\chi_{0V}, \chi_{1V}, \chi_{2V}, \chi_{3V}, \chi_{4V}$	0.772	0.596	0.484	29.1874	5.314
20	Triplet	$\chi_{0V}, \chi_{1V}, \chi_{2V}, \chi_{3V}, \chi_{4V}, \chi_{5V}$	0.777	0.603	0.463	29.7597	4.312
21	Obsd	$I_{AC}\ V_{index}\ X_{index}\ W_{3D}, J_{3D},$ DDL, RCI	0.704	0.495	0.200	0.3587	1.680
22	Obsd	$I_{AC}\ U_{index}\ X_{index}\ Y_{index}\ W_{3D}, J_{3D}, H_{3D}$ DDL	0.726	0.527	0.182	0.3626	1.530
23	Singlet	X_{index} DDL	0.800	0.640	0.606	18.5143	18.692
24	Singlet	$X_{index}\ Y_{index}$ DDL	0.818	0.669	0.620	18.1920	13.490
25	Singlet	$X_{index}\ Y_{index}$ DDL ,RCI	0.835	0.697	0.633	17.8710	10.916
26	Singlet	$X_{index}\ Y_{index}\ J_{3D},$ DDL ,RCI	0.847	0.718	0.640	17.7022	9.173
27	Singlet	$I_{AC}\ X_{index}\ Y_{index}\ J_{3D},$ DDL ,RCI	0.852	0.726	0.629	17.9709	7.495
28	Singlet	$I_{AC}\ U_{index}\ X_{index}\ Y_{index}, J_{3D},$ DDL ,RCI	0.861	0.741	0.628	17.9997	6.538
29	Singlet	$I_{AC}\ U_{index}\ X_{index}\ Y_{index}\ W_{3D}, J_{3D},$ DDL ,RCI	0.869	0.755	0.624	18.0855	5.773
30	Triplet	$V_{index}\ W_{3D}\ J_{3D}$	0.718	0.515	0.442	30.3379	7.084
31	Triplet	$U_{index}\ V_{index}\ W_{3D}\ J_{3D}$	0.729	0.532	0.434	30.5763	5.403
32	Triplet	$X_{index}\ Y_{index}\ W_{3D}\ J_{3D}$ DDL	0.771	0.594	0.481	29.2574	5.271
33	Triplet	$I_{AC}\ X_{index}\ Y_{index}\ W_{3D}\ J_{3D}$ DDL	0.774	0.599	0.457	29.9390	4.226
34	Triplet	$I_{AC}\ V_{index}\ X_{index}\ Y_{index}\ W_{3D}\ J_{3D}$ DDL	0.774	0.599	0.424	30.8381	3.418
35	Triplet	$I_{AC}\ V_{index}\ X_{index}\ Y_{index}\ W_{3D}\ J_{3D}$ DDL ,RCI	0.774	0.600	0.386	31.8352	2.808
36	Obsd	χ_{2V}, χ_{3V} DDL	0.705	0.497	0.403	0.3099	5.277
37	Obsd	χ_{2V}, χ_{3V} , W_{3D} DDL	0.774	0.600	0.493	0.2855	5.621
38	Obsd	χ_{2V}, χ_{3V} , $U_{index}\ W_{3D}$ DDL	0.775	0.600	0.475	0.2954	4.205
39	Obsd	χ_{2V}, χ_{3V} , $U_{index}\ I_{AC}\ W_{3D}$ DDL,	0.799	0.638	0.471	0.2917	3.820
40	Obsd	$\chi_{0V}, \chi_{1V}, \chi_{2V}, \chi_{3V}, I_{AC}\ W_{3D}$ DDL	0.829	0.688	0.506	0.2819	3.778
41	Obsd	$\chi_{0V}, \chi_{1V}, \chi_{2V}, \chi_{3V}\ I_{AC}\ U_{index}\ W_{3D}$ DDL	0.822	0.676	0.488	0.2871	3.583
42	Singlet	X_{index} DDL,	0.800	0.640	0.606	18.5143	18.692
43	Singlet	$\chi_{2V}\ V_{index}$ DDL,	0.836	0.698	0.653	17.3747	15.431
44	Singlet	χ_{2V}, χ_{3V} , DDL, RCI	0.878	0.772	0.723	15.5138	16.038
