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QSPR ANALYSIS OF ANTI-ASTHMATIC DRUGS USING REDEFINED FIRST ZAGREB POWER INDEX

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Abstract. In this paper, we introduce a novel degree-based topological index, the Redefined First Zagreb Power Index ($ReZG_1PI(G)$). Explicit formulae for $ReZG_1PI(G)$ are derived for several standard graphs. Furthermore, we investigate the quantitative structure–property relationship (QSPR) of anti-asthmatic drugs. The study reveals a strong correlation between the physicochemical properties of these drugs and their corresponding $ReZG_1PI(G)$, reflecting the structural representation of molecules as graphs. Finally, we establish linear and quadratic regression models between the proposed molecular descriptor and the physicochemical properties of anti-asthmatic drugs.

1. Introduction

Asthma is a long-term lung disease that causes inflammation, too much mucus, and tightening of the airways, making it hard to breathe. In allergic asthma, the airways become extra sensitive to common allergens in the environment. Because it is a chronic condition, people with asthma often need daily medication, and it remains a major health problem worldwide.

According to the World Health Organization (WHO), about 262 million people had asthma in 2019, and the number is still rising. Inhaled steroids have helped lower asthma-related deaths, but the disease still causes major social and economic challenges. There is no known cure or way to prevent asthma, and about $5-10\%$ of patients continue to experience persistent symptoms even when using high-dose corticosteroids and following their treatment plans properly. Over the past 75 years, most drug developments for asthma have focused on improving the effectiveness and duration of existing medicines rather than creating completely new ones. Inhaled corticosteroids (ICS) are still the main treatment, but their "one-size-fits-all" approach doesn't suit every patient. Newer medicines, called leukotriene receptor antagonists (LTRAs) — such as Montelukast, Pranlukast, and Zafirlukast — can help some patients, but they are usually less effective and more expensive than corticosteroids [3, 13, 23].

Long-acting β_2-adrenergic agonists (LABAs) such as Salmeterol, Formoterol, Indacaterol, Olodaterol, and Vilanterol are used along with corticosteroids for long-term asthma control, as they help relax and widen the airways. Epinephrine,

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a short-acting form, is used to quickly relieve severe asthma attacks. Although research has improved natural products to make medicines safer and more effective, creating entirely new types of asthma drugs remains a difficult challenge.

This challenge highlights the urgent need for personalized medicines that can control symptoms and prevent flare-ups without harmful side effects. The discussion on chemical graph theory, Quantitative Structure Property/Activity Relationship (QSPR/QSAR) models, and topological indices correctly explains modern computational techniques used in drug discovery [4,16,24,29]. These methods analyze a molecule's structure to predict its properties, helping scientists design new compounds — an important direction for developing future asthma treatments [21,26]. For new topological indices we suggest the readers to refer the papers [1,2,12,15,17–19,25,27,28].

2. Preliminaries

In a molecular graph, atoms are represented as vertices, and the bonds connecting them are represented as edges. Let $G(V,E)$ be a graph where $V(G)$ denotes the set of vertices and $E(G)$ denotes the set of edges. The order of the graph is the number of its vertices, written as $|V(G)|$, and the size of the graph is the number of its edges, written as $|E(G)|$. The degree of a vertex u, denoted by d_u, is the number of edges connected to it. The standard graph-theoretical concepts used in this work, including bipartite graphs, regular graphs, wheel graphs, and friendship graph follow their usual definitions available in the literature and are presented below. For additional definitions and terminologies, the reader may refer to references [11,30].

Definition 2.1. [20] A graph in which vertex set can be partitioned into two non-empty subset V_1 i.e, $|V_1| = n$ and V_2 i.e $|V_2| = m$ and all vertices in vertex set V_1 is connected to all vertices in vertex set V_2 is called complete bipartite graph.

Definition 2.2. [32] A k-regular graph is a graph where every vertex degree is equal to k.

Definition 2.3. [8] A graph in which a single central vertex is connected to all vertices of a cycle C_{n-1} is called wheel graph W_n.

Definition 2.4. [7] A friendship graph F_n is a graph defined as a collection of n copies cycle graph C_3 with a common central vertex.

3. Redefined First Zagreb Power Index ($ReZG_1PI(G)$) of Graph and It's Computation on Some Standard Graph.

In the literature, most topological indices are formed using algebraic combinations of vertex degrees, often involving the maximum and minimum degree values. These indices are highly effective in relating the structural features of graphs to the physicochemical and biological properties of chemical compounds. As a result, they have become essential theoretical tools that have driven major progress in chemistry and related scientific fields. Among the earliest and most widely studied topological descriptors are the first and second Zagreb indices [6,14]. In 2013, Ranjini, Lokesha, and Usha introduced a new version known as the Redefined First Zagreb Index $ReZG_1(G)$ [9] for a graph G, it is defined as:

$$ReZG_1(G) = \sum_{uv \in E(G)} \frac{(d_u + d_v)}{(d_u \cdot d_v)}.$$

Motivated by the strong predictive performance of existing degree-based descriptors, we introduce a new topological index based on a distinct algebraic combination of a graph's minimum and maximum degrees, called the Redefined First Zagreb Power Index ($ReZG_1PI(G)$). It is defined for a graph G as follows:

Definition 3.1. Redefined First Zagreb Power Index ($ReZG_1PI(G)$) of graph G is defined as

$$ReZG_1PI(G) = \sum_{uv \in E(G)} \frac{[\Delta(G)^{max(d_u,d_v)} + \delta(G)^{min(d_u,d_v)}]}{[\Delta(G)^{max(d_u,d_v)} \cdot \delta(G)^{min(d_u,d_v)}]},$$

where $\Delta(G)$ is the maximum degree of graph G and $\delta(G)$ is minimum degree of graph G.

Empirical results demonstrate that this index exhibit superior correlation with the physicochemical properties of Anti-Asthmatic Drugs when compared to existing topological descriptors. Accordingly, the formulae of standard graphs for newly introduced index are provided below:

Theorem 3.2. *Let P_n be a path for $n \geq 3$ then*

$$ReZG_1PI(P_n) = \frac{5}{4}(n-1).$$

Proof. A path $P_n(\ n \geq 3)$ has n vertices and $n-1$ edges with maximum degree 2 and minimum degree 1. The edge partition of P_n on bases of degree is as follows:

$$|E(2,2)| = \{uv \in E(P_n)/\ d_u = 2 \ and \ d_v = 2\} = n-3$$

and

$$|E(2,1)| = \{uv \in E(P_n)/\ d_u = 2 \ and \ d_v = 1\} = 2.$$

By the definition of $ReZG_1PI(G)$ we get

$$\begin{aligned} ReZG_1PI(P_n) &= (n-3)\left(\frac{2^{max(2,2)} + 1^{min(2,2)}}{2^{max(2,2)} \cdot 1^{min(2,2)}}\right) + 2\left(\frac{2^{max(2,1)} + 1^{min(2,1)}}{2^{max(2,1)} \cdot 1^{min(2,1)}}\right) \\ &= (n-3)\left(\frac{2^2 + 1^2}{2^2 \cdot 1^2}\right) + 2\left(\frac{2^2 + 1^1}{2^2 \cdot 1^1}\right) \\ &= \frac{5}{4}\left(n-1\right). \end{aligned}$$

□

Theorem 3.3. *Let K_n be a complete graph for $n \geq 3$ then*

$$ReZG_1PI(K_n) = \frac{n(n-1)^2}{(n-1)^n}.$$

Proof. A complete graph $K_n(\ n \geq 3)$ has n vertices and $\frac{n(n-1)}{2}$ edges with maximum and minimum degree $(n-1)$. In K_n all end vertex are with degree $(n-1)$. Therefore by the definition of $ReZG_1PI(G)$, we get

$$\begin{aligned} ReZG_1PI(K_n) &= \frac{n(n-1)}{2}\left(\frac{(n-1)^{max(n-1,n-1)} + (n-1)^{min(n-1,n-1)}}{(n-1)^{max(n-1,n-1)} \cdot (n-1)^{min(n-1,n-1)}}\right) \\ &= \frac{n(n-1)}{2}\left(\frac{(n-1)^{(n-1)} + (n-1)^{(n-1)}}{(n-1)^{(n-1)} \cdot (n-1)^{(n-1)}}\right) \\ &= \frac{n(n-1)^2}{(n-1)^n}. \end{aligned}$$

□

Theorem 3.4. *Let $K_{m,n}$ be a complete bipartite graph for $\ n, m \geq 2$ then*

$$ReZG_1PI(K_{m,n}) = \begin{cases} 2n^{(-n+2)}, & for\ n = m; \\ nm\left(\frac{1}{m^m} + \frac{1}{n^n}\right), & for\ m < n. \end{cases}$$

Proof. A complete bipartite graph $K_{m,n}$, has $m+n$ vertices and mn edges. For $m = n$, in $K_{n,n}$ has $2n$ vertices with degree n. Then by the definition of $ReZG_1PI(G)$, we get

$$\begin{aligned} ReZG_1PI(K_{n,n}) &= n^2\left(\frac{n^{max(n,n)} + n^{min(n,n)}}{n^{max(n,n)} \cdot n^{min(n,n)}}\right) \\ &= n^2\left(\frac{n^n + n^n}{n^n \cdot n^n}\right) \\ &= 2n^{-n+2}. \end{aligned}$$

For $m < n$, $K_{m,n}$ has $\Delta(K_{m,n}) = n$ and $\delta(K_{m,n}) = m$. The edge partition of $K_{m,n}$ is given by

$$|E(m,n)| = \{uv \in E(K_{m,n})/\ d_{K_{m,n}}(u) = m\ and\ d_{K_{m,n}}(v) = n\} = nm.$$

