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FIRST MULTIPLICATIVE ZAGREB INDEX AS A MOLECULAR DESCRIPTOR FOR QSPR MODELING OF POLYCYCLIC AROMATIC HYDROCARBONS

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Abstract. In this research paper, we investigate the Quantitative Structure–Property Relationship (QSPR) analysis of polycyclic aromatic hydrocarbons (PAHs) using the first multiplicative Zagreb index, $FH_1(G)$. To examine the relationship between this topological descriptor and six selected physicochemical properties of PAHs, a logarithmic regression model is employed. The results demonstrate a strong correlation between the first multiplicative Zagreb index and the investigated physicochemical properties, indicating the effectiveness of $FH_1(G)$ as a molecular descriptor. Furthermore, detailed logarithmic regression analyses are presented and discussed to evaluate the predictive capability of the proposed index for the selected physicochemical properties of PAHs.

1. Introduction

Polycyclic aromatic hydrocarbons (PAHs) constitute an important group of organic compounds consisting exclusively of carbon and hydrogen atoms arranged in two or more fused aromatic rings. They are mainly formed during the incomplete combustion or pyrolysis of carbon-containing materials, including coal, petroleum products, wood, natural gas, and other fossil fuels. Owing to their widespread distribution and remarkable environmental stability, PAHs have become an important subject of investigation in environmental science, analytical chemistry, toxicology, and public health.

PAHs are frequently detected in various environmental compartments such as the atmosphere, aquatic systems, soils, sediments, and food chains. Their persistence and resistance to natural degradation enable them to remain in the environment for extended periods. Several members of this family possess mutagenic, teratogenic, and carcinogenic characteristics, leading to considerable concern regarding their ecological and human health impacts. Consequently, the United States Environmental Protection Agency (EPA) has designated sixteen PAHs as priority pollutants, including naphthalene, phenanthrene, anthracene, pyrene, chrysene, benzo[a]pyrene, and dibenz[a,h]anthracene, because of their environmental significance and toxicological effects.

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The physical and chemical behaviour of PAHs is strongly governed by their molecular architecture, particularly the number and arrangement of fused aromatic rings. Compounds containing fewer rings generally exhibit higher volatility and comparatively greater aqueous solubility, whereas larger PAHs possess lower solubility, stronger hydrophobicity, and greater chemical stability. These structural characteristics significantly influence their environmental transport, persistence, bioaccumulation, and degradation pathways.

Graph-theoretical methods have become increasingly valuable for analyzing molecular structures and predicting molecular properties through Quantitative Structure–Property Relationship (QSPR) and Quantitative Structure–Activity Relationship (QSAR) models. In these approaches, molecular graphs are represented mathematically, and numerical descriptors known as topological indices are employed to establish relationships between molecular structure and experimentally observed physicochemical or biological properties. Such predictive models reduce the dependence on costly experimental procedures while providing valuable insights into the environmental behaviour, toxicity, and reactivity of PAHs [1–3, 10].

PAHs comprise a diverse family of aromatic hydrocarbons ranging from simple two-ring systems such as naphthalene to more complex three-ring compounds including anthracene and phenanthrene, as well as higher fused-ring analogues. These molecules are generally neutral, non-polar, and predominantly colourless. Natural reservoirs of PAHs include crude oil, coal, and petroleum-derived products, while significant quantities are also released through the combustion of biomass, fossil fuels, municipal waste, and tobacco. Due to their semi-volatile and lipophilic nature, PAHs can accumulate in soils, sediments, and agricultural products, thereby entering the food chain. Although many PAHs exhibit relatively low acute toxicity, prolonged exposure to several high molecular weight PAHs has been strongly associated with carcinogenic effects, making them compounds of considerable environmental and biomedical importance [7–9].

2. QSRP Analysis of some Polycyclic Aromatic Hydrocarbons

Topological indices play a vital role in Quantitative Structure–Property Relationship (QSPR) studies by establishing mathematical relationships between molecular structures and their physicochemical properties. Combined with regression models, they provide efficient tools for predicting molecular properties, thereby supporting drug discovery and reducing experimental effort [8]. In this study, six physicochemical properties of 22 priority polycyclic aromatic hydrocarbons (PAHs), namely boiling point (BP), pi-electron count, molecular weight (MW), polarizability (P), molar volume (MV), and molar refractivity (MR), were analyzed. The corresponding experimental data were obtained from [5, 6] and are listed in Table 1.

