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

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Abstract. In this research paper, we discuss the Quantitative Structure–Property Relationship (QSPR) analysis of polycyclic aromatic hydrocarbons (PAHs) using the first multiplicative hyper-Zagreb index of a graph G. To investigate six physicochemical properties of PAH's, a logarithmic regression model is employed. The study reveals a strong correlation between the physicochemical properties of PAHs and the first multiplicative hyper-Zagreb index $FII_1(G)$. Furthermore, logarithmic regression analyses between the first multiplicative hyper-Zagreb index and various physicochemical properties of PAHs are presented and discussed.

1. Introduction

Polycyclic aromatic hydrocarbons (PAHs) are a large class of organic compounds composed of two or more fused aromatic rings containing only carbon and hydrogen atoms. These compounds are primarily generated during the incomplete combustion of organic materials such as coal, petroleum, wood, gasoline, and other fossil fuels. Due to their widespread occurrence and persistent nature, PAHs have attracted significant attention in environmental chemistry, toxicology, and public health research.

PAHs are commonly found in air, water, soil, sediments, and food products. Many PAHs exhibit toxic, mutagenic, and carcinogenic properties, making them hazardous pollutants of global concern. The United States Environmental Protection Agency (EPA) has identified sixteen priority PAHs, including naphthalene, anthracene, phenanthrene, pyrene, chrysene, benzo[a]pyrene, and dibenz[a,h]anthracene, because of their environmental persistence and adverse health effects.

The physicochemical properties of PAHs depend largely on their molecular structure and number of aromatic rings. Low molecular weight PAHs are relatively volatile and more soluble in water, whereas high molecular weight PAHs tend to be more hydrophobic, stable, and strongly adsorbed onto particulate matter. These characteristics influence their transport, bioaccumulation, and degradation

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in the environment.

In recent years, mathematical and computational approaches such as Quantitative Structure–Property Relationship (QSPR) and Quantitative Structure–Activity Relationship (QSAR) studies have been extensively employed to investigate the physicochemical and biological properties of PAHs. Topological indices derived from graph theory play an important role in predicting various chemical properties without the need for expensive laboratory experiments. Such studies help in understanding the structural behavior, environmental impact, and toxicity of PAHs, thereby contributing to the development of efficient predictive models in chemical research [1–3, 10].

Polycyclic aromatic hydrocarbons (PAHs) are a class of organic aromatic compounds composed of multiple aromatic rings. The simplest representative is naphthalene, which has two aromatic rings, while anthracene and phenanthrene represent three-ring compounds. These compounds are generally uncharged and nonpolar, and many are colorless. PAH's occur naturally in coal, crude oil, and gasoline. They are produced when coal, oil, gas, wood, garbage, and tobacco are burned. PAH's are semi-volatile, lipophilic, high molecular weight compounds that result from combustion and can accumulate in crops via contaminated soil. They typically exhibit a low degree of acute toxicity to humans, but the most significant endpoint of PAH's toxicity is cancer [7–9].

2. QSRP Analysis of some Polycyclic Aromatic Hydrocarbons

Topological indices and QSPR studies play a significant role in the discovery of new drugs by enabling scientists to analyze, compare, and predict the properties of chemical compounds, thereby accelerating the drug development process while minimizing extensive experimental work. In QSPR analysis, regression models are particularly important when combined with topological indices, as they help establish quantitative relationships between the molecular structure of a compound and its physicochemical properties. Such relationships are highly valuable in drug design, material science, and various other applications in chemistry and related disciplines. Consequently, topological indices have attracted considerable attention as effective mathematical tools for correlating the structural characteristics of chemical compounds with their experimentally determined physicochemical properties. QSPR analysis [8] has therefore emerged as a powerful computational technique in modern drug discovery and development. By constructing mathematical models that relate chemical structures to their physical and chemical properties, QSPR methods facilitate the prediction of important molecular characteristics, reduce experimental costs, and enhance the overall efficiency of drug design and development processes.

