

Topological Characterization of Line Graphs for Pazopanib and Belzutifan in Renal Cell Cancer Therapy

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Abstract: The topological indices calculated in a molecular network using the reciprocal (or inverse) of the degree of vertices are known as reverse degree-based topological indices of a graph. In situations where the connectivity of atoms or vertices with lower degrees significantly affects a compound's properties, these indices aim to provide a nuanced assessment of molecular topology. In this article, we calculate various topological indices of line graphs based on reverse degrees for Belzutifan and Pazopanib, which are used in the treatment of Renal Cell Cancer. Additionally, we plot 3D plots of their polynomials and describe their uses.

Keywords: reverse randic index; reverse atom bond connectivity index; reverse geometric arithmetic index; reverse first and second Zagreb indices; reverse hyper Zagreb index and forgotten index.

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1. Introduction

One of the most common tumors in the category of urological Cancers is Renal Cell Carcinoma (RCC), which is distinguished by its aggressiveness and resistance to standard chemotherapy. Pazopanib and Belzutifan have emerged as important medicines in the management of RCC, and recent developments in targeted treatments have completely changed the therapeutic landscape.

Graph theory is a field of mathematics that deals with the analysis of graphs, which consist of a set of points called vertices and lines connecting them, known as edges, used to represent relationships between objects. A line graph is constructed such that each vertex in the line graph represents an edge in the original graph G . Two vertices in the line graph are adjacent if and only if their corresponding edges in G share a common vertex. The analysis of line graphs provides a robust framework for investigating the structural properties, molecular interactions, and potential synergies of medicinal drugs. We aim to provide a fresh perspective on the molecular mechanisms of Belzutifan and Pazopanib in the fight against renal cell carcinoma (RCC) by employing topological indices and mathematical descriptors.

The following literature review highlights the important line graph studies. The computational characteristics of the carbon nanocone line graphs are investigated in detail [1].

Zeroth-order generalization of the Randic index for the line graphs of particular chemical components in pharmaceuticals is analyzed [2]. Topological indices for the line graphs of fullerene networks, k-subdivided linear tetracene, tetracene nanotori, and carbon nanotubes are covered [3]. Initially, the Line graphs were introduced by Estrada [4] and Tomovic [5].

Molecular graphs are simple graphs, meaning they don't have loops or multiple edges and are undirected. In this illustration, the vertices (nodes) of the molecule indicate atoms. The edges (lines) indicate the chemical bonds between the atoms.

The Reverse degree of graph G was first introduced by Kulli [6]. It is denoted by $R(v)$ and is defined as $R(v) = 1 + \Delta(G) - d(v)$, where $d(v)$ stands for the degree of the vertex v and $\Delta(G)$ stands for the highest degree of a vertex v in G.

The following literature review presents recent developments in reverse degree graphs. Zhao *et al.* [3] evaluated the Reverse Augmented Zagreb index for metal-organic networks TM-TCNB and further determined several reverse topological descriptors, including the Reverse General Randic, Reverse Balaban, Reverse Atom-Bond Connectivity, Reverse Geometric, and Reverse Zagreb indices. Similarly, Jung *et al.* [7] investigated TUC4 by computing the Reverse Atom-Bond Connectivity index, the Reverse Geometric-Arithmetic index, the First and Second Zagreb indices, and the First and Second Hyper Zagreb indices. Wei *et al.* [8] determined various reverse degree-based topological indices for the Remdesivir compound employed in COVID-19 treatment, including the Reverse General Randic, Reverse Atom-Bond Connectivity, Reverse Geometric-Arithmetic, Reverse Forgotten, Reverse Balaban, and Reverse Zagreb indices. Ravi *et al.* [9] investigated the QSPR of the reverse degree-based topological indices. Haoer and Virk [10] computed Reverse Zagreb indices, Reverse Hyper Zagreb indices, and Related polynomials for metal-organic networks. Hashmi *et al.* computed the Reverse ABC index for several dendrimer generations [11]. Rosary [12] computed many topological indices based on reverse degrees for the line graph of Remdesivir. Prasanna [13] computed Reverse Topological indices for some drugs used in the Treatment of H1N1. References [14-24] provide comprehensive insights into molecular topological indices and their applications in chemical graph theory and biological sciences. More recently, H.M. Nagesh *et al.* [25] investigated reverse degree-based topological indices for Zanamivir and Oseltamivir, which are used in the treatment of H1N1. This inspired us to calculate the reverse topological indices for the Pazopanib and Belzutifan molecular structure line graph.

In this paper, the degrees of the vertices u and v are represented by d_u and d_v respectively, while p and q denote the size and order of the graph $G = (V, E)$.

Initially, the degree-based topological index was proposed by Milan Randic [26]. The Reverse Randic index was proposed by Wei *et al.* [8], and is defined as:

$$RR\gamma(G) = \sum_{u,v \in E(G)} (d_u \times d_v)^\gamma, \text{ Where } \gamma = -1, -\frac{1}{2}, \frac{1}{2}, 1. \quad (1)$$

The polynomial of the Reverse Randic index is:

$$RR\gamma(G) = \sum_{u,v \in E(G)} x^{(d_u \times d_v)^\gamma} \quad (2)$$

The Atom Bond Connectivity index was proposed by Estrada *et al.* [27]. The Reverse Autom Bond Connectivity index was proposed by Wei *et al.* [8], and is defined as:

$$RABC(G) = \sum_{u,v \in E(G)} \sqrt{\frac{d_u + d_v - 2}{d_u \times d_v}} \quad (3)$$

The Geometric Arithmetic index was proposed by Vukicevic *et al.* [28]. The Reverse Geometric Arithmetic index was proposed by Wei *et al.* [8], which is defined as:

$$RGA(G) = \sum_{u,v \in E(G)} 2 \sqrt{\frac{d_u \times d_v}{d_u + d_v}} \quad (4)$$

The first and second Zagreb indices were proposed by Gutman [29,30]. The Reverse first and second Zagreb indices were proposed by Wei *et al.* [8] and are defined as:

$$RM_1(G) = \sum_{u,v \in E(G)} (d_u + d_v) \quad (5)$$

$$RM_2(G) = \sum_{u,v \in E(G)} (d_u \times d_v) \quad (6)$$

The polynomials of the reverse first and second Zagreb indices are:

$$RM_1(G) = \sum_{u,v \in E(G)} x^{(d_u + d_v)} \quad (7)$$

$$RM_2(G) = \sum_{u,v \in E(G)} x^{(d_u \times d_v)} \quad (8)$$

The first and second Zagreb co-indices are proposed by Doslic and Gutman [31,32]. The Reverse first and second Zagreb co-indices are proposed by Wei *et al.* [8] and are defined as:

$$\overline{RM_1(G)} = 2|E(G)|(|V(G)| - 1) - RM_1(G) \quad (9)$$

$$\overline{RM_2(G)} = 2|E(G)|^2 - \frac{1}{2}RM_1(G) - RM_2(G) \quad (10)$$

The Hyper Zagreb index was proposed by Shirdel *et al.* [33]. The Reverse Hyper Zagreb index was proposed by Wei *et al.* [8], and is defined as:

$$RHM(G) = \sum_{u,v \in E(G)} (d_u + d_v)^2 \quad (11)$$

The polynomial of the Reverse Hyper Zagreb index is:

$$RHM(G) = \sum_{u,v \in E(G)} x^{(d_u + d_v)^2} \quad (12)$$

The Forgotten index was proposed by Furtula and Gutman [29]. The Reverse Forgotten index was proposed by Wei *et al.* [8], and is defined as:

$$RHM(G) = \sum_{u,v \in E(G)} [(d_u)^2 + (d_v)^2] \quad (13)$$

The Reverse Forgotten polynomial index is:

$$RHM(G) = \sum_{u,v \in E(G)} x^{[(d_u)^2 + (d_v)^2]} \quad (14)$$

The Reverse Balaban index was proposed by Wei *et al.* [8] and is defined as:

$$RJ(G) = \frac{p}{p-q+2} \sum_{u,v \in E(G)} \frac{1}{\sqrt{d_u \times d_v}} \quad (15)$$

Where p represents the total number of vertices and q represents the total number of edges in the graph G .

The Reverse first and second Multiple Zagreb indices are proposed by Wei *et al.* [8] and are defined as:

$$RPM_1(G) = \prod_{u,v \in E(G)} (d_u + d_v) \quad (16)$$

$$RPM_2(G) = \prod_{u,v \in E(G)} (d_u \times d_v) \quad (17)$$

The redefined first, second, and third Zagreb indices were proposed by Gao *et al.* [34]. The Reverse redefined first, second, and third Zagreb indices are proposed by Wei *et al.* [8] and are defined as:

$$RR_eZG_1(G) = \sum_{u,v \in E(G)} \left(\frac{d_u + d_v}{d_u \times d_v} \right) \quad (18)$$

$$RR_eZG_2(G) = \sum_{u,v \in E(G)} \left(\frac{d_u \times d_v}{d_u + d_v} \right) \quad (19)$$

$$RR_eZG_3(G) = \sum_{u,v \in E(G)} [(d_u \times d_v) (d_u + d_v)] \quad (20)$$

The Reverse redefined third Zagreb polynomial index is defined as:

$$RR_eZG_3(G) = \sum_{u,v \in E(G)} x^{[(d_u + d_v)(d_u \times d_v)]} \quad (21)$$

In this article, we calculated the molecular structure of Reverse topological indices of Pazopanib and Belzutifan.

2. Materials and Methods

The techniques employed in this work include partitioning edges by the Reverse degree of end vertices, dividing vertices by reverse degree, and counting reverse vertex degrees. The topological indices, as indicated by formulae from (1) to (21), are computed using the partition of edges and reverse vertex degree counting methods. Using ChemDraw Pro 8.0, the 2D molecular structure and Line graphs of Pazopanib and Belzutifan are drawn, and their polynomials are computed. PYTHON is used to produce a graphic comparison of the reverse topological indices of the molecular structures of Pazopanib and Belzutifan.

3. Results and Discussion

3.1. Pazopanib's line graph's reverse topological indices.

There are 31 vertices and 42 edges in the Pazopanib molecular networks of the line graph. Table 1 shows the edge partition of the line graph of Pazopanib according to the degree pairs of adjacent vertices (d_u, d_v).

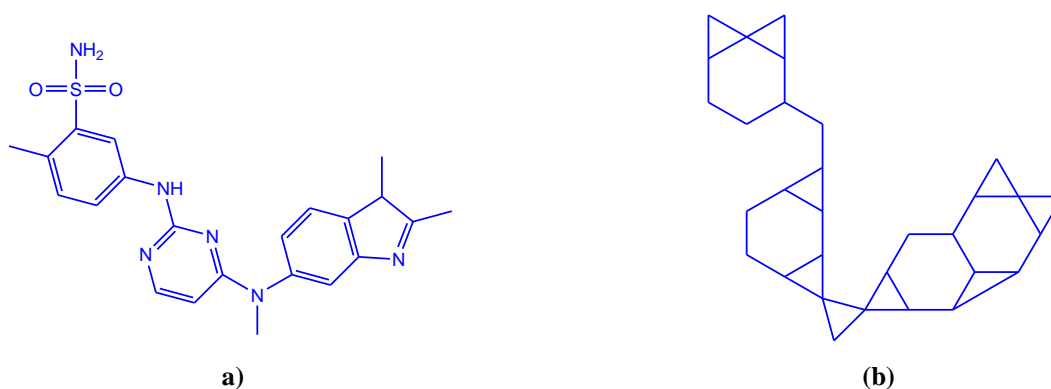


Figure 1. (a) 2D molecular structure of Pazopanib; (b) Line graph of Pazopanib.

