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RESOLVING -POLYNOMIAL AND QSPR STUDY OF COVID-19 DRUGS

CHANDRAKALA S. B., SOORYANARAYANA B., ROSHINI G. R.,
AND PRASANNA POOJARY*

Abstract. The emergence of COVID-19 virus is a serious public health concern that has erupted into a global pandemic. The therapy suggestions are diverse. Due to a lack of adequate medication, the condition has deteriorated. Scientists are looking into COVID-19 medications based on previous research for SARS and MERS. Topological indices (TIs) are helpful in research, to model a variety of physicochemical properties. In this paper, several degree-based TIs for several chemical compounds used in treating COVID-19, were obtained using a polynomial of two variables derived from the concept of resolving sets. A QSPR was developed between TIs and some of the properties of the chemical compound considered.

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1. Introduction

Contagious diseases, their cause, and their remedies have come to the focus of research in recent years. Especially virology is in the limelight and attracts attention from all quarters of research. Scientists across the globe had to aggressively work to discover therapeutic treatments, for the victims. The efforts have resulted in partial success. Few countries have successfully designed and brought out vaccines. The new virus SARS-CoV-2 has emerged as a severe public health risk that has spread over the world, which is popularly called COVID-19. Due to a lack of sufficient medication, the situation has gotten worse. Based on prior studies, scientists are looking into drugs for SARS and MERS that are based on medical therapy. Infected individuals are undergoing clinical trials to determine the effectiveness and safety profile of chemicals used in the development of vaccines and antiviral drugs [6]. Many researchers from various countries have worked on developing antiviral drugs and vaccines that make use of various chemical compounds such as lopinavir, arbidol, thalidomide, ritonavir, chloroquine, hydroxychloroquine, theaflavin, and remdesivir. For related work on topological indices and QSPR/QSAR analysis of chemical compounds used in the treatment of COVID-19 patients, we refer [13–15].

*Corresponding Author.

Throughout this paper, $G = G(V,E)$ is a simple, undirected, finite connected graph, with vertex set $V(G)$ and edge set $E(G)$, respectively, having n and m elements. Also, $d_G(a)$ be the degree of a vertex a and $d(a,\ b)$ be the distance between the vertices a and b in G. For the terms not defined here, we refer to the book [2].

The concept of metric dimension based on the resolving set was first studied by P. J. Slater [7] and independently by F. Harary and R. A. Melter [4]. A non-empty subset $S \subseteq V$ is said to be a *resolving set* if for every pair of vertices $a,\ b \in V - S$, there exists a vertex $x \in S$ such that $d(x,a) \neq d(x,b)$. A resolving set of minimum cardinality is called a *metric basis* of G and its cardinality, denoted by $\beta(G)$, is the metric dimension of G. The code or the coordinate of the vertex v with respect to the metric basis S is defined as, $\Gamma(v/S) = (d(v,\ s_1),\ d(v,\ s_2),\ldots,\ d(v,\ s_k))$.

Topological indices (TIs) are the numerical invariants of a molecular graph and are very useful for predicting the physio-chemical properties of chemical compounds. A great variety of such indices are studied and used in theoretical chemistry. The family of Zagreb indices [3] is one of the oldest degree based TIs given as $M_1(G) = \sum_{a \in V(G)} d_G(a)^2 = \sum_{ab \in E(G)} [d_G(a) + d_G(b)]$ and $M_2(G) = \sum_{ab \in E(G)} d_G(a)\ d_G(b)$.

In the literature, some distance-based graph polynomials were studied to reduce the computational complexity of TIs. Analogous to this in 2015, Deutsch and Klavzar [1] introduced M-polynomial to compute various degree-based TIs. