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Sharp Bounds on the Generalized Multiplicative First Zagreb Index of Graphs with Application to QSPR Modeling

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Abstract: Degree sequence measurements on graphs have attracted a lot of research interest in recent decades. Multiplying the degrees of adjacent vertices in graph Ω provides the multiplicative first Zagreb index of a graph. In the context of graph theory, the generalized multiplicative first Zagreb index of a graph Ω is defined as the product of the sum of the αth powers of the vertex degrees of Ω, where α is a real number such that $\alpha \neq 0$ and $\alpha \neq 1$. The focus of this work is on the extremal graphs for several classes of graphs including trees, unicyclic, and bicyclic graphs, with respect to the generalized multiplicative first Zagreb index. In the initial step, we identify a set of operations that either increases or decreases the generalized multiplicative first Zagreb index for graphs. We then involve analysis of the generalized multiplicative first Zagreb index achieving sharp bounds by characterizing the maximum or minimum graphs for those classes. We present applications of the generalized multiplicative first Zagreb index Π_1^α for predicting the π-electronic energy $E_\pi(\beta)$ of benzenoid hydrocarbons. In particular, we answer the question concerning the value of α for which the predictive potential of Π_1^α with E_π for lower benzenoid hydrocarbons is the strongest. In fact, our statistical analysis delivers that Π_1^α correlates with E_π of lower benzenoid hydrocarbons with correlation coefficient $\rho = -0.998$, if $\alpha = -0.00496$. In QSPR modeling, the value $\rho = -0.998$ is considered to be considerably significant.

Keywords: multiplicative Zagreb index; graph; unicyclic graph; bicyclic graph; extremal values

MSC: 05C92; 05C09; 05C76

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1. Introduction and Preliminaries

We call the "graphical invariant" a quantity associated with a graph whose value is preserved throughout automorphisms of the graph. These topological descriptors are also known as the topological invariants in chemical graph theory. Molecular descriptors may be useful for describing chemical and biological properties notably toxicity, physio-chemical, and thermodynamical characteristics, and for quantitative structure–property relationships (QSPR) and quantitative structure-activity relationships (QSAR) analysis.

Without exception, all of the graphs in this paper will be undirected and simple (no loops or multiple edges). We denote $\Omega = (V(\Omega), E(\Omega))$, to be any graph where $V(\Omega)$ (resp. $E(\Omega)$), is the collection of vertices (resp. edges). Gutman and Trinajstić [1] investigated the effect of molecular structure on the total π-electron energy, then introduced the significant indices named, "Zagreb indices". They further studied the significance of these indices in mathematical chemistry as discussed herein [2]. The first and second Zagreb indices $M_1(\Omega)$ and $M_2(\Omega)$ for any (molecular) graph Ω are defined as

$$M_1(\Omega) = \sum_{u \in V(\Omega)} deg_\Omega(u)^2,$$

$$M_2(\Omega) = \sum_{uv \in E(\Omega)} deg_\Omega(u) \cdot deg_\Omega(v).$$

The topological indices $M_1(\Omega)$ and $M_2(\Omega)$, are used to measure the degree of branching in the molecular carbon skeleton [3,4]. Multiple chemical and mathematical uses of Zagreb indices provided remarkable results, (see [5–7]). Additionally, the classical Zagreb indices $M_1(\Omega)$ and $M_2(\Omega)$ have been discussed by many researchers [8–11]. Similarly, many researchers explored the connection and comparison between $M_1(\Omega)$ and $M_2(\Omega)$ in [12–16]. It should be noted that some academics have also referred to the first Zagreb index $M_1(\Omega)$ as the Gutman index (see quote [3]). Specifically, a synopsis of the most essential characteristics of $M_1(\Omega)$ and $M_2(\Omega)$ have been discussed in [17–19]. Deng [18] provided a unified method for determining the maximum and minimum Zagreb indices for trees, unicyclic graphs, and bicyclic graphs. For further up-to-date information on regular Zagreb indices, we refer the reader to [20,21] and their corresponding cited works.

The multiplicative variants of the Zagreb indices are proposed in 2010 by Todeschini et al. [22]. They have been defined as follows:

$$\Pi_1 = \Pi_1(\Omega) = \prod_{u\in V(\Omega)} deg_\Omega(u)^2,$$

$$\Pi_2 = \Pi_2(\Omega) = \prod_{uv\in E(\Omega)} deg_\Omega(u)\cdot deg_\Omega(v),$$

Note that, $\Pi_2(\Omega) = \prod_{uv\in E(\Omega)} deg_\Omega(u)\cdot deg_\Omega(v) = \prod_{u\in V(\Omega)} deg_\Omega(u)^{deg_\Omega(u)}$

Multiplicative Zagreb indices with given order and size of different graphs such as bipartite graphs, trees and certain nanotubes have been extensively studied in [5,23–25]. Similarly, Wang et al. [26] discussed the multiplicative Zagreb indices of extremal trees with a given number of vertices of maximum degree and Bozovic et al. [27] defined chemical trees with extreme values of a few types of multiplicative Zagreb indices. Then, Eliasi et al. [28,29] discussed a simple approach to multiplicative Zagreb indices and multiplicative first Zagreb index for trees [28].

Using the definition $\Pi_1^* = \Pi_1^*(\Omega) = \prod_{uv\in E(\Omega)}(deg_\Omega(u) + deg_\Omega(v))$, Eliasi and Iranmanesh et al. [30] have recently presented a new index as the multiplicative form of conventional first Zagreb index $M_1(\Omega)$. For the same reason, the generalized multiplicative version of the standard first Zagreb index is defined as $\Pi_1^\alpha = \Pi_1^\alpha(\Omega) = \prod_{uv\in E(\Omega)} (deg_\Omega(u) + deg_\Omega(v))^\alpha$, where α is a real number such that $\alpha \neq 0$ and $\alpha \neq 1$.

Horoldagva and Xu [31] discussed the multiplicative first Zagreb index for extremal graphs and Xu and Das [32] defined the multiplicative first Zagreb index for trees, unicyclic, and bicyclic graphs. Similarly, Alfuraidan et al. and Vetrík et al. [24,33] discussed the general multiplicative Zagreb indices for trees and unicyclic graphs. In accordance with the concept, we refer to the generalized multiplicative first Zagreb index as $\Pi_1^\alpha(\Omega)$. According to the information provided in [22], the generalized multiplicative first Zagreb index is different from the first multiplicative Zagreb index. For instance, $\Pi_1^\alpha(P_3) = 9^{2\alpha}$, whereas $\Pi_1(P_3) = 4$.

Consider T_n, U_n, and B_n to be the collection of trees, unicyclic graphs, and bicyclic graph with n vertices, respectively. The structure of the article is as followed. In order to understand the notations in the main results, Section 1 explains the introduction and preliminaries. Section 2, auxiliary results and a few transformations of graphs that increase/decrease the generalized multiplicative first Zagreb index of graphs are classified. In Section 3, we illustrate proofs of the main results of the paper. Section 2 provides practical applicability of Π_1^α for QSPR modeling of benzenoid hydrocarbons for determining their π-electronic energy E_π measured in β units.

2. Auxiliary Results

Here, we discuss certain graph changes that can either increase or decrease a graph's generalized multiplicative first Zagreb index. The graphs of types T_n, U_n, and B_n that are extremal with respect to generalized multiplicative first Zagreb index are determined by using these transformations.

The following basic results has been shown in [30].

Theorem 1 ([30]). *The path graph P_n achieves the least multiplicative first Zagreb index among all connected graphs with given order n.*

Specifically, we present a modification to graphs that minimizes the generalized multiplicative first Zagreb index, Π_1^{α}. The following results can be easily derived by using the definition of generalized multiplicative first Zagreb index.

Lemma 1 ([32]). *Assume that Ω is a graph that comprises two nonadjacent vertices say u, v and $e \in E(\Omega)$. We obtain $\Pi_1^*(\Omega) < \Pi_1^*(\Omega + uv)$ and $\Pi_1^*(\Omega) > \Pi_1^*(\Omega - e)$.*

Lemma 2. *Suppose a graph Ω with non-adjacent vertices $u, v \in V(\Omega)$ and $e \in E(\Omega)$. Then by employing the definition of the generalized multiplicative first Zagreb, we have $\Pi_1^{\alpha *}(\Omega) < \Pi_1^{\alpha *}(\Omega + uv)$ and $\Pi_1^{\alpha *}(\Omega) > \Pi_1^{\alpha *}(\Omega - e)$ for $\alpha > 0$.*

Transformation 1. *Consider a connected graph Ω with vertex labeled by v. We deduce Ω' from Ω by affixing two paths at vertex v say, $X : \{vw_1w_2 \dots w_k\}$ (resp. $Y : \{vu_1u_2 \dots u_l\}$) of length k (resp. l). Next, $\Omega'' = \Omega' - vu_1 + w_ku_l$.*

Lemma 3. *Consider Ω' and Ω'' are two graphs as constructed in Transformation 1. Then, $\Pi_1^{\alpha}(\Omega'') < \Pi_1^{\alpha}(\Omega')$.*

Proof. Let v be a vertex with degree $y > 0$ in a connected graph say, Ω. Let $deg^1, deg^2, \dots, deg^y$ be the degrees of adjacent vertices of v. For some $k, l \geq 2$, according to the concept of the generalized multiplicative first Zagreb index,

$$\begin{aligned}
\Pi_1^{\alpha}(\Omega') - \Pi_1^{\alpha}(\Omega'') &= \prod_{j=1}^{y} (y + 2 + d_j)^{\alpha} (y+4)^{\alpha} (y+4)^{\alpha} 3^{\alpha} 3^{\alpha} 4^{(k+l-4)\alpha} \\
&- \prod_{j=1}^{y} (d_j + y + 1)^{\alpha} (y+3)^{\alpha} 3^{\alpha} 4^{(k+l-2)\alpha} \\
&= \prod_{j=1}^{y} (d_j + y + 1)^{\alpha} 3^{\alpha} 4^{(k+l-4)\alpha} \left((y+4)^{2\alpha} - (y+3)^{\alpha} 16^{\alpha} \right) \\
&\geq (y+4)^{2\alpha} - (y+3)^{\alpha} 16^{\alpha} \\
&> 0 \ for \ \alpha > 0, \ y > 0
\end{aligned}$$

This completes the proof. □

Remark 1. *It is easy to see that continuously applying Transformation 1 can transform any tree T with size m associated with a graph Ω into a path P_{m+1}. Within this analysis, we demonstrate that Lemma 3 minimizes the generalized multiplicative first Zagreb index.*

By combining Theorem 1 with Lemma 1, we construct the following result, where generalized multiplicative first Zagreb index of trees from T_n decreases.

Theorem 2. *Consider any tree $t_n \in \mathrm{T}_n$ with $n \geq 4$ different from P_n. Then $\Pi_1^{\alpha *}(P_n) < \Pi_1^{\alpha *}(t_n)$.*

By repeatedly employing Lemma 3 and Remark 1, we acquire Theorem 2. Next, we present some auxiliary operations.

Transformation 2. *Let Ω be a connected graph with uv edge such that $deg_{\Omega}(v) \geq 2$. Let $\{v, v_1, v_2, \ldots, v_t\}$ be adjacent vertices to u such that $\{uv_1, uv_2, \ldots, uv_t\}$ is a set of pendant edges.*

Next, we construct $\Omega' = \Omega - \{uv_1, uv_2, \ldots, uv_t\} + \{vv_1, vv_2, \ldots, vv_t\}$.

Lemma 4. *Suppose Ω and Ω' represent two different graphs. Then, $\Pi_1^{\alpha}(\Omega) < \Pi_1^{\alpha}(\Omega')$.*

Proof. Suppose $\Omega_o = \Omega - u, v_1, v_2, \ldots, v_t$. Suppose that $deg_{\Omega_o} = y > 0$

$$\begin{aligned}
\Pi_1^{\alpha}(\Omega') - \Pi_1^{\alpha}(\Omega) &= (y+t+2)^{t\alpha+\alpha} \prod_{j=1}^{y} (d_j + y + t + 1)^{\alpha} \\
&\quad - (y+t+1)^{\alpha}(t+2)^{t\alpha} \prod_{j=1}^{y} (d_j + y + 1)^{\alpha} \\
&= \prod_{j=1}^{y} (d_j + y + 1)^{\alpha} \left((y+t+2)^{t\alpha+\alpha} - (y+t+1)^{\alpha}(t+2)^{t\alpha} \right) \\
&\geq ((y+t+2)^{t\alpha+\alpha} - (y+t+1)^{\alpha}(t+2)^{t\alpha} \\
&> 0 \ for \ \alpha > 0, \ y > 0
\end{aligned}$$

□

Remark 2. *Note that, by repeatedly applying Transformation 2, any tree T of size m that is associated with Ω can be transformed to a star P_{m+1}. Generalized multiplicative first Zagreb index keeps increasing by employing Lemma 4, as long as, this analysis has been performed correctly.*