Table 1. Edge partition of the line graph of Pazopanib.

(d_u, d_v)	(1,1)	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
Number of edge partitions	1	8	6	13	12	2

We now find the reverse degree based topological indices for the line graph of Pazopanib.

Using equation (1), When $\gamma = -1$ we obtain:

$$RR_{-1}[L(C_{21}H_{23}N_7O_2S)] = (1 \times 1)^{-1} + 8(1 \times 2)^{-1} + 6(1 \times 3)^{-1} + 13(2 \times 2)^{-1} + 12(2 \times 3)^{-1} + 2(3 \times 3)^{-1}$$

$$RR_{-1}[L(C_{21}H_{23}N_7O_2S)] = \mathbf{12.4722}.$$

Using equation (1), When $\gamma = -\frac{1}{2}$ we obtain:

$$RR_{-\frac{1}{2}}[L(C_{21}H_{23}N_7O_2S)] = (1 \times 1)^{-\frac{1}{2}} + 8(1 \times 2)^{-\frac{1}{2}} + 6(1 \times 3)^{-\frac{1}{2}} + 13(2 \times 2)^{-\frac{1}{2}} + 12(2 \times 3)^{-\frac{1}{2}} + 2(3 \times 3)^{-\frac{1}{2}}$$

$$RR_{-\frac{1}{2}}[L(C_{21}H_{23}N_7O_2S)] = \mathbf{22.1866}.$$

Using equation (1), When $\gamma = \frac{1}{2}$ we obtain:

$$RR_1[L(C_{21}H_{23}N_7O_2S)] = (1 \times 1)^{\frac{1}{2}} + 8(1 \times 2)^{\frac{1}{2}} + 6(1 \times 3)^{\frac{1}{2}} + 13(2 \times 2)^{\frac{1}{2}} + 12(2 \times 3)^{\frac{1}{2}} + 2(3 \times 3)^{\frac{1}{2}}$$

$$RR_1[L(C_{21}H_{23}N_7O_2S)] = \mathbf{84.0999}.$$

Using equation (1), When $\gamma = 1$ we obtain:

$$RR_1[L(C_{21}H_{23}N_7O_2S)] = (1 \times 1)^1 + 8(1 \times 2)^1 + 6(1 \times 3)^1 + 13(2 \times 2)^1 + 12(2 \times 3)^1 + 2(3 \times 3)^1$$

$$RR_1[L(C_{21}H_{23}N_7O_2S)] = \mathbf{177}.$$

Using equation (2), we obtain:

$$RR\gamma(G) = x^{(1 \times 1)^1} + 8x^{(1 \times 2)^1} + 6x^{(1 \times 3)^1} + 13x^{(2 \times 2)^1} + 12x^{(2 \times 3)^1} + 2x^{(3 \times 3)^1}$$

$$RR\gamma(G) = \mathbf{2x^9 + 12x^6 + 13x^4 + 6x^3 + 8x^2 + x^1}.$$

Using equation (3), we obtain:

$$RABC[L(C_{21}H_{23}N_7O_2S)] = \sqrt{\frac{1+1-2}{1 \times 1}} + 8\sqrt{\frac{1+2-2}{1 \times 2}} + 6\sqrt{\frac{1+3-2}{1 \times 3}} + 13\sqrt{\frac{2+2-2}{2 \times 2}} + 2\sqrt{\frac{2+3-2}{2 \times 3}} + 2\sqrt{\frac{3+3-2}{3 \times 3}}$$

$$RABC[L(C_{21}H_{23}N_7O_2S)] = \mathbf{29.5668}.$$

Using equation (4), we obtain:

$$RGA[L(C_{21}H_{23}N_7O_2S)] = 2\left\{\frac{\sqrt{1 \times 1}}{1+1} + 8\frac{\sqrt{1 \times 2}}{1+2} + 6\frac{\sqrt{1 \times 3}}{1+3} + 13\frac{\sqrt{2 \times 2}}{2+2} + 12\frac{\sqrt{2 \times 3}}{2+3} + 2\frac{\sqrt{3 \times 3}}{3+3}\right\}$$

$$RGA[L(C_{21}H_{23}N_7O_2S)] = \mathbf{40.4961}.$$

Using equation (5), we obtain:

$$RM_1[L(C_{21}H_{23}N_7O_2S)] = (1+1) + 8(1+2) + 6(1+3) + 13(2+2) + 12(2+3) + 2(3+3)$$

$$RM_1[L(C_{21}H_{23}N_7O_2S)] = \mathbf{174}.$$

Using equation (6), we obtain:

$$RM_2[L(C_{21}H_{23}N_7O_2S)] = (1 \times 1) + 8(1 \times 2) + 6(1 \times 3) + 13(2 \times 2) + 12(2 \times 3) + 2(3 \times 3)$$

$$RM_2[L(C_{21}H_{23}N_7O_2S)] = \mathbf{177}.$$

Using equation (7), we obtain:

$$RM_1[L(C_{21}H_{23}N_7O_2S)] = x^{(1+1)} + 8x^{(1+2)} + 6x^{(1+3)} + 13x^{(2+2)} + 12x^{(2+3)} + 2x^{(3+3)}$$

$$RM_1[L(C_{21}H_{23}N_7O_2S)] = \mathbf{2x^6 + 12x^5 + 19x^4 + 8x^3 + x^2}.$$

Using equation (8), we obtain:

$$RM_2[L(C_{21}H_{23}N_7O_2S)] = x^{(1 \times 1)} + 8x^{(1 \times 2)} + 6x^{(1 \times 3)} + 13x^{(2 \times 2)} + 12x^{(2 \times 3)} + 2x^{(3 \times 3)}$$

$$RM_2[L(C_{21}H_{23}N_7O_2S)] = \mathbf{2x^9 + 12x^6 + 13x^4 + 6x^3 + 8x^2 + x}.$$