In this study, six physicochemical properties of the top-priority 22 polycyclic aromatic hydrocarbons (PAHs) were considered, namely 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 corresponding to these physicochemical properties were obtained from [5, 6], and the collected values are presented in Table 1.

To investigate and predict the physicochemical properties of PAHs, the first multiplicative hyper-Zagreb index $HII_1(G)$ was employed as a molecular descriptor. The first multiplicative hyper-Zagreb index of a graph was introduced by Kulli in [4] and is defined as follows:

$$HII_1(G) = \prod_{uv \in E(G)} \left(d_G(u) + d_G(v)\right)^2 .$$

Here, $d_u(G)$ and $d_v(G)$ denote the degrees of the vertices u and v in the graph G, respectively, while $E(G)$ represents the edge set of G. The computed values of the molecular descriptor corresponding to the molecular graphs of the considered PAHs are listed in Table 2.

Logarithmic Regression Model:

By utilizing the data of Table 1 and Table 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 $HII_1(G)$:

$$\begin{aligned}
BP &= 51.130 + 5.491 \cdot log(HII_1) \\
pi - ele &= 2.815 + 0.334 \cdot log(HII_1) \\
MW &= 36.396 + 2.846 \cdot log(HII_1) \\
PO &= 3.709 + 0.420 \cdot log(HII_1) \\
MV &= 73.526 + 1.659 \cdot log(HII_1) \\
MR &= 9.387 + 1.059 \cdot log(HII_1)
\end{aligned}$$

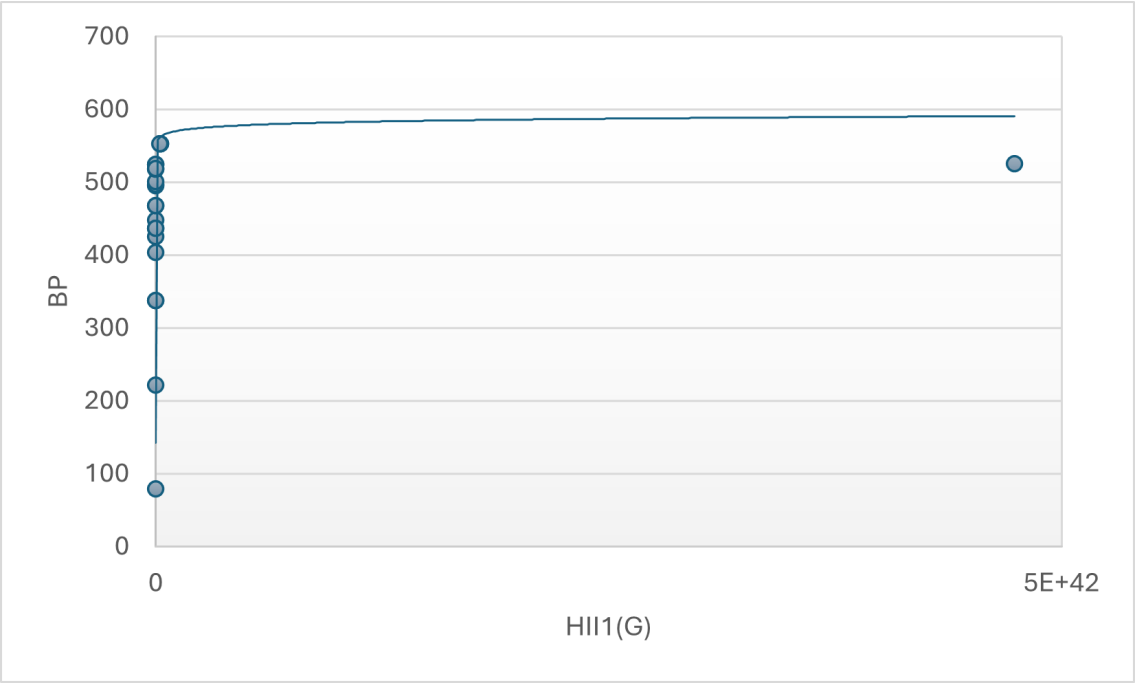
The correlation of first multiplicative hyper-Zagreb index $HII_1(G)$ with the above mentioned physical qualities of Polycyclic Aromatic Hydrocarbon compounds logarithmic models are depicted in the figures mentioned below:

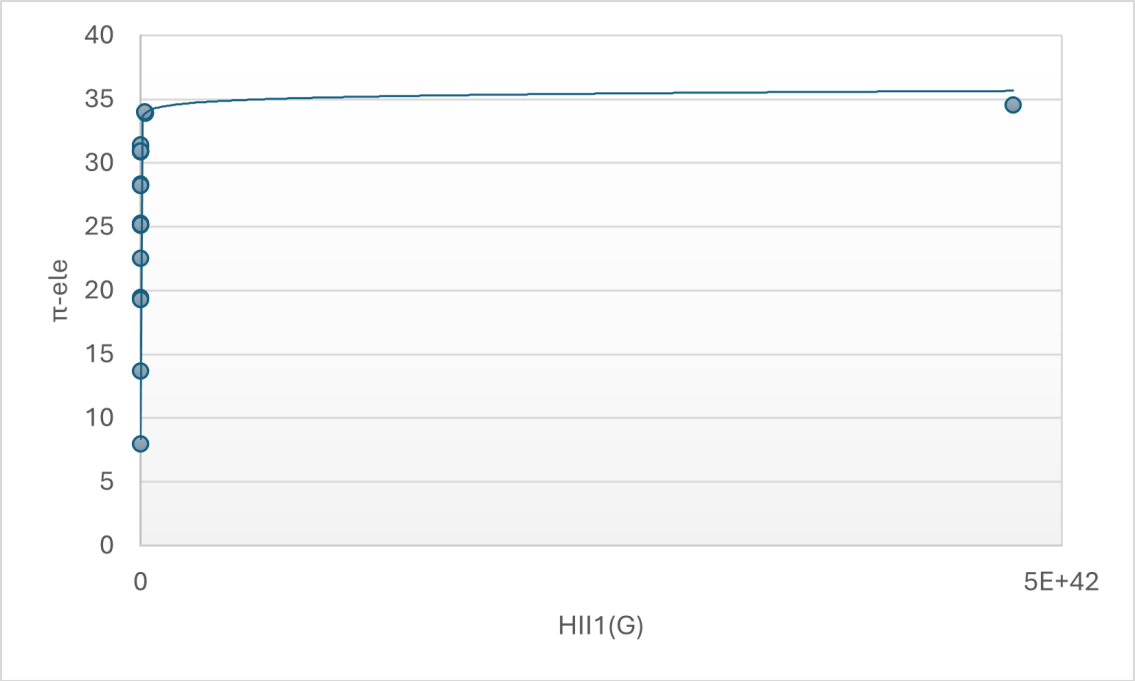
TABLE 1. Polycyclic Aromatic Hydrocarbons with their Physicochemical Properties.

Drug name	$HII_1(G)$	BP	π-ele	MW	PO	MV	MR
Benzene	16777216	78.8	8	78.11	10.4	89.4	26.3
Naphthalene	2.3593×10^{14}	221.5	13.683	128.17	17.5	123.5	44.1
Phenanthrene	3.05765×10^{21}	337.4	19.448	178.23	24.6	157.7	61.9
Anthracene	3.31776×10^{21}	337.4	19.314	178.23	24.6	157.7	61.9
Chrysene	3.96271×10^{28}	448	25.192	228.3	31.6	191.8	79.8
Benzo[a]anthracene	4.29982×10^{28}	436.7	25.101	228.3	31.6	191.8	79.8
Triphenylene	3.65203×10^{28}	425	25.275	228.3	31.6	191.8	79.8
Tetracene	4.6656×10^{28}	436.7	25.188	228.3	31.6	191.8	79.8
Benzo[a]pyrene	2.00612×10^{33}	495	28.222	252.3	35.8	196.1	90.3
Benzo[e]pyrene	1.84884×10^{33}	467.5	28.336	252.3	35.8	196.1	90.3
Perylene	1.84884×10^{33}	467.5	28.245	252.3	35.8	196.1	90.3
Anthanthrene	1.0156×10^{38}	497.1	31.253	276.3	40	200.4	100.8
Benzo[ghi]perylene	9.35977×10^{37}	501	31.425	276.3	40	200.4	100.8
Dibenz[a,c]anthracene	5.13567×10^{35}	518	30.942	278.3	38.7	225.9	97.6
Dibenz[a,h]anthracene	5.57256×10^{35}	524.7	30.881	278.3	38.7	225.9	97.6
Dibenz[a,j]anthracene	5.57256×10^{35}	524.7	30.88	278.3	38.7	225.9	97.6
Picene	5.13567×10^{35}	519	30.943	278.3	38.7	225.9	97.6
Coronene	4.73838×10^{42}	525.6	34.572	300.4	44.1	204.7	111.4
Dibenzo[a,h]pyrene	2.59993×10^{40}	552.3	33.928	302.4	42.9	230.2	108.1
Dibenzo[a,i]pyrene	2.60×10^{40}	552.3	33.954	302.4	42.9	230.2	108.1
Dibenzo[a,l]pyrene	2.3961×10^{40}	552.3	34.031	302.4	42.9	230.2	108.1
Pyrene	1.54793×10^{26}	404	22.506	202.25	28.7	162	72.5

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) $°C$	0.971	0.943	0.940	330.029	0.000
pi-electron count	0.998	0.995	0.995	4212.024	0.000
molecular weight (MW) g/mol	0.994	0.989	0.988	1752.594	0.000
polarizability (P) $dyne/cm$	0.999	0.998	0.998	12851.120	0.000
molar volumes (MV) cm^3	0.937	0.878	0.872	143.697	0.000
molar refractions (MR) cm^3	0.999	0.998	0.998	13203.800	0.000