Then by the definition of $ReZG_1PI(G)$ and edge partition of $K_{m,n}$ for $(m, n \geq 2)$, we get

$$\begin{aligned} ReZG_1PI(K_{m,n}) &= nm\left(\frac{n^{max(n,m)} + m^{min(n,m)}}{n^{max(n,m)} \cdot m^{min(n,m)}}\right) \\ &= nm\left(\frac{n^n + m^m}{n^n \cdot m^m}\right) \\ &= nm\left(\frac{1}{m^m} + \frac{1}{n^n}\right). \end{aligned}$$

□

Corollary 3.5. *For a star graph $S_{1,n}$ $(n \geq 2)$,*

$$ReZG_1PI(S_{1,n}) = n + n^{(1-n)}.$$

Theorem 3.6. *Let G be a $k-$regular graph with $n \geq 3$ vertices then*

$$ReZG_1PI(G) \quad = \quad nk^{(1-k)}.$$

Proof. The $k-$regular graph of $n \geq 3$ vertices has $\frac{kn}{2}$ edges with maximum and minimum degree k. Therefore by utilizing definition of $ReZG_1PI(G)$, we get

$$\begin{aligned} ReZG_1PI(G) &= \frac{kn}{2}\left(\frac{k^{max(k,k)} + k^{min(k,k)}}{k^{max(k,k)} \cdot k^{min(k,k)}}\right) \\ &= \frac{kn}{2}\left(\frac{k^k + k^k}{k^k \cdot k^k}\right) \\ &= nk^{(1-k)}. \end{aligned}$$

□

Corollary 3.7. *Let C_n be a cycle for $n \geq 3$ then*

$$ReZG_1PI(C_n) = \frac{n}{2}.$$

Theorem 3.8. *Let W_n be a wheel graph for $n \geq 4$ then*

$$ReZG_1PI(W_n) = \frac{n^3 - 3n^2 + 3n + 26}{27(n-1)^2}.$$

Proof. A wheel graph $W_n(\ n \geq 4)$ with n vertices and $2(n-1)$ edges has maximum degree $(n-1)$ minimum degree 3. The edge partition of Wheel Graph W_n is given as follows,

$$\begin{aligned} |E(n-1,3)| &= \{uv \in E(W_n)/\ d_u = n-1 \ and \ d_v = 3\} = n-1, \\ |E(3,3)| &= \{uv \in E(W_n)/\ d_u = 3 \ and \ d_v = 3\} = n-1. \end{aligned}$$

By definition of $ReZG_1PI(G)$ and edge partitions of W_n, For $(n \geq 4)$, we get

$$\begin{aligned} ReZG_1PI(W_n) &= (n-1)\left(\frac{(n-1)^{max(n-1,3)} + 3^{min(n-1,3)}}{(n-1)^{max(n-1,3)} \cdot 3^{min(n-1,3)}}\right) \\ &\quad +(n-1)\left(\frac{(n-1)^{max(3,3)} + 3^{min(3,3)}}{(n-1)^{max(3,3)} \cdot 3^{min(3,3)}}\right) \\ &= (n-1)\left(\frac{(n-1)^{(n-1)} + 3^3}{(n-1)^{(n-1)} \cdot 3^3}\right) + (n-1)\left(\frac{(n-1)^3 + 3^3}{(n-1)^3 \cdot 3^3}\right) \\ &= \frac{n^3 - 3n^2 + 3n + 26}{27(n-1)^2}. \end{aligned}$$

□

4. $ReZG_1PI(G)$ of well known graphs and their line graphs.

The following well known graphs are derived from graph operations on cycle C_n.

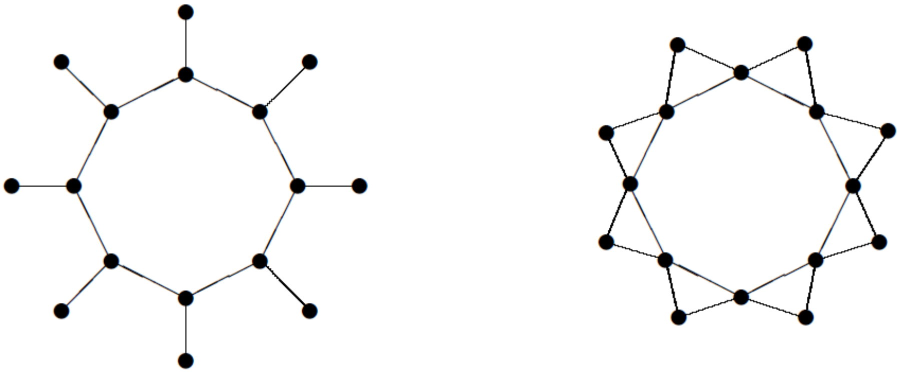

FIGURE 1. CW_8 and $L(CW_8)$

4.1. Crown Graph. The graph $C_n \circ K_1$ is called a crown graph CW_n [10]. The graph CW_8 and its corresponding line graph $L(CW_8)$ are shown in Figure 1.

Theorem 4.1. *For a crown graph* CW_n*,* $(n \geq 4)$*,*

$$ReZG_1PI(CW_n) = \frac{56}{27}n.$$

Proof. A crown graph CW_n has $2n$ vertices and $2n$ edges with $\Delta(CW_n) = 3$, $\delta(CW_n) = 1$. The edge partitions of crown graph CW_n is given by,

$$\begin{aligned} |E(3,3)| &= |\{uv \in E(CW_n)/\ d_{CW_n}(u) = 3 \ and \ d_{CW_n}(v) = 3\}| = n, \\ |E(1,3)| &= |\{uv \in E(CW_n)/\ d_{CW_n}(u) = 1 \ and \ d_{CW_n}(v) = 3\}| = n. \end{aligned}$$

By definition of $ReZG_1PI(G)$ and edge partitions of CW_n, For $(n \geq 4)$, we get

$$\begin{aligned} ReZG_1PI(CW_n) &= n\Big(\frac{3^{max(3,3)} + 1^{min(3,3)}}{3^{max(3,3)} \ . \ 1^{min(3,3)}}\Big) + n\Big(\frac{3^{max(1,3)} + 1^{min(1,3)}}{3^{max(1,3)} \ . \ 1^{min(1,3)}}\Big) \\ &= n\Big(\frac{3^3 + 1^3}{3^3 \cdot 1^3}\Big) + n\Big(\frac{3^3 + 1^1}{3^3 \cdot 1^1}\Big) \\ &= \frac{56}{27}n. \end{aligned}$$

□

Theorem 4.2. *For line graph of crown graph* $L(CW_n)$*,* $(n \geq 4)$*,*

$$ReZG_1PI(L(CW_n)) \quad = \quad \frac{147}{256}n.$$

Proof. A line graph of crown graph $L(CW_n)$ has $2n$ vertices and $3n$ edges with $\Delta(L(CW_n)) = 4$, $\delta(L(CW_n)) = 2$. The edge partitions of line graph of crown graph $L(CW_n)$ is given by,

$$|E(2,4)| = |\{uv \in E(L(CW_n))/\ d_{L(CW_n)}(u) = 2 \ and \ d_{L(CW_n)}(v) = 4\}| = 2n,$$
$$|E(4,4)| = |\{uv \in E(L(CW_n))/\ d_{L(CW_n)}(u) = 4 \ and \ d_{L(CW_n)}(v) = 4\}| = n.$$

By definition of $ReZG_1PI(G)$ and edge partitions of $L(CW_n)$, for $(n \geq 4)$ we get:

$$\begin{aligned} ReZG_1PI(L(CW_n)) &= 2n\Big(\frac{4^{max(2,4)}+2^{min(2,4)}}{4^{max(2,4)}\cdot 2^{min(2,4)}}\Big)+n\Big(\frac{4^{max(4,4)}+2^{min(4,4)}}{4^{max(4,4)}\cdot 2^{min(4,4)}}\Big) \\ &= 2n\Big(\frac{4^4+2^2}{4^4\cdot 2^2}\Big)+n\Big(\frac{4^4+2^4}{4^4\cdot 2^4}\Big) \\ &= \frac{147}{256}n. \end{aligned}$$

□

4.2. Gear Graph. The graph obtained by adding a vertex between every pair of adjacent vertices of the cycle C_n in the wheel W_{n+1} is called a gear graph G_n. The gear graph G_6 and its corresponding line graph $L(G_6)$ are shown in Figure 2.

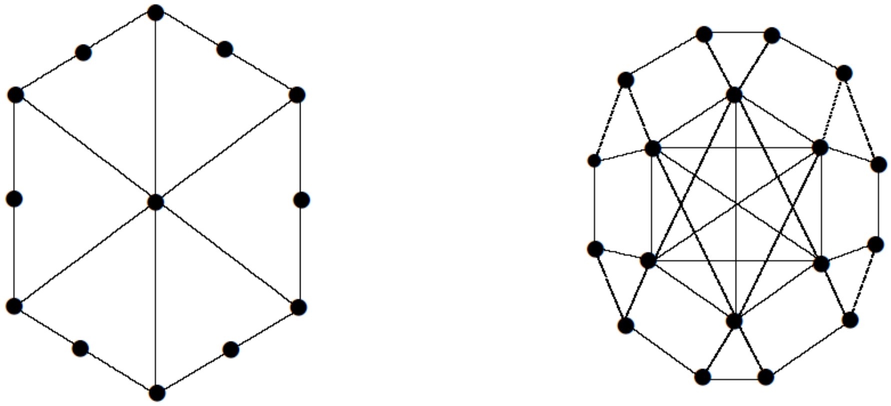

FIGURE 2. G_6 and $L(G_6)$

Theorem 4.3. *For a gear graph $G_n, (n \geq 4)$,*

$$ReZG_1PI(G_n) = \frac{16n^n+5n^{n+3}+8n^3}{8n^{n+2}}.$$

Proof. A gear graph G_n has $2n+1$ vertices and $3n$ edges with $\Delta(G_n) = n$, $\delta(G_n) = 2$. The edge partitions of gear graph G_n is given by,

$$\begin{aligned} |E(2,3)| &= |\{uv \in E(G_n)/\ d_{G_n}(u) = 2 \ and \ d_{G_n}(v) = 3\}| = 2n, \\ |E(3,n)| &= |\{uv \in E(G_n)/\ d_{G_n}(u) = 3 \ and \ d_{G_n}(v) = n\}| = n. \end{aligned}$$

