

Chapter 7

AL indices and their Applications

7.1 Introduction

In this chapter, we construct 8 novel topological indices, denoted by $AL_1, AL_2, AL_3, AL_4, AL_5, AL_6, AL_7$ and AL_8 , and we give a method to compute these indices from a neighborhood matrix of graphs. To establish our aim, we study the discriminating ability, regression, and correlation analysis of the indices against various physicochemical properties on widely available datasets, namely the octane isomers and polychlorobiphenyl (*PCB*) compounds. Further, we also make a comparative study with a few existing *VDB* indices to establish the potentiality and use them to predict expected values of the properties for *PCBs*.

The chapter is organized as follows: Section 7.2, we propose the new *AL* indices and give a method for computing these indices and the *VDB* indices. Section 7.3 tests the degeneracy of *AL* indices and compares the results with other *VDB* indices. In section 7.4, we give the correlation study and make a comparative analysis with *VDB* indices where subsection 7.4.1 focuses on comparing the physicochemical properties of octane isomer and subsection 7.4.2 studies the correlation of *AL* indices with the properties of *PCBs*.

We recall a graph matrix and a lemma, proposed in [130] that will be used to define the new indices is as shown below.

Definition 7.1. [130] The neighborhood matrix of a given graph G , denoted by $NM(G) = [b_{ij}]_{n \times n}$, is defined as

$$b_{ij} = \begin{cases} |N_G(j) \setminus N_G(i)| & : \text{if } (i, j) \in E(G), \\ -|N_G(i) \cap N_G(j)| & : \text{if } (i, j) \notin E(G) \\ -|N_G(i)| & : \text{if } i = j. \end{cases}$$

Computationally, this matrix can be obtained by the product of two well known graph matrices, namely the adjacency matrix and the Laplacian matrix. This was also proved in [130].

Lemma 7.2. [130] *The neighborhood matrix $NM(G)$ of a graph G can be obtained by the product of adjacency matrix $A(G)$ and Laplacian matrix $L(G)$ of graph.*

7.2 Novel AL Indices

In this section, we propose 8 new topological indices which are denoted by $AL_1, AL_2, AL_3, AL_4, AL_5, AL_6, AL_7, AL_8$, and give a method for computation of these indices directly and easily using the neighborhood matrix $NM(G)$.

For a given graph G , let $P_2(u)$ denotes the number of distinct vertices at distance two from vertex u .

$$\begin{aligned}
 AL_1(G) &= \sum_{u \in V(G)} P_2(u), & AL_2(G) &= \sum_{(u,v) \in E(G)} \{P_2(u) + P_2(v)\}, \\
 AL_3(G) &= \sum_{(u,v) \in E(G)} P_2(u)P_2(v), & AL_4(G) &= \sum_{(u,v) \in E(G)} \sqrt{P_2(u)P_2(v)} \\
 AL_5(G) &= \sum_{(u,v) \in E(G)} \frac{1}{\sqrt{P_2(u)P_2(v)}}, & AL_6(G) &= \sum_{(u,v) \in E(G)} \left\{ \frac{P_2(u)}{P_2(v)} + \frac{P_2(v)}{P_2(u)} \right\} \\
 AL_7(G) &= \sum_{(u,v) \in E(G)} \left\{ \frac{P_2(u)P_2(v)}{P_2(u) + P_2(v)} \right\}, & AL_8(G) &= \sum_{(u,v) \in E(G)} \frac{2}{P_2(u) + P_2(v)}.
 \end{aligned}$$

Example 7.1. Let G be a molecular graph of “2,5,4’-Trichloro-1-1’-biphenyl” then $P_2(a) = 2, P_2(b) = 2, P_2(c) = 3, P_2(d) = 3, P_2(e) = 4, P_2(f) = 3, P_2(g) = 3, P_2(h) = 5, P_2(i) = 3, P_2(j) = 2, P_2(k) = 3, P_2(l) = 3, P_2(m) = 2, P_2(o) = 4, P_2(n) = 2$, and the value of AL indices are $AL_1(G) = 44, AL_2(G) = 98, AL_3(G) = 155, AL_4(G) = 48.3718, AL_5(G) = 5.6026, AL_6(G) = 37.7, AL_7(G) = 23.8813, AL_8(G) = 5.5325$.

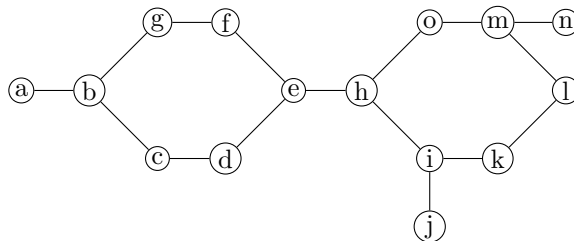


FIGURE 7.1: Molecular graph of “2,5,4’-Trichloro-1-1’-biphenyl”.

Note that from the above example, computing the values of P_2 for every vertex is crucial and time consuming. Computationally, we can use the all-pairs shortest paths algorithms to extract this information which will cost a lot of computational time. To overcome this, next, we give a method to compute the defined novel AL indices as well as the other VDB indices.

Method-: Let b_{ij} be any entry of the matrix NM , then from the definition of NM matrix, if $b_{ij} > 0$ then vertex i and j are adjacent and if $b_{ij} < 0$, then vertex i and j are separated by distance two. Now, first we define a function $g : V \times V \rightarrow \mathbb{R}$ defined by using a two-variable index-relation $f(\cdot, \cdot)$ defined on the diagonal elements of the NM matrix as follows.

$$\text{define, } g(i, j) = \begin{cases} f(b_{ii}, b_{jj}) & : \text{if } b_{ij} > 0, \\ 0 & : \text{Otherwise.} \end{cases} \quad (7.1)$$

Then, any VDB index can be obtained as sum of the elements g , that is

$$VDB = \sum_{i=1}^n \sum_{j=i+1}^n g_{ij}, \text{ for a suitably chosen index-relation } f.$$

For instance, for the Randić index, the index relation function f is given by $f(b_{ii}, b_{jj}) = \frac{1}{\sqrt{b_{ii} \cdot b_{jj}}}$

To compute the AL indices from NM matrix, we define

$$\text{define, } h(i, j) = \begin{cases} 1 & : \text{if } b_{ij} < 0, \\ 0 & : \text{Otherwise,} \end{cases} \quad (7.2)$$

$$C(i) = \sum_{j=1}^n h(i, j) - 1, \quad (7.3)$$

$$D(i, j) = \begin{cases} f(C(i), C(j)) & : \text{if } b_{ij} > 0 \\ 0 & : \text{Otherwise,} \end{cases} \quad (7.4)$$

where $f(C(i), C(j))$ is a index-relation.

Then the first AL index is defined as $AL_1(G) = \sum_{i=1}^n C(i)$,

and the other indices are defined as $AL_k(G) = \sum_{j=i+1}^n D(i, j)$, $2 \leq k \leq 8$, with the function $f_k(C(i), C(j))$ given by

For the second AL index, $AL_2(G)$, $f_2(C(i), C(j)) = C(i) + C(j)$.

For the third AL index, $AL_3(G)$, $f_3(C(i), C(j)) = C(i) \cdot C(j)$.

For the fourth AL index, $AL_4(G)$, $f_4(C(i), C(j)) = \sqrt{C(i) \cdot C(j)} = \sqrt{f_3(C(i), C(j))}$.

For the fifth AL index, $AL_5(G)$, $f_5(C(i), C(j)) = \frac{1}{\sqrt{C(i) \cdot C(j)}} = \frac{1}{f_4(C(i), C(j))}$.

For the sixth AL index, $AL_6(G)$, $f_6(C(i), C(j)) = \frac{C(j)}{C(i)} + \frac{C(i)}{C(j)}$.

For the seventh *AL* index, $AL_7(G)$, $f_7(C(i), C(j)) = \frac{C(i)C(j)}{C(i) + C(j)} = \frac{f_3(C(i), C(j))}{f_2(C(i), C(j))}$.

For the eight *AL* index, $AL_8(G)$, $f_8(C(i), C(j)) = \frac{C(i) + C(j)}{2} = \frac{f_2(C(i), C(j))}{2}$.

7.3 Degeneracy of AL Indices

The primary purpose of a molecular descriptor or topological index is to encode the structural features as much as possible. The vital study when one proposes a new topological index is to assess the capacity of the index to distinguish the molecules within the considered group. However, due to various limitations, such a unique topological index can never be realized. If two or more isomers of a molecule possess the same value for a topological index, then the index is degenerate. The measure of degeneracy, also known as sensitivity, was introduced by Konstantinova [131]. It is defined as

$$S_I = \frac{N - N_I}{N},$$

where N denotes the total number of isomers of a molecule, and N_I is the number of them that can not be distinguished by the topological index I . Note that $0 \leq S_I \leq 1$ and that if S_I is closer to 1, then the isomer discrimination power of the topological index is more. If a topological index has a lower degeneracy value, it has higher discriminative power and that it can capture more structural information.

We now study the discriminative ability of the VDB indices in order to understand the proposed *AL* indices. We consider two datasets to establish our views: octane isomers and PCB molecules. The data is given below in Table 7.1.

Topological Indices	S_I	
	Octane	PCB
AL_1	0.3333	0.0478
AL_2	0.5555	0.1435
AL_3	0.8888	0.4066
AL_4	1	0.9617
AL_5	1	0.8564
AL_6	0.7777	0.8229
AL_7	1	0.9617
AL_8	1	0.8086
R	0.8888	0.1435
AZI	0.8333	0.1435
H	0.7777	0.1435
ISI	0.7222	0.1435

TABLE 7.1: Measure of sensitivity of indices for octane isomers and *PCB* congeners.

From Table 7.1, it is immediate that the indices AL_4 , AL_5 , AL_7 , and AL_8 have the highest discriminative power for the set of octane isomers. AL_3 and R perform similarly with the same level of discrimination as they have the same sensitivity index (89%) for octane isomers.

On the other hand, for the *PCB* congeners, the indices AL_4 and AL_7 have the highest discriminative power. Following this, AL_5 , AL_6 , and AL_8 have a better discrimination ability with the sensitivity index of around 86%, 82%, and 81%, respectively, compared to other indices.

We also find that AL_1 index has the least discriminative power compared with the other investigated indices on both the sets of octane isomers and *PCBs*, which turns out against our expectation/intuition.

The degeneracy study shows that most of the proposed *AL* indices have a good discrimination ability or low degeneracy rate compared to the existing *VDB* indices. We shall focus more on the indices with higher discrimination power when analyzing the correlation ability.

Next, we turn our attention to analyzing the ability of the proposed *AL* indices in terms of their ability to correlate with the physicochemical properties of molecules.

7.4 Correlation of AL Indices

In this section, we study the comparative analysis of *AL* indices with other well studied *VDB* indices such as Randić index, Augmented Zagreb index, Harmonic Index, and Inverse sum index.

For our purpose, we consider the well-studied octane isomers and the polychlorobiphenyl congeners. The experimental data of various physico-chemical properties [namely Acentric factor (**Acent Fac.**), Entropy (**S**), enthalpy of vaporization (**HVAP**), Standard enthalpy of vaporization (**DHVAP**), Density (**DENS**), total surface area (**TSA**)] of the octane isomers are given in Table A.1 as an appendix at the end of this thesis is for a quick reference. These data are taken from the article [132] and are available in the website <http://www.moleculardescriptors.eu>. There are 18 isomers of octane with distinct properties are available in the data.

The experimental data of physicochemical properties such as melting point (**MP**), relative retention time (**RRT**), octanol-water-partition coefficient (**logP**), total surface area (**TSA**), log Henry constant (**logH**), log-water-solubility (**logSw**), log-water-activity coefficient (**logYw**), relative enthalpy of formation (**dHf**) for the *PCB* molecules are given in Table B.1 as an appendix. Note

that in Table B.1, blank space/empty cell represent that the experimental value of corresponding PCB molecules are not readily available. However, the missing experimental data of many PCB molecules makes it interesting to study and estimate if the AL indices correlate with physicochemical properties and can be used to predict them with confidence. Note that there are a total of 209 PCB congener molecules that have distinct properties. This can be observed from the data.

To test a physicochemical property against a topological index, we use the model given by the following linear regression equation $P = c + m \cdot TI$, where P is a physicochemical property, TI is a topological index (VDB index in our case), c is the intercept, and m is the slope of linear fit. Recall this model was defined in Section 5.3.1.

7.4.1 Linear Regression Model for Octane Isomer

Our focus is in computing the proposed *AL* indices for the considered datasets and to present a linear regression fit for the same.

As a first step, we compute the values of AL indices for the octane isomer data which is given in Table A.2 as an appendix. Secondly, the fitting of regression curve for each of the 6 physicochemical properties against the eight *AL*-indices are given below.

***AL*₁ Index-:**

$$\begin{aligned} \textit{Acent Fac.} &= 0.5347 - 0.0117AL_1(G), & S &= 130.2771 - 1.4722AL_1(G), \\ \textit{HVAP} &= 79.5175 - 0.613AL_1(G), & \textit{DHVAP} &= 11.1958 - 0.1225AL_1(G), \\ \textit{DENS} &= 0.6076 + 0.0063AL_1(G), & \textit{TSA} &= 418.3122 - 1.8364AL_1(G). \end{aligned}$$

***AL*₂ Index-:**

$$\begin{aligned} \textit{Acent Fac.} &= 0.5328 - 0.0064AL_2(G), & S &= 129.0092 - 0.7722AL_2(G), \\ \textit{HVAP} &= 76.3596 - 0.2355AL_2(G), & \textit{DHVAP} &= 10.7090 - 0.0518AL_2(G), \\ \textit{DENS} &= 0.5874 + 0.0041AL_2(G), & \textit{TSA} &= 444.0022 - 1.8558AL_2(G). \end{aligned}$$

***AL*₃ Index-:**

$$\begin{aligned}
Acent\ Fac. &= 0.4199 - 0.0025AL_3(G), & S &= 115.8167 - 0.3147AL_3(G), \\
HVAP &= 71.5809 - 0.0731AL_3(G), & DHVAP &= 9.7076 - 0.0175AL_3(G), \\
DENS &= 0.6480 + 0.0020AL_3(G), & TSA &= 411.9821 - 0.7468AL_3(G).
\end{aligned}$$

***AL*₄ Index-:**

$$\begin{aligned}
Acent\ Fac. &= 0.5001 - 0.0112AL_4(G), & S &= 125.4281 - 1.3752AL_4(G), \\
HVAP &= 74.0641 - 0.3367AL_4(G), & DHVAP &= 10.2822 - 0.0794AL_4(G), \\
DENS &= 0.5898 + 0.0086AL_4(G), & TSA &= 437.4955 - 3.4492AL_4(G).
\end{aligned}$$

***AL*₅ Index-:**

$$\begin{aligned}
Acent\ Fac. &= 0.1667 + 0.0451AL_5(G), & S &= 85.4339 + 5.3352AL_5(G), \\
HVAP &= 63.4211 + 1.5333AL_5(G), & DHVAP &= 7.8443 + 0.3423AL_5(G), \\
DENS &= 0.8275 - 0.0299AL_5(G), & TSA &= 331.7151 + 14.8421AL_5(G).
\end{aligned}$$

***AL*₆ Index-:**

$$\begin{aligned}
Acent\ Fac. &= 0.3522 - 0.0009AL_6(G), & S &= 105.8424 - 0.0248AL_6(G), \\
HVAP &= 76.1147 - 0.4027AL_6(G), & DHVAP &= 10.2240 - 0.0636AL_6(G), \\
DENS &= 0.8086 - 0.0054AL_6(G), & TSA &= 371.3679 + 0.9229AL_6(G).
\end{aligned}$$

***AL*₇ Index-:**

$$\begin{aligned}
Acent\ Fac. &= 0.4671 - 0.0189AL_7(G), & S &= 121.5595 - 2.3331AL_7(G), \\
HVAP &= 72.4486 - 0.4747AL_7(G), & DHVAP &= 9.9570 - 0.1200AL_7(G), \\
DENS &= 0.6045 + 0.0160AL_7(G), & TSA &= 428.7443 - 5.9893AL_7(G).
\end{aligned}$$

AL_8 Index-:

$$\begin{aligned}
 \text{Acent Fac.} &= 0.1559 + 0.0504AL_8(G), & S &= 84.2941 + 5.9305AL_8(G), \\
 \text{HVAP} &= 62.0846 + 1.9877AL_8(G), & \text{DHVAP} &= 7.6136 + 0.4247AL_8(G), \\
 \text{DENS} &= 0.8189 - 0.0291AL_8(G), & \text{TSA} &= 331.1528 + 15.7657AL_8(G).
 \end{aligned}$$

For a more clear understanding of the above data, we also present the statistical observation of these linear regression model in Tables 7.2 to 7.7 comparing the different VDB indices and the properties. Also, the graphical representation for the indices against each of the properties is given in Figures 7.2 to 7.7.

At the outset, we observe that over all the considered properties of octane isomer, the AL_1 -index has higher correlation except the total surface area and the density. In particular, AL_1 has higher correlation of 0.973 with the acentric factor among all the physicochemical properties considered.

Acentric Factor: From table 7.2 and Figure 7.2, we compare the correlation of Acentric factor with the AL and other VDB indices. We find that the higher value of correlation coefficient $r = 0.97$ is observed between AL_1 index and acentric factor with a standard error of estimate of 0.0084, while AL_2 and AL_8 follow closely with a correlation coefficient of 0.95. Among the latter two, with an absolute discrimination ability, we find that AL_8 with high confidence is comparatively better and hence has the potential viable to estimate the Acentric Factor of octanes. Note that other than

Index	C	m	r	SEE	F	SF
AL_1	0.5347	-0.0117	0.9730	0.0084	285.0641	1.28E-11
AL_2	0.5328	-0.0064	0.9488	0.0115	144.4143	2.02E-09
AL_3	0.4199	-0.0025	0.8618	0.0185	46.2101	4.28E-06
AL_4	0.5001	-0.0113	0.8736	0.0177	51.6016	2.18E-06
AL_5	0.1667	0.0451	0.9020	0.0158	69.9048	3.11E-07
AL_6	0.3522	-0.0009	0.0711	0.0364	0.0814	7.79E-01
AL_7	0.4671	-0.0189	0.8052	0.0216	29.5011	5.54E-05
AL_8	0.1559	0.0504	0.9494	0.0114	146.5033	1.82E-09
R	-0.3693	0.1934	0.9042	0.0156	71.7342	2.63E-07
AZI	0.1933	0.0031	0.6676	0.0272	12.8649	0.0025
H	-0.0286	0.1090	0.9069	0.0153	74.1347	2.11E-07
ISI	1.3696	-0.1569	0.7333	0.0248	18.6172	0.0005

TABLE 7.2: The statistical table of linear regression model comparing VDB indices with acentric factor of octane isomers.

AL_5 and AL_8 all the other indices have a negative slope implying that the index values decreases as the number of branching increases in the molecules. The linear regression fit with positive slope

can be recognized from the graph in Figure 7.2(h) for the index AL_8 , which is also having distinct values compared to other indices.

All the other VDB indices have a correlation value between 0.0711 to 0.90 with the least being AL_6 .

Thus we find that AL_1 and AL_8 indices are best suitable for studying the acentric factor of octane isomers.

Entropy: In Table 7.3 and Figure 7.3, we compare the entropy S of octane isomers with the AL indices and VDB indices. Here, we obtain that AL_1 index has the highest value of correlation coefficient $r = 0.9542$ while the Randic index follows with a correlation of 0.9058. The Harmonic index also has a correlation of 0.90. The other indices have correlation value between 0.0145 to 0.9053 with the least being obtained by AL_6 . However, with reference to the discriminating ability we see that the indices AL_4 , AL_5 have an moderate correlation ability.