700
600
500
400
300
200
100
0
BP
0
5E+42
HII1(G)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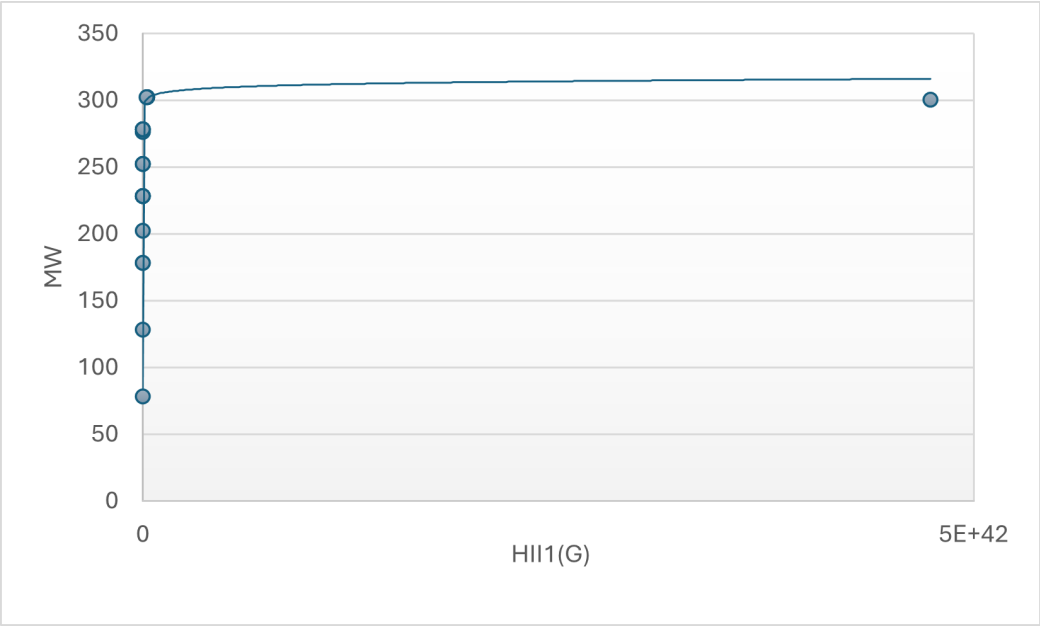
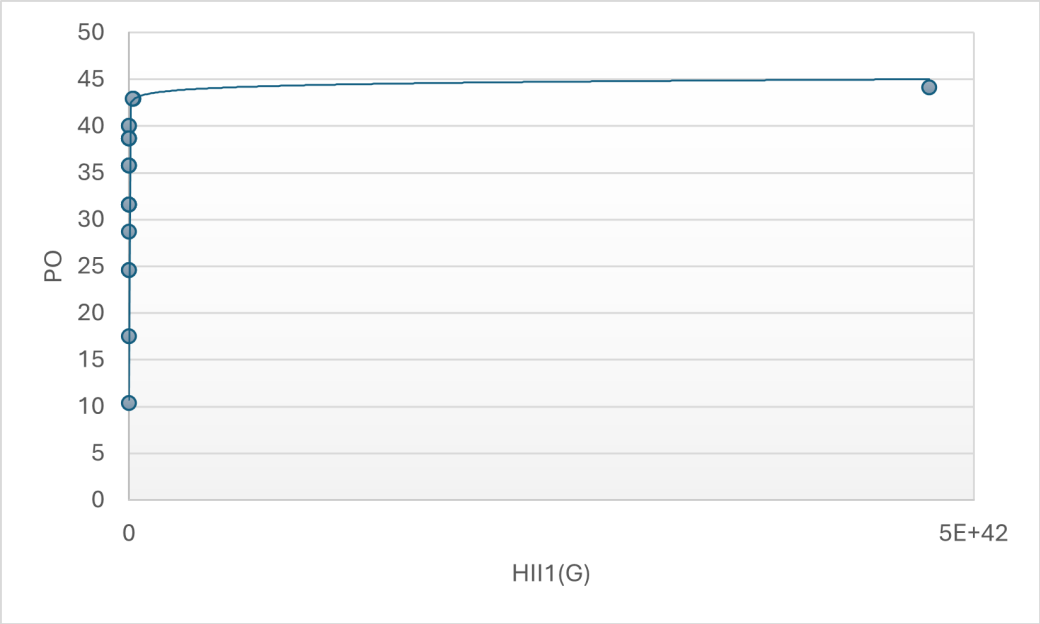
35
30
25
20
15
10
5
0
π-ele
0
5E+42
HII1(G)