Transformation 3. *Let u and w be a non-pendant adjacent vertex with different neighbor vertices in a non-trivial connected graph say, Ω. Next, we deduce a resulting graph symbolized by Ω', which is acquired by associating the vertices u and w to a new vertex by p and attaching a pendant vertex indicated by q to the vertex p.*

Lemma 5. *Suppose Ω and Ω' are two graphs. Then $\Pi_1^{\alpha}(\Omega) < \Pi_1^{\alpha}(\Omega')$.*

Proof. Suppose that the neighbors of u are $\{u_1, u_2 \ldots, u_s\}$ with degrees $\{deg(u_1), \ldots, deg(u_s)\}$, respectively, and the neighbors of w are $\{w_1, w_1 \ldots, w_t\}$ with degrees $\{deg(w_1), \ldots, deg(w_t)\}$, respectively.

$$\begin{aligned}
\Pi_1^{\alpha}(\Omega') - \Pi_1^{\alpha}(\Omega) &= (s+t+2)^{\alpha} \prod_{j=1}^{s} (deg_{\Omega'}(u_j) + s + t + 1)^{\alpha} \prod_{j=1}^{t} (deg_{\Omega'}(w_j) + s + t + 1)^{\alpha} \\
&\quad - (s+t+2)^{\alpha} \prod_{j=1}^{s} (deg_{\Omega}(u_j) + s + 1)^{\alpha} \prod_{j=1}^{t} (deg_{\Omega}(w_j) + t + 1)^{\alpha} \\
&\geq \prod_{j=1}^{s} (deg_{\Omega'}(u_j) + s + t + 1)^{\alpha} \prod_{j=1}^{t} (deg_{\Omega'}(w_j) + s + t + 1)^{\alpha} \\
&\quad - \prod_{j=1}^{s} (deg_{\Omega}(u_j) + s + 1)^{\alpha} \prod_{j=1}^{t} (deg_{\Omega}(w_j) + t + 1)^{\alpha} \\
&> 0 \ for \ \alpha > 0, \ s, t > 0
\end{aligned}$$

□

Transformation 4. *Let Ω be a connected graph that comprises pendant path $X = \{u_1 u_2 \ldots u_{t-1} u_t\}$ identifying at vertex u_1 such that u_1 is adjacent with two different vertices say w and x other than u_2. Next, we deduce $\Omega' = \Omega - \{wu_1 + wu_t\}$.*

Lemma 6. *Assume that the two graphs are labeled Ω and Ω'. Then $\Pi_1^{\alpha}(\Omega) > \Pi_1^{\alpha}(\Omega')$.*

Proof. Suppose that $deg_{\Omega}(w) = p > 1$ and $deg_{\Omega'}(x) = q > 1$. For $t \geq 2$, by using the concept of generalized multiplicative first Zagreb index,

$$\begin{aligned}\Pi_1^{\alpha}(\Omega) - \Pi_1^{\alpha}(\Omega') &= (p+3)^{\alpha}(q+3)^{\alpha}5^{\alpha}4^{(t-2)\alpha}3^{\alpha} - (p+2)^{\alpha}(q+2)^{\alpha}4^{t\alpha} \\ & 4^{(t-2)\alpha}[(p+3)^{\alpha}(q+3)^{\alpha}5^{\alpha}3^{\alpha} - 4^{2\alpha}(p+2)^{\alpha}(q+2)^{\alpha}] \\ & > 0 \; for \; \alpha > 0, \; 0 \leq p,q \leq 29\end{aligned}$$

□

Using Transformations 2 and 4, we can have the following transformation.

Transformation 5. *Let Ω be connected graph with path $X = \{xu_1u_2 \ldots u_ty\}$ such that $deg_{\Omega}(u_j) = 2$ and $deg_{\Omega}(p) \geq 2$, $deg_{\Omega}(q) \geq 2$, for some $j = 1, 2, .., t$. $\Omega' = \Omega - \{u_2u_3, u_3u_4, \ldots, u_{t-1}u_t, u_ty\}$ $+\{u_1u_3, u_1u_4, \ldots, u_1u_t, u_1y\}$.*

From Lemmas 4 and 6, the following lemma satisfies.

Lemma 7. *Consider connected graphs say, Ω and Ω'. then $\Pi_1^{\alpha}(\Omega) < \Pi_1^{\alpha}(\Omega')$*

Lemma 8. *Let $deg_1, deg_2, \ldots, deg_t$ be t non-negative integers. Now, we construct a function*

$$z(y) = (y+t+1)^{y\alpha} \prod_{j=1}^{t} (deg_j + y + t)$$

where $y > 0$ is a variant.

Lemma 9. *Suppose $z(y)$ be a function illustrated in Lemma 8. Then, for any non-negative integers p and q, we obtain $z(p+q)z(0) > z(p)z(q)$.*

Proof. Given that $z(y) > 0$ for some $y > 0$. Consequently, to reach a result, it is sufficient to show that $\ln z(p+q) + \ln z(0) > \ln z(p) + \ln z(q)$.

Now, we consider a new function $g(y) = \ln z(y) + \ln z(0) - \ln z(y_1) - \ln z(y - y_1)$ where $0 < y_1 < y$ is an invariant. Introduce new function $h(y) = \alpha \ln(y+t+1) + \frac{\alpha y}{y+t+1} + \sum_{j=1}^{m} \frac{\alpha}{deg_i + y + t}$, then we have

$$\begin{aligned} h'(y) &= \frac{\alpha}{(y+t+1)} - \frac{m+1}{(y+t+1)^2} + \frac{\alpha}{((\prod_{j=1}^{y} deg_j + y + t)^2)} \\ &= \frac{(y+1)\alpha + (\alpha-1)t + \alpha - 1}{(y+t+1)^2} + \frac{\alpha}{(\prod_{j=1}^{y} deg_j + y + t)^2} \\ & > 0 \; for \; \alpha \geq 1 \end{aligned}$$

Consequently, we claim that $h(y)$ is absolutely non-decreasing if $y > 0$. Hence, we obtain

$$\begin{aligned}
g(y) &= \ln(y+t+1)^{y\alpha} + \ln(\prod_{j=1}^{y} deg_j + y + t)^{\alpha} - \ln((y-y_1)+t+1)^{(y-y_1)\alpha} \\
&+ \ln(\prod_{j=1}^{y} deg_j + (y-y_1) + t)^{\alpha} \\
g^{'}(y) &= \frac{y\alpha}{(y+t+1)} + \alpha\ln(y+t+1) + \frac{\alpha}{(\prod_{j=1}^{y} d_j + y + t)} \\
&- \frac{(y-y_1)\alpha}{((y-y_1)+t+1)} + \alpha\ln((y-y_1)+t+1) + \frac{\alpha}{(\prod_{j=1}^{y} + (y-y_1)+t)} \\
&= h(y) - h(y-y_1) \\
&> 0
\end{aligned}$$