By the definition of $ReZG_1PI(G)$ and edge partitions of G_n, For $(n \geq 4)$, we get

$$\begin{aligned} ReZG_1PI(G_n)) &= 2n\Big(\frac{n^{max(2,3)}+2^{min(2,3)}}{n^{max(2,3)}\cdot 2^{min(2,3)}}\Big)+n\Big(\frac{n^{max(3,n)}+2^{min(3,n)}}{n^{max(3,n)}\cdot 2^{min(3,n)}}\Big) \\ &= 2n\Big(\frac{n^3+2^2}{n^3\cdot 2^2}\Big)+n\Big(\frac{n^n+2^3}{n^n\cdot 2^3}\Big) \\ &= \frac{16n^n+5n^{n+3}+8n^3}{8n^{n+2}}. \end{aligned}$$

□

Theorem 4.4. *For line graph of gear graph* $L(G_n), (n \geq 4)$,

$$ReZG_1PI(L(G_n)) \quad = \quad \frac{A}{54 \cdot 3^n \cdot (n+1)^3 \cdot (n+1)^n},$$

where,

$$\begin{aligned} A = n\big(&135 \cdot n^2\sigma_1 + 27 \cdot 3^n\sigma_2 + 180 \cdot n^3\sigma_1 + 135 \cdot n^4\sigma_1 + 54 \cdot n^4\sigma_1 + 9 \cdot n^6\sigma_1 \\ &+ 216 \cdot n \cdot 3^n + 54 \cdot n\sigma_1 + 116 \cdot 3^n(n+1)^n + 108 \cdot 3^n + 9\sigma_1 \\ &+ 108 \cdot 3^n \cdot n^2 + 24 \cdot 3^n \cdot n(n+1)^n \\ &+ 135 \cdot 3^n \cdot n\sigma_2 + 24 \cdot 3^n \cdot n^2(n+1)^n + 8 \cdot 3^n \cdot (n+1)^n \\ &+ 270 \cdot 3^n \cdot n^2\sigma_2 + 270 \cdot 3^n \cdot n^3\sigma_2 + 135 \cdot 3^n \cdot n^4\sigma_2 + 27 \cdot 3^n \cdot n^5\sigma_2\big), \end{aligned}$$

$\sigma_1 = (n+1)^{(3n)}$, *and* $\sigma_2 = (n+1)^{(2n)}$.

Proof. A line graph of gear graph $L(G_n)$ has $3n$ vertices and $\frac{n^2+7n}{2}$ edges with $\Delta(L(G_n)) = n+1$, $\delta(L(G_n)) = 3$. The edge partitions of line graph of gear graph $L(G_n)$ is given by,

$$\begin{aligned} |E(3,3)| &= |\{uv \in E(L(G_n))/\ d_{L(G_n)}(u) = 3 \ and\ d_{L(G_n)}(v) = 3\}| = 2n \\ |E(3,n+1)| &= |\{uv \in E(L(G_n))/\ d_{L(G_n)}(u) = 3 \ and\ d_{L(G_n)}(v) = n+1\}| = 2n \\ |E(n+1,n+1)| &= |\{uv \in E(L(G_n))/\ d_{L(G_n)}(u) = n+1 \ and\ d_{L(G_n)}(v) = n+1\}| \\ &= \frac{n(n-1)}{2}. \end{aligned}$$

By definition of $ReZG_1PI(G)$ and the edge partitions of $L(G_n)$, for $(n \geq 4)$, we get

$$\begin{aligned} ReZG_1PI(L(G_n)) \quad &= \quad 2n\Big(\frac{(n+1)^{max(3,3)} + 3^{min(3,3)}}{(n+1)^{max(3,3)} \cdot 3^{min(3,3)}}\Big) \\ &\quad +2n\Big(\frac{(n+1)^{max(n+1,3)} + 3^{min(n+1,3)}}{(n+1)^{max(n+1,3)} \cdot 3^{min(n+1,3)}}\Big) \\ &\quad +\frac{n(n-1)}{2}\Big(\frac{(n+1)^{max(n+1,n+1)} + 3^{min(n+1,n+1)}}{(n+1)^{max(n+1,n+1)} \cdot 3^{min(n+1,n+1)}}\Big) \\ &= \quad 2n\Big(\frac{(n+1)^3 + 3^3}{(n+1)^3 \cdot 3^3}\Big) + 2n\Big(\frac{(n+1)^{(n+1)} + 3^3}{(n+1)^{n+1} \cdot 3^3}\Big) \\ &\quad +\frac{n(n-1)}{2}\Big(\frac{(n+1)^{(n+1)} + 3^{(n+1)}}{(n+1)^{(n+1)} \cdot 3^{(n+1)}}\Big) \\ &= \quad \frac{A}{54 \cdot 3^n \cdot (n+1)^3 \cdot (n+1)^n}, \end{aligned}$$

where,

$$\begin{aligned} A = n\big(&135 \cdot n^2\sigma_1 + 27 \cdot 3^n\sigma_2 + 180 \cdot n^3\sigma_1 + 135 \cdot n^4\sigma_1 + 54 \cdot n^4\sigma_1 + 9 \cdot n^6\sigma_1 \\ &+ 216 \cdot n \cdot 3^n + 54 \cdot n\sigma_1 + 116 \cdot 3^n(n+1)^n + 108 \cdot 3^n + 9\sigma_1 \\ &+ 108 \cdot 3^n \cdot n^2 + 24 \cdot 3^n \cdot n(n+1)^n \end{aligned}$$

$$+ 135 \cdot 3^n \cdot n\sigma_2 + 24 \cdot 3^n \cdot n^2(n+1)^n + 8 \cdot 3^n \cdot (n+1)^n$$
$$+ 270 \cdot 3^n \cdot n^2\sigma_2 + 270 \cdot 3^n \cdot n^3\sigma_2 + 135 \cdot 3^n \cdot n^4\sigma_2 + 27 \cdot 3^n \cdot n^5\sigma_2\big),$$

$\sigma_1 = (n+1)^{(3n)}$, and $\sigma_2 = (n+1)^{(2n)}$. □

4.3. Friendship Graph. A friendship graph C_3^n [7], is a graph defined as a collection of n copies cycle graph C_3 with a common central vertex. The friendship graph C_3^4 and its corresponding line graph $L(C_3^4)$ are shown in Figure 3.

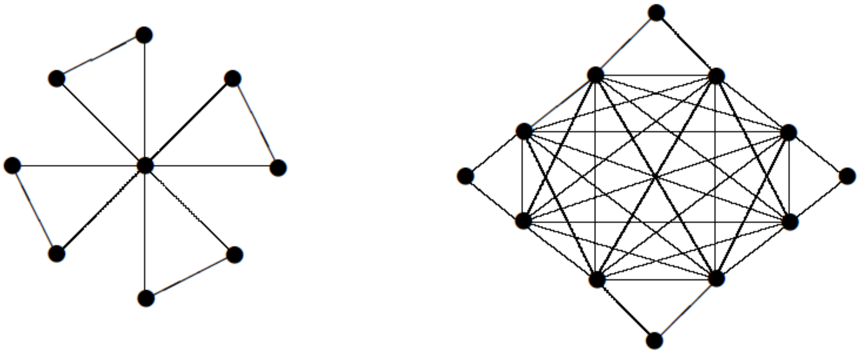

FIGURE 3. C_3^4 and $L(C_3^4)$

Theorem 4.5. *For a friendship graph* C_3^n, $n \geq 2$

$$ReZG_1PI(C_3^n) = \frac{3n^2(2n)^{2n} + 8n^2 + (2n)^{(2n)}}{4n(2n)^{2n}}.$$

Proof. A friendship graph C_3^n has $2n+1$ vertices and $3n$ edges with $\Delta(C_3^n) = 2n$, $\delta(C_3^n) = 2$. Edge partitions of C_3^n is given by,

$$|E(2,2n)| = |\{uv \in E(C_3^n) / \ d_{C_3^n}(u) = 2 \ and \ d_{C_3^n}(v) = 2n\}| = 2n,$$
$$|E(2,2)| = |\{uv \in E(C_3^n) / \ d_{C_3^n}(u) = 2 \ and \ d_{C_3^n}(v) = 2\}| = n.$$

By definition of $ReZG_1PI(G_n)$ and edge partitions of C_3^n, For $n \geq 2$ we get

$$\begin{aligned} ReZG_1PI(C_3^n) =& 2n\Big(\frac{(2n)^{max(2n,2)} + 2^{min(2n,2)}}{(2n)^{max(2n,2)} \cdot 2^{min(2n,2)}}\Big) + n\Big(\frac{(2n)^{max(2,2)} + 2^{min(2,2)}}{(2n)^{max(2,2)} \cdot 2^{min(2,2)}}\Big) \\ =& 2n\Big(\frac{(2n)^{2n} + 2^2}{(2n)^{2n} \cdot 2^2}\Big) + n\Big(\frac{(2n)^2 + 2^2}{(2n)^2 \cdot 2^2}\Big) \\ =& \frac{3n^2(2n)^{2n} + 8n^2 + (2n)^{(2n)}}{4n(2n)^{2n}}. \end{aligned}$$

□

Theorem 4.6. *For line graph of friendship graph* $L(C_3^n)$, $n \geq 2$

$$ReZG_1PI(C_3^n) = \frac{n\big(2 \cdot 2^{(2n)} + 2^{2n}(2n)^{2n} + 4n(2n)^{(2n)} + 4n \cdot 2^{2n} - 2(2n)^{2n}\big)}{2(2)^{2n}(2n)^{2n}}.$$