To investigate and predict the physicochemical properties of PAHs, the first multiplicative Zagreb index $FH_1(G)$ was employed as a molecular descriptor. The first multiplicative Zagreb index of a graph G is defined as follows:

TABLE 1. Polycyclic Aromatic Hydrocarbons with their Physicochemical Properties

Drug name	BP	π-ele	MW	PO	MV	MR
Benzene	78.8	8	78.11	10.4	89.4	26.3
Naphthalene	221.5	13.683	128.17	17.5	123.5	44.1
Phenanthrene	337.4	19.448	178.23	24.6	157.7	61.9
Anthracene	337.4	19.314	178.23	24.6	157.7	61.9
Chrysene	448	25.192	228.3	31.6	191.8	79.8
Benzo[a]anthracene	436.7	25.101	228.3	31.6	191.8	79.8
Triphenylene	425	25.275	228.3	31.6	191.8	79.8
Tetracene	436.7	25.188	228.3	31.6	191.8	79.8
Benzo[a]pyrene	495	28.222	252.3	35.8	196.1	90.3
Benzo[e]pyrene	467.5	28.336	252.3	35.8	196.1	90.3
Perylene	467.5	28.245	252.3	35.8	196.1	90.3
Anthanthrene	497.1	31.253	276.3	40	200.4	100.8
Benzo[ghi]perylene	501	31.425	276.3	40	200.4	100.8
Dibenz[a,c]anthracene	518	30.942	278.3	38.7	225.9	97.6
Dibenz[a,h]anthracene	524.7	30.881	278.3	38.7	225.9	97.6
Dibenz[a,j]anthracene	524.7	30.880	278.3	38.7	225.9	97.6
Picene	519	30.943	278.3	38.7	225.9	97.6
Coronene	525.6	34.572	300.4	44.1	204.7	111.4
Dibenzo[a,h]pyrene	552.3	33.928	302.4	42.9	230.2	108.1
Dibenzo[a,i]pyrene	552.3	33.954	302.4	42.9	230.2	108.1
Dibenzo[a,l]pyrene	552.3	34.031	302.4	42.9	230.2	108.1
Pyrene	404	22.506	202.25	28.7	162	72.5

$$FH_1(G) = \prod_{uv \in E(G)} \left(d_G(u) + d_G(v)\right),$$

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.

TABLE 2. Polycyclic Aromatic Hydrocarbons and the First Multiplicative Zagreb Index

Drug name	$\mathbf{FH_1(G)}$
Benzene	4096
Naphthalene	15360000
Phenanthrene	55296000000
Anthracene	57600000000
Chrysene	1.99×10^{14}
Benzo[a]anthracene	2.07×10^{14}
Triphenylene	1.91×10^{14}
Tetracene	2.16×10^{14}
Benzo[a]pyrene	4.48×10^{16}
Benzo[e]pyrene	4.30×10^{16}
Perylene	4.30×10^{16}
Anthanthrene	1.01×10^{19}
Benzo[ghi]perylene	9.67×10^{18}
Dibenz[a,c]anthracene	7.17×10^{17}
Dibenz[a,h]anthracene	7.46×10^{17}
Dibenz[a,j]anthracene	7.46×10^{17}
Picene	7.17×10^{17}
Coronene	2.18×10^{21}
Dibenzo[a,h]pyrene	1.61×10^{20}
Dibenzo[a,i]pyrene	1.61×10^{20}
Dibenzo[a,l]pyrene	1.55×10^{20}
Pyrene	1.24×10^{13}