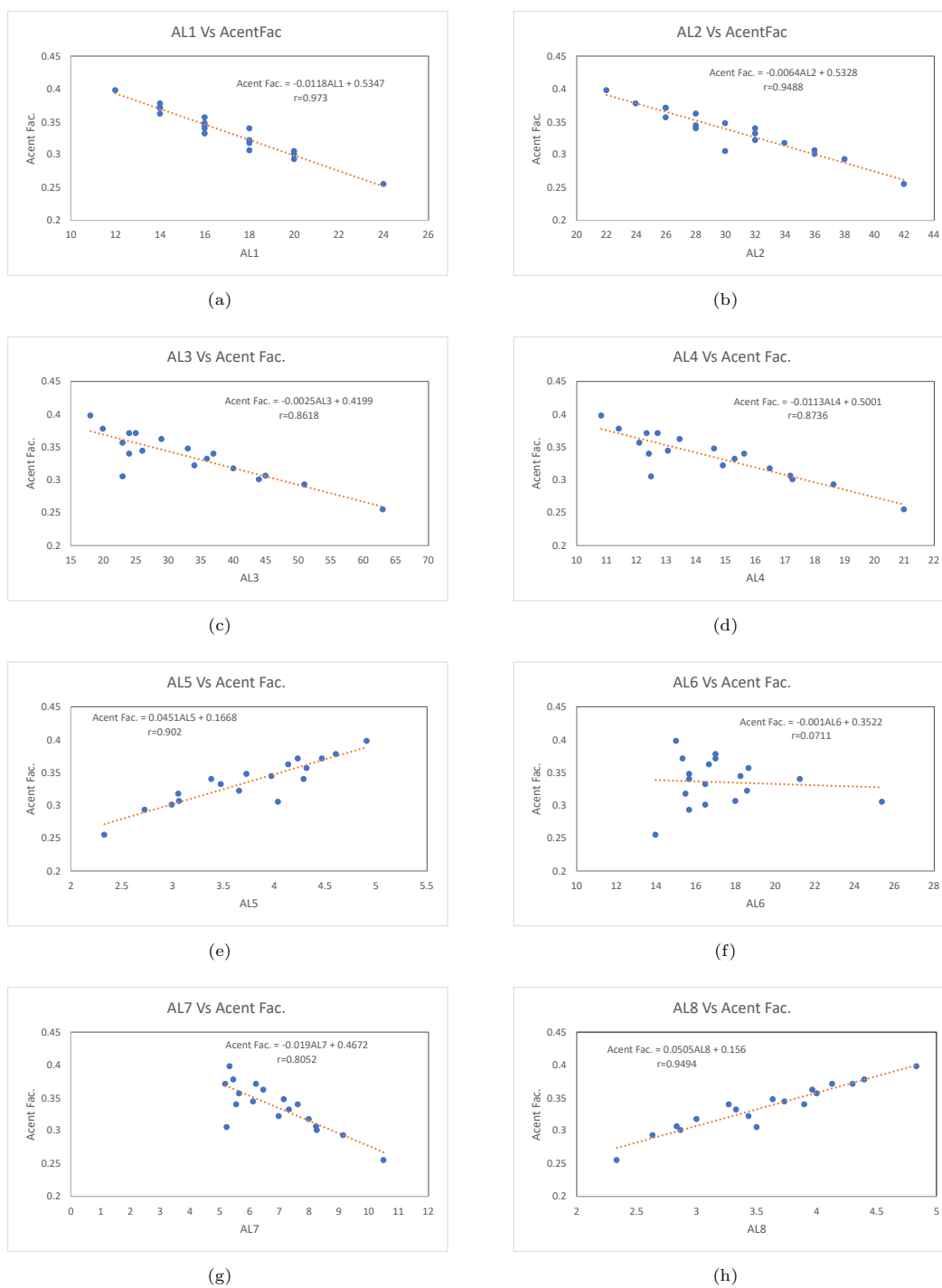
Index	C	m	r	SEE	F	SF
AL_1	130.2771	-1.4722	0.9542	1.3917	163.1234	8.30E-10
AL_2	129.0092	-0.7722	0.8915	2.1090	61.99815	6.81E-07
AL_3	115.8167	-0.3147	0.8361	2.5540	37.1861	1.54E-05
AL_4	125.4281	-1.3752	0.8347	2.5638	36.7785	1.64E-05
AL_5	85.4339	5.3352	0.8368	2.5489	37.3991	1.49E-05
AL_6	105.8424	-0.0248	0.0145	4.6561	0.0033	9.54E-01
AL_7	121.5595	-2.3331	0.7765	2.9341	24.2978	1.00E-04
AL_8	84.2941	5.9305	0.8752	2.2525	52.3748	1.98E-06
R	15.3921	24.6919	0.9058	1.9726	73.1554	2.31E-07
AZI	86.7686	0.4166	0.6855	3.3900	14.1896	0.0017
H	59.0568	13.8711	0.9053	1.9772	72.7446	2.39E-07
ISI	219.6857	-17.3439	0.6360	3.5932	10.8706	0.0046

TABLE 7.3: The statistical table of linear regression model comparing VDB indices with entropy of octane isomers.

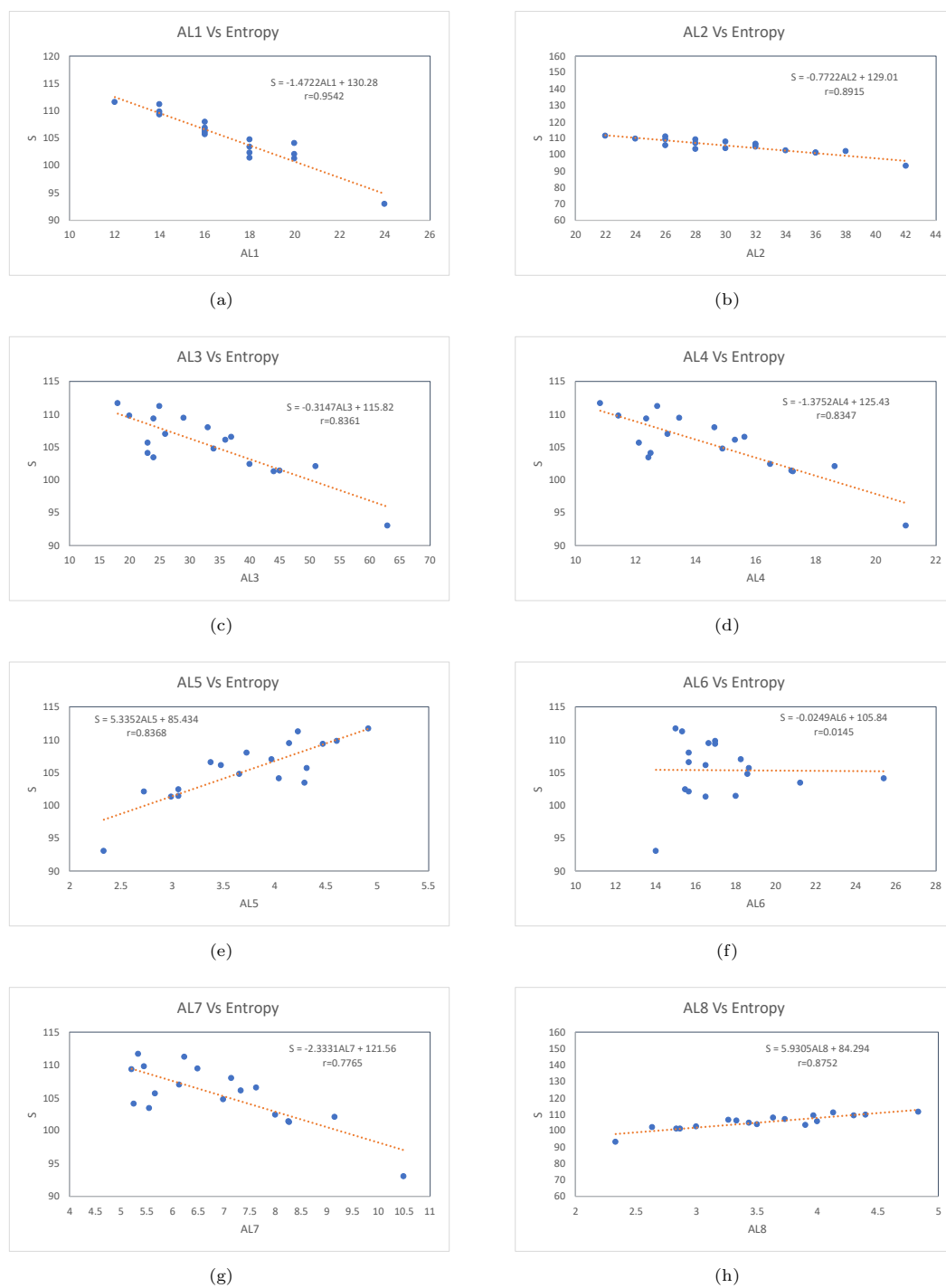
Thus, we conclude that AL_1 index have higher correlation in estimating the entropy of octane isomers.

Enthalpy of Vaporization: In Table 7.4 and Figure 7.4 we compare the enthalpy of vaporization $HVAP$ of octane isomer with the VDB indices. Our first observation is that the highest value of correlation coefficient of $r = 0.9389$ is displayed by Harmonic index H followed by Randić index R and Augmented Zagreb index AZI with a correlation value 0.9360 and 0.9377 respectively. Among the proposed AL indices, AL_1 index has a better correlation value of 0.8860. Overall, the other indices have correlation value between 0.2707 to 0.6540.

AL indices does not perform very well in representing the enthalpy of vaporization.

FIGURE 7.2: *AL* indices Vs Acentric factor of octane isomer.

Standard Enthalpy of Vaporization: In Table 7.5 and Figure 7.5, we present the regression analysis of the standard enthalpy of vaporization DH_{VAP} of octane isomer with the *VDB* indices. For this physicochemical property, we observe that the highest value of correlation coefficient of $r = 0.9607$

FIGURE 7.3: *AL* indices Vs entropy of octane isomer.

is displayed by Harmonic index H followed by Randić R and AL_1 with a correlation of 0.9581 and 0.9361 respectively. While the other indices have correlation value between 0.3836 to 0.8997. Here again, we observe that the AL indices do not correlate well with the standard enthalpy of

Index	C	m	r	SEE	F	SF
AL_1	79.5175	-0.6130	0.8860	0.9684	58.4268	9.96E-07
AL_2	76.3596	-0.2355	0.6062	1.6610	9.2965	0.0076
AL_3	71.5809	-0.0731	0.4332	1.8824	3.6968	0.0725
AL_4	74.0641	-0.3367	0.4557	1.8591	4.1938	0.0573
AL_5	63.4211	1.5333	0.5362	1.7629	6.4582	0.0217
AL_6	76.1147	-0.4027	0.5264	1.7757	6.1348	0.0248
AL_7	72.4486	-0.4747	0.3522	1.9547	2.2665	0.1516
AL_8	62.0846	1.9877	0.6540	1.5799	11.9600	0.0032
R	27.4372	11.445	0.9360	0.7346	113.3223	1.43E-08
AZI	57.7241	0.2556	0.9377	0.7251	116.7253	9.26E-09
H	47.6	6.4522	0.9389	0.7186	119.1285	8.02E-09
ISI	90.9833	-3.3117	0.2707	2.0106	1.2659	0.2771

TABLE 7.4: The statistical table of linear regression model comparing *VDB* indices with enthalpy of vaporization of octane isomer.

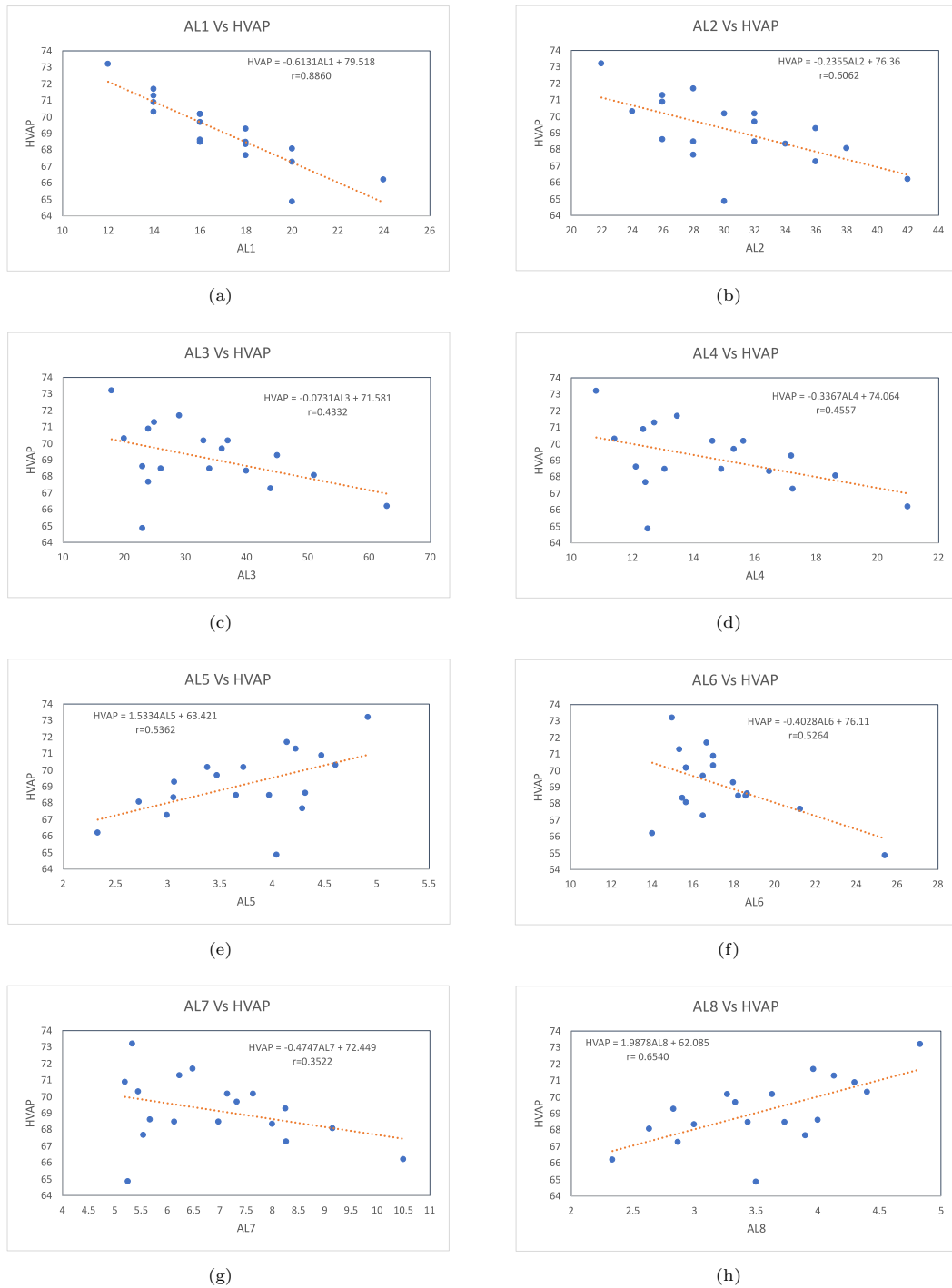
vaporization.

Index	C	m	r	SEE	F	SF
AL_1	11.1958	-0.1225	0.9361	0.1389	113.4059	1.14E-08
AL_2	10.7090	-0.0518	0.7049	0.2802	15.8025	0.0011
AL_3	9.7076	-0.0175	0.5506	0.3298	6.9615	0.0179
AL_4	10.2822	-0.0794	0.5682	0.3251	7.6284	0.0139
AL_5	7.8443	0.3423	0.6328	0.3059	10.6898	0.0048
AL_6	10.2240	-0.0636	0.4394	0.3549	3.8301	0.0680
AL_7	9.9570	-0.1200	0.4708	0.3458	4.5571	0.0486
AL_8	7.6136	0.4247	0.7388	0.2662	19.2310	0.0004
R	1.0467	2.2161	0.9581	0.1130	179.3953	4.12E-10
AZI	7.0502	0.0463	0.8997	0.1724	67.9939	3.74E-07
H	4.9523	1.2489	0.9607	0.1095	192.0475	2.49E-10
ISI	14.9752	-0.8877	0.3836	0.3648	2.7620	0.1160

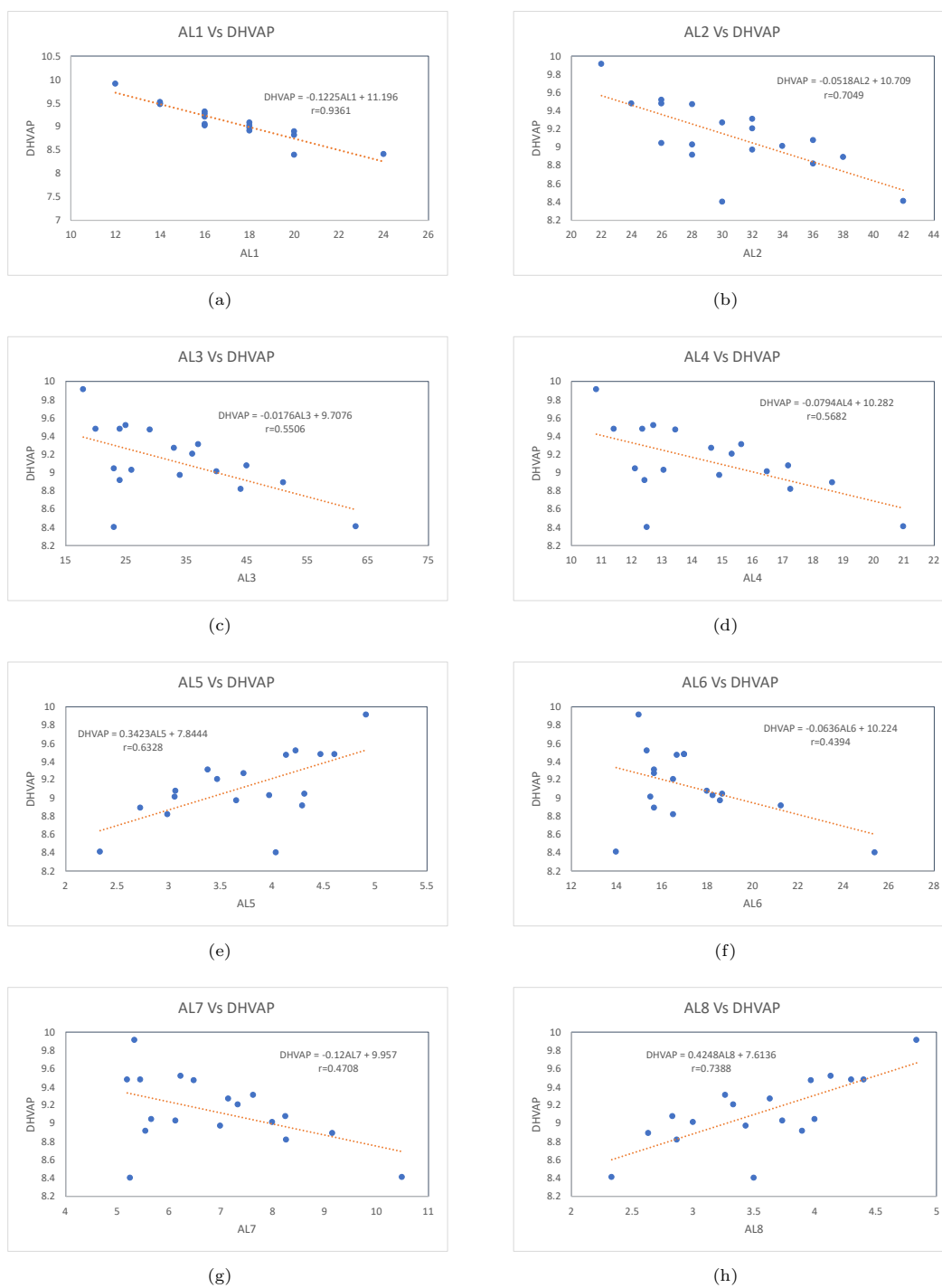
TABLE 7.5: The statistical table of linear regression model comparing *VDB* indices with standard enthalpy of vaporization for octane isomer.

Total Surface Area: In Table 7.6 and Figure 7.6, we present the regression analysis data for the total surface area *TSA* of octane isomer with the *VDB* indices. From the table our first observation is that the maximum value of correlation coefficient of $r = 0.8678$ is displayed by Inverse sum index *ISI* followed by the AL_5 -index with a value of 0.7391. While the other indices have correlation value between 0.0224 to 0.7386. Among the *AL* indices, apart from AL_5 , the index AL_8 also performs well with a correlation of 0.7386. Again with higher discriminating power, AL_5 and AL_8 can be considered as a good estimator. However, *ISI* overtakes and hence is better than any other indices.

Density: In Table 7.7 and Figure 7.7, we compare the density (*DENS*) of octane isomer with the *VDB* indices and present their regression analysis. From the table, we have that AL_3 index has

FIGURE 7.4: *AL* indices Vs Enthalpy of vaporization of octane isomer.

the highest value of correlation coefficient $r = 0.8384$ followed by AL_7 with a value of 0.8247. While the other indices have value of correlation coefficient between 0.2383 to 0.8099. Further, AL_4 also has a good correlation. Especially with higher discrimination power, AL_4 and AL_8 can

FIGURE 7.5: *AL* indices Vs Standard enthalpy of vaporization of octane isomer.

be considered as viable descriptors for analyzing density of octane isomers. We find that AL_3 index have higher value of correlation coefficient with the density of octane isomer and shall be considered.

Index	C	m	r	SEE	F	SF
AL_1	418.3122	-1.8365	0.3779	13.5798	2.6660	0.1220
AL_2	444.0022	-1.8558	0.6802	10.7515	13.7784	0.0018
AL_3	411.9821	-0.7468	0.6299	11.3919	10.5242	0.0050
AL_4	437.4955	-3.4492	0.6646	10.9583	12.6647	0.0026
AL_5	331.7151	14.8422	0.7391	9.8796	19.2659	0.0005
AL_6	371.3679	0.9229	0.1717	14.4496	0.4864	0.4955
AL_7	428.7443	-5.9893	0.6328	11.3569	10.6878	0.0048
AL_8	331.1528	15.7657	0.7386	9.8871	19.2125	0.0005
R	308.8024	21.5300	0.2507	14.1990	1.0735	0.3155
AZI	385.3767	0.0428	0.0224	14.6600	0.0080	0.9296
H	344.3126	12.8618	0.2665	14.1371	1.2234	0.2850
ISI	878.4261	-74.5421	0.8678	7.2869	48.8268	3.06E-06

TABLE 7.6: The statistical table of linear regression model comparing *VDB* indices with the total surface area of octane isomer.

Index	C	m	r	SEE	F	SF
AL_1	0.6076	0.0063	0.6397	0.0231	11.0862	0.0042
AL_2	0.5874	0.0041	0.7477	0.0200	20.2886	0.0004
AL_3	0.6480	0.0020	0.8384	0.0164	37.8614	1.39E-05
AL_4	0.5898	0.0086	0.8099	0.0176	30.5162	4.62E-05
AL_5	0.8275	-0.0299	0.7246	0.0208	17.6906	0.0007
AL_6	0.8086	-0.0054	0.4887	0.0263	5.0215	0.0395
AL_7	0.6045	0.0160	0.8247	0.0170	34.0364	2.54E-05
AL_8	0.8189	-0.0291	0.6623	0.0225	12.5064	2.70E-03
R	1.0748	-0.0985	0.5586	0.0249	7.2580	0.0159
AZI	0.7574	-0.0009	0.2383	0.0292	0.9634	0.3409
H	0.8985	-0.0547	0.5523	0.0251	7.0239	0.0174
ISI	-0.0141	0.1107	0.6276	0.0234	10.3989	0.0053

TABLE 7.7: The statistical table of linear regression model comparing *VDB* indices with density of octane isomer.

Finally, from the comparative study on octane isomers, we observe that the AL_1 -index has an excellent correlation with acentric factor, entropy of octane isomer and displays a good correlation with standard enthalpy of vaporization. AL_3 -index have a good correlation with density of octane isomers. The other AL indices also display a relatively better performance for most of the considered properties. However, combining the discrimination power and the correlation, we find that AL_4 , AL_7 , and AL_8 can also be very useful in analysis of properties other than enthalpy and standard enthalpy of vaporization.