Proof. A line graph of friendship graph $L(C_3^n)$ has $3n$ vertices and $n(2n+1)$ edges with $\Delta(L(C_3^n)) = 2n$, $\delta(L(C_3^n)) = 2$. Edge partition of $L(C_3^n)$ is given by,

$$|E(2,2n)| = |\{uv \in E(L(C_3^n))/\ d_{L(C_3^n)}u = 2 \textit{ and } d_{L(C_3^n)}v = 2n\}| = 2n,$$
$$|E(2n,2n)| = |\{uv \in E(L(C_3^n))/\ d_{L(C_3^n)}(u) = 2n \textit{ and } d_{L(C_3^n)}v = 2n\}| = n(2n-1).$$

By definition of $ReZG_1PI(G))$ and edge partitions of $L(C_3^n)$ we get

$$\begin{aligned} ReZG_1PI(C_3^n) &= 2n\Big(\frac{(2n)^{max(2n,2)} + 2^{min(2n,2)}}{(2n)^{max(2n,2)} \,.\, 2^{min(2n,2)}}\Big) \\ &\quad + n(2n-1)\Big(\frac{(2n)^{max(2n,2n)} + 2^{min(2n,2n)}}{(2n)^{max(2n,2n)} \,.\, 2^{min(2n,2n)}}\Big) \\ &= 2n\Big(\frac{(2n)^{2n} + 2^2}{(2n)^{2n} \cdot 2^2}\Big) + n(2n-1)\Big(\frac{(2n)^{2n} + 2^{2n}}{(2n)^{2n} \cdot 2^{2n}}\Big) \\ &= \frac{n\big(2 \cdot 2^{(2n)} + 2^{2n}(2n)^{2n} + 4n(2n)^{(2n)} + 4n \cdot 2^{2n} - 2(2n)^{2n}\big)}{2(2)^{2n}(2n)^{2n}}. \end{aligned}$$

□

4.4. Helm Graph. The helm graph H_n [31], is the graph constructed by adjoining a pendant edge at each vertex of the cycle C_n in a wheel graph W_{n+1}.The helm graph H_6 and its corresponding line graph $L(H_6)$ are shown in Figure 4.

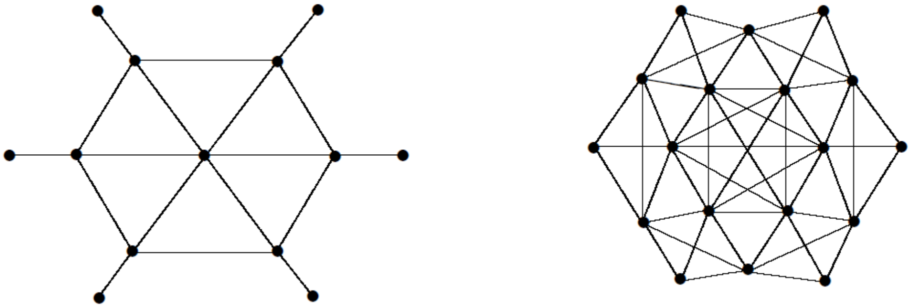

FIGURE 4. H_6 and $L(H_6)$

Theorem 4.7. *For helm graph H_n, $n \geq 4$,*

$$ReZG_1PI(H_n)) = \frac{2n^n + 3n^{n+4} + n^4}{(n)^{n+3}}.$$

Proof. A helm graph H_n has $2n+1$ vertices and $3n$ edges with $\Delta(H_n) = n$, $\delta(H_n) = 1$. Edge partition of H_n is given by

$$\begin{aligned} |E(1,4)| &= |\{uv \in E(H_n)/\ d_{H_n}(u) = 1 \textit{ and } d_{H_n}(v) = 4\}| = n, \\ |E(4,4)| &= |\{uv \in E(H_n)/\ d_{H_n}(u) = 4 \textit{ and } d_{H_n}(v) = 4\}| = n, \\ |E(4,n)| &= |\{uv \in E(H_n)/\ d_{H_n}(u) = 4 \textit{ and } d_{H_n}(v) = n\}| = n. \end{aligned}$$

By definition of $ReZG_1PI(G)$ and edge partition of H_n, for $n \geq 4$, we get

$$\begin{aligned} ReZG_1PI(H_n) &= 2n\Big(\frac{(n)^{max(1,4)} + 1^{min(1,4)}}{(n)^{max(1,4)} \cdot 1^{min(1,4)}}\Big) + n\Big(\frac{(n)^{max(4,4)} + 1^{min(4,4)}}{(n)^{max(4,4)} \cdot 1^{min(4,4)}}\Big) \\ &\quad + n\Big(\frac{(n)^{max(4,n)} + 1^{min(4,n)}}{(n)^{max(4,n)} \cdot 1^{min(4,n)}}\Big) \\ &= n\Big(\frac{n^4 + 1^1}{n^4 \cdot 1^1}\Big) + n\Big(\frac{n^4 + 1^4}{n^4 \cdot 1^4}\Big) + n\Big(\frac{n^n + 1^4}{n^n \cdot 1^4}\Big) \\ &= \frac{2n^n + 3n^{n+4} + n^4}{(n)^{n+3}}. \end{aligned}$$

□

Theorem 4.8. *For line graph of helm graph $L(H_n)$, $n \geq 4$,*

$$ReZG_1PI(L(H_n)) = \frac{B}{486 \cdot 3^n \cdot (n+2)^6 (n+2)^n},$$

where

$$\begin{aligned} B = &19440 \cdot 3^n \cdot n - 1728 \cdot n(n+2)^n - 3456 \cdot n^2(n+2)^n - 1296 \cdot n^3(n+2)^n \\ &+ 2160 \cdot n^4(n+2)^4 + 2700 \cdot n^5(n+2) + 1296 \cdot n^6(n+2)^n + 297 \cdot n^7(n+2)^n \\ &+ 27 \cdot n^8(n+2)^n + 42768 \cdot 3^n \cdot n^2 + 36936 \cdot 3^n \cdot n^3 + 15552 \cdot 3^n \cdot n^4 \\ &+ 3159 \cdot 3^n \cdot n^5 + 2433 \cdot 3^n \cdot n^6 + 5042 \cdot 3^n \cdot n(n+2)^n + 10752 \cdot 3^n \cdot n^2(n+2)^n \\ &+ 13440 \cdot 3^n \cdot n^3(n+2)^n + 8960 \cdot n^4(n+2)^n + 3360 \cdot 3^n \cdot n^5(n+2)^n \\ &+ 672 \cdot 3^n \cdot n^6(n+2)^n + 56 \cdot 3^n \cdot n^7(n+2)^n. \end{aligned}$$

Proof. A line graph of helm graph $L(H_n)$ has $3n$ vertices and $\frac{n(n+11)}{2}$ edges with $\Delta(L(H_n)) = n+2$, $\delta(L(H_n)) = 3$. Edge partition of $L(H_n)$ is given by

$$\begin{aligned} |E(n+2, n+2)| &= |\{uv \in E(L(H_n))/\ d_{L(H_n)}(u) = n+2 \ and \ d_{L(H_n)}(v) = n+2\}| \\ &= \frac{n(n-1)}{2}, \\ |E(n+2, 6)| &= |\{uv \in E(L(H_n))/\ d_{L(H_n)}(u) = n+2 \ and \ d_{L(H_n)}(v) = 6\}| = 2n, \\ |E(6, 3)| &= |\{uv \in E(L(H_n))/\ d_{L(H_n)}(u) = 6 \ and \ d_{L(H_n)}(v) = 3\}| = 2n, \\ |E(n+2, 3)| &= |\{uv \in E(L(H_n))/\ d_{L(H_n)}(u) = n+2 \ and \ d_{L(H_n)}(v) = 3\}| = n, \\ |E(6, 6)| &= |\{uv \in E(L(H_n))/\ d_{L(H_n)}(u) = 6 \ and \ d_{L(H_n)}(v) = 6\}| = n. \end{aligned}$$

By definition of $ReZG_1PI(G)$ and edge partition of $L(H_n)$, For $n \geq 4$, we get

$$\begin{aligned} ReZG_1PI(L(H_n)) = &\frac{n(n-1)}{2}\Big(\frac{(n+2)^{max((n+2),(n+2))} + 3^{min((n+2),(n+2))}}{(n+2)^{max((n+2),(n+2))}) \cdot 3^{min((n+2),(n+2))}}\Big) \\ &+ 2n\Big(\frac{(n+2)^{max((n+2),6)} + 3^{min((n+2),6)}}{(n+2)^{max((n+2),6)}) \cdot 3^{min((n+2),6)}}\Big) \\ &+ 2n\Big(\frac{(n+2)^{max(6,3)} + 3^{min(6,3)}}{(n+2)^{max(6,3)}) \cdot 3^{min((6,3)}}\Big) \end{aligned}$$

$$
\begin{aligned}
&+ n\Big(\frac{(n+2)^{max((n+2),3)} + 3^{min((n+2),3)}}{(n+2)^{max((n+2),3)}) \cdot 3^{min((n+2),3)}}\Big)\\
&+ n\Big(\frac{(n+2)^{max(6,6)} + 3^{min(6,6)}}{(n+2)^{max(6,6)}) \cdot 3^{min((6,6)}}\Big)\\
=&\frac{n(n-1)}{2}\Big(\frac{(n+2)^{(n+2)} + 3^{(n+2)}}{(n+2)^{(n+2)}) \cdot 3^{(n+2)}}\Big) + 2n\Big(\frac{(n+2)^{(n+2)} + 3^{6}}{(n+2)^{(n+2)}) \cdot 3^{6}}\Big)\\
&+ 2n\Big(\frac{(n+2)^{6} + 3^{3}}{(n+2)^{6} \cdot 3^{3}}\Big) + n\Big(\frac{(n+2)^{(n+2)} + 3^{3}}{(n+2)^{(n+2)}) \cdot 3^{3}}\Big)\\
&+ n\Big(\frac{(n+2)^{6} + 3^{6}}{(n+2)^{6} \cdot 3^{6}}\Big)\\
=&\frac{n(n-1)\big((n+2)^{(n+2)} + 3^{(n+2)}\big)}{2 \cdot (n+2)^{(n+2)}) \cdot 3^{(n+2)}} + \frac{2n\big((n+2)^{(n+2)} + 729\big)}{(n+2)^{729 \cdot (n+2)}}\\
&+ \frac{2n\big((n+2)^{6} + 27\big)}{27 \cdot (n+2)^{6}} + \frac{n\big((n+2)^{(n+2)} + 27\big)}{27 \cdot (n+2)^{(n+2)}}\\
&+ \frac{n\big((n+2)^{6} + 729\big)}{729 \cdot (n+2)^{6}}\\
=&\frac{B}{486 \cdot 3^{n} \cdot (n+2)^{6}(n+2)^{n}},
\end{aligned}
$$