45	Singlet	χ_{2V}, χ_{3V} ,X_{index} DDL, RCI	0.895	0.801	0.746	14.8693	14.503
46	Singlet	$\chi_{2V}, \chi_{3V}, \chi_{4V}$, $V_{index}\ W_{3D}$, DDL, RCI	0.908	0.825	0.763	14.3720	13.315
47	Singlet	$\chi_{2V}, \chi_{3V}, \chi_{4V}$, V_{index} DDL, RCI	0.927	0.859	0.798	13.2666	13.958
48	Singlet	$\chi_{1V}, \chi_{2V}, \chi_{3V}, \chi_{4V}, V_{index},$ DDL, RCI	0.932	0.869	0.799	13.2324	12.412
49	Triplet	$V_{index}\ W_{3D}\ J_{3D}$	0.718	0.515	0.442	30.3379	7.084
50	Triplet	U_{index} ,$V_{index}\ W_{3D}\ J_{3D}$	0.729	0.532	0.434	30.5763	5.403
51	Triplet	$\chi_{2V}, \chi_{3V}, \chi_{4V}\ \chi_{5V}$ DDL	0.903	0.816	0.765	19.7167	15.933
52	Triplet	$\chi_{2V}, \chi_{3V}, \chi_{4V}, \chi_{5V}\ J_{3D}$ DDL	0.928	0.860	0.811	17.6570	17.464
53	Triplet	$\chi_{2V}, \chi_{3V}, \chi_{4V}, \chi_{5V}, W_{3D}\ J_{3D}$ DDL	0.936	0.876	0.822	17.1630	16.127
54	Triplet	$\chi_{2V}, \chi_{3V}, \chi_{4V}, \chi_{5V}, I_{AC}\ W_{3D}\ J_{3D}$ DDL	0.943	0.890	0.831	16.7030	15.136
55	Obsd	χ_5, χ_{3V} , Y_{index}	0.700	0.490	0.394	0.3122	5.115
56	Obsd	$\chi_5, \chi_{1V}, \chi_{4V}$, Y_{index}	0.750	0.563	0.446	0.2985	4.825
57	Obsd	$\chi_5, \chi_{1V}, \chi_{3V}\ \chi_{4V}$, Y_{index}	0.764	0.584	0.435	0.3015	3.925
58	Obsd	$\chi_0\ \chi_5, \chi_{1V}, \chi_{3V}\ \chi_{4V}$,Y_{index}	0.778	0.605	0.422	0.3048	3.316
59	Obsd	$\chi_4, \chi_5, \chi_{1V}, \chi_{3V}, \chi_{4V}, \chi_{5V}$, Y_{index}	0.790	0.625	0.452	0.2970	3.608
60	Obsd	$\chi_1, \chi_4, \chi_5, \chi_{1V}, \chi_{2V}, \chi_{3V}, \chi_{4V}, \chi_{5V}\ V_{index}\ Y_{index}$	0.800	0.639	0.429	0.3031	3.038
61	Singlet	χ_5 , χ_{0V} , χ_{1V} , X_{index}	0.875	0.766	0.717	15.7028	15.540
62	Singlet	χ_0, χ_5 , χ_{1V}, χ_{3V} , X_{index}	0.888	0.789	0.731	15.3058	13.485
63	Singlet	χ_0, χ_5 , $\chi_{1V}, \chi_{2V}\ \chi_{3V}$, X_{index}	0.891	0.794	0.721	15.5739	10.918
64	Singlet	χ_0, χ_5 , $\chi_{1V}, \chi_{2V}\ \chi_{3V}\ \chi_{4V}$, ,$X_{index}$	0.898	0.807	0.722	15.5436	9.547
65	Singlet	χ_0, χ_5 , χ_{0V} , $\chi_{1V}, \chi_{2V}\ \chi_{3V}\ \chi_{4V}\ V_{index}$	0.905	0.819	0.722	15.5422	8.481
66	Triplet	$\chi_{3V}\ \chi_{5V}\ X_{index}$	0.729	0.531	0.461	29.8374	7.549
67	Triplet	$\chi_{2V}\ \chi_{3V}\ \chi_{5V}\ X_{index}$	0.739	0.545	0.450	30.1373	5.701
68	Triplet	$\chi_{2V}, \chi_{3V}, \chi_{4V}, \chi_{5V}$, X_{index}	0.769	0.591	0.478	29.3565	5.211

Reg. model	Dependent	Parameters	R	R Square	Adjusted R Square	Std. Error of the Estimate	F
69	Triplet	χ_5 , χ_{1V}, χ_{2V}, χ_{3V}, χ_{4V} V_{index}	0.807	0.651	0.528	27.9070	5.292
70	Triplet	χ_1, χ_2 , χ_{0V} , χ_{1V}, χ_{2V}, χ_{3V} ,I_{AC}	0.712	0.507	0.370	32.2415	3.705
71	Triplet	χ_1, χ_2, χ_{0V}, χ_{2V}, χ_{4V}, I_{AC}, U_{index}, Y_{index}	0.755	0.570	0.382	31.9465	3.029
72	Obsd	χ_0 , χ_3 χ_{3V} X_{3V}, J_{3D} RCI	0.709	0.503	0.326	0.3293	2.838
73	Obsd	χ_0, χ_{2V}, χ_{3V}, χ_{4V} , W_{3D} ,DDL	0.785	0.616	0.439	0.3003	3.483
74	Obsd	χ_1, χ_3, χ_{1V}, χ_{2V}, χ_{3V}, χ_{4V}, χ_{5V} W_{3D} ,	0.796	0.634	0.465	0.2934	3.751
75	Obsd	χ_0 χ_1, χ_3 χ_{1V}, χ_{2V}, χ_{3V} W_{3D} ,DDL	0.801	0.641	0.432	0.3023	3.064
76	Singlet	χ_2 ,χ_{1V}	0.704	0.495	0.447	21.9339	10.299
77	Singlet	χ_2, χ_3 DDL	0.831	0.691	0.644	17.5925	14.887
78	Singlet	χ_2, χ_3, DDL,RCI	0.866	0.750	0.697	16.2309	14.241
79	Singlet	χ_1, χ_2, χ_3 ,DDL,RCI	0.889	0.791	0.732	15.2613	13.585
80	Singlet	χ_1, χ_2, χ_3, χ_4 DDL,RCI	0.901	0.812	0.746	14.8609	12.269
81	Singlet	χ_1, χ_2, χ_3, χ_4, χ_5 , DDL,RCI	0.926	0.857	0.795	13.3708	13.706
82	Singlet	χ_0 χ_1, χ_2, χ_3, χ_4, χ_5 , DDL,RCI	0.935	0.874	0.807	12.9529	13.035
83	Triplet	χ_2, χ_3,W_{3D}	0.821	0.674	0.626	24.8590	13.813
84	Triplet	χ_2, χ_3, χ_{4V},,DDL	0.881	0.776	0.729	21.1657	16.438
85	Triplet	χ_2, χ_3, χ_{4V}, W_{3D} ,DDL	0.902	0.814	0.762	19.8046	15.760
86	Triplet	χ_2, χ_3, χ_4, χ_{4V} , W_{3D} ,DDL	0.922	0.851	0.798	18.2652	16.134
87	Triplet	, χ_2, χ_3, χ_5 χ_{3V}, χ_{4V}, W_{3D},X_3 DDL	0.935	0.875	0.820	17.2227	16.000
88	Triplet	χ_1, χ_4, χ_5 χ_{2V}, χ_{3V}, χ_{5V} DDI, W_{3D},	0.962	0.925	0.885	13.7485	23.233