7.4.2 Linear Regression Model for PCB Congeners

In this subsection, we present the linear regression model and its analysis for 8 different physico-chemical properties of PCB compounds by using the model $P = C + m \cdot TI$.

For this model, we first compute the value of *AL* indices for all the 209 PCB compounds and present them in the Table B.2 as an appendix. Following this we fit the linear regression model for the eight physicochemical properties against the eight *AL* indices. The regression fit is given below:

***AL*₁ Index-:**

$$\begin{array}{ll}
 MP = 5.0508AL_1(G) - 154.0400, & \log Yw = 0.1027AL_1(G) + 1.3104, \\
 RRT = 0.0247AL_1(G) - 0.6907, & \log P = 0.0997AL_1(G) + 1.0733, \\
 TSA = 3.8522AL_1(G) - 72.0340, & \log H = 0.0456AL_1(G) + 1.4026, \\
 \log Sw = 0.1538AL_1(G) - 0.4446, & dHf = 0.3113AL_1(G) + 4.5039.
 \end{array}$$

***AL*₂ Index-:**

$$\begin{array}{ll}
 MP = 1.9141AL_2(G) - 121.8094, & \log Yw = 0.0387AL_2(G) + 1.9842, \\
 RRT = 0.0092AL_2(G) - 0.5183, & \log P = 0.0376AL_2(G) + 1.7450, \\
 TSA = 1.4612AL_2(G) + 96.4197, & \log H = 0.0194AL_1(G) + 1.4718, \\
 \log Sw = 0.0584AL_2(G) + 0.5321, & dHf = 0.1201AL_1(G) + 6.1224.
 \end{array}$$

***AL*₃ Index-:**

$$\begin{array}{ll}
 MP = 0.8244AL_3(G) - 61.8034, & \log Yw = 0.0167AL_4(G) + 3.1936, \\
 RRT = 0.0039AL_3(G) - 0.2099, & \log P = 0.0161AL_4(G) + 2.9563, \\
 TSA = 0.6310AL_3(G) + 141.8355, & \log H = 0.0102AL_3(G) + 1.7543, \\
 \log Sw = 0.0252AL_3(G) + 2.3573, & dHf = 0.0517AL_3(G) + 9.7872.
 \end{array}$$

***AL*₄ Index-:**

$$\begin{array}{ll}
 MP = 3.9533AL_4(G) - 125.0218, & \log Yw = 0.0796AL_4(G) + 1.9460, \\
 RRT = 0.0192AL_4(G) - 0.5368, & \log P = 0.0778AL_4(G) + 1.6766, \\
 TSA = 3.0088AL_4(G) + 94.5777, & \log H = 0.0262AL_4(G) + 2.1617, \\
 \log Sw = 0.1206AL_4(G) + 0.4480, & dHf = 0.2502AL_4(G) + 5.8107.
 \end{array}$$

***AL*₅ Index-:**

$$\begin{aligned}
 MP &= 119.0312AL_5(G) - 587.6203, & \log Yw &= 2.6525AL_5(G) - 8.8433, \\
 RRT &= 0.5488AL_5(G) - 2.6220, & \log P &= 2.3714AL_5(G) - 7.6206, \\
 TSA &= 96.0261AL_5(G) - 289.3495, & \log H &= 3.7340AL_5(G) - 17.6434, \\
 \log Sw &= 3.7380AL_5(G) - 14.3156, & dHf &= 6.6011AL_5(G) - 17.8277.
 \end{aligned}$$

***AL*₆ Index-:**

$$\begin{aligned}
 MP &= 8.2256AL_6(G) - 211.5567, & \log Yw &= 0.1707AL_6(G) + 0.0063, \\
 RRT &= 0.0393AL_6(G) - 0.9415, & \log P &= 0.1605AL_6(G) + 0.0040, \\
 TSA &= 6.3364AL_6(G) + 25.6229, & \log H &= 0.1839AL_6(G) - 3.0353, \\
 \log Sw &= 0.25091AL_6(G) - 2.2255, & dHf &= 0.4880AL_6(G) + 1.5970.
 \end{aligned}$$

***AL*₇ Index-:**

$$\begin{aligned}
 MP &= 8.1526AL_7(G) - 128.0171, & \log Yw &= 0.1632AL_7(G) + 1.9155, \\
 RRT &= 0.0398AL_7(G) - 0.5536, & \log P &= 0.1609AL_7(G) + 1.6148, \\
 TSA &= 6.1824AL_7(G) + 93.0078, & \log H &= 0.0245AL_7(G) + 2.8946, \\
 \log Sw &= 0.2483AL_7(G) + 0.3747, & dHf &= 0.5207AL_7(G) + 5.5101.
 \end{aligned}$$

***AL*₈ Index-:**

$$\begin{aligned}
 MP &= 132.6224AL_8(G) - 651.7273, & \log Yw &= 2.9423AL_8(G) - 10.2000, \\
 RRT &= 0.6180AL_8(G) - 2.9539, & \log P &= 2.6587AL_8(G) - 8.9936, \\
 TSA &= 107.0610AL_8(G) - 341.5288, & \log H &= 3.6726AL_8(G) - 16.9459, \\
 \log Sw &= 4.1699AL_8(G) - 16.3591, & dHf &= 7.3653AL_8(G) - 21.3949.
 \end{aligned}$$

A detailed regression analysis for the corresponding data is presented as tables comparing the behaviour of different VDB indices for each of the physicochemical properties; see Tables 7.8 to 7.15. We also give the respective graphical representations of *AL* indices for each physicochemical property in Figures 7.8 to 7.15.

At the outset, we find that for the PCB molecules, the AL_1 -index have highest correlation with total surface area among all the physicochemical properties and other *VDB* indices considered.

Total Surface Area: In Table 7.8 and Figure 7.8, we compare the total surface area of PCB molecules against the *VDB* indices. Here, we observe that the higher value of correlation coefficient $r = 0.9973$ is obtained by AL_1 index which is followed by Randić R index with a value of 0.9962. The indices AL_4 and AL_7 which have the highest discrimination power also have higher correlation of 0.98. While the other considered *VDB* indices follow closely with a correlation value ranging between 0.9397 to 0.9956.

Index	C	m	r	SEE	F	SF
AL_1	72.0340	3.8522	0.9973	2.2542	13360.84	1.19E-81
AL_2	96.4197	1.4612	0.9890	4.6039	3149.8730	6.12E-60
AL_3	141.8355	0.6310	0.9783	6.4549	1568.0130	1.16E-49
AL_4	94.5777	3.0088	0.9891	4.5775	3187.2460	4.08E-60
AL_5	-289.3500	96.0261	0.9397	10.6772	528.6732	2.40E-34
AL_6	25.6229	6.3364	0.9865	5.1099	2543.7640	9.07E-57
AL_7	93.0078	6.1824	0.9886	4.6921	3029.9480	2.31E-59
AL_8	-341.5288	107.0610	0.9424	10.4418	555.9691	5.03E-35
R	-25.1214	37.1564	0.9962	2.6870	9382.3710	2.59E-76
AZI	1.5569	1.9538	0.9656	8.1134	966.7878	1.05E-42
H	-69.1267	45.0919	0.9941	3.3783	5909.9057	2.36E-69
ISI	24.9296	12.0879	0.9949	3.1386	6858.2048	1.37E-71

TABLE 7.8: The statistical table of linear regression model comparing *VDB* indices with the total surface area of PCBs.

Thus we find that AL_1 -index have higher correlation value with the total surface area of PCBs and the other proposed AL indices also perform well with more than 93% correlation ability.

Log-Water Solubility: In Table 7.9 and Figure 7.9, we present the regression analysis of log-water-solubility ($logSw$) of PCBs with the *VDB* indices. Here again we obtain that AL_1 index has the highest value of correlation coefficient $r = 0.9614$ followed by Randić R index with a value of 0.9596.

Further, combined with higher discrimination ability, AL_4 and AL_7 also have high correlation value of 0.95, which makes them more interesting and suitable for the study of molecular characterization. While the other indices have correlation value ranging between 0.9105 to 0.9576.

Thus, we find that AL_1 , AL_4 and AL_7 indices are more suitable to predict log-water-solubility $logSw$ for PCB molecules. In addition, other proposed AL indices also show a promising performance with more than 91% correlation ability.

Index	C	m	r	SEE	F	SF
AL_1	-0.4446	0.1538	0.9614	0.3137	1637.8180	5.33E-77
AL_2	0.5321	0.0584	0.9502	0.3552	1247.7290	9.27E-70
AL_3	2.3573	0.0252	0.9354	0.4030	939.2095	2.12E-62
AL_4	0.4480	0.1206	0.9510	0.3526	1267.8670	3.51E-70
AL_5	-14.3156	3.7380	0.9105	0.4714	650.4905	2.86E-53
AL_6	-2.2255	0.2509	0.9501	0.3557	1243.5760	1.13E-69
AL_7	0.3747	0.2483	0.9511	0.3522	1271.6130	2.94E-70
AL_8	-16.3591	4.1699	0.9128	0.4656	670.0806	5.46E-54
R	-4.3232	1.4839	0.9596	0.3209	1559.3630	1.11E-75
AZI	-3.2953	0.0785	0.9250	0.4334	794.3363	3.55E-58
H	-6.0820	1.8015	0.9565	0.3326	1442.1670	1.36E-73
ISI	-2.3240	0.4828	0.9576	0.3284	1482.1050	2.54E-74

TABLE 7.9: The statistical table of linear regression model comparing *VDB* indices with the log-water-solubility of PCBs.

Relative Retention Time: In Table 7.10 and Figure 7.10, we present the regression analysis of relative retention time (*RRT*) of PCB molecules with the *VDB* indices. Our first observation is that the highest value of correlation coefficient $r = 0.95$ is displayed by AL_1 index followed by the Randić R index with a correlation value of 0.9478. Indices AL_4 and AL_7 closely follow with a correlation of 0.94. While the other indices have correlation value between 0.8256 to 0.9454.

Index	C	m	r	SEE	F	SF
AL_1	-0.6907	0.0247	0.9500	0.0560	1916.601	1.3E-106
AL_2	-0.5183	0.0092	0.9361	0.0630	1466.586	6.72E-96
AL_3	-0.2099	0.0039	0.9129	0.0731	1036.540	1.54E-82
AL_4	-0.5368	0.0192	0.9412	0.0605	1607.256	1.57E-99
AL_5	-2.6220	0.5488	0.8256	0.1012	443.182	2.40E-53
AL_6	-0.9415	0.0393	0.9173	0.0714	1098.749	9.82E-85
AL_7	-0.5536	0.0398	0.9456	0.0583	1752.267	5.5E-103
AL_8	-2.9539	0.6180	0.8334	0.0991	470.868	3.17E-55
R	-1.3108	0.2383	0.9478	0.0571	1830.349	9.54E-105
AZI	-1.0827	0.0121	0.9036	0.0768	921.679	3.54E-78
H	-1.5855	0.2884	0.9440	0.0591	1696.451	1.09E-101
ISI	-0.9859	0.0774	0.9454	0.0584	1742.576	9.2E-103

TABLE 7.10: The statistical table of linear regression model comparing *VDB* indices with the relative retention time of PCBs.

Thus, here again we find that AL_1 index have higher correlation value with the relative retention time and the other AL indices, except AL_5 and AL_8 , have at least 90% correlation ability.

Octanol-Water-Partition Coefficient: In Table 7.11 and Figure 7.11, we compare the behaviour of AL and *VDB* indices against the octanol-water-partition coefficient ($\log P$) of PCB molecules. We find that the highest correlation coefficient value of $r = 0.9209$ is displayed by AL_1 index followed by Randić R index with correlation of 0.9175 and ISI index with 0.9141. AL_4 and AL_7 are also

performing well with correlation 0.90. While the other indices have correlation value between 0.866 to 0.9141.

Index	C	m	r	SEE	F	SF
AL_1	1.0733	0.0997	0.9209	0.2995	765.4899	6.10E-58
AL_2	1.7450	0.0376	0.9023	0.3313	600.4690	6.33E-52
AL_3	2.9563	0.0161	0.8790	0.3664	466.0169	6.32E-46
AL_4	1.6766	0.0778	0.9057	0.3257	626.0675	6.09E-53
AL_5	-7.6206	2.3714	0.8590	0.3935	385.8035	1.14E-41
AL_6	0.0040	0.1605	0.8978	0.3384	569.6820	1.18E-50
AL_7	1.6148	0.1609	0.9086	0.3209	649.0523	7.96E-54
AL_8	-8.9936	2.6587	0.8660	0.3843	411.0298	4.48E-43
R	-1.4300	0.9610	0.9175	0.3050	729.8739	9.66E-57
AZI	-0.6280	0.0490	0.8668	0.3832	414.2623	2.99E-43
H	-2.5480	1.1642	0.9120	0.3148	679.8153	5.71E-55
ISI	-0.1250	0.3123	0.9141	0.3116	696.5609	1.42E-55

TABLE 7.11: The statistical table of linear regression model comparing *VDB* indices with the octanol-water-partition coefficient of PCBs.

Thus, here again we find that AL_1 index have higher correlation value with the octanol-water-partition $\log P$ of PCBs among the newly proposed indices and the other AL indices also relatively well with a correlation ability of at least 86%.

Log-Water-Activity Coefficient:Next, in Table 7.12 and Figure 7.12, we compare the behaviour of AL and VDB indices against the log-water-activity coefficient ($\log Yw$) of PCB compounds.

Index	C	m	r	SEE	F	SF
AL_1	1.3104	0.1027	0.8993	0.3713	363.9553	1.19E-32
AL_2	1.9842	0.0387	0.8839	0.3971	307.3383	3.93E-30
AL_3	3.1936	0.0167	0.8699	0.4189	267.6107	3.88E-28
AL_4	1.9460	0.0796	0.8828	0.3988	303.9664	5.69E-30
AL_5	-8.8433	2.6525	0.8812	0.4015	298.8631	1.01E-29
AL_6	0.0063	0.1707	0.8961	0.3769	350.7208	4.31E-32
AL_7	1.9155	0.1632	0.8811	0.4015	298.8087	1.01E-29
AL_8	-10.2000	2.9423	0.8817	0.4007	300.4365	8.43E-30
R	-1.2716	0.9896	0.8966	0.3760	352.8851	3.48E-32
AZI	-0.4801	0.0514	0.8523	0.4442	228.3820	6.22E-26
H	-2.4297	1.1991	0.8923	0.3833	336.2308	1.85E-31
ISI	0.0682	0.3216	0.8938	0.3807	341.9432	1.03E-31

TABLE 7.12: The statistical table of linear regression model comparing *VDB* indices with the log-water-activity coefficient of PCBs.

Here again, we get that AL_1 index has the highest value of correlation coefficient of $r = 0.8993$ followed by Randić R index with a value of 0.8966. Here again, AL_4 and AL_7 perform well by having a correlation of 0.88. While the other indices have correlation value ranging between 0.8523 to 0.8961.

Further, all the proposed *AL* indices show a good correlation ability with the log-water-activity coefficient ($\log Yw$) of PCB molecules.

Melting Point: Next, in Table 7.13 and Figure 7.13, we present the comparison of the behaviour of *AL* and *VDB* indices against the melting point of PCB molecules. The highest value of correlation coefficient $r = 0.7798$ is displayed by AL_1 index followed by Randić R index with a value of 0.7787. While the other indices have correlation coefficient value between 0.6962 to 0.7774.

Even though the correlation ability of none of the indices is more than 78%, it is indeed interesting to note that the highest correlation is obtained by AL_1 index and all the other *AL* indices perform closely well for the melting point.

Index	C	m	r	SEE	F	SF
AL_1	-154.0400	5.0508	0.7798	31.9168	122.6528	9.57E-18
AL_2	-121.8094	1.9141	0.7720	32.4133	116.5226	3.27E-17
AL_3	-61.8034	0.8244	0.7581	33.2491	106.8157	2.49E-16
AL_4	-125.0218	3.9533	0.7741	32.2806	118.1336	2.36E-17
AL_5	-587.6203	119.0312	0.6962	36.6002	74.3471	5.32E-13
AL_6	-211.5567	8.2256	0.7648	32.8475	111.3878	9.44E-17
AL_7	-128.0171	8.1526	0.7760	32.1621	119.5882	1.76E-17
AL_8	-651.7273	132.6224	0.6974	36.5440	74.8192	4.70E-13
R	-281.3859	48.7132	0.7787	31.9874	121.7642	1.14E-17
AZI	-244.7811	2.5499	0.7509	33.6744	102.1516	6.85E-16
H	-338.9597	59.1030	0.7766	32.1193	120.1180	1.58E-17
ISI	-215.7138	15.8454	0.7774	32.0707	120.7226	1.40E-17

TABLE 7.13: The statistical table of linear regression model comparing *VDB* indices with the melting point of PCBs.

Relative Enthalpy of Formation: In Table 7.14 and Figure 7.14, we compare the performance of the *AL* and *VDB* indices against the relative enthalpy of formation (dHf) of PCB molecules. At the outset the correlation ability of the considered indices is relatively good and not the best. However, we want to highlight here that one of the reason could be the non-availability of sufficient experimental data for studying this property for PCBs. Even with the minimum data set, we see that the *AL* and *VDB* indices have a better correlation.

Having said that, we find that the highest value of correlation coefficient of $r = 0.6917$ is displayed by AL_7 index followed by AL_4 index with a value of 0.6852. With their good discrimination ability, we propose that the relative enthalpy of formation can be studied through AL_4 and AL_7 .

Further we also note that the correlation value r lies between 0.5505 to 0.6785 for the other indices. Except AL_5 and AL_8 indices, all the considered indices performs relatively well with a correlation ability of at least 67%.

Index	C	m	r	SEE	F	SF
AL_1	4.5039	0.3113	0.6746	3.7848	11.6931	0.0041
AL_2	6.1224	0.1201	0.6785	3.7663	11.9461	0.0038
AL_3	9.7872	0.0517	0.6721	3.7961	11.5396	0.0043
AL_4	5.8107	0.2502	0.6852	3.7343	12.3928	0.0033
AL_5	-17.8277	6.6011	0.5517	4.2761	6.1276	0.0267
AL_6	1.5970	0.4880	0.6456	3.9154	10.0077	0.0069
AL_7	5.5101	0.5207	0.6917	3.7028	12.8436	0.0029
AL_8	-21.3949	7.3653	0.5505	4.2801	6.0903	0.0270
R	-3.4455	3.0119	0.6757	3.7795	11.7644	0.0040
AZI	-2.5159	0.1655	0.6783	3.7671	11.9343	0.0038
H	-7.1770	3.6722	0.6770	3.7733	11.8490	0.0039
ISI	0.5269	0.9828	0.6766	3.7752	11.8230	0.0039

TABLE 7.14: The statistical table of linear regression model comparing *VDB* indices with the relative enthalpy of formation of PCBs.

Log-Henry Constant: Finally, in Table 7.15 and Figure 7.15, we study the behaviour of considered indices with the log-Henry constant ($\log H$). Here, we first show that neither *AL* indices nor *VDB* indices have a good correlation with log-Henry constant, since, the highest value of correlation coefficient is only 0.4467.

Index	C	m	r	SEE	F	SF
AL_1	1.4026	0.0456	0.1195	2.2257	0.2608	0.6157
AL_2	1.4718	0.0194	0.1272	2.2235	0.2961	0.5929
AL_3	1.7543	0.0102	0.1474	2.2172	0.3998	0.5351
AL_4	2.1617	0.0262	0.0826	2.2341	0.1237	0.7290
AL_5	-17.6434	3.7340	0.4467	2.0056	4.4883	0.0482
AL_6	-3.0353	0.1839	0.3007	2.1379	1.7903	0.1975
AL_7	2.8946	0.0245	0.0373	2.2402	0.0251	0.8757
AL_8	-16.9459	3.6726	0.3976	2.0569	3.3800	0.0825
R	0.1711	0.4510	0.1212	2.2252	0.2684	0.6106
AZI	-0.2930	0.0299	0.1357	2.2210	0.3380	0.5681
H	-0.4994	0.5660	0.1235	2.2245	0.2791	0.6036
ISI	0.7155	0.1501	0.1227	2.2248	0.2755	0.6060

TABLE 7.15: The statistical table of linear regression model comparing *VDB* indices with the log-Henry constant of PCBs.

However, we want to highlight here that one of the reasons could be the non-availability of sufficient experimental data for studying this property of PCBs. With this minimum data set, we see that the *AL* and *VDB* indices do not correlate well with the PCB's log Henry constant values. Thus, one may study the behaviour of AL_5 -index for this property as it performs better with a moderate 0.44 correlation value.

Finally as an overall observation for the PCB molecules, we have seen that AL_1 , AL_4 and AL_7 indices has an excellent correlation with the total surface area (*TSA*), log-water-solubility $\log Sw$,

Octanol water partition coefficient ($\log P$) and log-water-activity coefficient ($\log Y_w$) of PCBs. AL_5 does correlate moderately with log-Henry coefficient. While the other AL indices are performing relatively better.

Predictability Analysis

As a next step, we would like to focus on the four properties, namely the total surface area (TSA), log-water-solubility $\log Sw$, Octanol water partition coefficient ($\log P$) and log-water-activity coefficient ($\log Y_w$) and utilize the highest correlation ability of AL_1 to extend and predict the values of PCB compounds for which the experimental values does not exist.

