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QSPR ANALYSIS OF POLYCYCLIC AROMATIC HYDROCARBONS OF SECOND MULTIPLICATIVE HYPER-ZAGREB INDEX

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Abstract. In this research paper, we present a Quantitative Structure–Property Relationship (QSPR) analysis of polycyclic aromatic hydrocarbons (PAHs) using the second multiplicative hyper-Zagreb index of a graph G. To examine six physicochemical properties of PAHs, a logarithmic regression model is employed. The study demonstrates a strong correlation between the physicochemical properties of PAHs and the second multiplicative hyper-Zagreb index $FII_2(G)$. Furthermore, detailed logarithmic regression analyses between the second multiplicative hyper-Zagreb index and the selected physicochemical properties of PAHs are carried out and discussed.

1. Introduction

Polycyclic aromatic hydrocarbons (PAHs) constitute an important class of organic compounds consisting of two or more fused aromatic rings made exclusively of carbon and hydrogen atoms. These compounds are mainly formed during the incomplete combustion of organic substances such as coal, petroleum, gasoline, wood, tobacco, and other fossil fuels. PAHs naturally occur in crude oil, coal, and gasoline, and they are widely distributed in the environment due to both natural and anthropogenic activities.

PAHs are commonly detected in air, water, soil, sediments, and food materials. Because of their persistent nature and widespread distribution, they have become a major subject of study in environmental chemistry, toxicology, and public health. Several PAHs possess toxic, mutagenic, and carcinogenic characteristics, making them hazardous environmental pollutants. Owing to their harmful effects, the United States Environmental Protection Agency (EPA) has listed sixteen PAHs, including naphthalene, anthracene, phenanthrene, pyrene, chrysene, benzo[a]pyrene, and dibenz[a,h]anthracene, as priority pollutants.

The physicochemical behavior of PAHs is strongly influenced by their molecular structure and the number of aromatic rings present in the compound. Low molecular weight PAHs are generally more volatile and relatively soluble in water, whereas

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high molecular weight PAHs are more hydrophobic, lipophilic, chemically stable, and strongly adsorbed onto particulate matter. These properties significantly affect their environmental transport, degradation, persistence, and bioaccumulation in living organisms. Although many PAHs exhibit low acute toxicity, prolonged exposure to certain PAHs is associated with serious health risks, particularly cancer [1–3, 10].

In recent years, computational and mathematical approaches such as Quantitative Structure–Property Relationship (QSPR) and Quantitative Structure–Activity Relationship (QSAR) analyses have been extensively used to study the physicochemical and biological properties of PAHs. Among these approaches, graph-theoretical topological indices have gained considerable importance for predicting chemical properties and molecular behavior without performing expensive and time-consuming laboratory experiments. Such studies provide valuable insights into the structural characteristics, environmental impact, and toxicological behavior of PAHs, thereby contributing to the development of reliable predictive models in chemical and pharmaceutical research [7–9].

2. QSRP Analysis of some Polycyclic Aromatic Hydrocarbons

Topological indices and Quantitative Structure–Property Relationship (QSPR) studies have become essential tools in modern drug discovery and chemical research. These approaches enable researchers to analyze molecular structures, compare chemical compounds, and predict their physicochemical properties with high efficiency, thereby reducing the need for extensive experimental investigations. In particular, regression models used in QSPR analysis [8], together with topological indices, establish quantitative relationships between the structure of a molecule and its corresponding physicochemical characteristics. Such correlations are highly useful in drug design, material science, medicinal chemistry, and several other scientific fields.

Due to their strong predictive capability, topological indices have gained considerable importance as mathematical descriptors that effectively relate the structural features of chemical compounds to experimentally measured physicochemical properties. Consequently, QSPR analysis [8] has emerged as a powerful computational methodology in contemporary drug discovery and development. By developing mathematical models that connect molecular structures with their physical and chemical properties, QSPR techniques help predict significant molecular parameters, minimize experimental costs, and improve the efficiency of the overall drug development process. In the present study, six physicochemical properties of twenty-two top-priority polycyclic aromatic hydrocarbons (PAHs) were analyzed. These properties include boiling point (BP) in °C, pi-electron count, molecular weight (MW, g/mol), polarizability (P, dyne/cm), molar volume (MV, cm^3), and molar refractivity (MR, cm^3). The data associated with these physicochemical properties were collected from [5,6], and the corresponding values are summarized in Table 1.

TABLE 1. Polycyclic Aromatic Hydrocarbons with their physicochemical properties.

Drug name	$HII_2(G)$	BP	π-ele	MW	PO	MV	MR
Benzene	16777216	78.8	8	78.11	10.4	89.4	26.3
Naphthalene	2.28252×10^{15}	221.5	13.683	128.17	17.5	123.5	44.1
Phenanthrene	3.10535×10^{23}	337.4	19.448	178.23	24.6	157.7	61.9
Anthracene	3.10535×10^{23}	337.4	19.314	178.23	24.6	157.7	61.9
Chrysene	4.22479×10^{31}	448	25.192	228.3	31.6	191.8	79.8
Benzo[a]anthracene	4.22479×10^{31}	436.7	25.101	228.3	31.6	191.8	79.8
Triphenylene	4.22479×10^{31}	425	25.275	228.3	31.6	191.8	79.8
Tetracene	4.22479×10^{31}	436.7	25.188	228.3	31.6	191.8	79.8
Benzo[a]pyrene	2.24523×10^{37}	495	28.222	252.3	35.8	196.1	90.3
Benzo[e]pyrene	2.24523×10^{37}	467.5	28.336	252.3	35.8	196.1	90.3
Perylene	2.24523×10^{37}	467.5	28.245	252.3	35.8	196.1	90.3
Anthanthrene	1.19321×10^{43}	497.1	31.253	276.3	40	200.4	100.8
Benzo[ghi]perylene	1.19321×10^{43}	501	31.425	276.3	40	200.4	100.8
Dibenz[a,c]anthracene	5.74778×10^{39}	518	30.942	278.3	38.7	225.9	97.6
Dibenz[a,h]anthracene	5.74778×10^{39}	524.7	30.881	278.3	38.7	225.9	97.6
Dibenz[a,j]anthracene	5.74778×10^{39}	524.7	30.88	278.3	38.7	225.9	97.6
Picene	5.74778×10^{39}	519	30.943	278.3	38.7	225.9	97.6
Coronene	6.34118×10^{48}	525.6	34.572	300.4	44.1	204.7	111.4
Dibenzo[a,h]pyrene	3.0546×10^{45}	552.3	33.928	302.4	42.9	230.2	108.1
Dibenzo[a,i]pyrene	3.0546×10^{45}	552.3	33.954	302.4	42.9	230.2	108.1
Dibenzo[a,l]pyrene	3.0546×10^{45}	552.3	34.031	302.4	42.9	230.2	108.1
Pyrene	1.65031×10^{29}	404	22.506	202.25	28.7	162	72.5

To model and predict the physicochemical properties of the selected PAHs, the second multiplicative hyper-Zagreb index $HII_2(G)$ was utilized as a molecular descriptor. This graph invariant was introduced by Kulli in [4]. The second multiplicative hyper-Zagreb index of a graph G is defined by

$$HII_2(G) = \prod_{uv \in E(G)} \left(d_G(u) \cdot d_G(v)\right)^2,$$

where $d_G(u)$ and $d_G(v)$ represent the degrees of the vertices u and v in the graph G, respectively, and $E(G)$ denotes the edge set of G. The calculated values of this molecular descriptor for the molecular graphs of the considered PAHs are presented in Table 2.