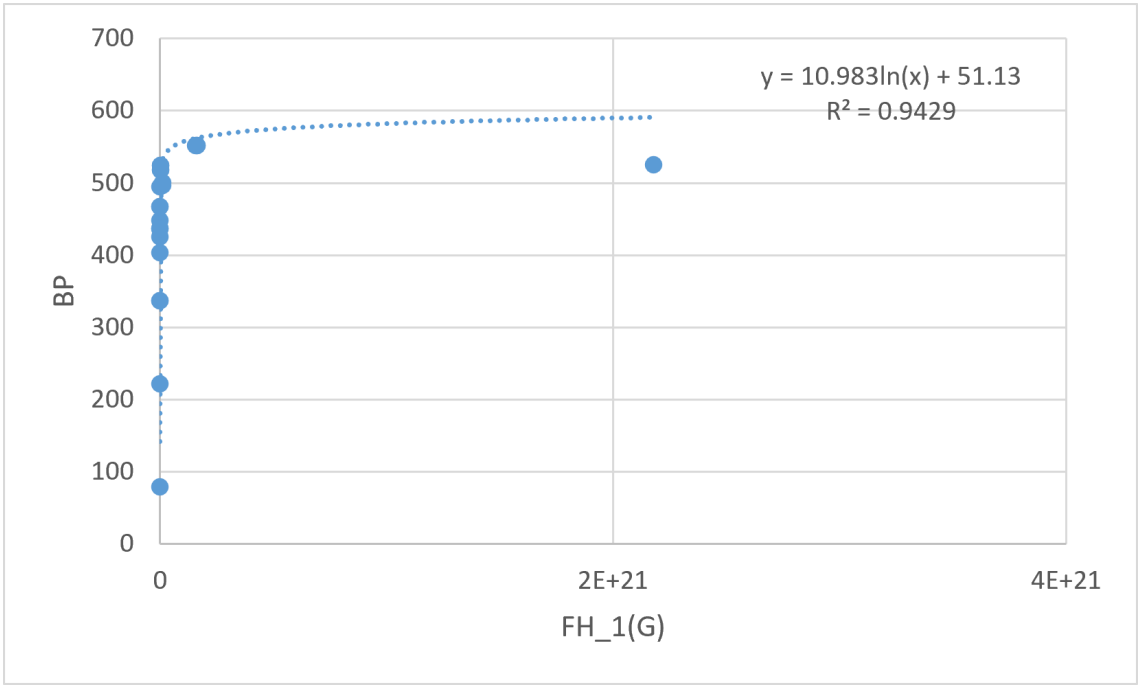
TABLE 3. Correlation coefficients (R) between the first multiplicative Hyper-Zagreb index $FH_1(G)$ and the physicochemical properties of PAHs

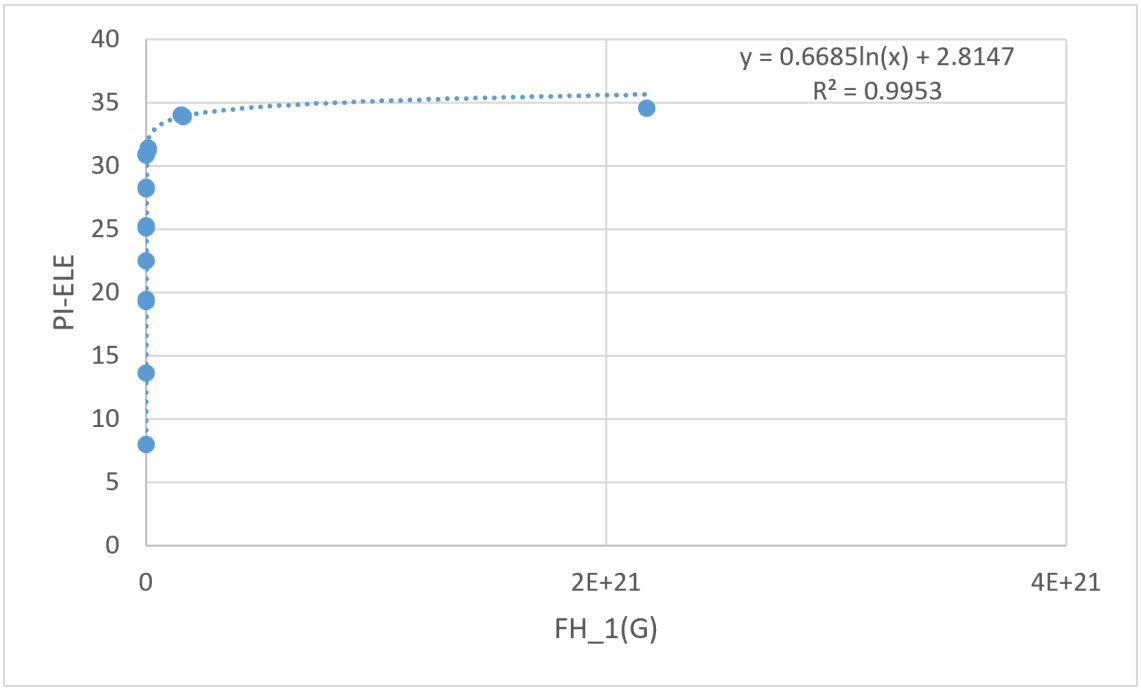
Physicochemical Property	R
Boiling point (BP) (°C)	0.971
Pi-electron count	0.997
Molecular weight (MW) (g/mol)	0.999
Polarizability (P) (dyne/cm)	0.999
Molar volume (MV) (cm^3)	0.936
Molar refraction (MR) (cm^3)	0.999