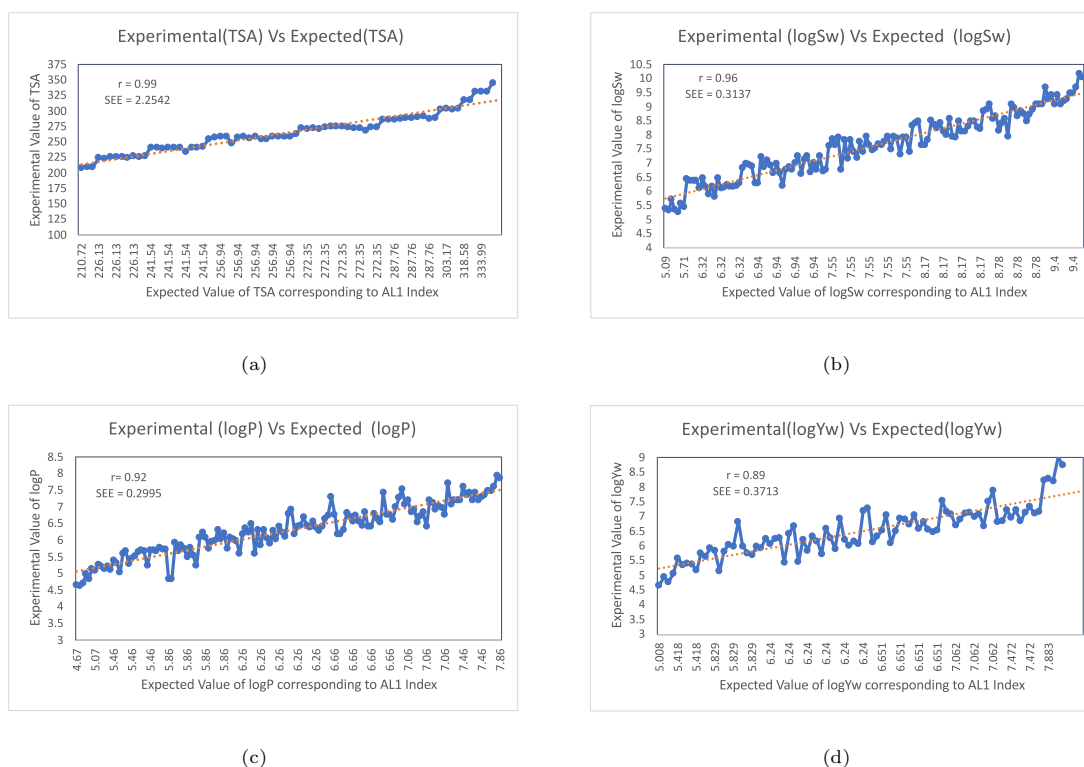


FIGURE 7.16: Experimental versus Expected Value of TSA , $\log Sw$, $\log P$ and $\log Y_w$ of PCBs.

To do this, firstly we compute the expected value for the TSA , $\log Sw$, $\log P$ and $\log Y_w$ by using the parameters obtained in Table 7.8, Table 7.9, Table 7.11 and Table 7.12. Next we compare the experimental and expected value of TSA , $\log Sw$, $\log P$ and $\log Y_w$ respectively, from the available data on PCB molecules.

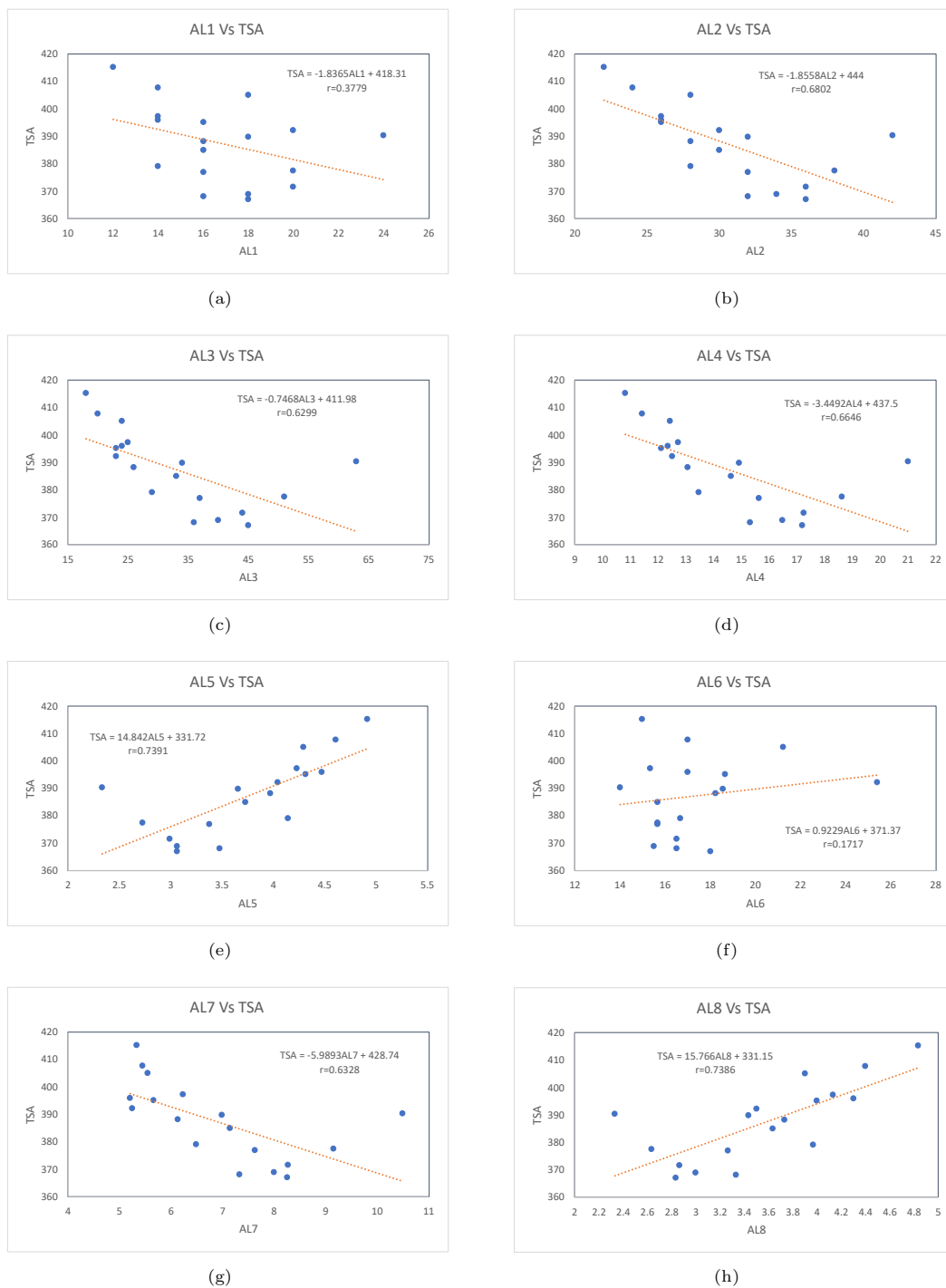
In Figure 7.16, we present the experimental vs expected plot for these 4 physicochemical properties against the AL_1 -index.

From the figure, it is pretty evident that the error (less than 0.37) between the experimental and expected values is significantly less for the $\log Sw$, $\log P$ and $\log Yw$ and the TSA has higher correlation of 99% which is significant high even though the error of 2.25 for a F value of 13360 is insignificant.

7.5 Summary

This chapter has introduced eight new topological indices labeled as AL_1 to AL_8 . We also have provided an easy method for computation of AL and VDB indices with the help of neighborhood matrix NM . We have studied the discriminative power of the proposed AL indices and compared the results with a few of the existing VDB indices. Among all the considered indices, four indices, namely AL_4 , AL_5 , AL_7 , and AL_8 have shown the highest discriminative power on the set of octane isomers. The indices AL_4 and AL_7 have the highest discriminative power on the set of PCB molecules compared to the other VDB indices. Further, the degeneracy study finds that the AL indices perform much better than the existing VDB indices in general.

Secondly, we also studied the correlation of AL indices with octane isomers and PCBs' physicochemical properties by fitting a linear regression curve for the data. As a result, we obtained that among all the proposed indices, AL_1 index correlates well with many physicochemical properties and that it exceeds the well-studied Randić index in all such cases. In particular, from the data, we find that AL_1 index has better-predicting power for acentric factor and entropy of octane isomers with a correlation value of 0.97 and 0.95, respectively. Similarly, for the PCBs, we find that AL_1 index has better predictive power for total surface area, log-water-solubility, relative retention time, octanol-water-partition, and log-water-activity coefficients with a correlation value of 0.997, 0.96, 0.95, 0.92, and 0.90, respectively.

FIGURE 7.6: *AL* indices Vs Total surface area of octane isomer.

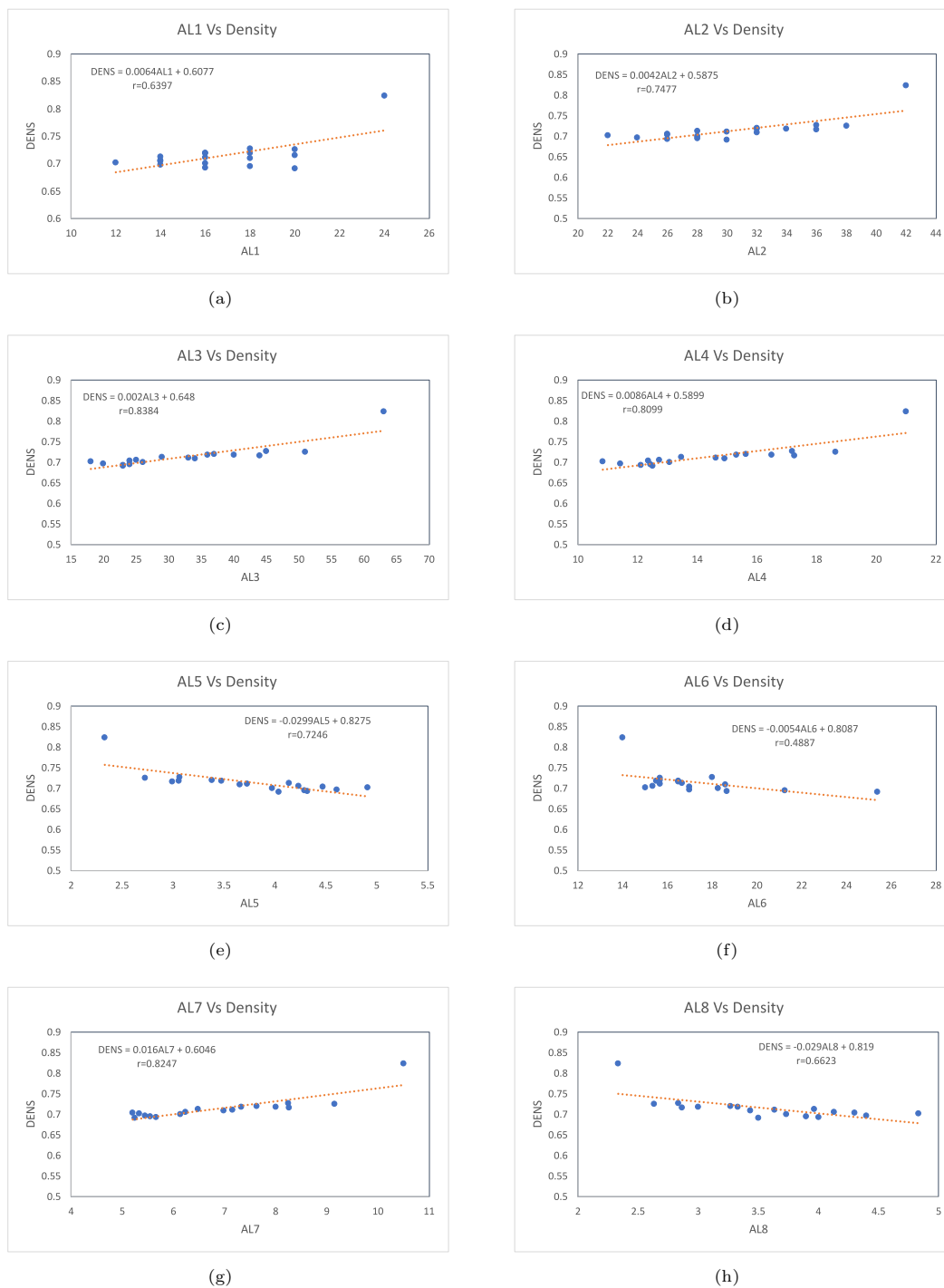


FIGURE 7.7: AL indices Vs Density of octane isomer.

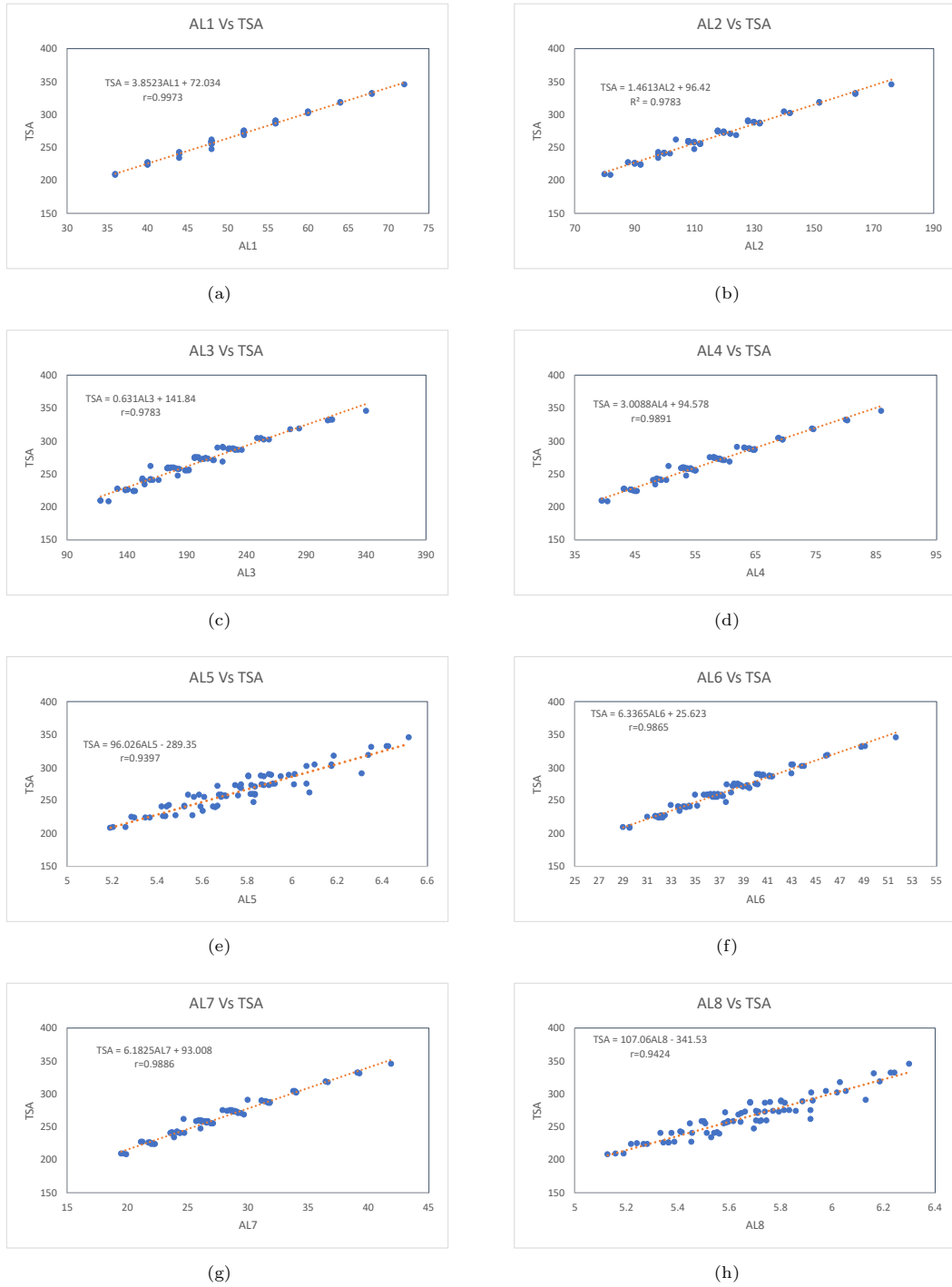
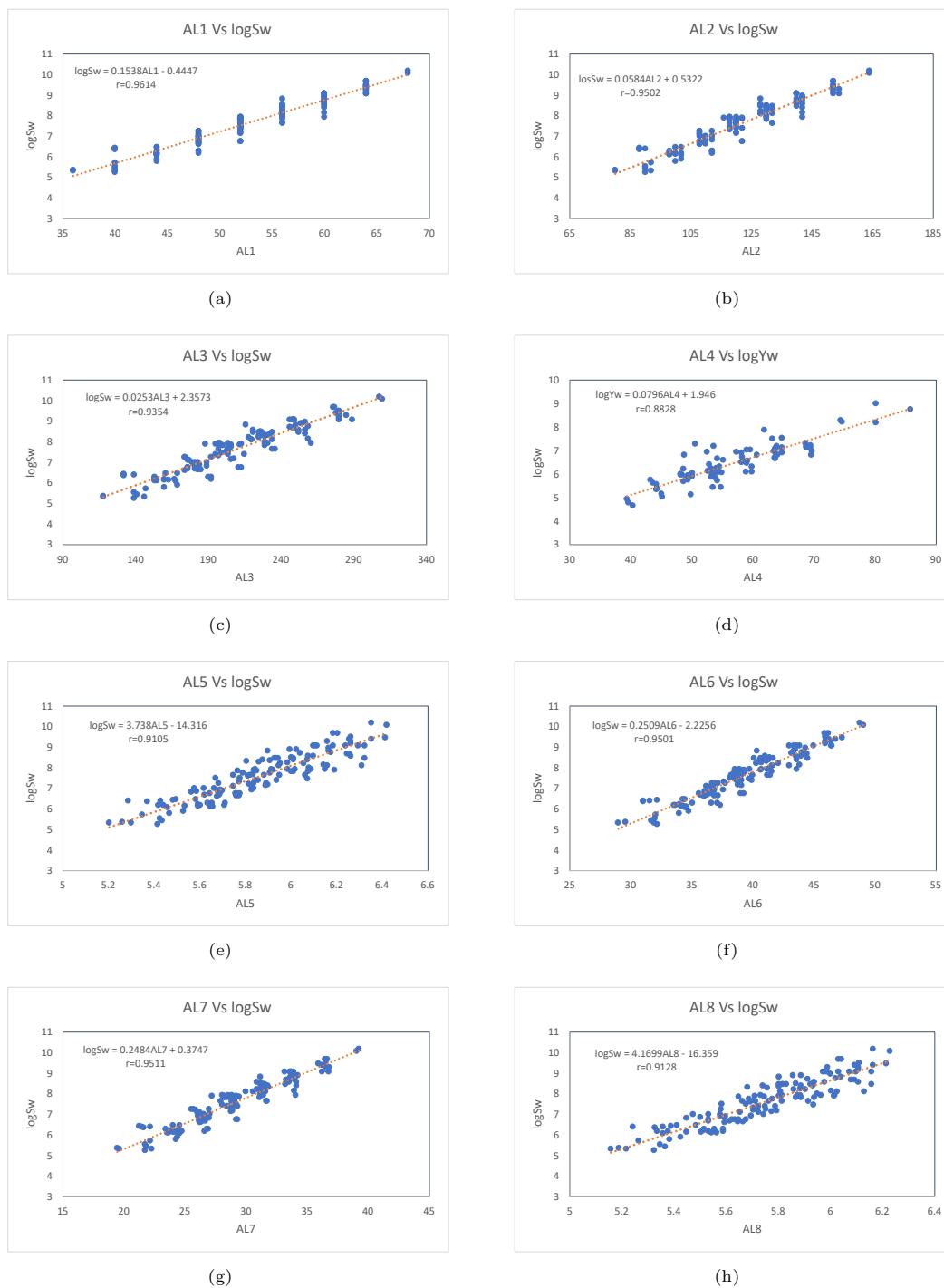


FIGURE 7.8: *AL* indices Vs total surface area (*TSA*) of PCBs.

FIGURE 7.9: AL indices Vs log water solubility ($\log Sw$) of PCBs.