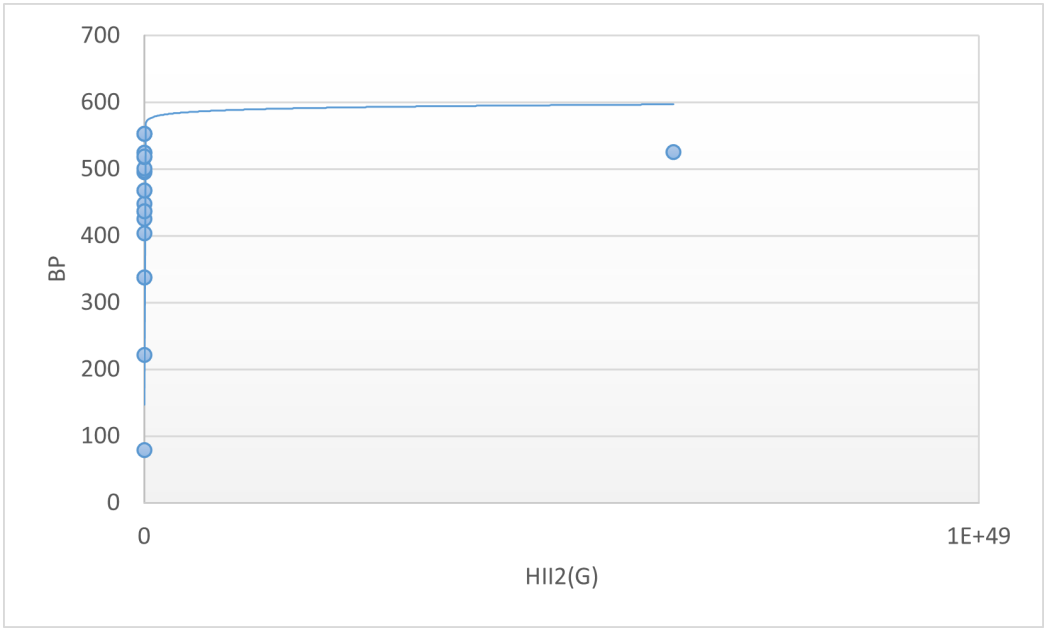
TABLE 2. Statical parameters for the logarithmic QSPR model for first multiplicative hyper-Zagreb index $HII_1(G)$ and physicochemical properties of PAHs.

Physiochemical properties	R	R^2	Adjusted R^2	F	Sig
boiling points (BP) $^\circ C$	0.966	0.933	0.930	278.209	0.000
pi-electron count	0.996	0.991	0.991	2275.045	0.000
molecular weight (MW) g/mol	0.991	0.983	0.982	1143.341	0.000
polarizability (P) $dyne/cm$	0.998	0.996	0.996	4810.575	0.000
molar volumes (MV) cm^3	0.928	0.861	0.854	123.794	0.000
molar refractions (MR) cm^3	0.998	0.996	0.996	4883.933	0.000

Logarithmic Regression Model:
By utilizing the data of Tables 1 and 2, we have the regression model for considered physiochemical properties of compounds as in the list. The evaluation of logarithmic regression model is considered as $y = a + b.log(x)$. Here, y denotes chemical property, a denotes regression co-efficient, b denotes regression constant and x is taken as molecular descriptor. Using Table 1 and Table 2 we can obtain the logarithmic regression models for degree-based indices as follows: **The logarithmic Regression Model for first multiplicative hyper-Zagreb index $HII_2(G)$:**

$$\begin{aligned} BP &= 68.971 + 4.698 \cdot log(HII_2) \\ pi - ele &= 3.825 + 0.287 \cdot log(HII_2) \\ MW &= 45.193 + 2.440 \cdot log(HII_2) \\ PO &= 4.958 + 0.361 \cdot log(HII_2) \\ MV &= 79.421 + 1.413 \cdot log(HII_2) \\ MR &= 12.536 + 0.910 \cdot log(HII_2) \end{aligned}$$

The correlation of first multiplicative hyper-Zagreb index $HII_2(G)$ with the above mentioned physical qualities of Polycyclic Aromatic Hydrocarbon compounds logarithmic models are depicted in the figures mentioned below:


700
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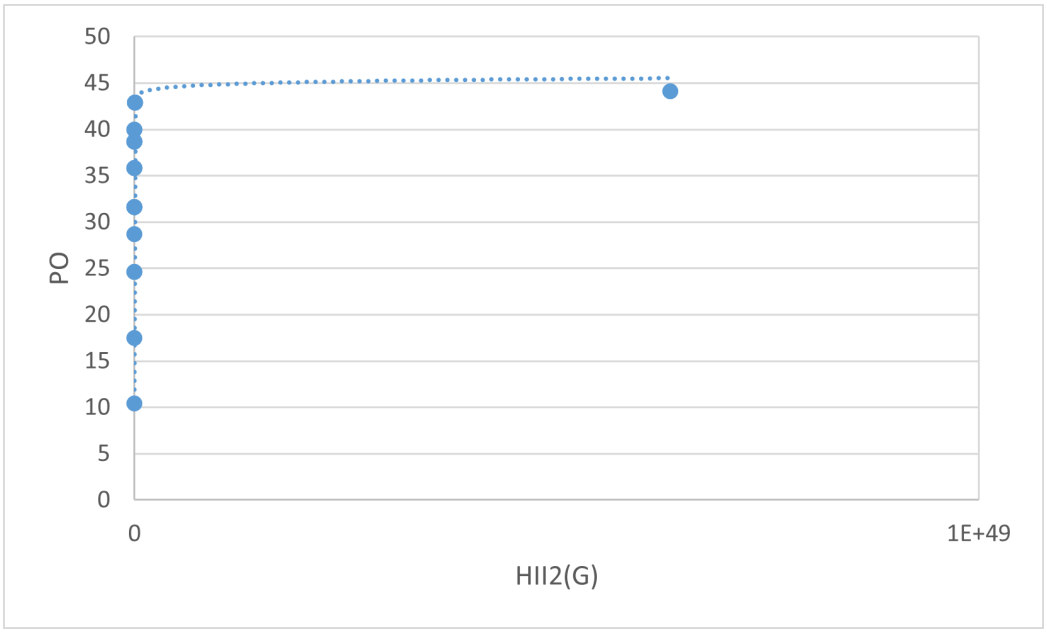
500
400
300
200
100
0
BP
0
1E+49
HII2(G)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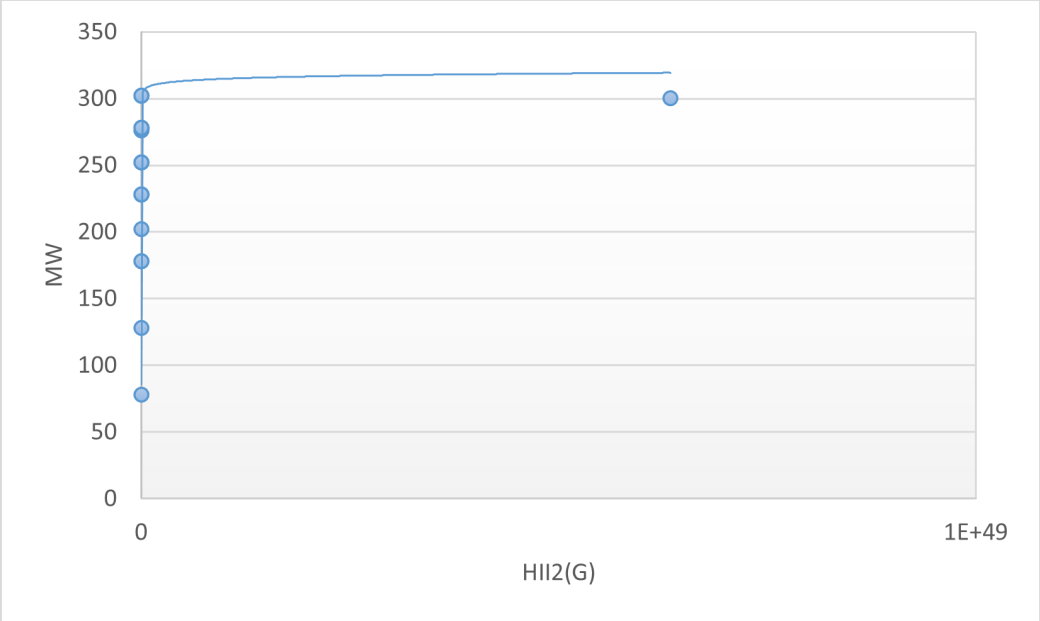
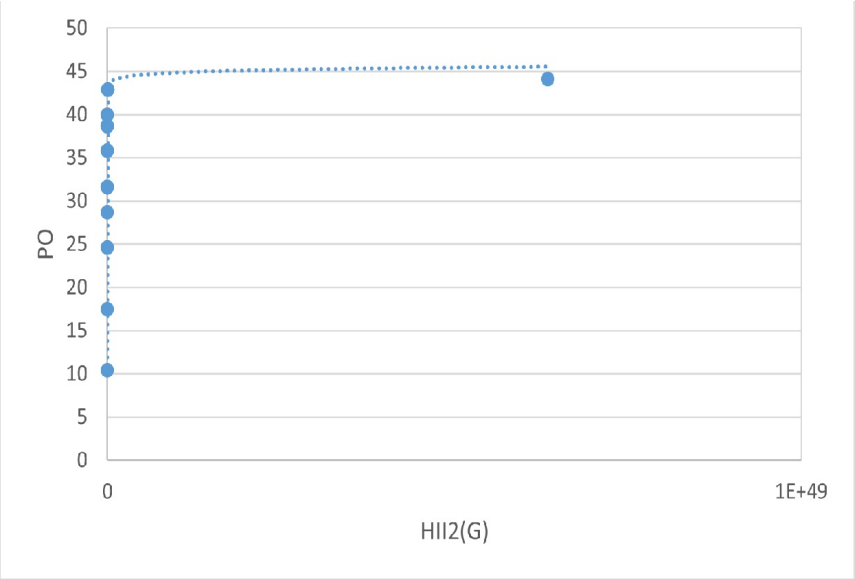
45
40
35
30
25
20
15
10
5
0
PO
0
1E+49
HII2(G)