Using equation (9), we obtain:

$$\overline{RM}_1[L(C_{21}H_{23}N_7O_2S)] = 2(42) (31-1) - 174$$

$$\overline{RM}_1[L(C_{21}H_{23}N_7O_2S)] = \mathbf{2346}.$$

Using equation (10), we obtain:

$$\overline{RM}_2[L(C_{21}H_{23}N_7O_2S)] = 2(42)^2 - \frac{1}{2}(174) - 177$$

$$\overline{RM}_2[L(C_{21}H_{23}N_7O_2S)] = \mathbf{3264}.$$

Using equation (11), we obtain:

$$RHM[L(C_{21}H_{23}N_7O_2S)] = (1+1)^2 + 8(1+2)^2 + 6(1+3)^2 + 13(2+2)^2 + 12(2+3)^2 + 2(3+3)^2$$

$$RHM[L(C_{21}H_{23}N_7O_2S)] = \mathbf{752}.$$

Using equation (12), we obtain:

$$\text{RHM}[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]=x^{(1+1)^2} + 8x^{(1+2)^2} + 6x^{(1+3)^2} + 13x^{(2+2)^2} + 12x^{(2+3)^2} + 2x^{(3+3)^2}$$

$$\text{RHM}[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]=2x^{36}+12x^{25}+19x^{16}+8x^9+x^4.$$

Using equation (13), we obtain:

$$\text{RHM}[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]= (1^2+1^2)+8(1^2+2^2)+6(1^2+3^2)+13(2^2+2^2)+12(2^2+3^2)+2(3^2+3^2)$$

$$\text{RHM}[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]= \mathbf{398}.$$

Using equation (14), we obtain:

$$\text{RHM}[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]=x^{(1^2+1^2)}+8x^{(1^2+2^2)} + 6x^{(1^2+3^2)} + 13x^{(2^2+2^2)} + 12x^{(2^2+3^2)} + 2x^{(3^2+3^2)}$$

$$\text{RF}[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]= 2x^{18}+12x^{13}+13x^8+6x^{10}+8x^5+x^2.$$

Using equation (15), we obtain:

$$\text{RJ}[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]=\frac{42}{42-31+2} \left\{ \frac{1}{\sqrt{1 \times 1}} + 8 \frac{1}{\sqrt{1 \times 2}} + 6 \frac{1}{\sqrt{1 \times 3}} + 13 \frac{1}{\sqrt{2 \times 2}} + 12 \frac{1}{\sqrt{2 \times 3}} + 2 \frac{1}{\sqrt{3 \times 3}} \right\}$$

$$\text{RJ}[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})] = \mathbf{71.6801}.$$

Using equation (16), we obtain:

$$\text{RPM}_1[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]=(1+1) \times 8(1+2) \times 6(1+3) \times 13(2+2) \times 12(2+3) \times 2(3+3)$$

$$\text{RPM}_1[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]= \mathbf{43130880}.$$

Using equation (17), we obtain:

$$\text{RPM}_2[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]=(1 \times 1) \times 8(1 \times 2) \times 6(1 \times 3) \times 13(2 \times 2) \times 12(2 \times 3) \times 2(3 \times 3)$$

$$\text{RPM}_2[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]= \mathbf{19408896}.$$

Using equation (18), we obtain:

$$\text{RR}_e\text{ZG}_1[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]=\left(\frac{1+1}{1 \times 1}\right) + 8 \left(\frac{1+2}{1 \times 2}\right) + 6 \left(\frac{1+3}{1 \times 3}\right) + 13 \left(\frac{2+2}{2 \times 2}\right) + 12 \left(\frac{2+3}{2 \times 3}\right) + 2 \left(\frac{3+3}{3 \times 3}\right)$$

$$\text{RR}_e\text{ZG}_1[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]= \mathbf{46.3333}.$$

Using equation (19), we obtain:

$$\text{RR}_e\text{ZG}_2[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]=\left(\frac{1 \times 1}{1+1}\right) + 8 \left(\frac{1 \times 2}{1+2}\right) + 6 \left(\frac{1 \times 3}{1+3}\right) + 13 \left(\frac{2 \times 2}{2+2}\right) + 12 \left(\frac{2 \times 3}{2+3}\right) + 2 \left(\frac{3 \times 3}{3+3}\right)$$

$$\text{RR}_e\text{ZG}_2[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]= \mathbf{40.7333}.$$

Using equation (20), we obtain:

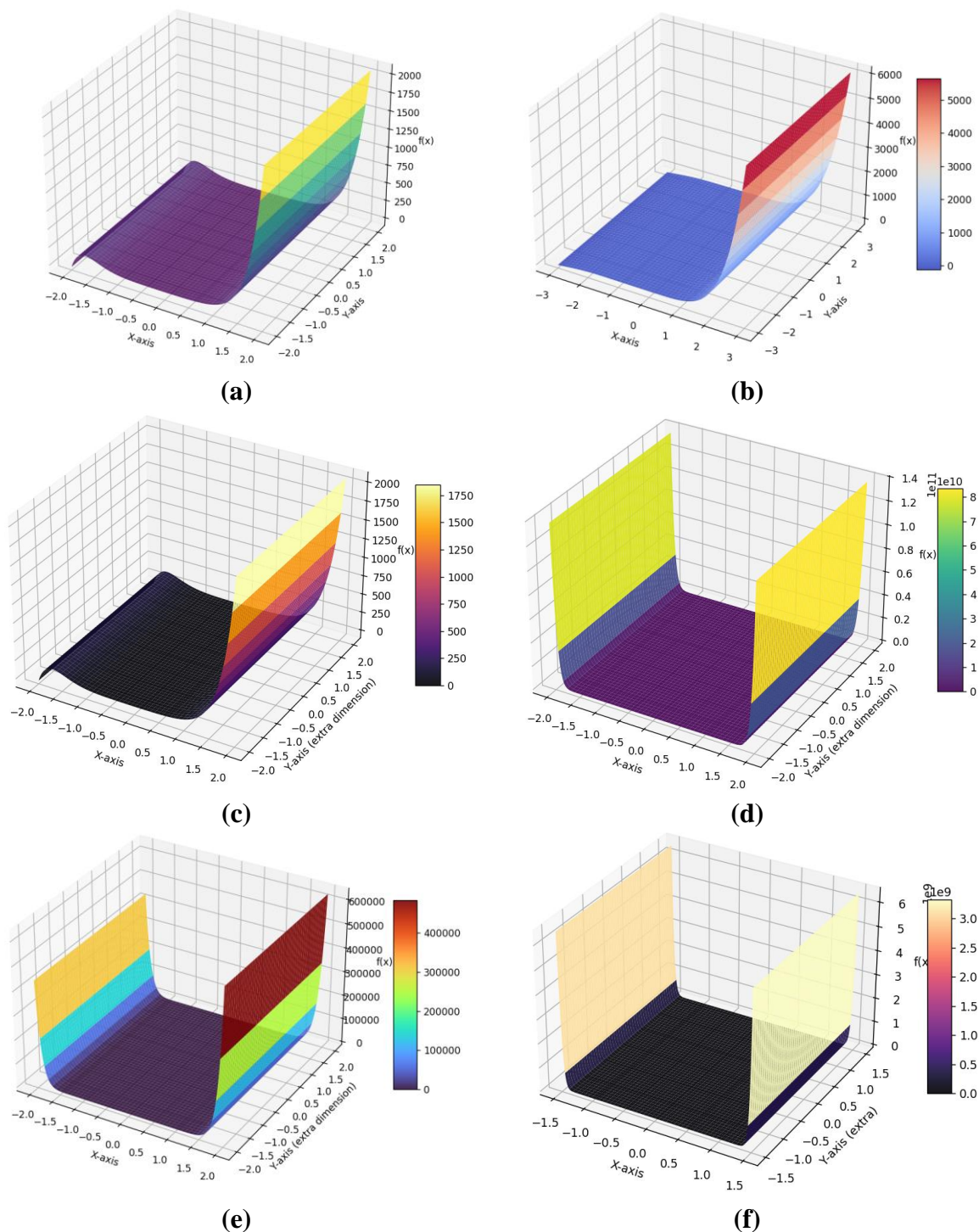
$$\text{RR}_e\text{ZG}_3[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]=[(1 \times 1)(1+1)]+8[(1 \times 2)(1+2)]+6[(1 \times 3)(1+3)]+13[(2 \times 2)(2+2)]+12[(2 \times 3)(2+3)]+2[(3 \times 3)(3+3)]$$

$$\text{RR}_e\text{ZG}_3[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]= \mathbf{798}.$$

Using equation (21), we obtain:

$$\text{RR}_e\text{ZG}_3[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]=x^{[(1 \times 1)(1+1)]}+8x^{[(1 \times 2)(1+2)]}+6x^{[(1 \times 3)(1+3)]}+13x^{[(2 \times 2)(2+2)]}+12x^{[(2 \times 3)(2+3)]}+2x^{[(3 \times 3)(3+3)]}$$

$$\text{RR}_e\text{ZG}_3[\text{L}(\text{C}_{21}\text{H}_{23}\text{N}_7\text{O}_2\text{S})]= 2x^{54}+12x^{30}+13x^{16}+6x^{12}+8x^6+x^2.$$



Graph 1. Pazopanib’s graphical representation of the polynomials (a) Reverse Randic index; (b) Reverse first Zagreb index; (c) Reverse second Zagreb index; (d) Reverse Hyper Zagreb index; (e) Reverse Forgotten index; (f) Reverse third refined Zagreb index.

3.2. Belzutifan’s line graphs’ reverse topological indices.

There are 25 vertices and 37 edges in the Belzutifan molecular networks of the line graph. Table 2 shows the edge partition of the line graph of Belzutifan according to the degree pairs of adjacent vertices (d_u, d_v).

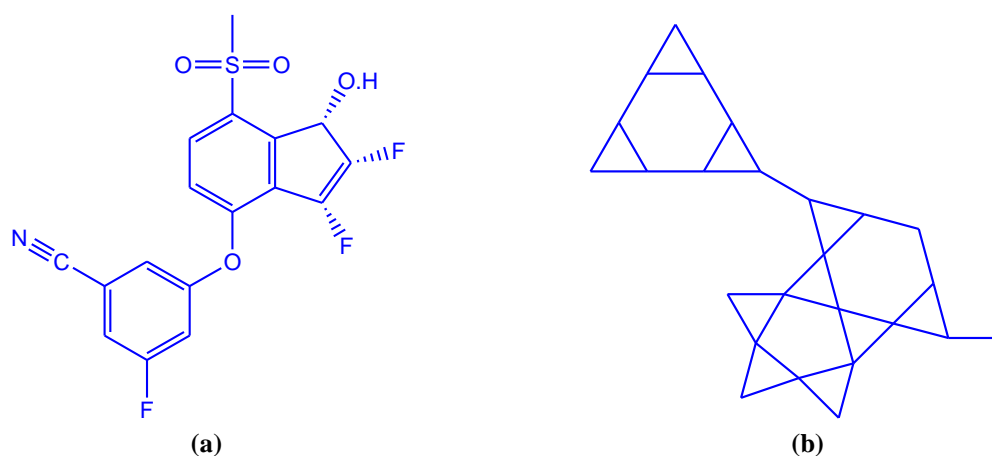


Figure 2. (a) 2D molecular structure of Belzutifan; (b) Line graph of Belzutifan.

Table 2. Edge partition of the line graph of Belzutifan.