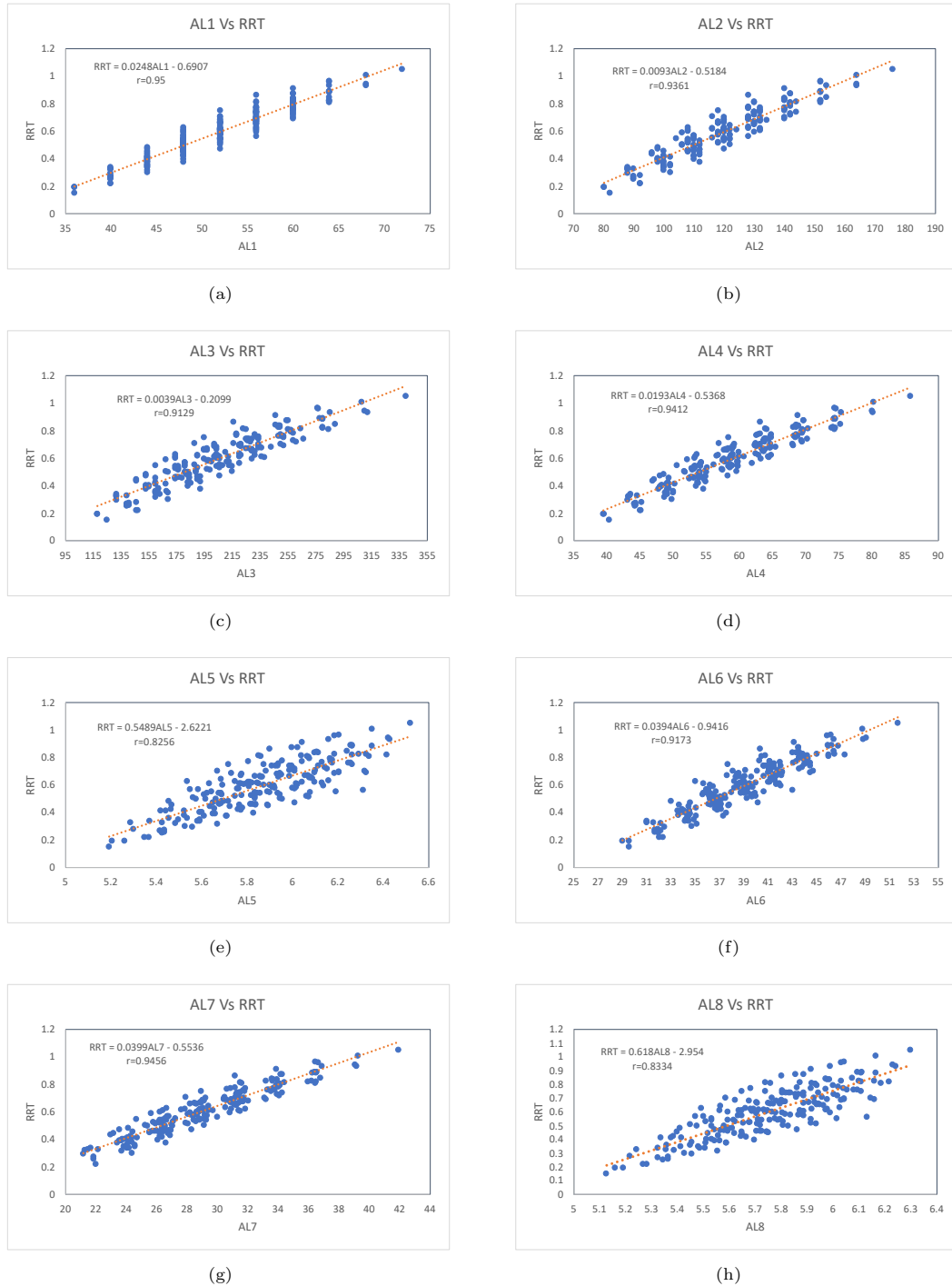
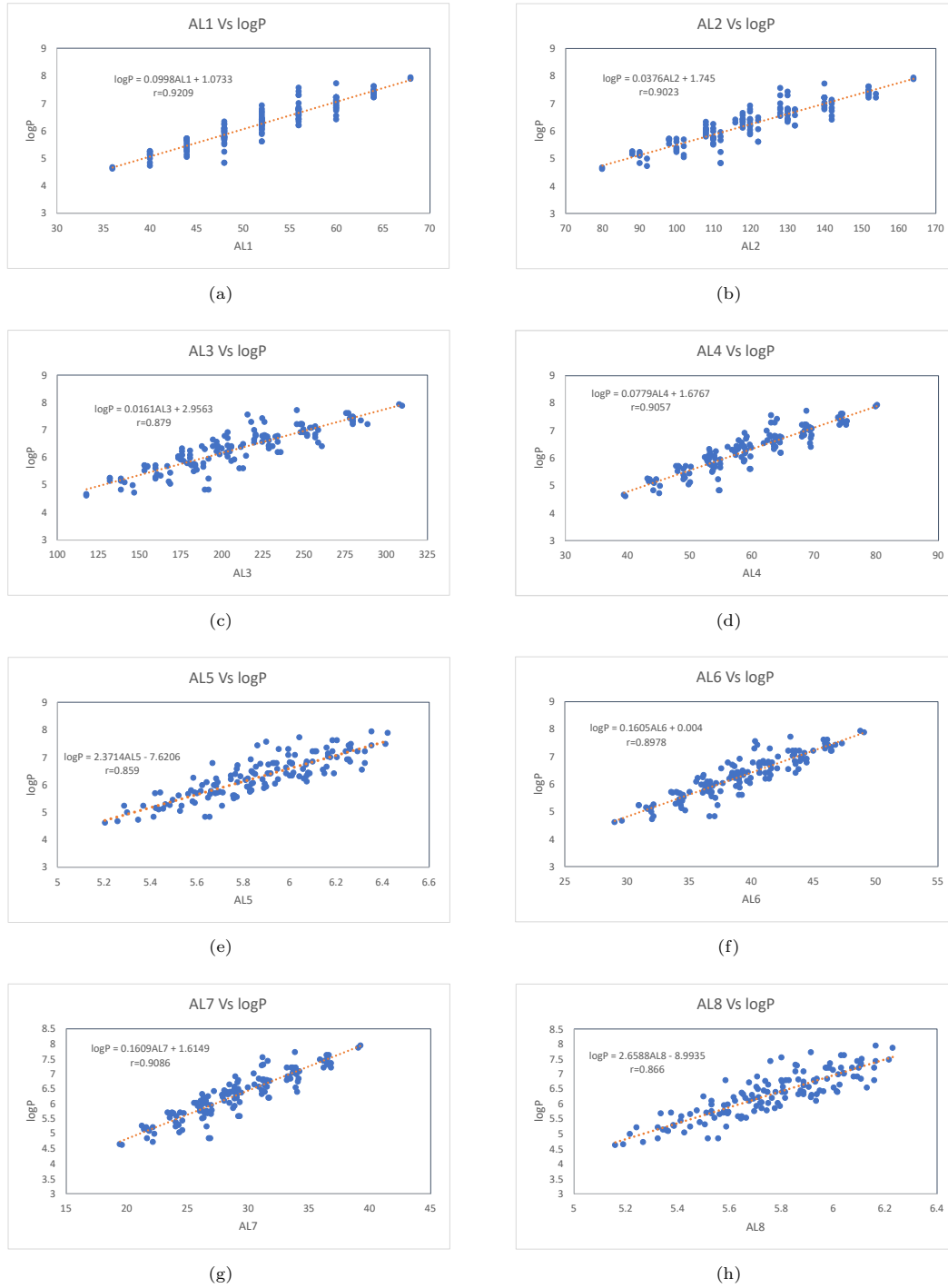
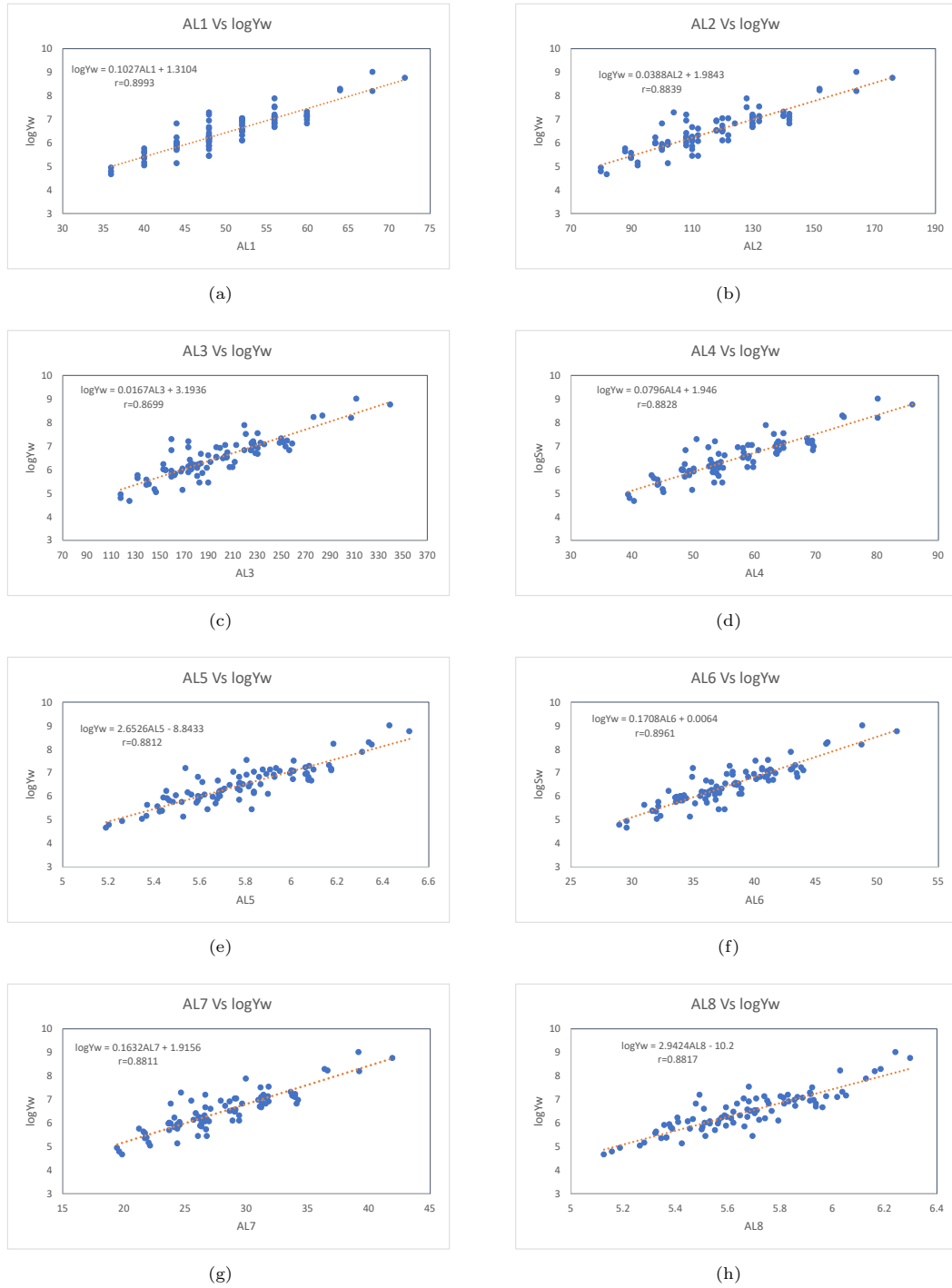


FIGURE 7.10: AL indices Vs relative retention time (RRT) of PCBs.

FIGURE 7.11: AL indices Vs octanol-water partition coefficient ($\log P$) of PCBs.

FIGURE 7.12: AL indices Vs log water activity coefficient ($\log Y_w$) PCB.

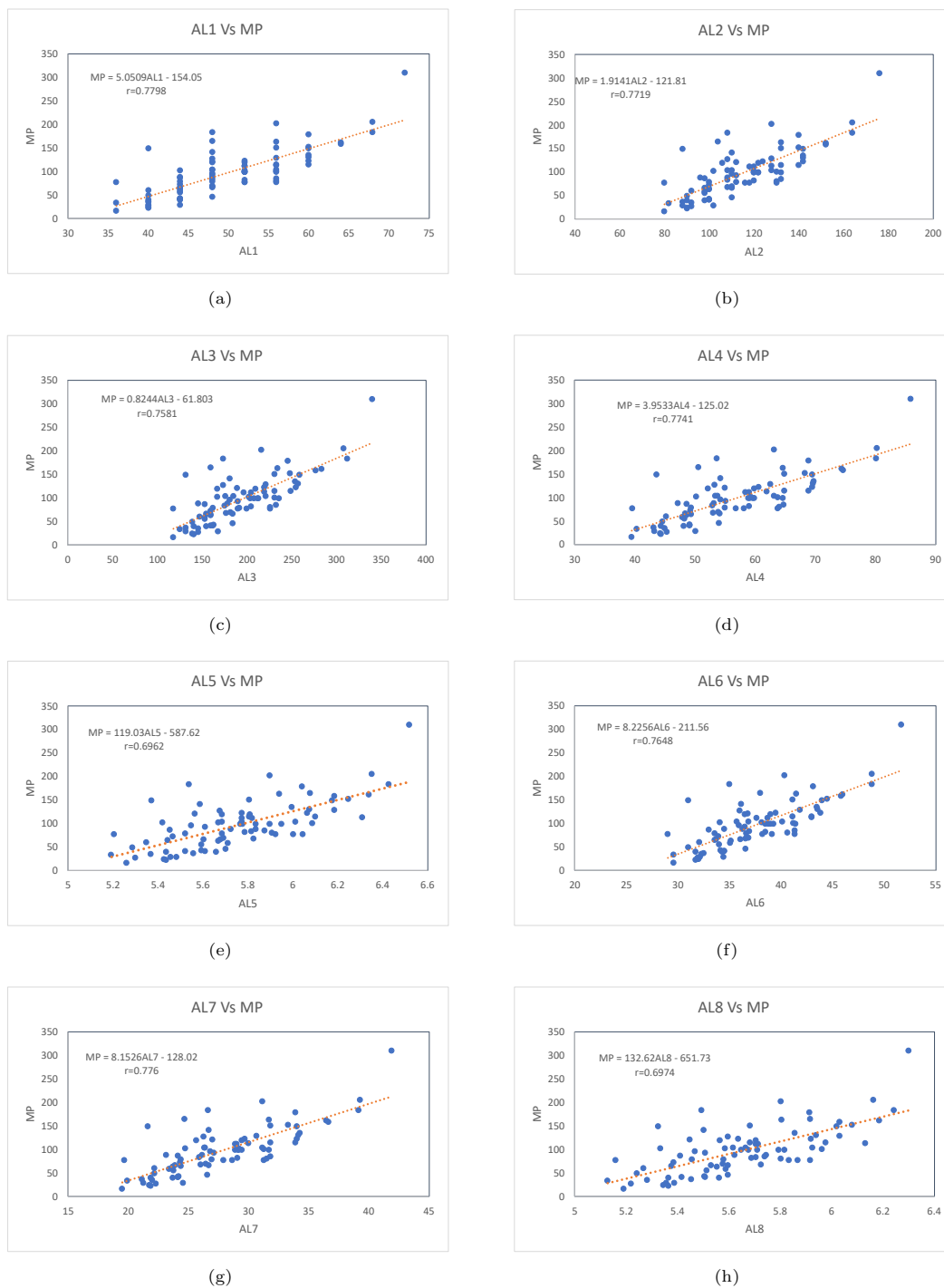
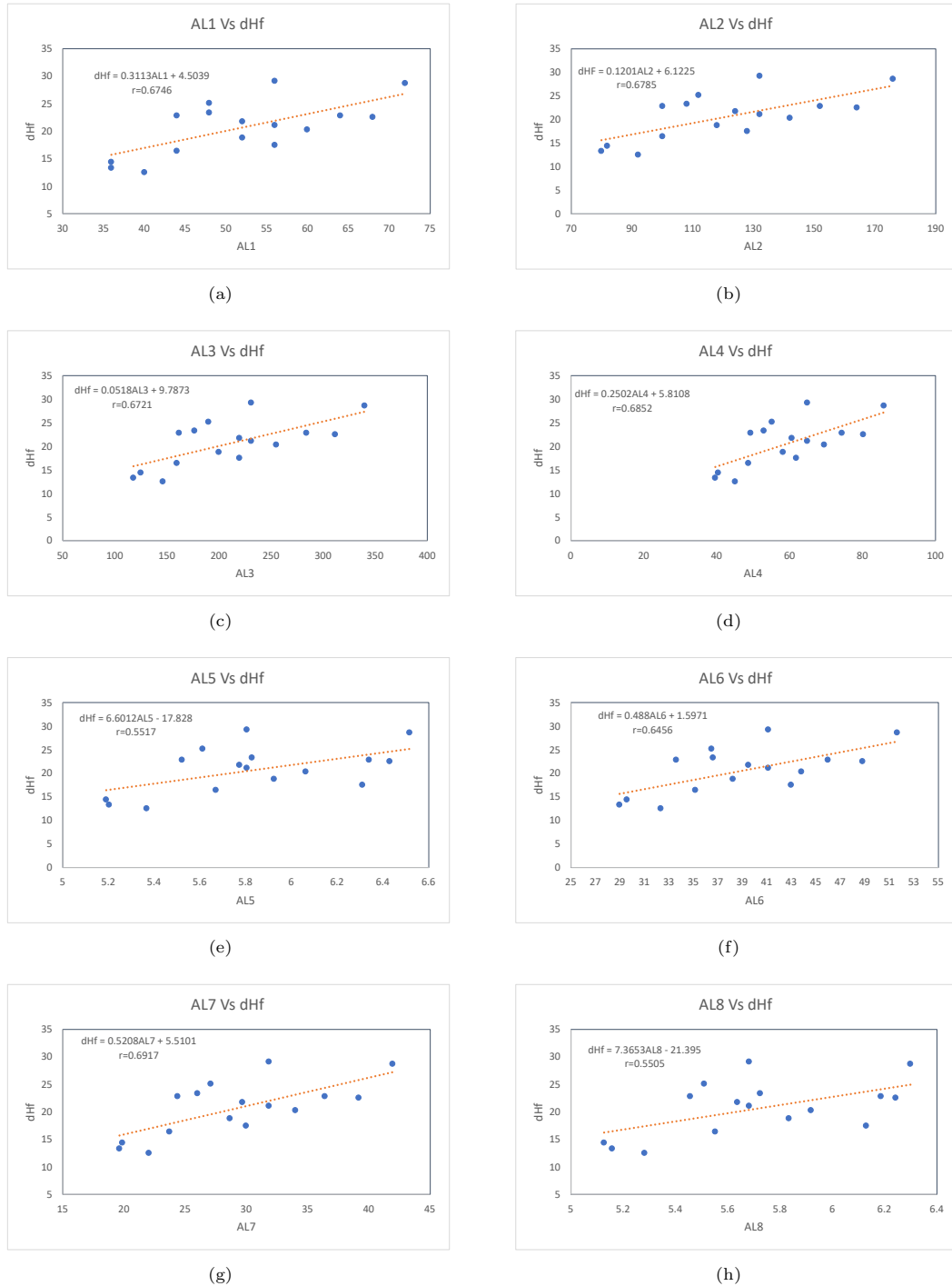
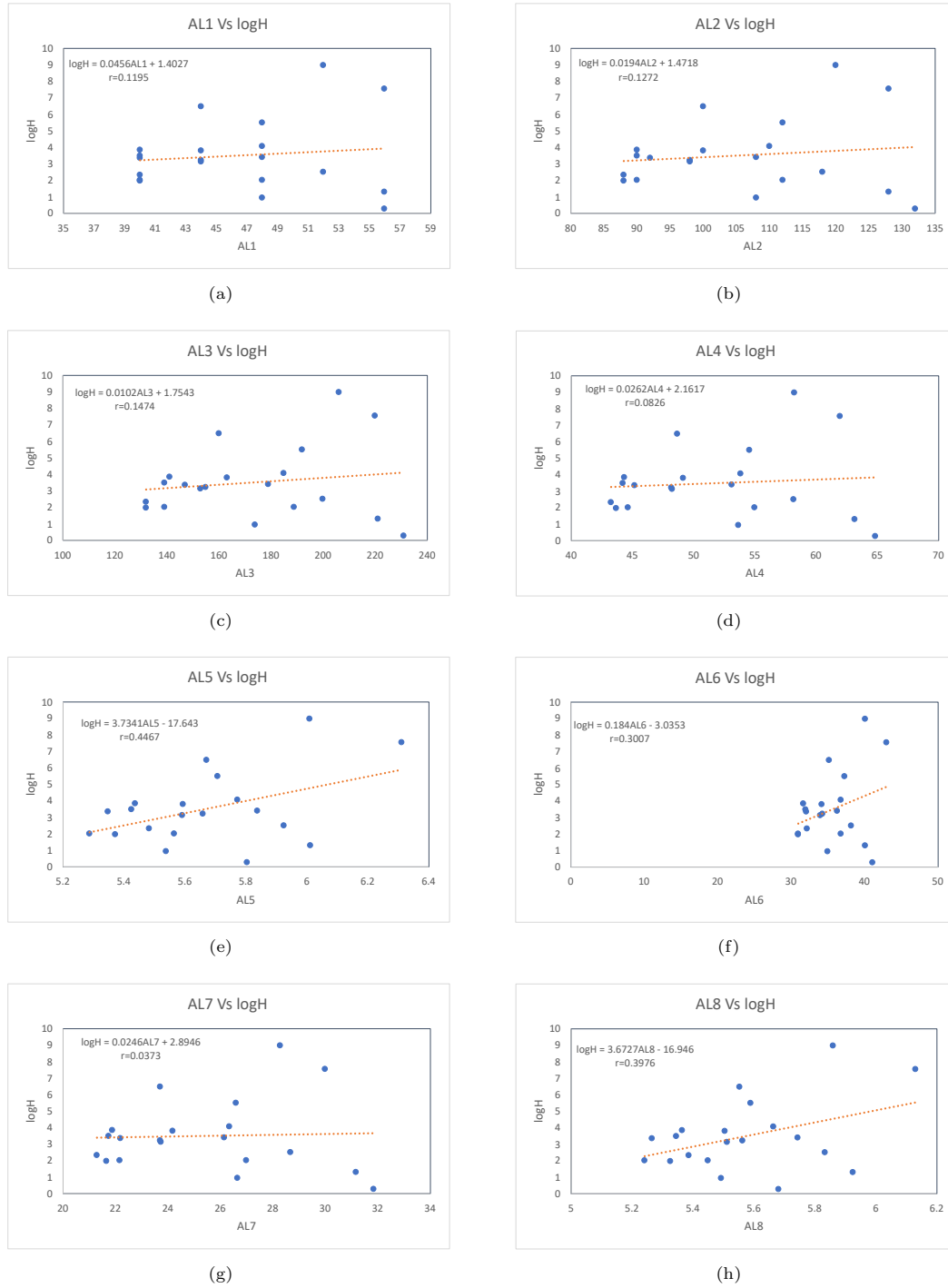


FIGURE 7.13: AL indices Vs Melting point of PCBs.

FIGURE 7.14: AL indices Vs relative enthalpy of formation (dHf) of PCBs.

FIGURE 7.15: *AL* indices Vs log Henry constant ($\log H$) of PCBs.

Appendix A

Octane Isomer

A.1 Physicochemical Properties of Octane Isomer

The data of physicochemical properties of octane isomer taken from the article [132] and the website <http://www.moleculardescriptors.eu>.