So, $g(y)$ is also absolutely non-decreasing for $y > 0$. Therefore, as a result $g(y) > g(y_1) = 0$. Consider $y = p+q$, $y_1 = p$, then we have $g(p+q) > g(p) = 0$, which shows $\ln z(p+q) + \ln z(0) - \ln z(p) - \ln z(q) > 0$. The proof is complete. □

Transformation 6. *Let Ω be connected graph comprises two vertices u and w such that pendent vertices $u_1u_2,\dots,u_p$ (resp. $w_1w_2,\dots,w_q$) identifying at vertex u (resp. w). Construct $\Omega_o = \Omega - \{u_1u_2,\dots,u_k,w_1w_2,\dots,w_l\}$. In Ω_o, vertex u (resp. w) has adjacent vertices say, $u_1^{'}u_2^{'},\dots,u_r^{'}$ (resp. $w_1^{'}w_2^{'},\dots,w_r^{'}$) with $deg_{\Omega_o}(u_j) = deg_{\Omega_o}(w_j) = deg^j$ for $j = 1,2,..,r$.*

Next, we derive $\Omega^{'} = \Omega - \{uu_1,uu_2,\dots,uu_p\} + \{wu_1,wu_2,\dots,wu_p\}$. Similarly, $\Omega^{''} = \Omega - \{ww_1,ww_2,\dots,ww_q\} + \{uw_1,uw_2,\dots,uw_q\}$.

Lemma 10. *Let Ω, $\Omega^{'}$, and $\Omega^{''}$ be a non-trivial connected graphs. Then $\Pi_1^{\alpha}(\Omega) < \Pi_1^{\alpha}(\Omega^{'}) = \Pi_1^{\alpha}(\Omega^{''})$*

Proof. By employing the definition of generalized multiplicative first Zagreb, we have

$$\begin{aligned}
&\Pi_1^{\alpha}(\Omega^{'}) - \Pi_1^{\alpha}(\Omega) = \Pi_1^{\alpha}(\Omega^{''}) - \Pi_1^{\alpha}(\Omega) \\
&\geq (p+q+t+1)^{p\alpha+q\alpha} \prod_{j=1}^{t}(deg^j + p + q + t)^{\alpha} \prod_{j=1}^{t}(deg^j + t)^{\alpha} \\
&- (p+t+1)^{p\alpha}(q+t+1)^{q\alpha} \prod_{j=1}^{t}(deg^j + p + t)^{\alpha} \prod_{j=1}^{t}(deg^j + q + t)^{\alpha} \\
&> 0
\end{aligned}$$

by employing Lemma 9. The proof is complete. □

3. Main Results

If T is a tree, then it can be transformed into a path, usually described as a caterpillar, by removing all of the pendant vertices that are attached to it. The caterpillar tree is also recognized as the Gutman tree (for references, see [2,5]. Now we evaluate the T_n tree with the maximum generalized multiplicative first Zagreb index.

Theorem 3. *Consider a tree $t_n \in \mathrm{T}_n$ with $n \geq 4$ dissimilar from S_n. Then $\Pi_1^{\alpha*}(t_n) < \Pi_1^{\alpha*}(S_n)$.*

Proof. The maximum generalized multiplicative first Zagreb index of a tree in T_n is a caterpillar, as determined by employing Lemma 4 and Remark 2. We illustrate that any caterpillar can be transformed into a star S_n with a bigger generalized multiplicative first Zagreb index by considering Transformations 3 and 5 derived from Lemmas 5 and 7. Consequently, the conclusion of this theorem follows directly. □

Similarly, we can obtain the following result.

Theorem 4. *Consider a graph $\Omega \in T_n$ dissimilar from S_n and P_n. Therefore, $\Pi_1^{\alpha*}(P_n) < \Pi_1^{\alpha}(\Omega) < \Pi_1^{\alpha}(S_n)$.*

Let $T_n^{'}$ be a collection of trees with vertices n such that there exists a vertex of degree at most 3. Consider that $S_n^{'}$ is a resulting graph from S_{n-1} by identifying isolated edges to isolated vertex of S_{n-1}. Eliasi and Iranmanesh [32] established the second minimum multiplicative first Zagreb index for all connected graphs with vertices n. The following result classifies the second maximum or the minimum generalized multiplicative first Zagreb index for graphs T_n.

Theorem 5. *Consider $\Omega \in T_n$ to be a graph dissimilar from S_n, P_n, $S_n^{'}$ and any tree $t_n^{'} \in T_n^{'}$. Then we have $\Pi_1^{\alpha*}(t_n^{'}) < \Pi_1^{\alpha*}(\Omega) < \Pi_1^{\alpha*}(S_n^{'})$.*

Proof. Let $t_n \in T_n$ be a graph different from S_n, P_n, $S_n^{'}$, and any tree $t_n^{'} \in T_n^{'}$. By repeatedly employing Remark 1 and Lemma 3, t_n can be transformed to any tree with n vertices such that there exists a vertex of degree at most 3, where the generalized multiplicative first Zagreb index decreases. Consequently, the left inequality, is satisfied.

Equivalently, the generalized multiplicative first Zagreb index increases when $t_n \in T_n$ is transformed to a caterpillar with diameter 3. A double star graph is basically a caterpillar with diameter 3, symbolized by S_{n_1,n_2} for $1 \leq n_1 \leq n_2$ and $n_1 + n_2 = n - 2$, which is generated by identifying n_1 (resp. n_2) isolated vertices to isolated vertex P_2 (resp. other vertex). Next, we claim that $\Pi_1^{\alpha} S_{n_1,n_2}$ have the largest value if $n_1 = 1$ and $n_2 = n - 3$. Otherwise, $n_1 = 2$. By employing Transformation 6 and Lemma 10, we obtain $S_{1,n-3}$ such that $\Pi_1^{\alpha}(S_{1,n-3}) > \Pi_1^{\alpha}(S_{1,n-3})(S_{n_1,n_2})$, which satisfies the right inequality. □

A graph Ω which comprises at most one cycle with a maximum degree of three and other vertices with a degree at most two is called a sun graph [34]. The following result shows the Π_1^{α} decreases for graphs in U_n.