(d_u, d_v)	(1,1)	(1,2)	(1,3)	(2,2)	(2,3)	(2,4)
Number of Edge partitions	9	4	6	11	6	1

We now find the reverse degree-based topological indices for Belzutifan.

Using equation(1), When $\gamma=-1$, we obtain:

$$RR_{-1}[L(C_{17}H_{12}F_3NO_4S)] = 9(1 \times 1)^{-1} + 4(1 \times 2)^{-1} + 6(1 \times 3)^{-1} + 11(2 \times 2)^{-1} + 6(2 \times 3)^{-1} + (2 \times 4)^{-1}$$

$$RR_{-1}[L(C_{17}H_{12}F_3NO_4S)] = \mathbf{16.875}.$$

Using equation (1), When $\gamma = -\frac{1}{2}$, we obtain:

$$RR_{-\frac{1}{2}}[L(C_{17}H_{12}F_3NO_4S)] = 9(1 \times 1)^{-\frac{1}{2}} + 4(1 \times 2)^{-\frac{1}{2}} + 6(1 \times 3)^{-\frac{1}{2}} + 11(2 \times 2)^{-\frac{1}{2}} + 6(2 \times 3)^{-\frac{1}{2}} + (2 \times 4)^{-\frac{1}{2}}$$

$$RR_{-\frac{1}{2}}[L(C_{17}H_{12}F_3NO_4S)] = \mathbf{23.5956}.$$

Using equation (1), When $\gamma = \frac{1}{2}$, we obtain:

$$RR_{\frac{1}{2}}[L(C_{17}H_{12}F_3NO_4S)] = 9(1 \times 1)^{\frac{1}{2}} + 4(1 \times 2)^{\frac{1}{2}} + 6(1 \times 3)^{\frac{1}{2}} + 11(2 \times 2)^{\frac{1}{2}} + 6(2 \times 3)^{\frac{1}{2}} + (2 \times 4)^{\frac{1}{2}}$$

$$RR_{\frac{1}{2}}[L(C_{17}H_{12}F_3NO_4S)] = \mathbf{64.5745}.$$

Using equation (1), When $\gamma = 1$, we obtain:

$$RR_1[L(C_{17}H_{12}F_3NO_4S)] = 9(1 \times 1)^1 + 4(1 \times 2)^1 + 6(1 \times 3)^1 + 11(2 \times 2)^1 + 6(2 \times 3)^1 + (2 \times 4)^1$$

$$RR_1[L(C_{17}H_{12}F_3NO_4S)] = \mathbf{123}.$$

Using equation (2), we obtain:

$$RR_1[L(C_{17}H_{12}F_3NO_4S)] = 9x^{(1 \times 1)^1} + 4x^{(1 \times 2)^1} + 6x^{(1 \times 3)^1} + 11x^{(2 \times 2)^1} + 6x^{(2 \times 3)^1} + x^{(2 \times 4)^1}$$

$$RR_1[L(C_{17}H_{12}F_3NO_4S)] = \mathbf{x^8 + 6x^6 + 11x^4 + 6x^3 + 4x^2 + 9x}.$$

Using equation (3), we obtain:

$$RABC[L(C_{17}H_{12}F_3NO_4S)] = 9\sqrt{\frac{1+1-2}{1 \times 1}} + 4\sqrt{\frac{1+2-2}{1 \times 2}} + 6\sqrt{\frac{1+3-2}{1 \times 3}} + 11\sqrt{\frac{2+2-2}{2 \times 2}} + 6\sqrt{\frac{2+3-2}{2 \times 3}} + \sqrt{\frac{2+4-2}{2 \times 4}}$$

$$RABC[L(C_{17}H_{12}F_3NO_4S)] = \mathbf{20.4553}.$$

Using equation (4), we obtain:

$$\text{RGA}[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = 2 \left\{ 9 \frac{\sqrt{1 \times 1}}{1+1} + 4 \frac{\sqrt{1 \times 2}}{1+2} + 6 \frac{\sqrt{1 \times 3}}{1+3} + 11 \frac{\sqrt{2 \times 2}}{2+2} + 6 \frac{\sqrt{2 \times 3}}{2+3} + \frac{\sqrt{2 \times 4}}{2+4} \right\}$$

$$\text{RGA}[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = \mathbf{35.789}.$$

Using equation (5), we obtain:

$$\text{RM}_1[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = 9(1+1)+4(1+2)+6(1+3)+11(2+2)+6(2+3)+(2+4)$$

$$\text{RM}_1[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = \mathbf{134}.$$

Using equation (6), we obtain:

$$\text{RM}_2[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = 9(1 \times 1)+4(1 \times 2)+6(1 \times 3)+11(2 \times 2)+6(2 \times 3)+(2 \times 4)$$

$$\text{RM}_2[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = \mathbf{123}.$$

Using equation (7), we obtain:

$$\text{RM}_1[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = 9x^{(1+1)}+4x^{(1+2)}+6x^{(1+3)}+11x^{(2+2)}+6x^{(2+3)}+x^{(2+4)}$$

$$\text{RM}_1[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = \mathbf{x^6+6x^5+17x^4+4x^3+9x^2}.$$

Using equation (8), we obtain:

$$\text{RM}_2[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = 9x^{(1 \times 1)} + 4x^{(1 \times 2)} + 6x^{(1 \times 3)} + 11x^{(2 \times 2)} + 6x^{(2 \times 3)} + x^{(2 \times 4)}$$

$$\text{RM}_2[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = \mathbf{x^8 + 6x^6 + 11x^4 + 6x^3 + 4x^2 + 9x^1}.$$

Using equation (9), we obtain:

$$\overline{\text{RM}}_1[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = 2(37)(25-1)-134$$

$$\overline{\text{RM}}_1[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = \mathbf{1642}.$$

Using equation (10), we obtain:

$$\overline{\text{RM}}_2[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = 2(37)^2 - \frac{1}{2}(134) - 123$$

$$\overline{\text{RM}}_2[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = \mathbf{2548}.$$