TABLE A.1: Experimental value of physicochemical properties of octane isomers

No.	MolID	Molecule	Acent Fac	S	HVAP	DHVAP	DENS	TSA
1	C8_01.hin	n-octane	0.397898	111.67	73.19	9.915	0.7025	415.3
2	C8_02.hin	2-methyl-heptane	0.377916	109.84	70.3	9.484	0.698	407.85
3	C8_03.hin	3-methyl-heptane	0.371002	111.26	71.3	9.521	0.7058	397.34
4	C8_04.hin	4-methyl-heptane	0.371504	109.32	70.91	9.483	0.7046	396.04
5	C8_05.hin	3-ethyl-hexane	0.362472	109.43	71.7	9.476	0.7136	379.04
6	C8_06.hin	2,2-dimethyl-hexane	0.339426	103.42	67.7	8.915	0.6953	405.11
7	C8_07.hin	2,3-dimethyl-hexane	0.348247	108.02	70.2	9.272	0.7121	384.93
8	C8_08.hin	2,4-dimethyl-hexane	0.344223	106.98	68.5	9.029	0.7004	388.11
9	C8_09.hin	2,5-dimethyl-hexane	0.35683	105.72	68.6	9.051	0.6935	395.08
10	C8_10.hin	3,3-dimethyl-hexane	0.322596	104.74	68.5	8.973	0.71	389.79
11	C8_11.hin	3,4-dimethyl-hexane	0.340345	106.59	70.2	9.316	0.72	376.91
12	C8_12.hin	2-methyl-3-ethyl-pentane	0.332433	106.06	69.7	9.209	0.7193	368.1
13	C8_13.hin	3-methyl-3-ethyl-pentane	0.306899	101.48	69.3	9.081	0.7274	366.99
14	C8_14.hin	2,2,3-trimethyl-pentane	0.300816	101.31	67.3	8.826	0.7161	371.75
15	C8_15.hin	2,2,4-trimethyl-pentane	0.30537	104.09	64.87	8.402	0.6919	392.19
16	C8_16.hin	2,3,3-trimethyl-pentane	0.293177	102.06	68.1	8.897	0.7262	377.4
17	C8_17.hin	2,3,4-trimethyl-pentane	0.317422	102.39	68.37	9.014	0.7191	368.93
18	C8_18.hin	2,2,3,3-tetramethylbutane	0.255294	93.06	66.2	8.41	0.8242	390.47

A.2 AL Indices for Octane Isomer

TABLE A.2: AL Index value of Octane isomers.

No.	MolID	Molecule	AL_1	AL_2	AL_3	AL_4	AL_5	AL_6	AL_7	AL_8
1	C8_01.hin	n-octane	12	22	18	10.8284	4.9142	15	5.3333	4.8333
2	C8_02.hin	2-methyl-heptane	14	24	20	11.4242	4.6069	17	5.45	4.4
3	C8_03.hin	3-methyl-heptane	14	26	25	12.7274	4.2307	15.3333	6.2333	4.1333
4	C8_04.hin	4-methyl-heptane	14	26	24	12.3631	4.4712	17	5.2	4.3
5	C8_05.hin	3-ethyl-hexane	14	28	29	13.4595	4.1414	16.6667	6.4833	3.9667
6	C8_06.hin	2,2-dimethyl-hexane	18	28	24	12.4388	4.2927	21.25	5.55	3.9
7	C8_07.hin	2,3-dimethyl-hexane	16	30	33	14.631	3.7272	15.6667	7.15	3.6333
8	C8_08.hin	2,4-dimethyl-hexane	16	28	26	13.0711	3.9749	18.25	6.1333	3.7333
9	C8_09.hin	2,5-dimethyl-hexane	16	26	23	12.121	4.3165	18.6667	5.6667	4
10	C8_10.hin	3,3-dimethyl-hexane	18	32	34	14.9089	3.6556	18.5833	6.9833	3.4333
11	C8_11.hin	3,4-dimethyl-hexane	16	32	37	15.6264	3.3805	15.6667	7.6333	3.2667
12	C8_12.hin	2-methyl-3-ethyl-pentane	16	32	36	15.3137	3.4749	16.5	7.3333	3.3333
13	C8_13.hin	3-methyl-3-ethyl-pentane	18	36	45	17.1962	3.0654	18	8.25	2.8333
14	C8_14.hin	2,2,3-trimethyl-pentane	20	36	44	17.248	2.9925	16.5	8.2667	2.8667
15	C8_15.hin	2,2,4-trimethyl-pentane	20	30	23	12.4967	4.0407	25.4	5.25	3.5
16	C8_16.hin	2,3,3-trimethyl-pentane	20	38	51	18.631	2.7272	15.6667	9.15	2.6333
17	C8_17.hin	2,3,4-trimethyl-pentane	18	34	40	16.4853	3.0607	15.5	8	3
18	C8_18.hin	2,2,3,3-tetramethylbutane	24	42	63	21	2.3333	14	10.5	2.3333

Appendix B

PolyChloroBiphenyl Congeners

B.1 Physicochemical Properties of PCB Congeners

In Table B.1, we present the experimental value of the physicochemical property of PCB taken from [126] and the expected values from our analysis (represented in bold font).

TABLE B.1: The bold values indicate the expected values of the PCB congeners for log-water solubility and octanol-water partition coefficient while the others are experimental data.

No.	MolID	Molecule	<i>MP</i>	<i>logH</i>	<i>dHf</i>	<i>logSw</i>	<i>logP</i>
1	PCB.001.HIN	2-chloro-1,1'-biphenyl	34		14.5	4.98	4.587
2	PCB.002.HIN	3-chloro-1,1'-biphenyl	16.5			5.39	4.66
3	PCB.003.HIN	4-chloro-1,1'-biphenyl	77.7		13.3	5.33	4.63
4	PCB.004.HIN	2,2'-dichloro-1,1'-biphenyl	60.5	3.37		5.72	4.72
5	PCB.005.HIN	2,3-dichloro-1,1'-biphenyl	28			5.35	4.99
6	PCB.006.HIN	2,3'-dichloro-1,1'-biphenyl				5.26	4.84
7	PCB.007.HIN	2,4-dichloro-1,1'-biphenyl	24.3	3.48		5.56	5.15
8	PCB.008.HIN	2,4'-dichloro-1,1'-biphenyl	40.5			5.46	5.09
9	PCB.009.HIN	2,5-dichloro-1,1'-biphenyl	23	3.88		5.67	5.037
10	PCB.010.HIN	2,6-dichloro-1,1'-biphenyl	35.5		12.6	5.67	4.996
11	PCB.011.HIN	3,3'-dichloro-1,1'-biphenyl	29	2.33		6.45	5.27
12	PCB.012.HIN	3,4-dichloro-1,1'-biphenyl	49.5	2.05		6.39	5.23
13	PCB.013.HIN	3,4'-dichloro-1,1'-biphenyl				6.4	5.15
14	PCB.014.HIN	3,5-dichloro-1,1'-biphenyl	36			5.73	5.078
15	PCB.015.HIN	4,4'-dichloro-1,1'-biphenyl	148.5	1.99		6.37	5.23
16	PCB.016.HIN	2,3,2'-trichloro-1,1'-biphenyl	28.5			6.1	5.12
17	PCB.017.HIN	2,4,2'-trichloro-1,1'-biphenyl				6.49	5.39
18	PCB.018.HIN	2,5,2'-trichloro-1,1'-biphenyl	43.5	3.8		6.17	5.33
19	PCB.019.HIN	2,6,2'-trichloro-1,1'-biphenyl				5.9	5.04
20	PCB.020.HIN	2,3,3'-trichloro-1,1'-biphenyl	42			6.3	5.6
21	PCB.021.HIN	2,3,4-trichloro-1,1'-biphenyl	101.5			6.18	5.68
22	PCB.022.HIN	2,3,4'-trichloro-1,1'-biphenyl	73.1			5.8	5.29
23	PCB.023.HIN	2,3,5-trichloro-1,1'-biphenyl	41			6.3	5.447
24	PCB.024.HIN	2,3,6-trichloro-1,1'-biphenyl				6.49	5.44
25	PCB.025.HIN	2,4,3'-trichloro-1,1'-biphenyl				6.11	5.54

No.	MolID	Molecule	MP	logH	dHf	logSw	logP
26	PCB_026.HIN	2,5,3'-trichloro-1,1'-biphenyl	40.3	3.25		6.14	5.65
27	PCB_027.HIN	2,6,3'-trichloro-1,1'-biphenyl				6.3	5.447
28	PCB_028.HIN	2,4,4'-trichloro-1,1'-biphenyl	56	3.16		6.22	5.71
29	PCB_029.HIN	2,4,5-trichloro-1,1'-biphenyl	78.5		22.8	6.3	5.447
30	PCB_030.HIN	2,4,6-trichloro-1,1'-biphenyl	62.5	6.49	16.5	6.3	5.447
31	PCB_031.HIN	2,5,4'-trichloro-1,1'-biphenyl	67			6.18	5.68
32	PCB_032.HIN	2,6,4'-trichloro-1,1'-biphenyl				6.16	5.24
33	PCB_033.HIN	2,3',4'-trichloro-1,1'-biphenyl	65.5			6.21	5.71
34	PCB_034.HIN	2,3',5'-trichloro-1,1'-biphenyl	58			6.3	5.71
35	PCB_035.HIN	3,4,3'-trichloro-1,1'-biphenyl				6.36	5.488
36	PCB_036.HIN	3,5,3'-trichloro-1,1'-biphenyl				6.42	5.529
37	PCB_037.HIN	3,4,4'-trichloro-1,1'-biphenyl	87.3			6.36	5.488
38	PCB_038.HIN	3,4,5-trichloro-1,1'-biphenyl				6.3	5.447
39	PCB_039.HIN	3,5,4'-trichloro-1,1'-biphenyl	88			6.42	5.529
40	PCB_040.HIN	2,3,2',3'-tetrachloro-1,1'-biphenyl	120.9	2.02		6.83	5.67
41	PCB_041.HIN	2,3,4,2'-tetrachloro-1,1'-biphenyl				7	5.79
42	PCB_042.HIN	2,3,2',4'-tetrachloro-1,1'-biphenyl	69			6.96	5.72
43	PCB_043.HIN	2,3,5,2'-tetrachloro-1,1'-biphenyl				6.93	5.856
44	PCB_044.HIN	2,3,2',5'-tetrachloro-1,1'-biphenyl	46.8			6.91	5.73
45	PCB_045.HIN	2,3,6,2'-tetrachloro-1,1'-biphenyl				6.3	4.84
46	PCB_046.HIN	2,3,2',6'-tetrachloro-1,1'-biphenyl				6.3	4.84
47	PCB_047.HIN	2,4,2',4'-tetrachloro-1,1'-biphenyl	83			7.23	5.94
48	PCB_048.HIN	2,4,5,2'-tetrachloro-1,1'-biphenyl	66			6.86	5.69
49	PCB_049.HIN	2,4,2',5'-tetrachloro-1,1'-biphenyl	67.8		23.4	7.12	5.87
50	PCB_050.HIN	2,4,6,2'-tetrachloro-1,1'-biphenyl				6.94	5.75
51	PCB_051.HIN	2,4,2',6'-tetrachloro-1,1'-biphenyl				6.65	5.51
52	PCB_052.HIN	2,5,2',5'-tetrachloro-1,1'-biphenyl	88	3.42		7	5.79
53	PCB_053.HIN	2,5,2',6'-tetrachloro-1,1'-biphenyl	103.7	4.06		6.65	5.55
54	PCB_054.HIN	2,6,2',6'-tetrachloro-1,1'-biphenyl		5.5		6.2	5.24
55	PCB_055.HIN	2,3,4,3'-tetrachloro-1,1'-biphenyl				6.77	6.1
56	PCB_056.HIN	2,3,3',4'-tetrachloro-1,1'-biphenyl	96.5			6.93	5.856
57	PCB_057.HIN	2,3,5,3'-tetrachloro-1,1'-biphenyl				6.99	5.897
58	PCB_058.HIN	2,3,3',5'-tetrachloro-1,1'-biphenyl				6.99	5.897
59	PCB_059.HIN	2,3,6,3'-tetrachloro-1,1'-biphenyl				6.93	5.856
60	PCB_060.HIN	2,3,4,4'-tetrachloro-1,1'-biphenyl	142			6.86	6.24
61	PCB_061.HIN	2,3,4,5-tetrachloro-1,1'-biphenyl	92.3		25.2	6.86	5.815
62	PCB_062.HIN	2,3,4,6-tetrachloro-1,1'-biphenyl				6.86	5.815
63	PCB_063.HIN	2,3,5,4'-tetrachloro-1,1'-biphenyl				6.77	6.1
64	PCB_064.HIN	2,3,6,4'-tetrachloro-1,1'-biphenyl				7.02	5.76
65	PCB_065.HIN	2,3,5,6-tetrachloro-1,1'-biphenyl	79			7.25	5.96

No.	MolID	Molecule	MP	logH	dHf	logSw	logP
66	PCB.066.HIN	2,4,3',4'-tetrachloro-1,1'-biphenyl	127.3			6.63	5.98
67	PCB.067.HIN	2,4,5,3'-tetrachloro-1,1'-biphenyl				7.13	6.32
68	PCB.068.HIN	2,4,3',5'-tetrachloro-1,1'-biphenyl				7.05	5.938
69	PCB.069.HIN	2,4,6,3'-tetrachloro-1,1'-biphenyl				7.26	6.03
70	PCB.070.HIN	2,5,3',4'-tetrachloro-1,1'-biphenyl	104			6.69	6.22
71	PCB.071.HIN	2,6,3',4'-tetrachloro-1,1'-biphenyl				7.02	5.76
72	PCB.072.HIN	2,5,3',5'-tetrachloro-1,1'-biphenyl				7.05	5.938
73	PCB.073.HIN	2,6,3',5'-tetrachloro-1,1'-biphenyl				6.991	5.897
74	PCB.074.HIN	2,4,5,4'-tetrachloro-1,1'-biphenyl				6.77	6.1
75	PCB.075.HIN	2,4,6,4'-tetrachloro-1,1'-biphenyl				7.26	6.03
76	PCB.076.HIN	2,3',4',5'-tetrachloro-1,1'-biphenyl				6.71	5.98
77	PCB.077.HIN	3,4,3',4'-tetrachloro-1,1'-biphenyl	183	0.94		6.991	5.897
78	PCB.078.HIN	3,4,5,3'-tetrachloro-1,1'-biphenyl				6.991	5.897
79	PCB.079.HIN	3,4,3',5'-tetrachloro-1,1'-biphenyl	119.5			7.05	5.938
80	PCB.080.HIN	3,5,3',5'-tetrachloro-1,1'-biphenyl	164			7.117	5.979
81	PCB.081.HIN	3,4,5,4'-tetrachloro-1,1'-biphenyl				6.992	5.897
82	PCB.082.HIN	2,3,4,2',3'-pentachloro-1,1'-biphenyl	119.7			7.494	6.224
83	PCB.083.HIN	2,3,5,2',3'-pentachloro-1,1'-biphenyl				7.557	6.265
84	PCB.084.HIN	2,3,6,2',3'-pentachloro-1,1'-biphenyl				6.78	5.6
85	PCB.085.HIN	2,3,4,2',4'-pentachloro-1,1'-biphenyl				7.62	6.18
86	PCB.086.HIN	2,3,4,5,2'-pentachloro-1,1'-biphenyl	99.9			7.87	6.38
87	PCB.087.HIN	2,3,4,2',5'-pentachloro-1,1'-biphenyl	112.3			7.66	6.23
88	PCB.088.HIN	2,3,4,6,2'-pentachloro-1,1'-biphenyl	99.9			7.92	6.5
89	PCB.089.HIN	2,3,4,2',6'-pentachloro-1,1'-biphenyl				6.78	5.6
90	PCB.090.HIN	2,3,5,2',4'-pentachloro-1,1'-biphenyl				7.82	6.32
91	PCB.091.HIN	2,3,6,2',4'-pentachloro-1,1'-biphenyl				7.17	5.87
92	PCB.092.HIN	2,3,5,2',5'-pentachloro-1,1'-biphenyl				7.82	6.32
93	PCB.093.HIN	2,3,5,6,2'-pentachloro-1,1'-biphenyl				7.4	6.06
94	PCB.094.HIN	2,3,5,2',6'-pentachloro-1,1'-biphenyl				7.557	6.265
95	PCB.095.HIN	2,3,6,2',5'-pentachloro-1,1'-biphenyl	99.2			7.19	5.92
96	PCB.096.HIN	2,3,6,2',6'-pentachloro-1,1'-biphenyl				7.494	6.225
97	PCB.097.HIN	2,3,2',4',5'-pentachloro-1,1'-biphenyl	81.5			7.76	6.3
98	PCB.098.HIN	2,3,2',4',6'-pentachloro-1,1'-biphenyl				7.4	6.04
99	PCB.099.HIN	2,4,5,2',4'-pentachloro-1,1'-biphenyl				7.95	6.41
100	PCB.100.HIN	2,4,6,2',4'-pentachloro-1,1'-biphenyl				7.66	6.23
101	PCB.101.HIN	2,4,5,2',5'-pentachloro-1,1'-biphenyl	77	2.51	18.8	7.62	6.306
102	PCB.102.HIN	2,4,5,2',6'-pentachloro-1,1'-biphenyl				7.557	6.265
103	PCB.103.HIN	2,4,6,2',5'-pentachloro-1,1'-biphenyl				7.47	6.11
104	PCB.104.HIN	2,4,6,2',6'-pentachloro-1,1'-biphenyl		8.97		7.557	6.265
105	PCB.105.HIN	2,3,4,3',4'-pentachloro-1,1'-biphenyl	103			7.52	6.79

No.	MolID	Molecule	MP	logH	dHf	logSw	logP
106	PCB.106.HIN	2,3,4,5,3'-pentachloro-1,1'-biphenyl				7.68	6.92
107	PCB.107.HIN	2,3,5,3',4'-pentachloro-1,1'-biphenyl				7.62	6.306
108	PCB.108.HIN	2,3,4,3',5'-pentachloro-1,1'-biphenyl				7.62	6.306
109	PCB.109.HIN	2,3,4,6,3'-pentachloro-1,1'-biphenyl				7.557	6.265
110	PCB.110.HIN	2,3,6,3',4'-pentachloro-1,1'-biphenyl				7.65	6.2
111	PCB.111.HIN	2,3,5,3',5'-pentachloro-1,1'-biphenyl				7.683	6.347
112	PCB.112.HIN	2,3,5,6,3'-pentachloro-1,1'-biphenyl				7.76	6.41
113	PCB.113.HIN	2,3,6,3',5'-pentachloro-1,1'-biphenyl				7.95	6.45
114	PCB.114.HIN	2,3,4,5,4'-pentachloro-1,1'-biphenyl	98.5			7.5	6.71
115	PCB.115.HIN	2,3,4,6,4'-pentachloro-1,1'-biphenyl				7.96	6.44
116	PCB.116.HIN	2,3,4,5,6-pentachloro-1,1'-biphenyl	123		21.8	7.43	6.184
117	PCB.117.HIN	2,3,5,6,4'-pentachloro-1,1'-biphenyl				7.88	6.39
118	PCB.118.HIN	2,4,5,3',4'-pentachloro-1,1'-biphenyl	111.5			7.33	6.57
119	PCB.119.HIN	2,4,6,3',4'-pentachloro-1,1'-biphenyl				7.91	6.4
120	PCB.120.HIN	2,4,5,3',5'-pentachloro-1,1'-biphenyl	76.9			7.683	6.3
121	PCB.121.HIN	2,4,6,3',5'-pentachloro-1,1'-biphenyl				7.92	6.42
122	PCB.122.HIN	2,3,3',4',5'-pentachloro-1,1'-biphenyl				7.557	6.265
123	Pcb.123.hin	2,4,3',4',5'-pentachloro-1,1'-biphenyl				7.42	6.64
124	PCB.124.HIN	2,5,3',4',5'-pentachloro-1,1'-biphenyl				7.62	6.306
125	PCB.125.HIN	2,6,3',4',5'-pentachloro-1,1'-biphenyl				7.557	6.266
126	PCB.126.HIN	3,4,5,3',4'-pentachloro-1,1'-biphenyl				7.62	6.306
127	PCB.127.HIN	3,4,5,3',5'-pentachloro-1,1'-biphenyl				7.683	6.347
128	PCB.128.HIN	2,3,4,2',3',4'-hexachloro-1,1'-biphenyl	150	0.302	29.2	8.33	6.634
129	PCB.129.HIN	2,3,4,5,2',3'-hexachloro-1,1'-biphenyl	84.9			8.42	6.76
130	PCB.130.HIN	2,3,4,2',3',5'-hexachloro-1,1'-biphenyl				8.185	7.3
131	PCB.131.HIN	2,3,4,6,2',3'-hexachloro-1,1'-biphenyl				8.48	6.78
132	PCB.132.HIN	2,3,4,2',3',6'-hexachloro-1,1'-biphenyl				7.65	6.2
133	PCB.133.HIN	2,3,5,2',3',5'-hexachloro-1,1'-biphenyl	128.5			8.248	6.716
134	PCB.134.HIN	2,3,5,6,2',3'-hexachloro-1,1'-biphenyl	99.9			7.65	6.2
135	PCB.135.HIN	2,3,5,2',3',6'-hexachloro-1,1'-biphenyl				7.82	6.32
136	PCB.136.HIN	2,3,6,2',3',6'-hexachloro-1,1'-biphenyl	114.3		21.1	8.123	6.634
137	PCB.137.HIN	2,3,4,5,2',4'-hexachloro-1,1'-biphenyl	77.5			8.52	6.82
138	PCB.138.HIN	2,3,4,2',4',5'-hexachloro-1,1'-biphenyl	81			8.38	6.73
139	PCB.139.HIN	2,3,4,6,2',4'-hexachloro-1,1'-biphenyl				8.185	6.675
140	PCB.140.HIN	2,3,4,2',4',6'-hexachloro-1,1'-biphenyl				8.24	6.58
141	PCB.141.HIN	2,3,4,5,2',5'-hexachloro-1,1'-biphenyl				8.42	6.75
142	PCB.142.HIN	2,3,4,5,6,2'-hexachloro-1,1'-biphenyl				8.06	6.593
143	PCB.143.HIN	2,3,4,5,2',6'-hexachloro-1,1'-biphenyl				8.13	6.56
144	PCB.144.HIN	2,3,4,6,2',5'-hexachloro-1,1'-biphenyl				8.01	6.45
145	PCB.145.HIN	2,3,4,6,2',6'-hexachloro-1,1'-biphenyl				8.123	6.634