Theorem 6. *Consider $\Omega \in U_n$ is a graph that is dissimilar from $C_n^{'}$. Then, $\Pi_1^{\alpha}(C_n^{'}) < \Pi_1^{\alpha}(\Omega)$.*

Proof. Given that the unicyclic graph Ω can be transformed to a sun graph which decreases the generalized multiplicative first Zagreb index Π_1^{α} by employing Lemma 3 and Remark 1. The generalized multiplicative first Zagreb index Π_1^{α} gets decreased by repeatedly employing Lemma 6 to any sun graph as long as it is not the cycle $C_n^{'}$. Then $\Pi_1^{\alpha}(C_n^{'}) < \Pi_1^{\alpha}(\Omega)$ is satisfied. □

A graph Ω which comprises at most one cycle and all its isolated vertices transform it into a cycle, called cycle-caterpillar. Consider cycle-caterpillar with cycle C_p if p is its girth. Consider $C_{n,p}$ is a resulting graph by joining $n - p$ isolated edges to a vertex of C_p. The following result shows that the generalized multiplicative first Zagreb index Π_1^{α} increases for graphs in U_n.

Theorem 7. *Assume that $\Omega \in U_n$ is a graph with at most one cycle that is dissimilar from $C_{n,3}$. Then $\Pi_1^{\alpha}(C_{n,3}) > \Pi_1^{\alpha}(\Omega)$.*

Proof. We claim that the generalized multiplicative first Zagreb index increases for graphs in U_n are cyclic caterpillar by repeatedly employing Lemma 4 and Remark 2. Next, the generalized multiplicative first Zagreb index increases when any cyclic caterpillar can be transformed to a cyclic caterpillar with triangle $C_3^{'} = u_1u_2u_3u_1$, by employing Transformations 3 and 5 and Lemmas 7 and 5.

Consider, $C_3^{'}(n_1, n_2, n_3)$ be the cyclic caterpillar with n vertices generated by joining n_k isolated vertices to vertex v_k for some $k = 1, 2, 3$. By employing Transformation 6 at most twice and Lemma 10, we can construct the graph $C_{n,3}$ with $\Pi_1^{\alpha}(C_n^{'3}) > \Pi_1^{*\alpha}(C_3^{'}(n_1, n_2, n_3))$, ending the proof of this result. □

The following result immediately follows by combining Theorems 6 and 7, where extremal graphs from U_n with respect to the generalized multiplicative first Zagreb index are classified.

Theorem 8. *Let $\Omega \in U_n$ be a graph that is dissimilar from $C_3^{'}$ and $C_n^{'}$. Then we have $\Pi_1^{\alpha}(C_n^{'}) < \Pi_1^{\alpha}(\Omega) < \Pi_1^{\alpha}(C_n^{'3})$.*

Next, we discuss extremal graphs from B_n with respect to the generalized multiplicative first Zagreb index. Let $\Omega \in B_n$ be a graph with at least two cycles. The following three cases classified its structure of cycles [35].

1. Let v_o be a common vertex for two cycles C_a and C_b.
2. There exists a path graph of length $m > 0$ attached with cycles C_a and C_b.
3. There exists a common path of length $m > 0$ between C_{m+n} and C_{m+p} cycles.

The graphs $C_{a,b}$, $C_{a,m,b}$ and $C_{n,m,p}$ (where $1 \leq m \leq min\{n, p\}$) corresponding to the cases above are called main subgraphs of $\Omega^{'} \in B_n$ of type (1), (2) and (3), respectively.

Consider $B_n^{'}$ is a resulting graph generated from joining two adjacent edges in S_n among its three isolated vertices. B_n comprises only those graphs which are generated by the removal of an edge of a complete graph K_4 for $n = 4$. Otherwise, for $n = 5$, the generalized multiplicative first Zagreb index Π_1^{α} increases for $B_n^{'}$ among all graphs of B_n.

Next, we will discuss graphs in B_n for $n \geq 6$.

Theorem 9. *Consider $\Omega \in B_n$ is a graph with $n \geq 6$ dissimilar from $B_n^{'}$. Then $\Pi_1^{\alpha}(\Omega) < \Pi_1^{\alpha}(B_n^{'})$.*

Proof. Consider $\Omega^{''} \in B_n$ is a graph achieving largest generalized multiplicative first Zagreb index Π_1^{α}. Let $B_n^{''}$ be a subgraph of $\Omega^{''}$ and its structure similar to any type of case defined in Theorem 8. By employing Remark 2, it is obvious that $\Omega^{''}$ can be construct by joining some isolated edges to some vertices of the graph $B_n^{''}$. Considering the Transformations 3 and 5 and consequently Lemmas 5 and 7, any graph $\Omega \in B_n$ of type (2) can be transformed to $\Omega^{'}$ of type (1) achieving maximum generalized multiplicative first Zagreb index.

Next, consider that type (1) and (3) in B_n.

Claim 1. *Any cycle of $B_n^{''}$ comprises the length less than 5.*

Proof. Otherwise, if $B_n^{''}$ is of type (1), we can construct a different graph $\Omega_1^{''}$ from $\Omega^{''}$ such that $\Pi_1^{\alpha}(\Omega^{''}) < \Pi_1^{\alpha}(\Omega_1^{''})$, by employing Transformations 3, 5 and Lemmas 5, 7, which is contradiction to our choice of $\Omega^{''}$.

Next, we assume that $B_n^{''}$ is of type 3. Let $B_n^{''} \cong \vartheta_{n,m,p}$ with $1 \leq m \leq min\{n, p\}$ and $n + p \geq 5$, where $n, p \nleq 3$. According to formation of $\Omega^{''}$, by employing Transformation 3 or Transformation 5 to $B_n^{''} \in \Omega^{''}$, there exist another graph $\Omega_2^{''} \in B_n$ achieving minimum generalized multiplicative first Zagreb index by Lemmas 5 and 7, which is again contradiction to our choice of $\Omega^{''}$. The proof of Claim 1 is complete. □