Using equation (11), we obtain:

$$\text{RHM}[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = 9(1+1)^2+4(1+2)^2+6(1+3)^2+11(2+2)^2+6(2+3)^2+(2+4)^2$$

$$\text{RHM}[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = \mathbf{530}.$$

Using equation (12), we obtain:

$$\text{RHM}[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = 9x^{(1+1)^2}+4x^{(1+2)^2}+6x^{(1+3)^2}+11x^{(2+2)^2}+6x^{(2+3)^2}+x^{(2+4)^2}$$

$$\text{RHM}[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = \mathbf{x^{36}+6x^{25}+17x^{16}+4x^9+9x^4}.$$

Using equation (13), we obtain:

$$\text{RHM}[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = 9(1^2+1^2)+4(1^2+2^2)+6(1^2+3^2)+11(2^2+2^2)+6(2^2+3^2)+(2^2+4^2)$$

$$\text{RHM}[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = \mathbf{284}.$$

Using equation (14), we obtain:

$$\text{RHM}[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = 9x^{(1^2+1^2)}+4x^{(1^2+2^2)}+6x^{(1^2+3^2)}+11x^{(2^2+2^2)}+6x^{(2^2+3^2)}+x^{(2^2+4^2)}$$

$$\text{RF}[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = \mathbf{x^{20}+6x^{13}+6x^{10}+11x^8+4x^5+9x^2}.$$

Using equation (15), we obtain:

$$\text{RJ}[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = \frac{37}{37-25+2} \left\{ 9 \frac{1}{\sqrt{1 \times 1}} + 4 \frac{1}{\sqrt{1 \times 2}} + 6 \frac{1}{\sqrt{1 \times 3}} + 11 \frac{1}{\sqrt{2 \times 2}} + 6 \frac{1}{\sqrt{2 \times 3}} + \frac{1}{\sqrt{2 \times 4}} \right\}$$

$$\text{RJ}[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = \mathbf{62.3597}.$$

Using equation (16), we obtain:

$$\text{RPM}_1[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = 9(1+1) \times 4(1+2) \times 6(1+3) \times 11(2+2) \times 6(2+3) \times (2+4)$$

$$\text{RPM}_1[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = \mathbf{41057280}.$$

Using equation (17), we obtain:

$$\text{RPM}_2[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})]=9(1 \times 1) \times 4(1 \times 2) \times 6(1 \times 3) \times 11(2 \times 2) \times 6(2 \times 3) \times (2 \times 4)$$

$$\text{RPM}_2[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})]= \mathbf{16422912}.$$

Using equation (18), we obtain:

$$\text{RR}_e\text{ZG}_1[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})]= 9\left(\frac{1+1}{1 \times 1}\right)+4\left(\frac{1+2}{1 \times 2}\right)+6\left(\frac{1+3}{1 \times 3}\right)+11\left(\frac{2+2}{2 \times 2}\right)+6\left(\frac{2+3}{2 \times 3}\right)+\left(\frac{2+4}{2 \times 4}\right)$$

$$\text{RR}_e\text{ZG}_1[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})]= \mathbf{48.75}.$$

Using equation (19), we obtain:

$$\text{RR}_e\text{ZG}_2[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})]= 9\left(\frac{1 \times 1}{1+1}\right)+4\left(\frac{1 \times 2}{1+2}\right)+6\left(\frac{1 \times 3}{1+3}\right)+11\left(\frac{2 \times 2}{2+2}\right)+6\left(\frac{2 \times 3}{2+3}\right)+\left(\frac{2 \times 4}{2+4}\right)$$

$$\text{RR}_e\text{ZG}_2[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})]= \mathbf{31.2}.$$

Using equation (20), we obtain:

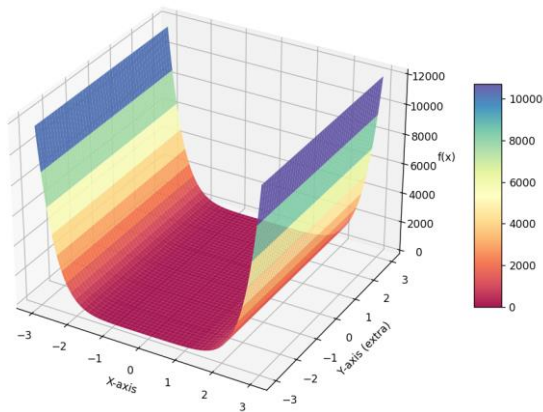
$$\text{RR}_e\text{ZG}_3[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})]=9[(1 \times 1)(1+1)]+4[(1 \times 2)(1+2)]+6[(1 \times 3)(1+3)]+11[(2 \times 2)(2+2)]+6[(2 \times 3)(2+3)]+ [(2 \times 4)(2+4)]$$

$$\text{RR}_e\text{ZG}_3[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})]= \mathbf{518}.$$

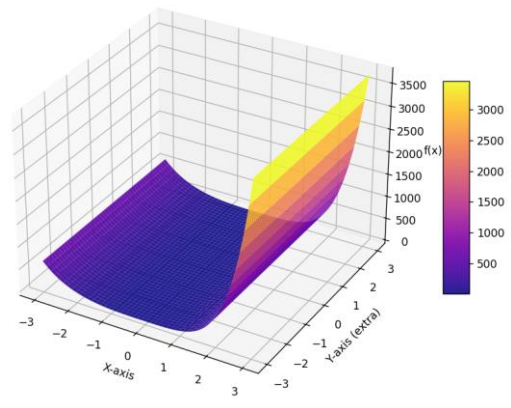
Using equation (21), we obtain:

$$\text{RR}_e\text{ZG}_3[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})]=9x^{[(1 \times 1)(1+1)]} + 4x^{[(1 \times 2)(1+2)]} + 6x^{[(1 \times 3)(1+3)]} + 11x^{[(2 \times 2)(2+2)]} + 6x^{[(2 \times 3)(2+3)]} + x^{[(2 \times 4)(2+4)]}$$