No.	MolID	Molecule	MP	logH	dHf	logSw	logP
146	PCB_146.HIN	2,3,5,2',4',5'-hexachloro-1,1'-biphenyl				8.58	6.85
147	PCB_147.HIN	2,3,5,6,2',4'-hexachloro-1,1'-biphenyl				8.185	6.675
148	PCB_148.HIN	2,3,5,2',4',6'-hexachloro-1,1'-biphenyl				8.248	6.716
149	PCB_149.HIN	2,3,6,2',4',5'-hexachloro-1,1'-biphenyl				7.94	6.41
150	PCB_150.HIN	2,3,6,2',4',6'-hexachloro-1,1'-biphenyl				8.185	6.675
151	PCB_151.HIN	2,3,5,6,2',5'-hexachloro-1,1'-biphenyl	100.5			7.93	6.42
152	PCB_152.HIN	2,3,5,6,2',6'-hexachloro-1,1'-biphenyl				8.123	6.634
153	PCB_153.HIN	2,4,5,2',4',5'-hexachloro-1,1'-biphenyl	103.5	1.32		8.49	6.8
154	PCB_154.HIN	2,4,5,2',4',6'-hexachloro-1,1'-biphenyl				8.12	6.65
155	PCB_155.HIN	2,4,6,2',4',6'-hexachloro-1,1'-biphenyl	112.5	7.55	17.5	8.12	6.54
156	PCB_156.HIN	2,3,4,5,3',4'-hexachloro-1,1'-biphenyl				8.31	7.44
157	PCB_157.HIN	2,3,4,3',4',5'-hexachloro-1,1'-biphenyl				8.185	6.675
158	PCB_158.HIN	2,3,4,6,3',4'-hexachloro-1,1'-biphenyl				8.48	6.78
159	PCB_159.HIN	2,3,4,5,3',5'-hexachloro-1,1'-biphenyl				8.248	6.716
160	PCB_160.HIN	2,3,4,5,6,3'-hexachloro-1,1'-biphenyl				8.123	6.634
161	PCB_161.HIN	2,3,4,6,3',5'-hexachloro-1,1'-biphenyl				8.248	6.716
162	PCB_162.HIN	2,3,5,3',4',5'-hexachloro-1,1'-biphenyl				8.248	6.716
163	PCB_163.HIN	2,3,5,6,3',4'-hexachloro-1,1'-biphenyl				8.48	6.78
164	PCB_164.HIN	2,3,6,3',4',5'-hexachloro-1,1'-biphenyl				8.27	6.63
165	PCB_165.HIN	2,3,5,6,3',5'-hexachloro-1,1'-biphenyl				8.248	7
166	PCB_166.HIN	2,3,4,5,6,4'-hexachloro-1,1'-biphenyl	162.5			8.123	6.634
167	PCB_167.HIN	2,4,5,3',4',5'-hexachloro-1,1'-biphenyl				8.21	7.29
168	PCB_168.HIN	2,4,6,3',4',5'-hexachloro-1,1'-biphenyl				8.248	6.716
169	PCB_169.HIN	3,4,5,3',4',5'-hexachloro-1,1'-biphenyl	201.5			8.85	7.55
170	PCB_170.HIN	2,3,4,5,2',3',4'-heptachloro-1,1'-biphenyl	135			8.9	7.08
171	PCB_171.HIN	2,3,4,6,2',3',4'-heptachloro-1,1'-biphenyl	122.3		20.3	8.751	7.043
172	PCB_172.HIN	2,3,4,5,2',3',5'-heptachloro-1,1'-biphenyl				9.1	7.21
173	PCB_173.HIN	2,3,4,5,6,2',3'-heptachloro-1,1'-biphenyl				8.688	7.002
174	PCB_174.HIN	2,3,4,5,2',3',6'-heptachloro-1,1'-biphenyl	130.6			8.59	6.85
175	PCB_175.HIN	2,3,4,6,2',3',5'-heptachloro-1,1'-biphenyl				8.68	6.92
176	PCB_176.HIN	2,3,4,6,2',3',6'-heptachloro-1,1'-biphenyl				8.15	6.55
177	PCB_177.HIN	2,3,4,2',3',5',6'-heptachloro-1,1'-biphenyl				8.42	6.73
178	PCB_178.HIN	2,3,5,6,2',3',5'-heptachloro-1,1'-biphenyl				8.59	6.85
179	PCB_179.HIN	2,3,5,6,2',3',6'-heptachloro-1,1'-biphenyl				7.94	6.41
180	PCB_180.HIN	2,3,4,5,2',4',5'-heptachloro-1,1'-biphenyl	114.5			9.1	7.21
181	PCB_181.HIN	2,3,4,5,6,2',4'-heptachloro-1,1'-biphenyl				8.97	7.13
182	PCB_182.HIN	2,3,4,5,2',4',6'-heptachloro-1,1'-biphenyl	152.5			8.68	6.92
183	PCB_183.HIN	2,3,4,6,2',4',5'-heptachloro-1,1'-biphenyl				8.85	7.04
184	PCB_184.HIN	2,3,4,6,2',4',6'-heptachloro-1,1'-biphenyl				8.814	7.084
185	PCB_185.HIN	2,3,4,5,6,2',5'-heptachloro-1,1'-biphenyl	148.5			8.75	6.99

No.	MolID	Molecule	MP	logH	dHf	logSw	logP
186	PCB.186.HIN	2,3,4,5,6,2',6'-heptachloro-1,1'-biphenyl				8.688	7.002
187	PCB.187.HIN	2,3,5,6,2',4',5'-heptachloro-1,1'-biphenyl				8.814	7.084
188	PCB.188.HIN	2,3,5,6,2',4',6'-heptachloro-1,1'-biphenyl				8.49	6.78
189	PCB.189.HIN	2,3,4,5,3',4',5'-heptachloro-1,1'-biphenyl	178			8.72	7.72
190	PCB.190.HIN	2,3,4,5,6,3',4'-heptachloro-1,1'-biphenyl				8.9	7.08
191	PCB.191.HIN	2,3,4,6,3',4',5'-heptachloro-1,1'-biphenyl				9.1	7.21
192	PCB.192.HIN	2,3,4,5,6,3',5'-heptachloro-1,1'-biphenyl				9.1	7.21
193	PCB.193.HIN	2,3,5,6,3',4',5'-heptachloro-1,1'-biphenyl				9.1	7.21
194	PCB.194.HIN	2,3,4,5,2',3',4',5'-octachloro-1,1'-biphenyl	159			9.7	7.62
195	PCB.195.HIN	2,3,4,5,6,2',3',4'-octachloro-1,1'-biphenyl				9.29	7.35
196	PCB.196.HIN	2,3,4,5,2',3',4',6'-octachloro-1,1'-biphenyl				9.42	7.43
197	PCB.197.HIN	2,3,4,6,2',3',4',6'-octachloro-1,1'-biphenyl				9.1	7.21
198	PCB.198.HIN	2,3,4,5,6,2',3',5'-octachloro-1,1'-biphenyl				9.42	7.43
199	PCB.199.HIN	2,3,4,5,6,2',3',6'-octachloro-1,1'-biphenyl				9.1	7.21
200	PCB.200.HIN	2,3,4,6,2',3',5',6'-octachloro-1,1'-biphenyl				9.2	7.3
201	PCB.201.HIN	2,3,4,5,2',3',5',6'-octachloro-1,1'-biphenyl				9.29	7.35
202	PCB.202.HIN	2,3,5,6,2',3',5',6'-octachloro-1,1'-biphenyl	161		22.8	9.379	7.452
203	PCB.203.HIN	2,3,4,5,6,2',4',5'-octachloro-1,1'-biphenyl				9.5	7.49
204	PCB.204.HIN	2,3,4,5,6,2',4',6'-octachloro-1,1'-biphenyl				9.48	7.48
205	PCB.205.HIN	2,3,4,5,6,3',4',5'-octachloro-1,1'-biphenyl				9.7	7.62
206	PCB.206.HIN	2,3,4,5,6,2',3',4',5'-nonachloro-1,1'-biphenyl	206			10.18	7.94
207	PCB.207.HIN	2,3,4,5,6,2',3',4',6'-nonachloro-1,1'-biphenyl				10.07	7.88
208	PCB.208.HIN	2,3,4,5,6,2',3',5',6'-nonachloro-1,1'-biphenyl	182.7		22.6	9.945	7.821
209	PCB.209.HIN	2,3,4,5,6,2',3',4',5',6'-decachloro-1,1'-biphenyl	310		28.7	10.51	8.189

B.2 AL Indices for PCB Congeners

TABLE B.2: AL Index value of Polychlorobiphenyls (PCBs).

No.	MolID	Molecule	AL_1	AL_2	AL_3	AL_4	AL_5	AL_6	AL_7	AL_8
1	PCB_001.HIN	2-chloro-1,1'-biphenyl	36	82	125	40.3938	5.1919	29.5833	19.9008	5.127
2	PCB_002.HIN	3-chloro-1,1'-biphenyl	36	80	118	39.4682	5.2608	29.5833	19.4762	5.1905
3	PCB_003.HIN	4-chloro-1,1'-biphenyl	36	80	118	39.6544	5.2044	29	19.6571	5.1595
4	PCB_004.HIN	2,2'-dichloro-1,1'-biphenyl	40	92	147	45.1889	5.349	32.0667	22.2	5.2667
5	PCB_005.HIN	2,3-dichloro-1,1'-biphenyl	40	92	146	45.2854	5.2996	31.95	22.2956	5.2183
6	PCB_006.HIN	2,3'-dichloro-1,1'-biphenyl	40	90	139	44.2076	5.4151	32.1667	21.7198	5.3246
7	PCB_007.HIN	2,4-dichloro-1,1'-biphenyl	40	90	139	44.2368	5.4259	32	21.7484	5.346
8	PCB_008.HIN	2,4'-dichloro-1,1'-biphenyl	40	90	141	44.3718	5.436	31.7	21.8813	5.3659
9	PCB_009.HIN	2,5-dichloro-1,1'-biphenyl	40	90	141	44.3718	5.436	31.7	21.8813	5.3659
10	PCB_010.HIN	2,6-dichloro-1,1'-biphenyl	40	92	146	45.0094	5.369	32.3333	22.0286	5.2825
11	PCB_011.HIN	3,3'-dichloro-1,1'-biphenyl	40	88	132	43.282	5.4839	32.1667	21.2952	5.3881
12	PCB_012.HIN	3,4-dichloro-1,1'-biphenyl	40	90	139	44.6544	5.2877	31	22.1571	5.2429
13	PCB_013.HIN	3,4'-dichloro-1,1'-biphenyl	40	88	132	43.4682	5.4275	31.5833	21.4762	5.3571
14	PCB_014.HIN	3,5-dichloro-1,1'-biphenyl	40	88	132	43.1409	5.5581	32.5	21.1619	5.4548
15	PCB_015.HIN	4,4'-dichloro-1,1'-biphenyl	40	88	132	43.6544	5.371	31	21.6571	5.3262
16	PCB_016.HIN	2,3,2'-trichloro-1,1'-biphenyl	44	102	168	50.0806	5.4566	34.4333	24.5948	5.3579
17	PCB_017.HIN	2,4,2'-trichloro-1,1'-biphenyl	44	100	161	49.0319	5.5829	34.4833	24.0476	5.4857
18	PCB_018.HIN	2,5,2'-trichloro-1,1'-biphenyl	44	100	163	49.167	5.593	34.1833	24.1806	5.5056
19	PCB_019.HIN	2,6,2'-trichloro-1,1'-biphenyl	44	102	169	49.8549	5.5281	34.7333	24.3773	5.4263
20	PCB_020.HIN	2,3,3'-trichloro-1,1'-biphenyl	44	100	160	49.0993	5.5227	34.5333	24.1147	5.4159
21	PCB_021.HIN	2,3,4-trichloro-1,1'-biphenyl	44	102	167	50.2149	5.42	34.1167	24.729	5.3349
22	PCB_022.HIN	2,3,4'-trichloro-1,1'-biphenyl	44	100	160	49.2854	5.4662	33.95	24.2956	5.3849
23	PCB_023.HIN	2,3,5-trichloro-1,1'-biphenyl	44	100	162	49.1066	5.6109	34.4833	24.1238	5.5095
24	PCB_024.HIN	2,3,6-trichloro-1,1'-biphenyl	44	102	169	50.0593	5.4965	34.25	24.5762	5.4127
25	PCB_025.HIN	2,4,3'-trichloro-1,1'-biphenyl	44	98	153	48.0506	5.649	34.5833	23.5675	5.5437
26	PCB_026.HIN	2,5,3'-trichloro-1,1'-biphenyl	44	98	155	48.1857	5.6591	34.2833	23.7004	5.5635
27	PCB_027.HIN	2,6,3'-trichloro-1,1'-biphenyl	44	100	160	48.8232	5.5922	34.9167	23.8476	5.4802
28	PCB_028.HIN	2,4,4'-trichloro-1,1'-biphenyl	44	98	153	48.2368	5.5926	34	23.7484	5.5127
29	PCB_029.HIN	2,4,5-trichloro-1,1'-biphenyl	44	100	162	49.3852	5.5234	33.6167	24.3909	5.4563
30	PCB_030.HIN	2,4,6-trichloro-1,1'-biphenyl	44	100	160	48.6955	5.6703	35.1667	23.7238	5.554
31	PCB_031.HIN	2,5,4'-trichloro-1,1'-biphenyl	44	98	155	48.3718	5.6026	33.7	23.8813	5.5325
32	PCB_032.HIN	2,6,4'-trichloro-1,1'-biphenyl	44	100	160	49.0094	5.5357	34.3333	24.0286	5.4492
33	PCB_033.HIN	2,3',4'-trichloro-1,1'-biphenyl	44	100	160	49.3938	5.4419	33.5833	24.4008	5.377
34	PCB_034.HIN	2,3',5'-trichloro-1,1'-biphenyl	44	98	153	47.8803	5.7123	35.0833	23.4056	5.5889
35	PCB_035.HIN	3,4,3'-trichloro-1,1'-biphenyl	44	98	153	48.0506	5.649	34.5833	23.5675	5.5437
36	PCB_036.HIN	3,5,3'-trichloro-1,1'-biphenyl	44	96	146	46.9547	5.7812	35.0833	22.981	5.6524
37	PCB_037.HIN	3,4,4'-trichloro-1,1'-biphenyl	44	98	153	48.6544	5.4544	33	24.1571	5.4095
38	PCB_038.HIN	3,4,5-trichloro-1,1'-biphenyl	44	100	160	49.411	5.4686	33.6667	24.419	5.3976
39	PCB_039.HIN	3,5,4'-trichloro-1,1'-biphenyl	44	96	146	47.1409	5.7247	34.5	23.1619	5.6214

No.	MolID	Molecule	AL ₁	AL ₂	AL ₃	AL ₄	AL ₅	AL ₆	AL ₇	AL ₈
40	PCB_040.HIN	2,3,2',3'-tetrachloro-1,1'-biphenyl	48	112	189	54.9722	5.5642	36.8	26.9897	5.4492
41	PCB_041.HIN	2,3,4,2'-tetrachloro-1,1'-biphenyl	48	112	189	55.01	5.577	36.6	27.0282	5.4746
42	PCB_042.HIN	2,3,2',4'-tetrachloro-1,1'-biphenyl	48	110	182	53.9236	5.6906	36.85	26.4425	5.577
43	PCB_043.HIN	2,3,5,2'-tetrachloro-1,1'-biphenyl	48	110	184	53.9017	5.7679	36.9667	26.423	5.6492
44	PCB_044.HIN	2,3,2',5'-tetrachloro-1,1'-biphenyl	48	110	184	54.0586	5.7006	36.55	26.5754	5.5968
45	PCB_045.HIN	2,3,6,2'-tetrachloro-1,1'-biphenyl	48	112	192	54.9048	5.6556	36.65	26.9249	5.5564
46	PCB_046.HIN	2,3,2',6'-tetrachloro-1,1'-biphenyl	48	112	190	54.7466	5.6358	37.1	26.7721	5.5175
47	PCB_047.HIN	2,4,2',4'-tetrachloro-1,1'-biphenyl	48	108	175	52.8749	5.8169	36.9	25.8952	5.7048
48	PCB_048.HIN	2,4,5,2'-tetrachloro-1,1'-biphenyl	48	110	184	54.1803	5.6804	36.1	26.6901	5.596
49	PCB_049.HIN	2,4,2',5'-tetrachloro-1,1'-biphenyl	48	108	177	53.01	5.827	36.6	26.0282	5.7246
50	PCB_050.HIN	2,4,6,2'-tetrachloro-1,1'-biphenyl	48	110	183	53.541	5.8294	37.5667	26.0725	5.6977
51	PCB_051.HIN	2,4,2',6'-tetrachloro-1,1'-biphenyl	48	110	183	53.6979	5.7621	37.15	26.2249	5.6453
52	PCB_052.HIN	2,5,2',5'-tetrachloro-1,1'-biphenyl	48	108	179	53.1451	5.837	36.3	26.1611	5.7444
53	PCB_053.HIN	2,5,2',6'-tetrachloro-1,1'-biphenyl	48	110	185	53.833	5.7722	36.85	26.3578	5.6652
54	PCB_054.HIN	2,6,2',6'-tetrachloro-1,1'-biphenyl	48	112	192	54.5665	5.7088	37.3333	26.6	5.5889
55	PCB_055.HIN	2,3,4,3'-tetrachloro-1,1'-biphenyl	48	110	181	54.0287	5.6431	36.7	26.548	5.5325
56	PCB_056.HIN	2,3,3',4'-tetrachloro-1,1'-biphenyl	48	110	181	54.2854	5.5496	35.95	26.7956	5.4683
57	PCB_057.HIN	2,3,5,3'-tetrachloro-1,1'-biphenyl	48	108	176	52.9204	5.8341	37.0667	25.9429	5.7071
58	PCB_058.HIN	2,3,3',5'-tetrachloro-1,1'-biphenyl	48	108	174	52.772	5.8199	37.45	25.8004	5.6802
59	PCB_059.HIN	2,3,6,3'-tetrachloro-1,1'-biphenyl	48	110	183	53.8731	5.7196	36.8333	26.3952	5.6103
60	PCB_060.HIN	2,3,4,4'-tetrachloro-1,1'-biphenyl	48	110	181	54.2149	5.5866	36.1167	26.729	5.5016
61	PCB_061.HIN	2,3,4,5-tetrachloro-1,1'-biphenyl	48	112	190	55.1066	5.6109	36.4833	27.1238	5.5095
62	PCB_062.HIN	2,3,4,6-tetrachloro-1,1'-biphenyl	48	112	190	54.8159	5.6774	36.9167	26.8381	5.5675
63	PCB_063.HIN	2,3,5,4'-tetrachloro-1,1'-biphenyl	48	108	176	53.1066	5.7776	36.4833	26.1238	5.6762
64	PCB_064.HIN	2,3,6,4'-tetrachloro-1,1'-biphenyl	48	110	183	54.0593	5.6632	36.25	26.5762	5.5794
65	PCB_065.HIN	2,3,5,6-tetrachloro-1,1'-biphenyl	48	112	192	54.9364	5.6845	36.6667	26.9524	5.581
66	PCB_066.HIN	2,4,3',4'-tetrachloro-1,1'-biphenyl	48	108	174	53.2368	5.6759	36	26.2484	5.596
67	PCB_067.HIN	2,4,5,3'-tetrachloro-1,1'-biphenyl	48	108	176	53.199	5.7465	36.2	26.2099	5.654
68	PCB_068.HIN	2,4,3',5'-tetrachloro-1,1'-biphenyl	48	106	167	51.7233	5.9463	37.5	25.2532	5.8079
69	PCB_069.HIN	2,4,6,3'-tetrachloro-1,1'-biphenyl	48	108	174	52.5093	5.8935	37.75	25.5429	5.7516
70	PCB_070.HIN	2,5,3',4'-tetrachloro-1,1'-biphenyl	48	108	176	53.3718	5.686	35.7	26.3813	5.6159
71	PCB_071.HIN	2,6,3',4'-tetrachloro-1,1'-biphenyl	48	110	181	54.0094	5.619	36.3333	26.5286	5.5325
72	PCB_072.HIN	2,5,3',5'-tetrachloro-1,1'-biphenyl	48	106	169	51.8584	5.9563	37.2	25.3861	5.8278
73	PCB_073.HIN	2,6,3',5'-tetrachloro-1,1'-biphenyl	48	108	174	52.4959	5.8894	37.8333	25.5333	5.7444
74	PCB_074.HIN	2,4,5,4'-tetrachloro-1,1'-biphenyl	48	108	176	53.3852	5.69	35.6167	26.3909	5.623
75	PCB_075.HIN	2,4,6,4'-tetrachloro-1,1'-biphenyl	48	108	174	52.6955	5.837	37.1667	25.7238	5.7206
76	PCB_076.HIN	2,3',4',5'-tetrachloro-1,1'-biphenyl	48	110	181	54.1504	5.6228	36.25	26.6627	5.5317
77	PCB_077.HIN	3,4,3',4'-tetrachloro-1,1'-biphenyl	48	108	174	53.6544	5.5377	35	26.6571	5.4929
78	PCB_078.HIN	3,4,5,3'-tetrachloro-1,1'-biphenyl	48	108	174	53.2248	5.6917	36.25	26.2381	5.5952
79	PCB_079.HIN	3,4,3',5'-tetrachloro-1,1'-biphenyl	48	106	167	52.1409	5.8081	36.5	25.6619	5.7048
80	PCB_080.HIN	3,5,3',5'-tetrachloro-1,1'-biphenyl	48	104	160	50.6274	6.0784	38	24.6667	5.9167
81	PCB_081.HIN	3,4,5,4'-tetrachloro-1,1'-biphenyl	48	108	174	53.411	5.6353	35.6667	26.419	5.5643
82	PCB_082.HIN	2,3,4,2',3'-pentachloro-1,1'-biphenyl	52	122	210	59.9017	5.6846	38.9667	29.423	5.5659
83	PCB_083.HIN	2,3,5,2',3'-pentachloro-1,1'-biphenyl	52	120	205	58.7934	5.8756	39.3333	28.8179	5.7405
84	PCB_084.HIN	2,3,6,2',3'-pentachloro-1,1'-biphenyl	52	122	213	59.7965	5.7632	39.0167	29.3197	5.6477
85	PCB_085.HIN	2,3,4,2',4'-pentachloro-1,1'-biphenyl	52	120	203	58.853	5.811	39.0167	28.8758	5.6937