It is obvious any cycle in $B_n^{''}$ has length 3 or 4, by By Claim 1. If $B_n^{''}$ is a graph of type (1) then $B_n^{''} \cong C_{3,3}^{'}$. Otherwise, $B_n^{''} \cong \vartheta_{2,1,2}$. Assume that $C_{3,3}^{'}(\eta_1, \eta_2)$ is a resulting graph generated by joining η_1 (resp. η_2) isolated vertices to a vertex of degree 2 (resp. degree 4). Similarly, $\vartheta_{2,1,2}(\eta_1, \eta_2)$ is a resulting graph generated by joining η_1 (resp. η_2) isolated vertices to a vertex of degree 2 (resp. degree 3). According to structure of $C_{3,3}^{'}$ and $\vartheta_{2,1,2}$, we deduce $\Omega^{''}$ graph in the form of $C_{3,3}^{'}(\eta_1, \eta_2)$ (resp. $\vartheta_{2,1,2}(\eta_1, \eta_2)$) with $\eta_1 + \eta_2 = n - 5$, (resp. $\eta_1 + \eta_2 = n - 4$). By employing the concept of generalized multiplicative first Zagreb index, we obtain

$$\begin{aligned}
\Pi_1^{\alpha}(C_{3,3}^{'}(\eta_1, \eta_2))^{\alpha} &= 4^{\alpha}(\eta_1 + 3)^{\eta_1\alpha}(\eta_1 + \eta_2 + 6)^{\alpha}(\eta_1 + 4)^{\alpha}(\eta_2 + 6)^{3\alpha}(\eta_2 + 5)^{\eta_2\alpha} \\
&= 4^{\alpha}(n + 1)^{\alpha}(\eta + 3)^{\eta_1\alpha}(\eta_1 + 4)^{\alpha}(\eta_2 + 6)^{3\alpha}(\eta_2 + 5)^{\eta_2\alpha} \\
\Pi_1^{\alpha}(\vartheta_{2,1,2}(\eta_1, \eta_2))^{\alpha} &= 5^{\alpha}(\eta_1 + 3)^{\eta_1\alpha}(\eta_2 + 4)^{\eta_2\alpha}(\eta_1 + \eta_2 + 5)^{\alpha}(\eta_1 + 5)^{\alpha} \\
&= \cdot(\eta_2 + 6)^{\alpha}(\eta_2 + 5)^{\alpha} \\
&= 5^{\alpha}(\eta_1 + 3)^{\eta_1\alpha}(\eta_2 + 4)^{\eta_2\alpha}(n + 1)^{\alpha}(\eta_1 + 5)^{\alpha}(\eta_2 + 6)^{\alpha}(\eta_2 + 5)^{\alpha}
\end{aligned}$$

Claim 2. *If $\eta_1 = 0$. $\eta_2 = n - 5$, then $\Pi_1^{\alpha}(C_{3,3}^{'}(\eta_1, \eta_2))^{'\alpha}$ reduces its largest values.*

Proof. In order to prove this claim, it is sufficient to find the maximum values of $(\eta_1 + 3)^{\eta_1\alpha}(\eta_1 + 4)^{\alpha}(\eta_2 + 6)^{3\alpha}(\eta_2 + 5)^{\eta_2\alpha}$, where $\eta_1 + \eta_2 = n - 5$. It is clear from factors that maximum value achieve if $\eta_2 \geq \eta_1$, that is, $\eta_1 \leq (n - 5)/2$. Therefore, we only explain the maximum value of $(\eta_1 + 3)^{\eta_1\alpha}(\eta_1 + 4)^{\alpha}(n - \eta_1 + 1)^{3\alpha}(n - \eta_1)^{(n - \eta_1 - 5)\alpha}$. So, we assume a function,

$$f(x) = (y + 4)^{\alpha}(y + 3)^{\alpha y}(n - y + 1)^{3\alpha}(n - y)^{(n - y - 5)\alpha}$$

where $0 \leq y \leq \frac{n-5}{2}$ and $\alpha \geq 0$

$$\begin{aligned}
f^{'}(y) = f(y)\Big[&-\frac{\alpha}{(y + 4)(y + 3)} - \frac{2\alpha(n - 2y - 2)}{(n - y + 1)(y + 3)} + \frac{5\alpha}{(n - y + 1)(n - y)} \\
&+ \ln(\frac{(y + 3)}{(n - y)})^{\alpha}\Big]
\end{aligned}$$

As we know, $0 \leq y \leq \frac{n-5}{2}$ and $\alpha \geq 0$, then $(y + 3) < (n - y)$ and $(n - 2y - 2) \geq 3$ With the help of these results, we obtain

$$-\frac{2\alpha(n - 2y - 2)}{(n - y + 1)(y + 3)} + \frac{5\alpha}{(n - y + 1)(n - y)} < 0$$

Additionally,

$$0 \leq (\frac{(y + 3)}{(n - y)}) \leq 1$$

hence

$$\ln(\frac{(y + 3)}{(n - y)})^{\alpha} \leq 0$$

$$f^{'}(y) < 0,$$

Hence, $f(y)$ is a non-increasing function for $y \leq (n - 5)/2$ and $\alpha \geq 0$. Consequently, $f(y) \leq 4^{\alpha}(n + 1)^{3\alpha}n^{(n-5)\alpha}$ achieve maximum value if $y = 0$, equivalently, $\eta_1 = 0$, $\eta_2 = n - 5$. Which is the required result. □

Similarly, $\Pi_1^{\alpha}(\vartheta_{2,1,2}(n_1^{'}, n_2^{'}))$ achieving maximum values when $\eta_1 = 0$, $\eta_2 = n - 4$. From above discussion, we claim that $\Omega^{''}$ is one of two graphs $(C_{3,3}^{'}(0, n - 5))$ and

$(\vartheta_{2,1,2}(\eta_1, \eta_2)) \cong \mathrm{B}_n'$, In addition, $\Pi_1^{\alpha}(C_{3,3}'(0, n-5)) = 4^{2\alpha}n + 1^{4\alpha}(n)^{(n-5)\alpha}$
$\Pi_1^{\alpha}(\vartheta_{2,1,2}(0, n-4)) = 5^{\alpha}n + 1^{2\alpha}(n+2)(n)^{(n-4)\alpha}$

$$\begin{aligned}\Pi_1^{\alpha}(\vartheta_{2,1,2}(0, n-4)) - \Pi_1^{\alpha}(C_{3,3}'(0, n-5)) &= 5^{\alpha}n + 1^{2\alpha}(n+2)(n)^{(n-4)\alpha} \\ &\quad - 4^{2\alpha}n + 1^{4\alpha}(n)^{(n-5)\alpha} \\ &> 0, \ \alpha > 0\end{aligned}$$

□

Now we introduce three subsets of the set B_n as follows: $\mathrm{B}_{1_n} = C_{a,b} : a + b - 1 = n;$
$\mathrm{B}_{2_n} = C_{a,m,b}p, l, q : a + b + m - 1 = n;$
$\mathrm{B}_{3_n} = \vartheta_{n,m,p} : n + m + p - 1 = n.$