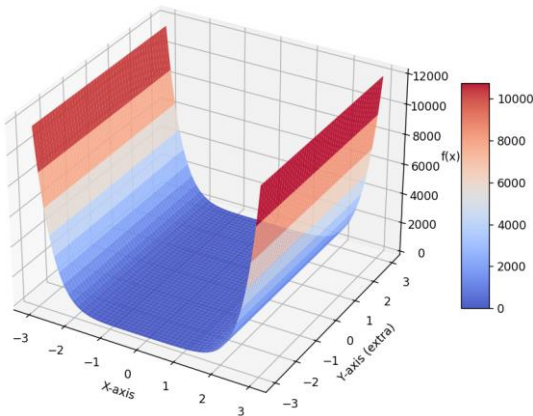
$$\text{RR}_e\text{ZG}_3[\text{L}(\text{C}_{17}\text{H}_{12}\text{F}_3\text{NO}_4\text{S})] = \mathbf{x^{48}+6x^{30}+11x^{16}+6x^{12}+4x^6+9x^2}.$$



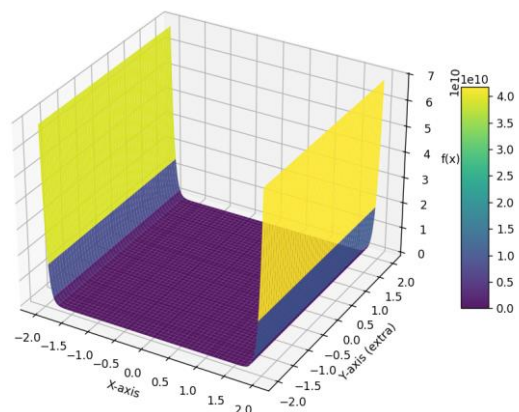
(a)



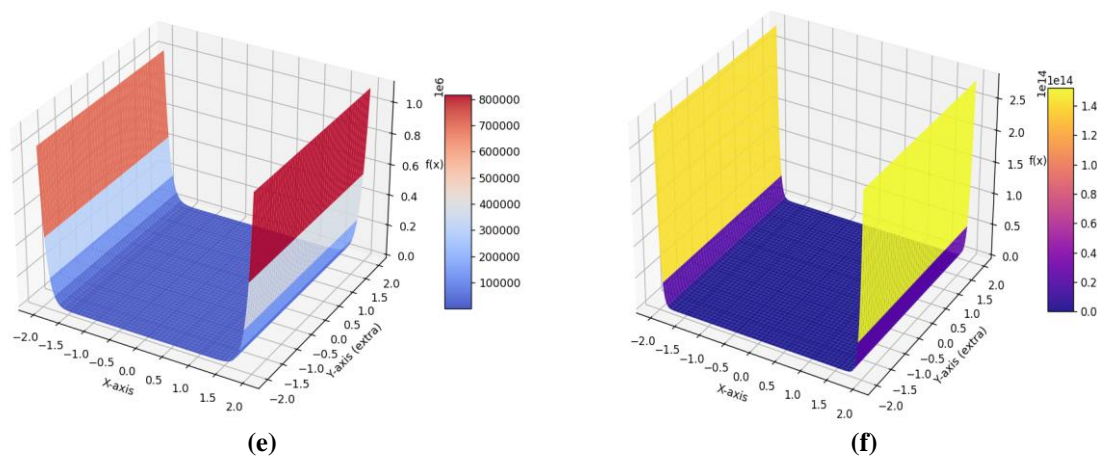
(b)



(c)



(d)



Graph 2. Belzutifan’s graphical representation of the polynomials (a) Reverse Randic index; (b) Reverse first Zagreb index; (c) Reverse second Zagreb index; (d) Reverse Hyper Zagreb index; (e) Reverse Forgotten index; (f) Reverse third Refined Zagreb index.

3.3. Applications.

The Reverse degree topological indices are an approach that explores the connections between atoms in molecules to analyze molecular topology. It is applicable in chemistry for understanding molecular branching arrangements, predicting physical properties, and distinguishing between isomers. To forecast therapeutic action, solubility, and enhance productivity, the pharmaceutical industry frequently uses QSAR/QSPR models. It also helps with lead optimization, where minor structural adjustments can improve medication effectiveness or reduce adverse effects. In addition, it supports safety screening and toxicity prediction, ensuring that substances meet pharmacological criteria. Overall, these indices offer a cost-effective and reliable way to support drug discovery, molecular design, and formulation research.

4. Conclusion

This work shows how useful reverse-degree-based topological indices are for capturing subtle molecular topology, especially for line graphs of the drugs Belzutifan and Pazopanib, which are used to treat renal cell carcinoma. We have offered a theoretical framework for comprehending their structural and functional characteristics by computing these indices and examining their polynomials. Without requiring extensive experimental work, these insights can help chemists and pharmaceutical industry professionals forecast key physicochemical and pharmacological properties of these drugs. This strategy provides an economical and effective way to progress drug development and enhance treatment approaches for Renal Cell Carcinoma.

Author Contribution

Conceptualization, R.J.; methodology, R.J.; software, R.J.; validation, R.J., J.R., and H.N.C.; formal analysis, R.J.; investigation, R.J.; resources, J.R. and H.N.C.; data curation, R.J.; writing—original draft preparation, R.J.; writing—review and editing, R.J., J.R., and H.N.C.; visualization, R.J.; supervision, J.R. and H.N.C.; project administration, J.R. All authors have read and agreed to the published version of the manuscript.

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Data Availability Statement

The data supporting the findings of this study are available upon reasonable request from the corresponding author.

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Conflicts of Interest

The authors declare no conflict of interest.

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