phototoxicicity of PAHs

Table 9. Regression details for the model -82

Variables Entered/Removed[b]

Model	Variables Entered	Variables Removed	Method
1	X_0, RCI, DDI, X_5, X_1, X_4, X_2, X_3[a]	.	Enter

a. All requested variables entered.

b. Dependent Variable: singlet energy

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	0.935[a]	0.874	0.807	12.9529

a. Predictors: (Constant), X_0, RCI, DDI, X_5, X_1, X_4, X_2, X_3

ANOVA[b]

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	17495.827	8	2186.978	13.035	0.000 [a]
	Residual	2516.673	15	167.778		
	Total	20012.500	23			

a. Predictors: (Constant), X_0, RCI, DDI, X_5, X_1, X_4, X_2, X_3

b. Dependent Variable: singlet energy

Coefficients[a]

Model		Unstandardized Coefficients		Standardized Coefficients		
		B	Std. Error	Beta	t	Sig.
1	(Constant)	730.071	59.490		12.272	.000
	X_2	-415.323	69.857	-22.645	-5.945	.000
	X_3	325.052	83.024	18.491	3.915	.001
	DDI	0.785	0.138	3.561	5.675	.000
	RCI	-20.462	8.102	-.239	-2.526	.023
	X_1	78.640	28.565	4.257	2.753	.015
	X_4	-130.117	45.436	-7.582	-2.864	.012
	X_5	56.258	26.944	3.464	2.088	.054
	X_0	1.495E-03	0.001	.142	1.431	.173

a. Dependent Variable: singlet energy

Table 10. Regression details for model -87

Variables Entered/Removed[b]

Model	Variables Entered	Variables Removed	Method
1	X_{3V}, W_{3D}, X_5, X_2, DDI, X_{4V}, X_3[a]	.	Enter

a. All requested variables entered.

b. Dependent Variable: Triplet energy

ANOVA[b]

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	33221.671	7	4745.953	16.000	0.000[a]
	Residual	4745.954	16	296.622		
	Total	37967.625	23			

a. Predictors: (Constant), X_{3V}, W_{3D}, X_5, X_2, DDI, X_{4V}, X_3

b. Dependent Variable: Triplet energy

Coefficients[a]

Model		Unstandardized Coefficients		Standardized Coefficients		
		B	Std. Error	Beta	t	Sig.
1	(Constant)	818.102	105.354		7.765	.000
	X_2	-758.430	88.668	-30.023	-8.554	.000
	X_3	603.454	90.249	24.923	6.687	.000
	X_{4V}	-764.481	185.066	-14.766	-4.131	.001
	DDI	3.718	0.818	12.253	4.546	.000
	W_{3D}	0-.319	0.117	-5.907	-2.738	.015
	X_5	67.254	35.095	3.006	1.916	.073
	X_{3V}	456.351	169.784	10.026	2.688	.016

a. Dependent Variable: Triplet energy

Table 11. Regression details for the model - 88

Variables Entered/Removed

Model	Variables Entered	Variables Removed	Method
1	DDI, X_{5V}, X_1, X_4, W_{3D}, X_{3V}, X_{2V}, X_5 [a]	.	Enter

a. All requested variables entered.

b. Dependent Variable: Triplet energy

Model Summary

Model	R	R Square	Adjusted R Square	Std. Error of the Estimate
1	0.962[a]	0.925	0.885	13.7485

a. Predictors: (Constant), DDI, X_{5V}, X_1, X_4, W_{3D}, X_{3V}, X_{2V}, X_5

ANOVA[b]

Model		Sum of Squares	df	Mean Square	F	Sig.
1	Regression	35132.291	8	4391.536	23.233	0.000 [a]
	Residual	2835.334	15	189.022		
	Total	37967.625	23			

a. Predictors: (Constant), DDI, X_{5V}, X_1, X_4, W_{3D}, X_{3V}, X_{2V}, X_5

b. Dependent Variable: Triplet energy

Coefficients[a]

Model		Unstandardized Coefficients		Standardized Coefficients	t	Sig.
		B	Std. Error	Beta		
1	(Constant)	801.192	88.190		9.085	.000
	X_1	-110.155	44.176	-4.329	-2.494	.025
	X_4	-638.406	91.765	-27.008	-6.957	.000
	X_5	870.699	134.362	38.920	6.480	.000
	X_{2V}	-1452.107	136.446	-35.686	-10.642	.000
	X_{3V}	2523.183	303.987	55.433	8.300	.000
	X_{5V}	-2041.427	347.790	-35.436	-5.870	.000
	W_{3D}	-.514	.122	-9.514	-4.197	.001
	DDI	5.140	.887	16.938	5.795	.000

a. Dependent Variable: Triplet energy