Let G_j be any graph from $\mathrm{B}_{\mathrm{j}_n}$ for $j = 1, 2, 3$. Then,
$\Pi_1^{\alpha}(\Omega_1) = 6^{4\alpha}4^{(n-3)\alpha}$
$\Pi_1^{\alpha}(\Omega_2) = 5^{4\alpha}4^{(n-4)\alpha}6^{\alpha}$ if $m = 1$
$\Pi_1^{\alpha}(\Omega_2) = 5^{6\alpha}4^{(n-4)\alpha}$ if $m > 1$
$\Pi_1^{\alpha}(\Omega_3) = 5^{4\alpha}4^{(n-4)\alpha}6^{\alpha}$ if $m = 1$
$\Pi_1^{\alpha}(\Omega_3) = 5^{6\alpha}4^{(n-4)\alpha}$ if $m > 1$

Theorem 10. *Assume that Ω_n is a graph in $\mathrm{B}_n \setminus \mathrm{B}_{2_n} \bigcup \mathrm{B}_{3_n}$ where $n \geq 6$ and K be a graph in $\mathrm{B}_{2_n} \bigcup \mathrm{B}_{3_n}$ with $m = 1$. Then we have $\Pi_1^{\alpha}(K) < \Pi_1^{\alpha}(\Omega_n)$.*

Proof. We claim that the graph from B_n achieving the minimum generalized multiplicative first Zagreb index must be a graph from the set $\mathrm{B}_{1_n} \bigcup \mathrm{B}_{2_n} \bigcup \mathrm{B}_{3_n}$, by employing the Lemmas 3 and 6 and Remark 1.

From the above calculation of graph Ω_j in B_{j_n}) with $j = 1, 2, 3$, we have $\Pi_1^{\alpha}(\Omega_1) - \Pi_1^{\alpha}(\Omega_2) > 0$ and $\Pi_1^{\alpha}(\Omega_1) - \Pi_1^{\alpha}(\Omega_3) > 0$ Considering the difference of $\Pi_1^{\alpha}(\Omega_j)$ for $j = 2, 3$ when m is different, which is the required result. □

The following result characterizes graphs from B_n with respect to the generalized multiplicative first Zagreb index.

Theorem 11. *Let K be a graph in $\mathrm{B}_{2_n} \bigcup \mathrm{B}_{3_n}$ with $m = 1$. Let Ω_n be a graph in $\mathrm{B}_n \setminus \mathrm{B}_{2_n} \bigcup \mathrm{B}_{3_n}$ different from B_n'. Then, $\Pi_1^{\alpha}(K) < \Pi_1^{\alpha}(\Omega_n) < \Pi_1^{\alpha}(\mathrm{B}_n')$.*

4. Applications of Π_1^{α} in QSPR Modeling of Benzenoid Hydrocarbons

This section intends to present the practical applicability of Π_1^{α} in QSPR modeling of benzenoid hydrocarbons. In [36], the authors investigated the predictive potential of commonly occurring degree-based topological indices for measuring $E_{\pi}(\beta)$ of lower benzenoid hydrocarbons. They consider Π_1^{α} with $\alpha = 1$ and showed that it correlated with $E_{\pi}(\beta)$ having the correlation coefficient $\rho = 0.2361$ which is very poor. They raised the question that for which value of α, for which the correlation coefficient between the index Π_1^{α} and E_{π} of lower benzenoid hydrocarbons is the strongest. This section answers that question and shows that for $\alpha = -0.00496$, we obtain the strongest correlation coefficient of $\rho = -0.998$ between the index Π_1^{α} and E_{π} of lower benzenoid hydrocarbons.

Chen [37] conducted a similar study on the general Randić R_{α} and general sum-connectivity index SCI_{α} and showed that $\alpha = -0.2661$ (resp. $\alpha = -0.5601$) provides the best correlation with E_{π} with R_{α} (resp. SCI_{α}) among all the values of $\alpha \in \mathbb{R}$. We extend that study to Π_1^{α} and show that for $\alpha = -0.00496$, we obtain the strongest correlation coefficient of $\rho = -0.998$ between the index Π_1^{α} and E_{π} of lower benzenoid hydrocarbons. At first, we retrieve the experimental data of E_{π} for the 30 lower benzenoid hydrocarbons from [38] and then compute their Π_1^{α} values. Table 1 present the molecules, their E_{π} and the corresponding Π_1^{α} index for 30 lower benzenoid hydrocarbons.

Table 1. The generalized multiplicative first Zagreb index Π_1^α, $\alpha \in \mathbb{R}$ of 30 lower benzenoid hydrocarbons with their $E_\pi(\beta)$.

Molecule	$E_\pi(\beta)$	Π_1^α
Benzene	8	4096^α
Naphthalene	13.6832	15360000^α
Anthracene	19.3137	57600000000^α
Phenanthrene	19.4483	55296000000^α
Tetracene	24.9308	216000000000000^α
Benzo[c]phenanthrene	25.1875	199065600000000^α
Benzo[a]anthracene	25.1012	207360000000000^α
Chrysene	25.1922	199065600000000^α
Triphenylene	25.2745	191102976000000^α
Pyrene	22.5055	12441600000000^α
Pentacene	30.544	$810000000000000000^\alpha$
Benzo[a]tetracene	30.7255	$777600000000000000^\alpha$
Dibenzo[a,h]anthracene	30.8805	$746496000000000000^\alpha$
Dibenzo[a,j]anthracene	30.8795	$746496000000000000^\alpha$
Pentaphene	30.7627	$777600000000000000^\alpha$
Benzo[g]chrysene	30.999	$687970713600000000^\alpha$
Pentahelicene	30.9362	$716636160000000000^\alpha$
Benzo[c]chrysene	30.9386	$716636160000000000^\alpha$
Picene	30.9432	$716636160000000000^\alpha$
Benzo[b]chrysene	30.839	$746496000000000000^\alpha$
Dibenzo[a,c]anthracene	30.9418	$716636160000000000^\alpha$
Dibenzo[b,g]phenanthrene	30.8336	$746496000000000000^\alpha$
Perylene	28.2453	42998169600000000^α
Benzo[e]pyrene	28.3361	44789760000000000^α
Benzo[a]pyrene	28.222	44789760000000000^α
Hexahelicene	36.6814	$25798901760000000000000^\alpha$
Benzo[ghi]perylene	31.4251	$9674588160000000000^\alpha$
Hexacene	36.1557	$30375000000000000131072^\alpha$
Coronene	34.5718	$21767823360000000000000^\alpha$
Ovalene	46.4974	$380849837506559992795192360960^\alpha$

Next, we executed the data in Table 1 in our Matlab program and show that for $\alpha = -0.00496$, the correlation coefficient $\rho = -0.998$ between the index Π_1^α and E_π of lower benzenoid hydrocarbons is the strongest. Figure 1 shows the curve depicting the α vs. ρ curve with the value of α for which the correlation coefficient ρ is the strongest. Figure 2 delivers a closer look at the curve explaining the dynamics of α vs. ρ values.