where

$$
\begin{aligned}
B =&19440 \cdot 3^{n} \cdot n - 1728 \cdot n(n+2)^{n} - 3456 \cdot n^{2}(n+2)^{n} - 1296 \cdot n^{3}(n+2)^{n}\\
&+ 2160 \cdot n^{4}(n+2)^{4} + 2700 \cdot n^{5}(n+2) + 1296 \cdot n^{6}(n+2)^{n} + 297 \cdot n^{7}(n+2)^{n}\\
&+ 27 \cdot n^{8}(n+2)^{n} + 42768 \cdot 3^{n} \cdot n^{2} + 36936 \cdot 3^{n} \cdot n^{3} + 15552 \cdot 3^{n} \cdot n^{4}\\
&+ 3159 \cdot 3^{n} \cdot n^{5} + 2433 \cdot 3^{n} \cdot n^{6} + 5042 \cdot 3^{n} \cdot n(n+2)^{n} + 10752 \cdot 3^{n} \cdot n^{2}(n+2)^{n}\\
&+ 13440 \cdot 3^{n} \cdot n^{3}(n+2)^{n} + 8960 \cdot n^{4}(n+2)^{n} + 3360 \cdot 3^{n} \cdot n^{5}(n+2)^{n}\\
&+ 672 \cdot 3^{n} \cdot n^{6}(n+2)^{n} + 56 \cdot 3^{n} \cdot n^{7}(n+2)^{n}.
\end{aligned}
$$

□

4.5. Flower Graph. A flower graph F_n [22] is generated by joining each pendant vertex to the central vertex of the helm graph. The flower graph F_6 and its corresponding line graph $L(F_6)$ are shown in Figure 5.

Theorem 4.9. *For a flower graph* $F_n, \ n \geq 4$

$$
ReZG_1PI(F_n) \quad = \quad \frac{5n^4(2n)^{2n} + 16n^4 + (2n)^{2n}}{8n^3(2n)^{2n}}.
$$

Proof. A flower graph F_n has $2n+1$ vertices and $4n$ edges with $\Delta(F_n) = 2n$, $\delta(F_n) = 2$. The edge partition of F_n is given by

$$
\begin{aligned}
|E(4,4)| =&|\{uv \in E(F_n)/ \ d_{F_n}(u) = 4 \ and \ d_{F_n}(v) = 4\}| = n,\\
|E(2n,4)| =&|\{uv \in E(F_n)/ \ d_{F_n}(u) = 2n \ and \ d_{F_n}(v) = 4\}| = n,
\end{aligned}
$$

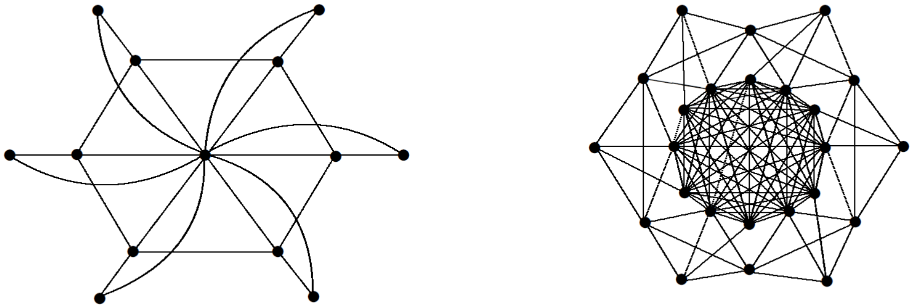

FIGURE 5. F_6 and $L(F_6)$

$$|E(4,2)| = |\{uv \in E(F_n)/\ d_{F_n}(u) = 4 \ and \ d_{F_n}(v) = 2\}| = n,$$
$$|E(2n,2)| = |\{uv \in E(F_n)/\ d_{F_n}(u) = 2n \ and \ d_{F_n}(v) = 2\}| = n.$$

By definition of $ReZG_1PI(F_n)$ and edge partitions of F_n, for $n \geq 4$, we get

$$\begin{aligned} ReZG_1PI(F_n) =& n\Big(\frac{(2n)^{max(4,4)} + 2^{min(4,4)}}{(2n)^{max(4,4)} \cdot 2^{min(4,4)}}\Big) + n\Big(\frac{(2n)^{max(2n,4)} + 2^{min(2n,4)}}{(2n)^{max(2n,4)} \cdot 2^{min(2n,4)}}\Big) \\ &+ n\Big(\frac{(2n)^{max(4,2)} + 2^{min(4,2)}}{(2n)^{max(4,2)} \cdot 2^{min(4,2)}}\Big) + n\Big(\frac{(2n)^{max(2n,2)} + 2^{min(2n,2)}}{(2n)^{max(2n,2)} \cdot 2^{min(2n,2)}}\Big) \\ =& n\Big(\frac{(2n)^4 + 2^4}{(2n)^4 \cdot 2^4}\Big) + n\Big(\frac{(2n)^{(2n)} + 2^4}{(2n)^{(2n)} \cdot 2^4}\Big) + n\Big(\frac{(2n)^4 + 2^2}{(2n)^4 \cdot 2^4}\Big) \\ &+ n\Big(\frac{(2n)^{(2n)} + 2^2}{(2n)^{(2n)} \cdot 2^2}\Big) \\ =& \frac{5n^4(2n)^{2n} + 16n^4 + (2n)^{2n}}{8n^3(2n)^{2n}}. \end{aligned}$$

□

Theorem 4.10. *For line graph of flower graph $L(F_n)$, $n \geq 4$*

$$ReZG_1PI(L(F_n)) \quad = \quad \frac{C}{4096 \cdot 4^{2n} \cdot \sigma_1 \cdot (n+1)^6}$$

where

$$\begin{aligned} C =& 36352 \cdot 4^{2n} \cdot n^2 - 128 \cdot n \cdot \sigma_1 + 82944 \cdot 4^{2n} \cdot n^3 + 101376 \cdot 4^{2n} \cdot n^4 \\ &+ 70144 \cdot 4^{2n} \cdot n^5 + 26112 \cdot 4^{2n} \cdot n^6 + 4096 \cdot 4^{2n} \cdot n^7 + 3456 \cdot n^2 \cdot \sigma_1 \\ &+ 3456 \cdot n^2 \cdot \sigma_1 + 23424 \cdot n^3 \cdot \sigma_1 + 60800 \cdot n^4 \cdot \sigma_1 + 82560 \cdot n^5 \cdot \sigma_1 \\ &+ 62592 \cdot n^6 \cdot \sigma_1 + 25216 \cdot n^7 \cdot \sigma_1 + 4224 \cdot n^8 \cdot \sigma_1 + 6656 \cdot 4^{2n} \cdot n \\ &+ 259 \cdot 4^{2n} \cdot n \cdot \sigma_1 + 402 \cdot 4^{2n} \cdot n^2\sigma_1 + 1005 \cdot 4^{2n} \cdot n^3\sigma_1 \\ &+ 1340 \cdot 4^{2n} \cdot n^4\sigma_1 + 1005 \cdot 4^{2n} \cdot n^5\sigma_1 + 402 \cdot 4^{2n} \cdot n^6 \cdot \sigma_1 + 67 \cdot 4^{2n} \cdot n^7 \cdot \sigma_1 \end{aligned}$$

with $\sigma_1 = (2n+2)^{(2n)}$.

Proof. A line graph of flower graph $L(F_n)$ has $4n$ vertices and $2n(n+3)$ edges with $\Delta(L(F_n)) = 2n+2$, $\delta(L(F_n)) = 4$. The edge partitions of $L(F_n)$ is given by

$$\begin{aligned}
|E(2n,2n)| =& |\{uv \in E(L(F_n))/\ d_{L(F_n)}(u) = 2n \ and \ d_{L(F_n)}(v) = 2n\}| \\
=& \frac{n(n-1)}{2}, \\
|E(2n+2,2n+2)| =& |\{uv \in E(L(F_n))/\ d_{L(F_n)}(u) = 2n+2 \ and \ d_{L(F_n)}(v) = 2n+2\}| \\
=& \frac{n(n-1)}{2}, \\
|E(2n,2n+2)| =& |\{uv \in E(L(F_n))/\ d_{L(F_n)}(u) = 2n \ and \ d_{L(F_n)}(v) = 2n+2\}| = n^2, \\
|E(2n+2,4)| =& |\{uv \in E(L(F_n))/\ d_{L(F_n)}(u) = 2n+2 \ and \ d_{L(F_n)}(v) = 4\}| = n, \\
|E(2n+2,6| =& |\{uv \in E(L(F_n))/\ d_{L(F_n)}(u) = 2n+2 \ and \ d_{L(F_n)}(v) = 6\}| = 2n, \\
|E(2n,4)| =& |\{uv \in E(L(F_n))/\ d_{L(F_n)}(u) = 2n \ and \ d_{L(F_n)}(v) = 4\}| = n, \\
|E(4,6)| =& |\{uv \in E(L(F_n))/\ d_{L(F_n)}(u) = 4 \ and \ d_{L(F_n)}(v) = 6\}| = 2n, \\
|E(6,6)| =& |\{uv \in E(L(F_n))/\ d_{L(F_n)}(u) = 6 \ and \ d_{L(F_n)}(v) = 6\}| = n.
\end{aligned}$$

By definition of $ReZG_1PI(G)$ and edge partitions of $L(F_n)$, For $n \geq 4$, we get

$$\begin{aligned}
ReZG_1PI(L(F_n)) \quad = \quad & \frac{n(n-1)}{2}\Big(\frac{(2n+2)^{max(2n,2n)} + 4^{min((2n,2n)}}{(2n+2)^{max(2n,2n)}) \cdot 4^{min((2n,2n)}}\Big) \\
&+ \frac{n(n-1)}{2}\Big(\frac{(2n+2)^{max((2n+2),(2n+2))} + 4^{min((2n+2),(2n+2))}}{(2n+2)^{max((2n+2),(2n+2))}) \cdot 4^{min((2n+2),(2n+2))}}\Big) \\
&+ n^2\Big(\frac{(2n+2)^{max(2n+2,2n)} + 4^{min((2n+2,2n)}}{(2n+2)^{max(2n+2,2n)}) \cdot 4^{min((2n+2,2n)}}\Big) \\
&+ n\Big(\frac{(2n+2)^{max((2n+2),4)} + 4^{min((2n+2),4)}}{(2n+2)^{max((2n+2),4)}) \cdot 4^{min((2n+2),4)}}\Big) \\
&+ 2n\Big(\frac{(2n+2)^{max(2n+2,6)} + 4^{min((2n+2,6)}}{(2n+2)^{max(2n+2,6)}) \cdot 4^{min((2n+2,6)}}\Big) \\
&+ n\Big(\frac{(2n+2)^{max((2n+2),4)} + 4^{min((2n+2),4)}}{(2n+2)^{max((2n+2),4)}) \cdot 4^{min((2n+2),4)}}\Big) \\
&+ 2n\Big(\frac{(2n+2)^{max(6,4)} + 4^{min((6,4)}}{(2n+2)^{max(6,4)}) \cdot 4^{min((6,4)}}\Big) \\
&+ n\Big(\frac{(2n+2)^{max((6,6)} + 4^{min((6,6)}}{(2n+2)^{max((6,6)}) \cdot 4^{min((6,6)}}\Big) \\
= \quad & \frac{n(n-1)}{2}\Big(\frac{(2n+2)^{2n} + 4^{2n}}{(2n+2)^{2n}) \cdot 4^{2n}}\Big) \\
&+ \frac{n(n-1)}{2}\Big(\frac{(2n+2)^{(2n+2)} + 4^{(2n+2)}}{(2n+2)^{(2n+2)}) \cdot 4^{(2n+2)}}\Big) \\
&+ n^2\Big(\frac{(2n+2)^{(2n+2)} + 4^{(2n)}}{(2n+2)^{max(2n+2)}) \cdot 4^{(2n)}}\Big) + n\Big(\frac{(2n+2)^{(2n+2)} + 4^4}{(2n+2)^{(2n+2)}) \cdot 4^4}\Big)
\end{aligned}$$

$$
\begin{aligned}
& +2n\Big(\frac{(2n+2)^{(2n+2)}+4^6}{(2n+2)^{(2n+2)})\cdot 4^6}\Big)+n\Big(\frac{(2n+2)^{(2n+2)}+4^4}{(2n+2)^{(2n+2)})\cdot 4^4}\Big)\\
& +2n\Big(\frac{(2n+2)^6+4^4}{(2n+2)^6)\cdot 4^4}\Big)+n\Big(\frac{(2n+2)^6+4^6}{(2n+2)^6)\cdot 4^6}\Big)\\
= \quad & \frac{C}{4096\cdot 4^{2n}\cdot \sigma_1\cdot (n+1)^6},
\end{aligned}
$$

where

$$
\begin{aligned}
C =& 36352\cdot 4^{2n}\cdot n^2-128\cdot n\cdot \sigma_1+82944\cdot 4^{2n}\cdot n^3+101376\cdot 4^{2n}\cdot n^4\\
&+70144\cdot 4^{2n}\cdot n^5+26112\cdot 4^{2n}\cdot n^6+4096\cdot 4^{2n}\cdot n^7+3456\cdot n^2\cdot \sigma_1\\
&+3456\cdot n^2\cdot \sigma_1+23424\cdot n^3\cdot \sigma_1+60800\cdot n^4\cdot \sigma_1+82560\cdot n^5\cdot \sigma_1\\
&+62592\cdot n^6\cdot \sigma_1+25216\cdot n^7\cdot \sigma_1+4224\cdot n^8\cdot \sigma_1+6656\cdot 4^{2n}\cdot n\\
&+259\cdot 4^{2n}\cdot n\cdot \sigma_1+402\cdot 4^{2n}\cdot n^2\sigma_1+1005\cdot 4^{2n}\cdot n^3\sigma_1\\
&+1340\cdot 4^{2n}\cdot n^4\sigma_1+1005\cdot 4^{2n}\cdot n^5\sigma_1+402\cdot 4^{2n}\cdot n^6\cdot \sigma_1+67\cdot 4^{2n}\cdot n^7\cdot \sigma_1
\end{aligned}
$$

with $\sigma_1=(2n+2)^{(2n)}$. □

5. QSRP Analysis of Anti-Asthmatic Drugs Using Redefined First Zagreb Power Index.

The development of anti-asthmatic drugs shows a clear move toward making medicines that act longer and more precisely on lung receptors. Early drugs like Epinephrine and Isoproterenol had simple molecular structures with a catechol base. They worked well to open airways but were quickly broken down in the body and often caused side effects like a fast heartbeat because they acted on both heart (β_1) and lung (β_1) receptors.

Later, chemists developed Short-Acting β_1-Agonists (SABAs) such as Salbutamol and Terbutaline by changing the chemical structure — replacing the catechol group with saligenin or resorcinol. These changes made the drugs more stable and longer-lasting. Adding a bulky tert-butyl group helped them act mainly on lung receptors, making them ideal for quick relief (“rescue inhalers”). Further improvements led to Long-Acting (LABA) and Ultra-Long-Acting (uLABA) drugs like Salmeterol, Indacaterol, and Vilanterol. These have more complex structures with long, oily (lipophilic) side chains or “tails” that help them stay near the receptor for 12–24 hours, allowing fewer doses. Indacaterol and Olodaterol are examples of once-daily treatments.

Finally, newer non-steroidal controller drugs such as Montelukast and the “Piprant” class (like Setipiprant, Fevipiprant, Abediterol, Bedoradrine, and Toreforant) target inflammation instead of just relaxing muscles. These drugs have larger, more complex structures with multiple rings, designed to block substances like leukotrienes or the CRTH2 receptor. Because of their properties, they can be taken as oral tablets to reduce lung inflammation and mucus production rather than providing immediate relief. The molecular graphs of these drugs are shown in Figure 6 : Anti-Asthmatic Drugs.

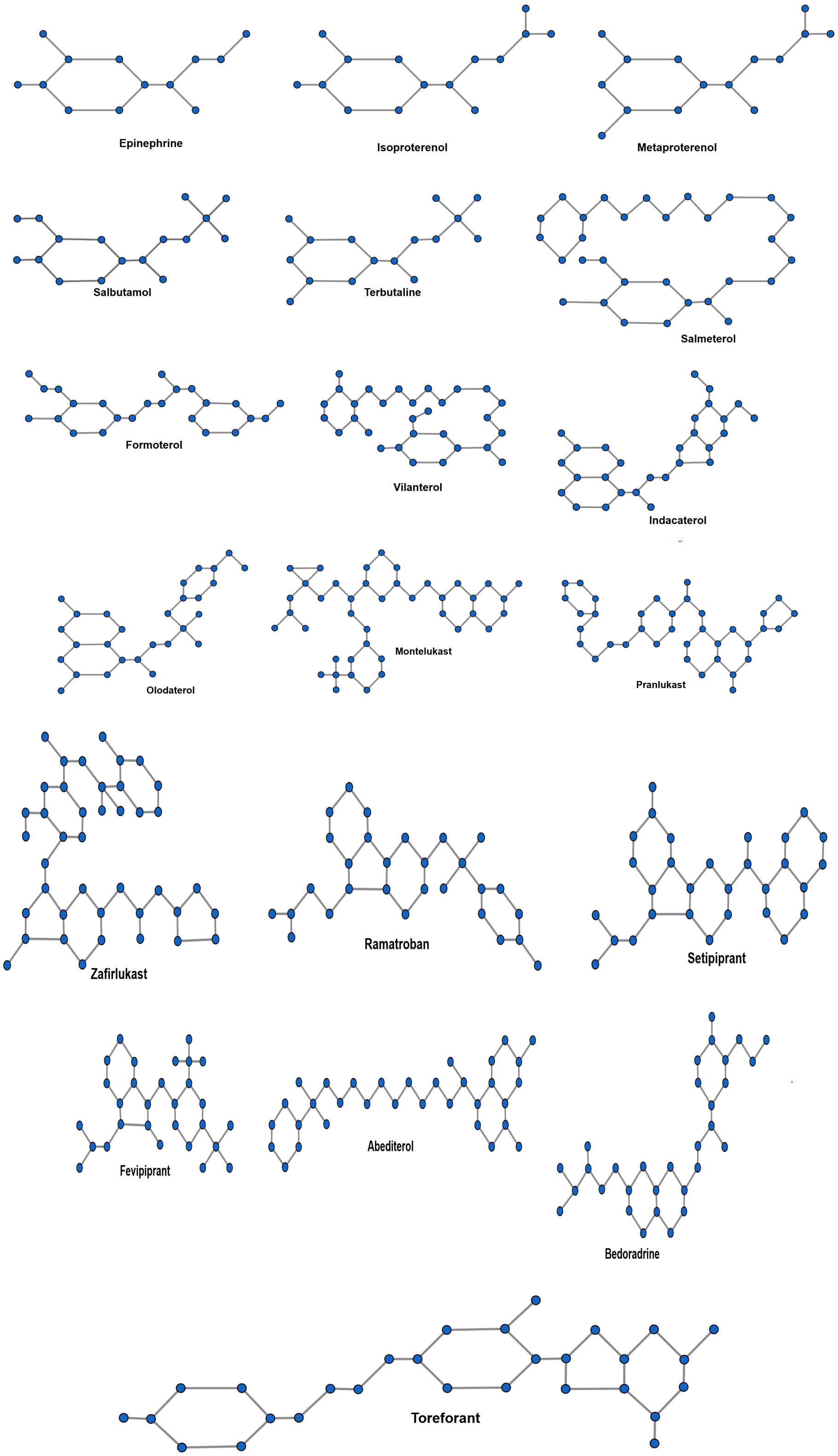

FIGURE 6. **Anti-Asthmatic Drugs.**

In this study, we examined six key physical and chemical properties of 19 major anti-asthmatic drugs: boiling point (BP), enthalpy of vaporization (E), flash point (FP), log(p), molar volume (MV), and molar refractivity (MR). The data for these properties were obtained from [5], and the values are presented in Table 1.