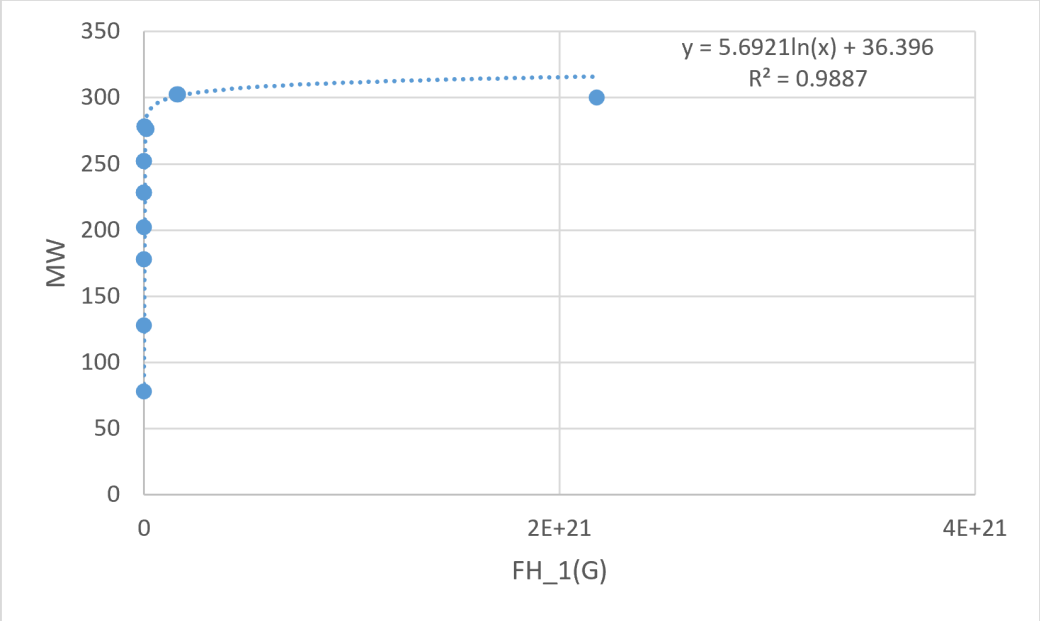
Logarithmic Regression Model:
By utilizing the data of Table 1 and Table 2 we have the regression model for considered physiochemical properties of compounds as in the list. The evaluation of logarithmic regression model is considered as $y = a + b.log(x)$. Here, y denotes chemical property, a denotes 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 Zagreb index $FH_1(G)$:

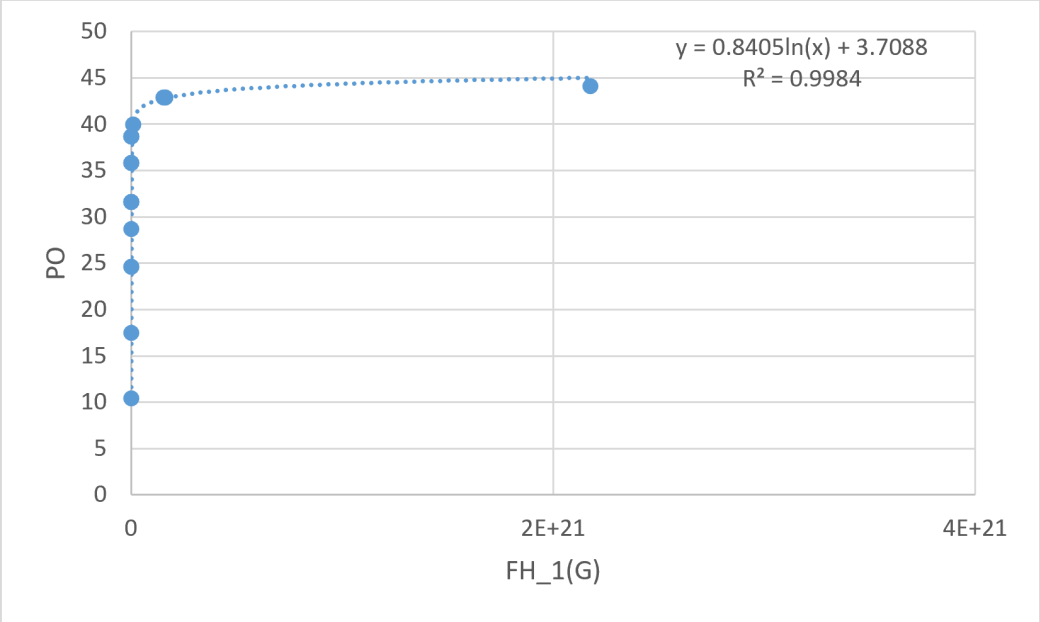
$$\begin{aligned} BP &= 51.13 + 10.983 \cdot log(FH_1(G)) \\ pi - ele &= 2.8147 + 0.6685 \cdot log(FH_1(G)) \\ MW &= 36.396 + 5.6921 \cdot log(FH_1(G)) \\ PO &= 3.7088 + 0.8405 \cdot log(FH_1(G)) \\ MV &= 73.526 + 3.3183 \cdot log(FH_1(G)) \\ MR &= 9.3867 + 2.1188 \cdot log(FH_1(G)) \end{aligned}$$

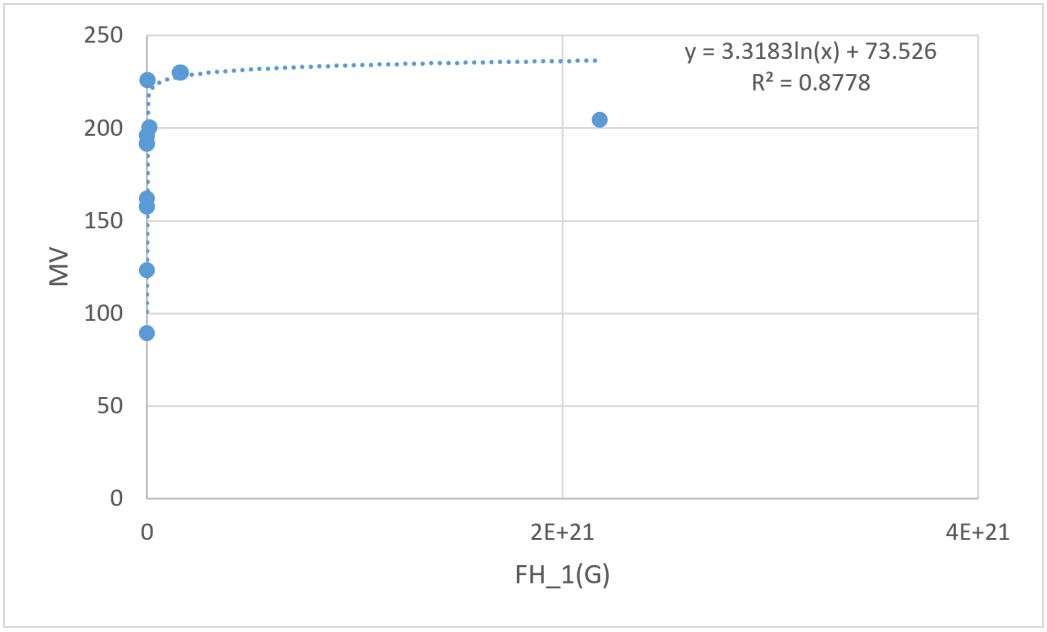
The correlation of first multiplicative Zagreb index $FH_1(G)$ with the above mentioned physical qualities of Polycyclic Aromatic Hydrocarbon compounds logarithmic models are depicted in the figures mentioned below:

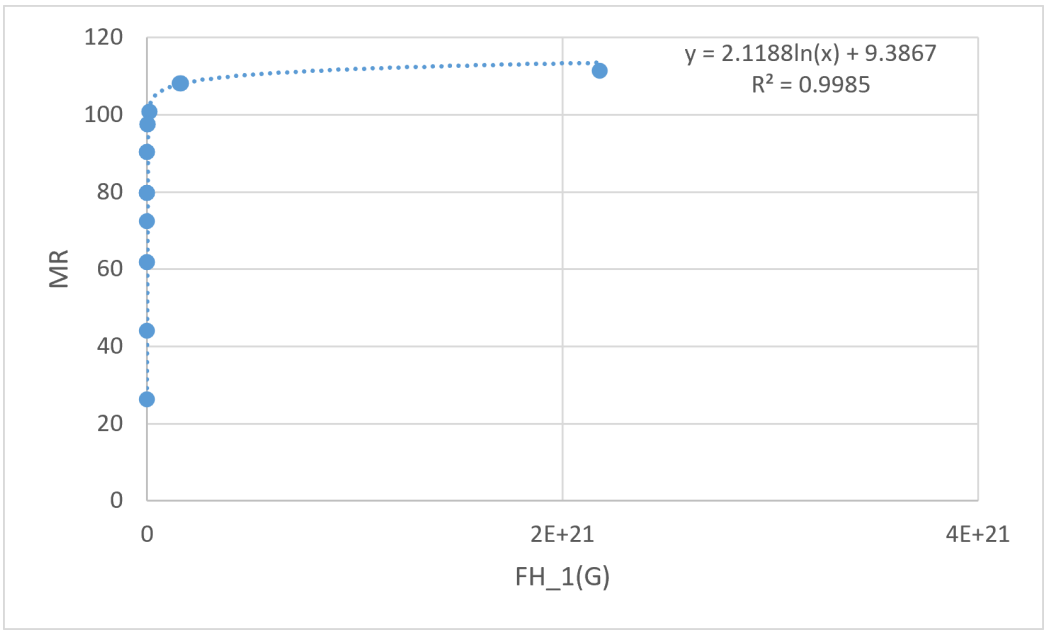

y = 10.983ln(x) + 51.13
R² = 0.9429
BP
700
600
500
400
300
200
100
0
0
2E+21
4E+21
FH_1(G)


y = 0.6685ln(x) + 2.8147
R² = 0.9953
PI-ELE
40
35
30
25
20
15
10
5
0
0
2E+21
4E+21
FH_1(G)


y = 5.6921ln(x) + 36.396
R² = 0.9887
MW
350
300
250
200
150
100
50
0
0
2E+21
4E+21
FH_1(G)


y = 0.8405ln(x) + 3.7088
R² = 0.9984
PO
50
45
40
35
30
25
20
15
10
5
0
0
2E+21
4E+21
FH_1(G)


y = 3.3183ln(x) + 73.526
R² = 0.8778
250
200
150
100
50
0
MV
0
2E+21
4E+21
FH_1(G)


y = 2.1188ln(x) + 9.3867
R² = 0.9985
120
100
80
60
40
20
0
MR
0
2E+21
4E+21
FH_1(G)

3. Conclusion

This study demonstrates that the first multiplicative Zagreb index $FH_1(G)$ is an effective molecular descriptor for the QSPR analysis of polycyclic aromatic hydrocarbons (PAHs). The logarithmic regression models exhibit strong correlations between $FH_1(G)$ and the six selected physicochemical properties, confirming its predictive capability. These findings highlight the potential of $FH_1(G)$ for efficient property prediction and encourage its application to other classes of chemical compounds in future QSPR studies.

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