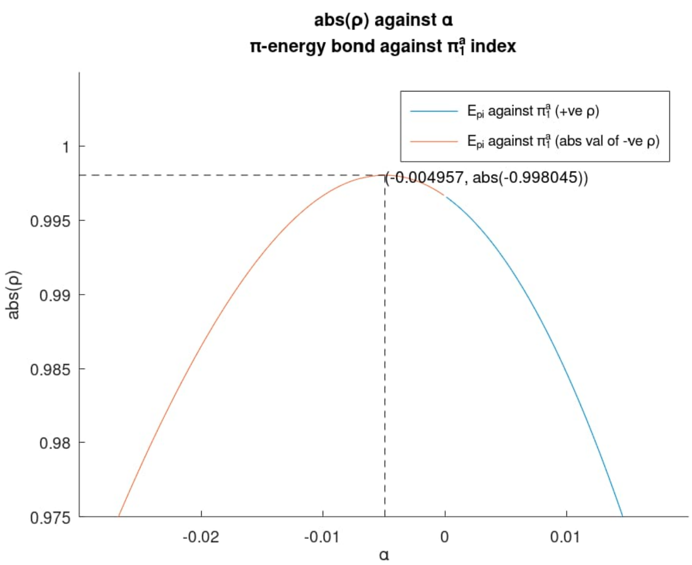

Figure 1. Curve incorporating the strongest ρ for benzenoid hydrocarbons.

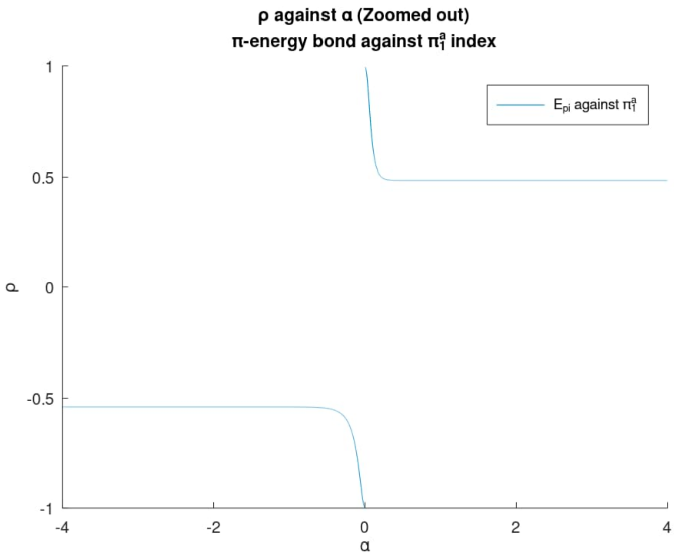

Figure 2. A closer look at the α vs. ρ curve.

The Π_1^α with $\alpha = -0.00496$ delivering the strongest correlation with E_π for benzenoid hydrocarbons has been studied further. We conduct a detailed statistical analysis between Π_1^α with $\alpha = -0.00496$ and E_π. Our statistical model shows that the most suitable regression model for Π_1^α and E_π is, in fact, linear. Next, we present the linear regression model with a 95% confidence interval for its slope and intercept, the determination coefficient r^2 and the standard error of fit s between Π_1^α and E_π.

$$E_\pi(\beta) = 160.5346_{\pm 3.2098} - 159.3616_{\pm 3.8629}\Pi_1^\alpha, \qquad \rho = -0.998,\ r^2 = 0.9960,\ s = 0.4511$$

Next, we construct the scatter plot between Π_1^α with $\alpha = -0.00496$ and E_π for the 30 lower benzenoid hydrocarbons. Figure 3 exhibits the scatter plot.

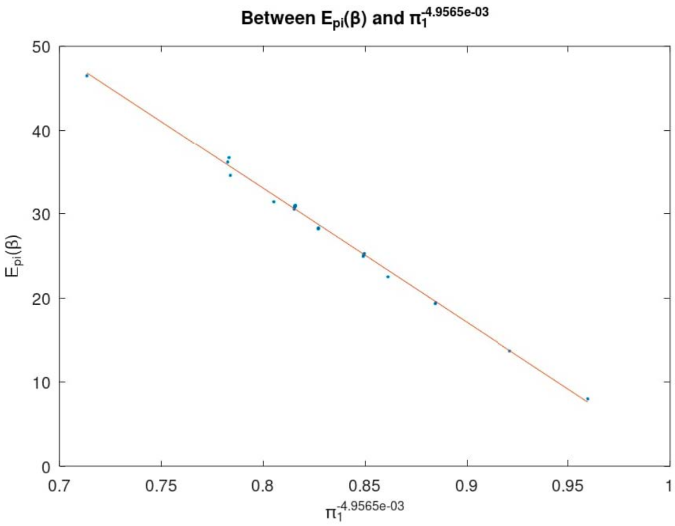

Figure 3. Scatter plot between Π_1^α with $\alpha = -0.00496$ and E_π.

Note that Gutman & Tošović [39] in their seminal work showed that if the correlation coefficient between a topological descriptor and a chemical property is $|\rho| > 0.95$, then the topological descriptor is considered significant and warrants its further usage in QSPR and QSAR modeling.

5. Concluding Remarks

This paper studied some extremal values of the generalized multiplicative first Zagreb index Π_1^α and derived sharp upper and lower bounds on it. In particular, we found sharp upper and lower bounds on Π_1^α, $\alpha \in \mathbb{R}$ for trees, unicylic and bicyclic graphs and characterized graphs achieving those bounds. Our results generalize some results in the literature studying Π_1^α. We also present the practical applicability of Π_1^α in QSPR modeling answering an open question asking for which value of α, the correlation between Π_1^α and the π-electronic energy is the strongest. Our statistical analysis shows that for $\alpha = -0.00496$, the correlation coefficient $\rho = -0.998$ between the index Π_1^α and E_π of lower benzenoid hydrocarbons is the strongest.

The correlation coefficient $\rho = -0.998$ strongly meets the criteria set up by Gutman & Tošović [39] and thus, Π_1^α warrants its further employability in QSPR and QSAR modeling.

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