No.	MolID	Molecule	AL ₁	AL ₂	AL ₃	AL ₄	AL ₅	AL ₆	AL ₇	AL ₈
86	PCB.086.HIN	2,3,4,5,2'-pentachloro-1,1'-biphenyl	52	122	212	59.9017	5.7679	38.9667	29.423	5.6492
87	PCB.087.HIN	2,3,4,2',5'-pentachloro-1,1'-biphenyl	52	120	205	58.9881	5.821	38.7167	29.0087	5.7135
88	PCB.088.HIN	2,3,4,6,2'-pentachloro-1,1'-biphenyl	52	122	213	59.6614	5.8365	39.3167	29.1868	5.7112
89	PCB.089.HIN	2,3,4,2',6'-pentachloro-1,1'-biphenyl	52	122	211	59.676	5.7561	39.2667	29.2054	5.6342
90	PCB.090.HIN	2,3,5,2',4'-pentachloro-1,1'-biphenyl	52	118	198	57.7447	6.0019	39.3833	28.2706	5.8683
91	PCB.091.HIN	2,3,6,2',4'-pentachloro-1,1'-biphenyl	52	120	206	58.7478	5.8896	39.0667	28.7725	5.7755
92	PCB.092.HIN	2,3,5,2',5'-pentachloro-1,1'-biphenyl	52	118	200	57.8798	6.012	39.0833	28.4036	5.8881
93	PCB.093.HIN	2,3,5,6,2'-pentachloro-1,1'-biphenyl	52	122	215	59.7819	5.8436	39.0667	29.3011	5.7247
94	PCB.094.HIN	2,3,5,2',6'-pentachloro-1,1'-biphenyl	52	120	206	58.5677	5.9471	39.6333	28.6003	5.8088
95	PCB.095.HIN	2,3,6,2',5'-pentachloro-1,1'-biphenyl	52	120	208	58.8829	5.8996	38.7667	28.9054	5.7953
96	PCB.096.HIN	2,3,6,2',6'-pentachloro-1,1'-biphenyl	52	122	215	59.6164	5.8363	39.25	29.1476	5.719
97	PCB.097.HIN	2,3,2',4',5'-pentachloro-1,1'-biphenyl	52	120	205	59.072	5.788	38.4667	29.0849	5.6873
98	PCB.098.HIN	2,3,2',4',6'-pentachloro-1,1'-biphenyl	52	120	204	58.4327	5.937	39.9333	28.4674	5.789
99	PCB.099.HIN	2,4,5,2',4'-pentachloro-1,1'-biphenyl	52	118	198	58.0234	5.9144	38.5167	28.5377	5.8151
100	PCB.100.HIN	2,4,6,2',4'-pentachloro-1,1'-biphenyl	52	118	197	57.384	6.0634	39.9833	27.9201	5.9167
101	PCB.101.HIN	2,4,5,2',5'-pentachloro-1,1'-biphenyl	52	118	200	58.1584	5.9244	38.2167	28.6706	5.8349
102	PCB.102.HIN	2,4,5,2',6'-pentachloro-1,1'-biphenyl	52	120	206	58.8464	5.8595	38.7667	28.8674	5.7556
103	PCB.103.HIN	2,4,6,2',5'-pentachloro-1,1'-biphenyl	52	118	199	57.5191	6.0735	39.6833	28.0531	5.9366
104	PCB.104.HIN	2,4,6,2',6'-pentachloro-1,1'-biphenyl	52	120	206	58.2526	6.0101	40.1667	28.2952	5.8603
105	PCB.105.HIN	2,3,4,3',4'-pentachloro-1,1'-biphenyl	52	120	202	59.2149	5.67	38.1167	29.229	5.5849
106	PCB.106.HIN	2,3,4,5,3'-pentachloro-1,1'-biphenyl	52	120	204	58.9204	5.8341	39.0667	28.9429	5.7071
107	PCB.107.HIN	2,3,5,3',4'-pentachloro-1,1'-biphenyl	52	118	197	58.1066	5.8609	38.4833	28.6238	5.7595
108	PCB.108.HIN	2,3,4,3',5'-pentachloro-1,1'-biphenyl	52	118	195	57.7014	5.9403	39.6167	28.2337	5.7968
109	PCB.109.HIN	2,3,4,6,3'-pentachloro-1,1'-biphenyl	52	120	204	58.6297	5.9006	39.5	28.6571	5.7651
110	PCB.110.HIN	2,3,6,3',4'-pentachloro-1,1'-biphenyl	52	120	204	59.0593	5.7465	38.25	29.0762	5.6627
111	PCB.111.HIN	2,3,5,3',5'-pentachloro-1,1'-biphenyl	52	116	190	56.5931	6.1313	39.9833	27.6286	5.9714
112	PCB.112.HIN	2,3,5,6,3'-pentachloro-1,1'-biphenyl	52	120	206	58.7502	5.9076	39.25	28.7714	5.7786
113	PCB.113.HIN	2,3,6,3',5'-pentachloro-1,1'-biphenyl	52	118	197	57.5458	6.0169	39.75	28.081	5.8746
114	PCB.114.HIN	2,3,4,5,4'-pentachloro-1,1'-biphenyl	52	120	204	59.1066	5.7776	38.4833	29.1238	5.6762
115	PCB.115.HIN	2,3,4,6,4'-pentachloro-1,1'-biphenyl	52	120	204	58.8159	5.8441	38.9167	28.8381	5.7341
116	PCB.116.HIN	2,3,4,5,6-pentachloro-1,1'-biphenyl	52	124	220	60.6663	5.774	39.5	29.6952	5.6381
117	PCB.117.HIN	2,3,5,6,4'-pentachloro-1,1'-biphenyl	52	120	206	58.9364	5.8512	38.6667	28.9524	5.7476
118	PCB.118.HIN	2,4,5,3',4'-pentachloro-1,1'-biphenyl	52	118	197	58.3852	5.7734	37.6167	28.8909	5.7063
119	PCB.119.HIN	2,4,6,3',4'-pentachloro-1,1'-biphenyl	52	118	195	57.6955	5.9203	39.1667	28.2238	5.804
120	PCB.120.HIN	2,4,5,3',5'-pentachloro-1,1'-biphenyl	52	116	190	56.8717	6.0437	39.1167	27.8956	5.9183
121	PCB.121.HIN	2,4,6,3',5'-pentachloro-1,1'-biphenyl	52	116	188	56.182	6.1907	40.6667	27.2286	6.0159
122	PCB.122.HIN	2,3,3',4',5'-pentachloro-1,1'-biphenyl	52	120	202	59.0421	5.7305	38.6167	29.0575	5.623
123	Pcb.123.hin	2,4,3',4',5'-pentachloro-1,1'-biphenyl	52	118	195	57.9934	5.8568	38.6667	28.5103	5.7508
124	PCB.124.HIN	2,5,3',4',5'-pentachloro-1,1'-biphenyl	52	118	197	58.1285	5.8669	38.3667	28.6433	5.7706
125	PCB.125.HIN	2,6,3',4',5'-pentachloro-1,1'-biphenyl	52	120	202	58.766	5.7999	39	28.7905	5.6873
126	PCB.126.HIN	3,4,5,3',4'-pentachloro-1,1'-biphenyl	52	118	195	58.411	5.7186	37.6667	28.919	5.6476
127	PCB.127.HIN	3,4,5,3',5'-pentachloro-1,1'-biphenyl	52	116	188	56.8975	5.989	39.1667	27.9238	5.8595
128	PCB.128.HIN	2,3,4,2',3',4'-hexachloro-1,1'-biphenyl	56	132	231	64.8311	5.805	41.1333	31.8563	5.6825
129	PCB.129.HIN	2,3,4,5,2',3'-hexachloro-1,1'-biphenyl	56	132	233	64.7934	5.8756	41.3333	31.8179	5.7405
130	PCB.130.HIN	2,3,4,2',3',5'-hexachloro-1,1'-biphenyl	56	130	226	63.7228	5.996	41.5	31.2512	5.8571

No.	MolID	Molecule	AL ₁	AL ₂	AL ₃	AL ₄	AL ₅	AL ₆	AL ₇	AL ₈
131	PCB_131.HIN	2,3,4,6,2',3'-hexachloro-1,1'-biphenyl	56	132	234	64.5531	5.9441	41.6833	31.5816	5.8025
132	PCB_132.HIN	2,3,4,2',3',6'-hexachloro-1,1'-biphenyl	56	132	234	64.7259	5.8836	41.1833	31.7531	5.7644
133	PCB_133.HIN	2,3,5,2',3',5'-hexachloro-1,1'-biphenyl	56	128	221	62.6145	6.1869	41.8667	30.646	6.0317
134	PCB_134.HIN	2,3,5,6,2',3'-hexachloro-1,1'-biphenyl	56	132	236	64.6735	5.9512	41.4333	31.6959	5.8159
135	PCB_135.HIN	2,3,5,2',3',6'-hexachloro-1,1'-biphenyl	56	130	229	63.6176	6.0746	41.55	31.1479	5.939
136	PCB_136.HIN	2,3,6,2',3',6'-hexachloro-1,1'-biphenyl	56	132	231	64.8311	5.805	41.1333	31.8563	5.6825
137	PCB_137.HIN	2,3,4,5,2',4'-hexachloro-1,1'-biphenyl	56	130	226	63.7447	6.0019	41.3833	31.2706	5.8683
138	PCB_138.HIN	2,3,4,2',4',5'-hexachloro-1,1'-biphenyl	56	130	226	64.0015	5.9084	40.6333	31.5183	5.804
139	PCB_139.HIN	2,3,4,6,2',4'-hexachloro-1,1'-biphenyl	56	130	227	63.5045	6.0705	41.7333	31.0344	5.9302
140	PCB_140.HIN	2,3,4,2',4',6'-hexachloro-1,1'-biphenyl	56	130	225	63.3621	6.0574	42.1	30.9007	5.9056
141	PCB_141.HIN	2,3,4,5,2',5'-hexachloro-1,1'-biphenyl	56	130	228	63.8798	6.012	41.0833	31.4036	5.8881
142	PCB_142.HIN	2,3,4,5,6,2'-hexachloro-1,1'-biphenyl	56	134	243	65.5118	5.9331	41.9	32.0439	5.7818
143	PCB_143.HIN	2,3,4,5,2',6'-hexachloro-1,1'-biphenyl	56	132	234	64.5677	5.9471	41.6333	31.6003	5.8088
144	PCB_144.HIN	2,3,4,6,2',5'-hexachloro-1,1'-biphenyl	56	130	229	63.6395	6.0806	41.4333	31.1674	5.9501
145	PCB_145.HIN	2,3,4,6,2',6'-hexachloro-1,1'-biphenyl	56	132	236	64.373	6.0172	41.9167	31.4095	5.8738
146	PCB_146.HIN	2,3,5,2',4',5'-hexachloro-1,1'-biphenyl	56	128	221	62.8931	6.0994	41	30.9131	5.9786
147	PCB_147.HIN	2,3,5,6,2',4'-hexachloro-1,1'-biphenyl	56	130	229	63.6249	6.0776	41.4833	31.1487	5.9437
148	PCB_148.HIN	2,3,5,2',4',6'-hexachloro-1,1'-biphenyl	56	128	221	62.8931	6.0994	41	30.9131	5.9786
149	PCB_149.HIN	2,3,6,2',4',5'-hexachloro-1,1'-biphenyl	56	130	229	63.8962	5.987	40.6833	31.415	5.8858
150	PCB_150.HIN	2,3,6,2',4',6'-hexachloro-1,1'-biphenyl	56	130	229	63.3024	6.1376	42.0833	30.8429	5.9905
151	PCB_151.HIN	2,3,5,6,2',5'-hexachloro-1,1'-biphenyl	56	130	231	63.76	6.0876	41.1833	31.2816	5.9636
152	PCB_152.HIN	2,3,5,6,2',6'-hexachloro-1,1'-biphenyl	56	132	238	64.4934	6.0243	41.6667	31.5238	5.8873
153	PCB_153.HIN	2,4,5,2',4',5'-hexachloro-1,1'-biphenyl	56	128	221	63.1718	6.0118	40.1333	31.1802	5.9254
154	PCB_154.HIN	2,4,5,2',4',6'-hexachloro-1,1'-biphenyl	56	128	220	62.5324	6.1608	41.6	30.5626	6.0271
155	PCB_155.HIN	2,4,6,2',4',6'-hexachloro-1,1'-biphenyl	56	128	220	61.9386	6.3114	43	29.9905	6.1317
156	PCB_156.HIN	2,3,4,5,3',4'-hexachloro-1,1'-biphenyl	56	130	225	64.1066	5.8609	40.4833	31.6238	5.7595
157	PCB_157.HIN	2,3,4,3',4',5'-hexachloro-1,1'-biphenyl	56	130	223	63.9715	5.8509	40.7833	31.4909	5.7397
158	PCB_158.HIN	2,3,4,6,3',4'-hexachloro-1,1'-biphenyl	56	130	225	63.8159	5.9274	40.9167	31.3381	5.8175
159	PCB_159.HIN	2,3,4,5,3',5'-hexachloro-1,1'-biphenyl	56	128	218	62.5931	6.1313	41.9833	30.6286	5.9714
160	PCB_160.HIN	2,3,4,5,6,3'-hexachloro-1,1'-biphenyl	56	132	234	64.4801	5.9971	42.0833	31.5143	5.8357
161	PCB_161.HIN	2,3,4,6,3',5'-hexachloro-1,1'-biphenyl	56	128	220	62.4229	6.2049	42.1667	30.4571	6.0429
162	PCB_162.HIN	2,3,5,3',4',5'-hexachloro-1,1'-biphenyl	56	128	218	62.8632	6.0418	41.15	30.8857	5.9143
163	PCB_163.HIN	2,3,5,6,3',4'-hexachloro-1,1'-biphenyl	56	130	227	63.9364	5.9345	40.6667	31.4524	5.831
164	PCB_164.HIN	2,3,6,3',4',5'-hexachloro-1,1'-biphenyl	56	130	229	63.8962	5.987	40.6833	31.415	5.8858
165	PCB_165.HIN	2,3,5,6,3',5'-hexachloro-1,1'-biphenyl	56	128	220	62.4229	6.2049	42.1667	30.4571	6.0429
166	PCB_166.HIN	2,3,4,5,6,4'-hexachloro-1,1'-biphenyl	56	132	234	64.6663	5.9407	41.5	31.6952	5.8048
167	PCB_167.HIN	2,4,5,3',4',5'-hexachloro-1,1'-biphenyl	56	128	218	63.1418	5.9543	40.2833	31.1528	5.8611
168	PCB_168.HIN	2,4,6,3',4',5'-hexachloro-1,1'-biphenyl	56	128	216	62.4521	6.1012	41.8333	30.4857	5.9587
169	PCB_169.HIN	3,4,5,3',4',5'-hexachloro-1,1'-biphenyl	56	128	216	63.1676	5.8995	40.3333	31.181	5.8024
170	PCB_170.HIN	2,3,4,5,2',3',4'-heptachloro-1,1'-biphenyl	60	142	254	69.7228	5.996	43.5	34.2512	5.8571
171	PCB_171.HIN	2,3,4,6,2',3',4'-heptachloro-1,1'-biphenyl	60	142	255	69.4825	6.0645	43.85	34.015	5.9191
172	PCB_172.HIN	2,3,4,5,2',3',5'-heptachloro-1,1'-biphenyl	60	140	249	68.6145	6.1869	43.8667	33.646	6.0317
173	PCB_173.HIN	2,3,4,5,6,2',3'-heptachloro-1,1'-biphenyl	60	144	264	70.4034	6.0407	44.2667	34.4388	5.8731
174	PCB_174.HIN	2,3,4,5,2',3',6'-heptachloro-1,1'-biphenyl	60	142	257	69.6176	6.0746	43.55	34.1479	5.939
175	PCB_175.HIN	2,3,4,6,2',3',5'-heptachloro-1,1'-biphenyl	60	140	250	68.3742	6.2555	44.2167	33.4098	6.0937

No.	MolID	Molecule	AL ₁	AL ₂	AL ₃	AL ₄	AL ₅	AL ₆	AL ₇	AL ₈
176	PCB_176.HIN	2,3,4,6,2',3',6'-heptachloro-1,1'-biphenyl	60	142	259	69.4229	6.1447	43.8333	33.9571	6.004
177	PCB_177.HIN	2,3,4,2',3',5',6'-heptachloro-1,1'-biphenyl	60	142	257	69.603	6.0716	43.6	34.1293	5.9326
178	PCB_178.HIN	2,3,5,6,2',3',5'-heptachloro-1,1'-biphenyl	60	140	252	68.4947	6.2626	43.9667	33.5241	6.1072
179	PCB_179.HIN	2,3,5,6,2',3',6'-heptachloro-1,1'-biphenyl	60	142	261	69.5433	6.1518	43.5833	34.0714	6.0175
180	PCB_180.HIN	2,3,4,5,2',4',5'-heptachloro-1,1'-biphenyl	60	140	249	68.8931	6.0994	43	33.9131	5.9786
181	PCB_181.HIN	2,3,4,5,6,2',4'-heptachloro-1,1'-biphenyl	60	142	257	69.3548	6.167	44.3167	33.8916	6.0009
182	PCB_182.HIN	2,3,4,5,2',4',6'-heptachloro-1,1'-biphenyl	60	140	248	68.2538	6.2484	44.4667	33.2955	6.0802
183	PCB_183.HIN	2,3,4,6,2',4',5'-heptachloro-1,1'-biphenyl	60	140	250	68.6529	6.1679	43.35	33.6769	6.0405
184	PCB_184.HIN	2,3,4,6,2',4',6'-heptachloro-1,1'-biphenyl	60	140	250	68.0591	6.3185	44.75	33.1048	6.1452
185	PCB_185.HIN	2,3,4,5,6,2',5'-heptachloro-1,1'-biphenyl	60	142	259	69.4898	6.1771	44.0167	34.0245	6.0207
186	PCB_186.HIN	2,3,4,5,6,2',6'-heptachloro-1,1'-biphenyl	60	144	266	70.2233	6.1137	44.5	34.2667	5.9444
187	PCB_187.HIN	2,3,5,6,2',4',5'-heptachloro-1,1'-biphenyl	60	140	252	68.7733	6.175	43.1	33.7912	6.054
188	PCB_188.HIN	2,3,5,6,2',4',6'-heptachloro-1,1'-biphenyl	60	140	252	68.1795	6.3256	44.5	33.219	6.1587
189	PCB_189.HIN	2,3,4,5,3',4',5'-heptachloro-1,1'-biphenyl	60	140	246	68.8632	6.0418	43.15	33.8857	5.9143
190	PCB_190.HIN	2,3,4,5,6,3',4'-heptachloro-1,1'-biphenyl	60	142	255	69.6663	6.024	43.5	34.1952	5.8881
191	PCB_191.HIN	2,3,4,6,3',4',5'-heptachloro-1,1'-biphenyl	60	140	246	68.5726	6.1083	43.5833	33.6	5.9722
192	PCB_192.HIN	2,3,4,5,6,3',5'-heptachloro-1,1'-biphenyl	60	140	248	68.1528	6.2944	45	33.2	6.1
193	PCB_193.HIN	2,3,5,6,3',4',5'-heptachloro-1,1'-biphenyl	60	140	248	68.693	6.1154	43.3333	33.7143	5.9857
194	PCB_194.HIN	2,3,4,5,2',3',4',5'-octachloro-1,1'-biphenyl	64	152	277	74.6145	6.1869	45.8667	36.646	6.0317
195	PCB_195.HIN	2,3,4,5,6,2',3',4'-octachloro-1,1'-biphenyl	64	154	285	75.3329	6.1611	46.4333	36.8721	5.9898
196	PCB_196.HIN	2,3,4,5,2',3',4',6'-octachloro-1,1'-biphenyl	64	152	278	74.3742	6.2555	46.2167	36.4098	6.0937
197	PCB_197.HIN	2,3,4,6,2',3',4',6'-octachloro-1,1'-biphenyl	64	152	280	74.1795	6.3256	46.5	36.219	6.1587
198	PCB_198.HIN	2,3,4,5,6,2',3',5'-octachloro-1,1'-biphenyl	64	152	280	74.2246	6.3521	46.8	36.267	6.1644
199	PCB_199.HIN	2,3,4,5,6,2',3',6'-octachloro-1,1'-biphenyl	64	154	289	75.2732	6.2412	46.4167	36.8143	6.0746
200	PCB_200.HIN	2,3,4,6,2',3',5',6'-octachloro-1,1'-biphenyl	64	152	280	74.4947	6.2626	45.9667	36.5241	6.1072
201	PCB_201.HIN	2,3,4,5,2',3',5',6'-octachloro-1,1'-biphenyl	64	152	280	74.4947	6.2626	45.9667	36.5241	6.1072
202	PCB_202.HIN	2,3,5,6,2',3',5',6'-octachloro-1,1'-biphenyl	64	152	284	74.4204	6.3398	46	36.4476	6.1857
203	PCB_203.HIN	2,3,4,5,6,2',4',5'-octachloro-1,1'-biphenyl	64	152	280	74.5032	6.2645	45.9333	36.534	6.1112
204	PCB_204.HIN	2,3,4,5,6,2',4',6'-octachloro-1,1'-biphenyl	64	152	280	73.9094	6.415	47.3333	35.9619	6.2159
205	PCB_205.HIN	2,3,4,5,6,3',4',5'-octachloro-1,1'-biphenyl	64	152	276	74.4229	6.2049	46.1667	36.4571	6.0429
206	PCB_206.HIN	2,3,4,5,6,2',3',4',5'-nonachloro-1,1'-biphenyl	68	164	308	80.2246	6.3521	48.8	39.267	6.1644
207	PCB_207.HIN	2,3,4,5,6,2',3',4',6'-nonachloro-1,1'-biphenyl	68	164	310	80.0299	6.4221	49.0833	39.0762	6.2294
208	PCB_208.HIN	2,3,4,5,6,2',3',5',6'-nonachloro-1,1'-biphenyl	68	164	312	80.1503	6.4292	48.8333	39.1905	6.2429
209	PCB_209.HIN	2,3,4,5,6,2',3',4',5',6'-decachloro-1,1'-biphenyl	72	176	340	85.8802	6.5187	51.6667	41.9333	6.3