350
300
250
200
150
100
50
0
MW
0
5E+42
HII1(G)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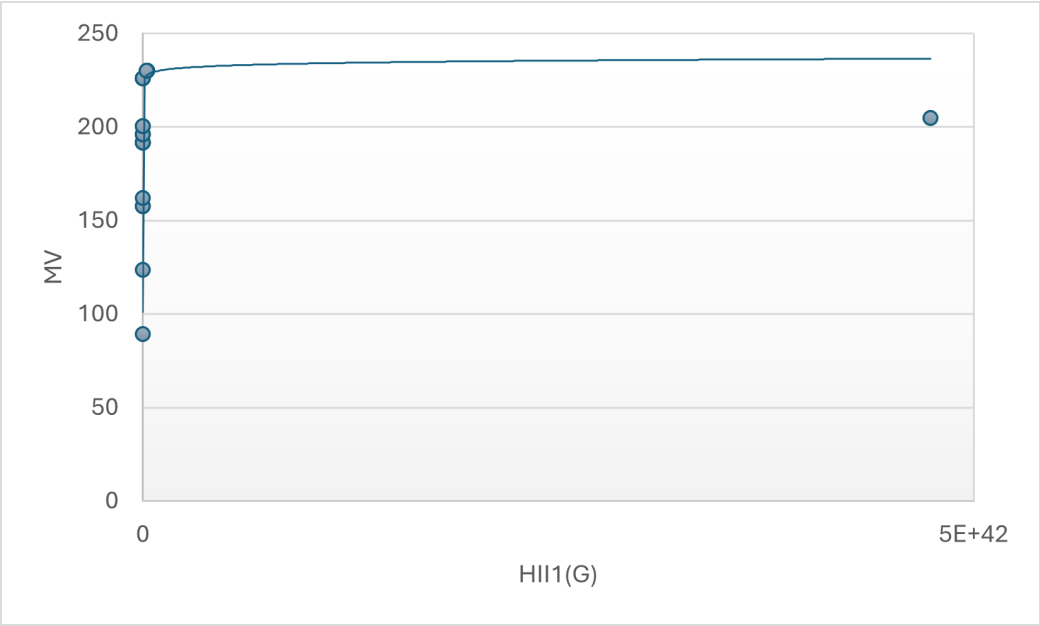
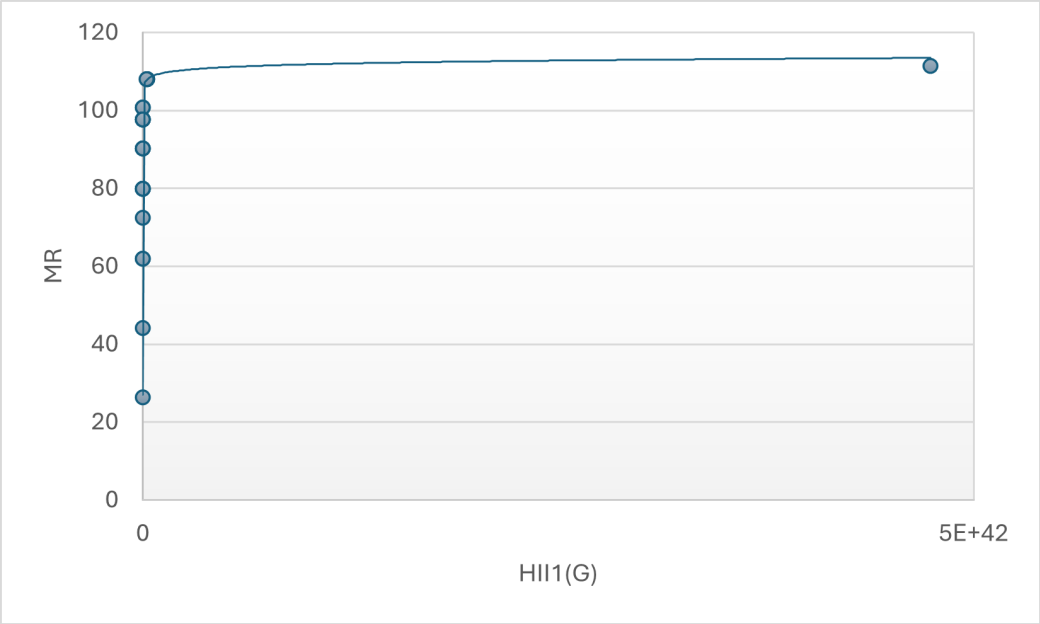
45
40
35
30
25
20
15
10
5
0
PO
0
5E+42
HII1(G)


250
200
150
100
50
0
MV
0
5E+42
HII1(G)


120
100
80
60
40
20
0
MR
0
5E+42
HII1(G)

3. Conclusion

This study demonstrates the effectiveness of the first multiplicative hyper-Zagreb index $FII_1(G)$ 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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