350
300
250
200
150
100
50
0
MW
0
1E+49
HII2(G)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45
40
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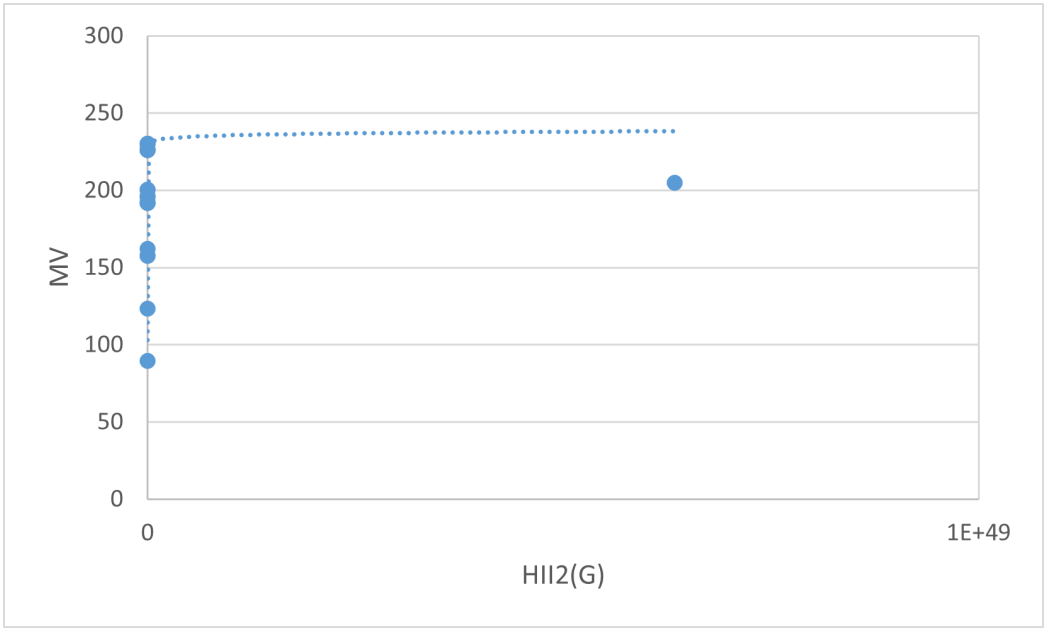
25
20
15
10
5
0
PO
0
1E+49
HII2(G)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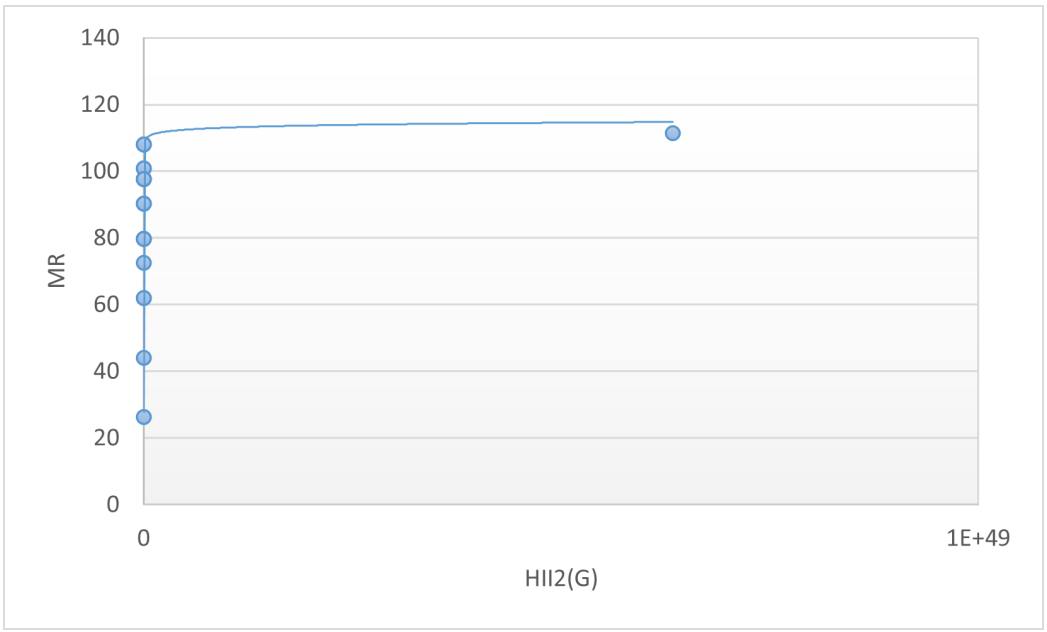
250
200
150
100
50
0
MV
0
1E+49
HII2(G)


140
120
100
80
60
40
20
0
MR
0
1E+49
HII2(G)

3. Conclusion

This study demonstrates the effectiveness of the second multiplicative hyper-Zagreb index $FII_2(G)$ in the QSPR analysis of polycyclic aromatic hydrocarbons (PAHs). By employing logarithmic regression models, strong correlations were observed between the selected topological descriptor and the six considered physicochemical properties of PAHs. The obtained results indicate that the first multiplicative hyper-Zagreb index can serve as a reliable molecular descriptor for predicting important physicochemical characteristics of PAHs. The developed logarithmic regression models provide an efficient mathematical approach for estimating these properties with reduced experimental effort, thereby contributing to the advancement of computational chemistry and molecular modeling. Furthermore, the study highlights the significance of topological indices in QSPR investigations and suggests that such descriptors may be effectively applied to other classes of chemical compounds in future research.

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