TABLE 1. The $ReZG_1PI(G)$ and Drug properties like BP, E, FP, logP, MV, MR for anti-asthmatic drugs.

Drug	$ReZG_1PI(G)$	BP	E	FP	logP	MV	MR
Epinephrine	14.09	413.1	70.2	207.9	-0.63	142.7	49.3
Isoproterenol	15.7	417.5	70.7	179.7	0.25	176.1	58.6
Metaproterenol	15.63	417.5	70.7	179.7	0.13	176.1	58.6
Salbutamol.	16.34	433.5	72.7	159.5	0.01	207.6	67.8
Terbutaline	16.25	419.2	70.9	165.3	0.48	192.3	63.2
Salmeterol	33.48	603.0	94.3	318.5	3.07	373.7	121.8
Formoterol	27.48	603.2	94.3	318.6	1.57	279.1	97.6
Vilanterol	35.41	646.7	100.2	344.9	2.97	387.5	128.7
Indacaterol	33.35	660.3	102.1	353.1	3.88	306.9	113.3
Olodaterol	30.66	649.0	100.5	346.3	1.17	308.9	105.1
Montelukast	46.13	750.5	114.8	407.7	7.80	460.8	173.7
Pranlukast.	40.33	–	–	–	3.88	350.4	132.6
Zafirlukast	46.07	–	–	–	6.15	433.6	156.4
Ramatroban.	32.78	654.7	101.3	349.7	4.09	289.7	107.5
Setipiprant	35.85	690.4	106.3	371.4	3.39	292.4	110.7
Fevipiprant	31.67	637.6	99.0	339.4	2.85	295.4	100.7
Abediterol	36.2	681.6	105.0	366.0	3.67	371.3	121.3
Bedoradrine	35.07	695.9	107.0	374.7	0.12	335.4	118.9
Toreforant	33.7	611.2	90.8	323.4	4.22	341.7	120.1

Linear Regression Model: Using the data presented in tables 1 and 2, we developed a regression model to describe the relationship between the physicochemical properties of the selected compounds and their molecular descriptors. The linear regression model is expressed as

$$y = ax + b,$$

where y represents the chemical property, a is the regression coefficient, b is the regression constant, and x denotes the molecular descriptor. Based on the data from tables 1 and 2, the linear regression equations for Redefined First Zagreb Power Index $ReZG_1PI(G)$ is follows.

The Linear Regression Model Redefined First Zagreb Power Index ($ReZG_1PI(G)$) of Graph G :

$$\begin{aligned} BP &= 12.044 \cdot ReZG_1PI(G) + 240.764 \\ E &= 1.558 \cdot ReZG_1PI(G) + 47.577 \\ FP &= 8.543 \cdot ReZG_1PI(G) + 54.507 \end{aligned}$$

TABLE 2. Statical parameters for the linear QSPR model for Redefined First Zagreb Power Index $ReZG_1PI(G)$ and physicochemical properties of Anti-Asthmatic Drugs.

Physiochemical properties	R	R^2	Adjusted R^2	F	Sig
Boiling Point (BP)	0.975	0.951	0.947	289.16	0.000
Enthalpy of Vaporization (E)	0.969	0.939	0.934	229.07	0.000
Flash Point (FP)	0.957	0.916	0.910	163.702	0.000
logp	0.843	0.711	0.692	36.881	0.000
Molar Volume (MV)	0.955	0.912	0.906	155.474	0.000
Molar Refraction (MR)	0.978	0.957	0.954	329.945	0.000

$$\begin{aligned} logp &= 0.195 \cdot ReZG_1PI(G) - 3.315 \\ MV &= 8.804 \cdot ReZG_1PI(G) + 37.104 \\ MR &= 3.338 \cdot ReZG_1PI(G) + 4.929 \end{aligned}$$

The correlation of Redefined First Zagreb Power Index with the above mentioned physical qualities of Anti-Asthmatic Drugs compounds linear model is depicted in the figures below.

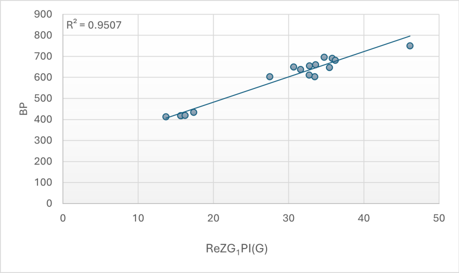

FIGURE 7. The linear fit using $ReZG_1PI(G)$ for boiling point (BP) of Anti-Asthmatic Drugs.

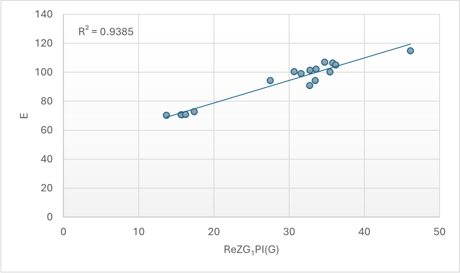

FIGURE 8. The linear fit using $ReZG_1PI(G)$ for enthalpy (E) of Anti-Asthmatic Drugs.

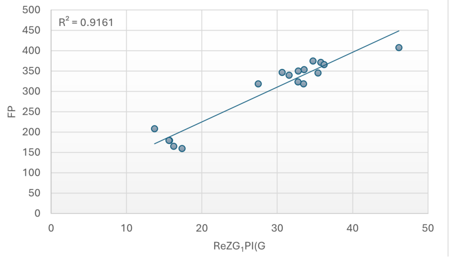

FIGURE 9. The linear fit using $ReZG_1PI(G)$ for flash point (FP) of Anti-Asthmatic Drugs.

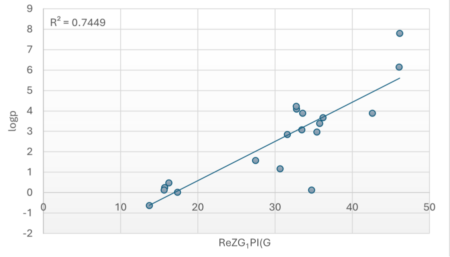

FIGURE 10. The linear fit using $ReZG_1PI(G)$ for logp of Anti-Asthmatic Drugs.

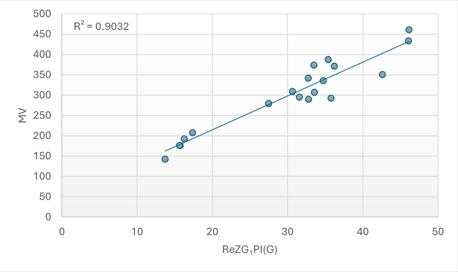

FIGURE 11. The linear fit using $ReZG_1PI(G)$ for molar volume (MV) of Anti-Asthmatic Drugs.

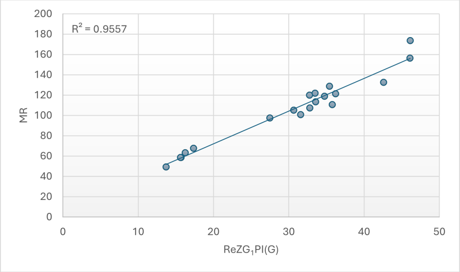

FIGURE 12. The linear fit using $ReZG_1PI(G)$ for molar refractivity (MR) of Anti-Asthmatic Drugs.

6. Predictive Efficiency of Linear Regression Analysis:

TABLE 3. Drug properties transposed: BP, E, FP, logP, MV, MR for Anti-Asthmatic Drugs.

Drug	BP	E	FP	logP	MV	MR
Epinephrine	405.77	68.92	171.55	-0.64	157.72	50.66
Isoproterenol	429.85	72.04	188.63	-0.25	175.33	57.34
Metaproterenol	429.01	71.93	188.03	-0.27	174.71	57.10
Salbutamol	449.85	74.62	202.81	0.07	189.94	62.88
Terbutaline	436.48	72.89	193.33	-0.15	180.17	59.17
Salmeterol	644.00	99.74	340.53	3.21	331.86	116.69
Formoterol	571.73	90.39	289.27	2.04	279.04	96.66
Vilanterol	667.24	102.75	357.01	3.59	348.85	123.13
Indacaterol	644.96	99.86	341.21	3.23	332.57	116.95
Olodaterol	610.03	95.35	316.44	2.66	307.03	107.27
Montelukast	796.35	119.45	448.60	5.68	443.23	158.91
Pranlukast	–	–	–	4.99	412.07	147.09
Zafirlukast	–	–	–	5.67	442.79	158.74
Ramatroban	635.57	98.65	334.55	3.08	325.70	114.35
Setipiprant	671.70	103.32	360.18	3.66	352.11	124.36
Fevipiprant	621.11	96.78	324.29	2.84	315.13	110.34
Abediterol	676.76	103.98	363.76	3.74	355.81	125.76
Bedoradrine	659.17	101.70	351.29	3.46	342.95	120.89
Toreforant	635.08	98.59	334.20	3.07	325.35	114.22

Table 4. Summary of best predictive fits from LRM.

Physiochemical properties	R	R^2	F	$RMSE$	$NRMSE$
Boiling Point (BP)	0.975	0.951	289.16	25.187	4.288
Enthalpy of Vaporization (E)	0.969	0.939	228.977	3.659	3.961
Flash Point (FP)	0.957	0.916	163.716	23.744	7.906
logp	0.863	0.745	49.681	1.115	43.177
Molar Volumes (MV)	0.950	0.903	158.59	27.725	9.207
Molar Refraction (MR)	0.978	0.956	366.642	7.040	6.668

7. The Quadratic Regression Model for Redefined First Zagreb Power Index ($ReZG_1PI(G)$) :

Using the data from Tables 1 and 5, we have developed a quadratic regression model that accounts for the physiochemical properties of the compounds in the list. The evaluation of the quadratic regression model is considered as $y = ax^2 + bx + c$. Here, y denotes chemical property, a, b denotes regression coefficient, b denotes regression constant, and x is taken as molecular descriptor. Using table 1 and 5, we can obtain the quadratic regression models for degree-based indices as follows.

Table 5. Statistical parameters for the Quadratic QSPR model for Redefined First Zagreb Power Index ($ReZG_1PI(G)$) and physicochemical properties of Anti-Asthmatic Drugs.

Physiochemical properties	R	R^2	Adjusted R^2	F	Sig
Boiling Points (BP)	0.983	0.966	0.961	198.223	0.000
Enthalpy of Vaporization (E)	0.973	0.947	0.939	125.21	0.000
Flash Point (FP)	0.967	0.935	0.926	100.63	0.000
logP	0.880	0.775	0.743	24.126	0.000
Molar Volume (MV)	0.956	0.914	0.902	74.630	0.000
Molar Refraction (MR)	0.985	0.970	0.965	222.668	0.000

The Quadratic Redefined First Zagreb Power Index G:

$$\begin{aligned}
BP &= -0.168 \cdot (ReZG_1PI(G))^2 + 21.169 \cdot ReZG_1PI(G) + 131.26 \\
E &= -0.016 \cdot (ReZG_1PI(G))^2 + 2.446 \cdot ReZG_1PI(G) + 36.913 \\
FP &= -0.135 \cdot (ReZG_1PI(G))^2 + 15.894 \cdot ReZG_1PI(G) - 33.709 \\
logp &= 0.006 \cdot (ReZG_1PI(G))^2 - 0.156 \cdot ReZG_1PI(G) + 0.899 \\
MV &= 0.048 \cdot (ReZG_1PI(G))^2 + 6.192 \cdot ReZG_1PI(G) + 68.45 \\
logp &= 0.043 \cdot (ReZG_1PI(G))^2 + 1.007 \cdot ReZG_1PI(G) + 32.914
\end{aligned}$$

The correlation of Redefined First Zagreb Power Index with the above mentioned physical qualities of Anti-Asthmatic Drugs compounds Quadratic model is depicted in the figures below:

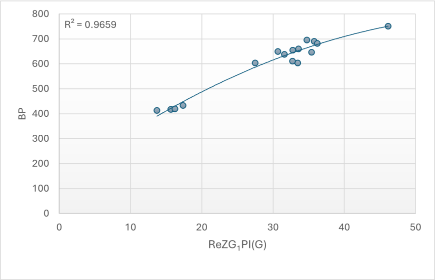

FIGURE 13. The Quadratic fit using $ReZG_1PI(G)$ for boiling point (BP) of Anti-Asthmatic Drugs.

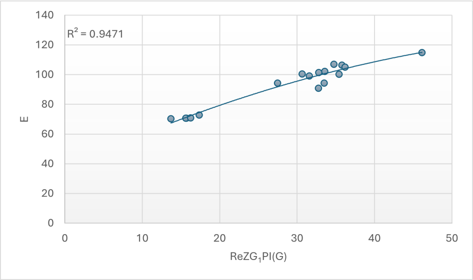

FIGURE 14. The Quadratic fit using $ReZG_1PI(G)$ for enthalpy (E) of Anti-Asthmatic Drugs.

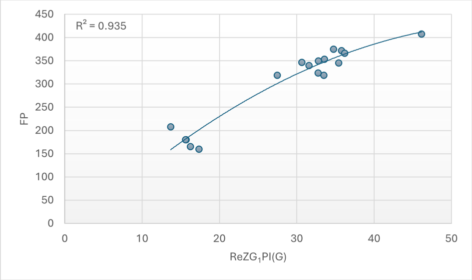

FIGURE 15. The Quadratic fit using $ReZG_1PI(G)$ for flash point (FP) of Anti-Asthmatic Drugs.

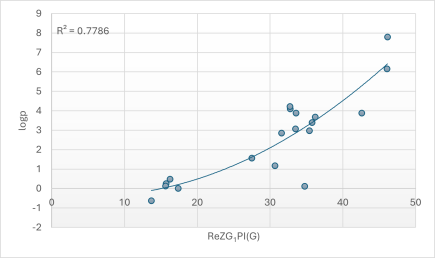

FIGURE 16. The Quadratic fit using $ReZG_1PI(G)$ for logp of Anti-Asthmatic Drugs.

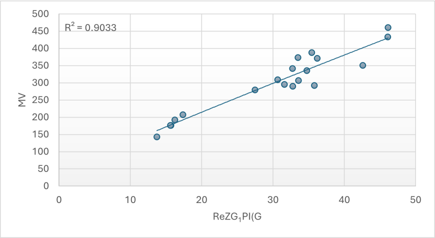

FIGURE 17. The Quadratic fit using $ReZG_1PI(G)$ for molar volume (MV) of Anti-Asthmatic Drugs.

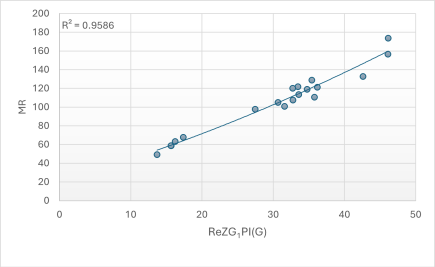

FIGURE 18. The Quadratic fit using $ReZG_1PI(G)$ for molar refractivity (MR) of Anti-Asthmatic Drugs.

8. Predictive Efficiency of Quadratic Regression Analysis

Table 6. Drug properties transposed: BP, E, FP, logP, MV, MR for Anti-Asthmatic Drugs.

Epinephrine	389.74	67.42	158.70	-0.11	162.29	56.78
Isoproterenol	422.20	71.37	182.55	-0.07	177.50	59.32
Metaproterenol	421.09	71.24	181.73	-0.07	176.96	59.16
Salbutamol	448.12	74.55	201.53	0.00	190.41	63.35
Terbutaline	430.89	72.44	188.92	-0.05	181.75	60.63
Salmeterol	651.69	100.87	347.10	2.40	329.56	114.83
Formoterol	586.12	92.05	301.11	1.14	274.85	93.06
Vilanterol	670.20	103.46	359.83	2.90	347.89	122.49
Indacaterol	652.48	100.98	347.65	2.42	330.31	115.14
Olodaterol	622.38	96.87	326.70	1.76	303.42	104.21
Montelukast	750.29	115.70	412.20	6.47	456.23	170.87
Pranlukast	–	–	–	5.14	419.23	153.80
Zafirlukast	–	–	–	6.45	455.70	170.62
Ramatroban	644.66	99.90	342.23	2.23	323.00	112.13
Setipiprant	673.61	103.95	362.15	3.00	351.45	123.99
Fevipiprant	632.23	98.20	333.59	1.96	311.86	107.60
Abediterol	677.42	104.49	364.74	3.11	355.50	125.72
Bedoradrine	663.92	102.58	355.52	2.72	341.49	119.79
Toreforant	644.25	99.84	341.95	2.22	322.63	111.98

Table 7. Summary of best predictive fits from QRM.

Physiochemical properties	R	R^2	F	$RMSE$	$NRMSE$
Boiling Point (BP)	0.983	0.996	424.784	20.95	3.566
Enthalpy of Vaporization (E)	0.973	0.947	268.517	3.41	3.695
Flash Point (FP)	0.967	0.935	215.622	20.90	6.959
logp	0.878	0.771	57.327	1.09	42.300
Molar Volumes (MV)	0.948	0.900	152.394	28.72	9.537
Molar Refraction (MR)	0.977	0.954	355.214	7.82	7.404

9. Conclusion

In this study, a novel topological index based on the maximum and minimum degrees of vertices, called the Redefined First Zagreb Power Index, is proposed. Explicit formulas for $ReZG_1PI(G)$ are derived for several standard graph structures, well-known graphs, and their corresponding line graphs. Furthermore, the predictive capability of the proposed index is evaluated through QSPR analysis to identify the best predictors for six physicochemical properties of 19 anti-asthmatic drugs. The results demonstrate that the proposed index exhibits significant predictive potential and can serve as a useful molecular descriptor in QSPR studies. The main findings of this study are summarized as follows:

- The theoretical estimation of the considered physicochemical properties is carried out using linear and quadratic regression models based on $ReZG_1PI(G)$.
- In the linear regression model, the Redefined First Zagreb Power Index $ReZG_1PI(G)$ demonstrates strong predictive ability for all six physicochemical properties of anti-asthmatic drugs, with correlation coefficients ranging from r=0.843 to r=0.978. Furthermore, in all cases, $p = 0.0000$, indicating that the linear regression model with respect to $ReZG_1PI(G)$ is highly significant.
- In the quadratic regression model, the Redefined First Zagreb Power Index $ReZG_1PI(G)$ also exhibits strong predictive performance for all six physicochemical properties of anti-asthmatic drugs, with correlation coefficients ranging from $r = 0.88$ to $r = 0.985$. Additionally, in all cases, p=0.0000, which confirms that the quadratic regression model with respect to $ReZG_1PI(G)$ is highly significant.

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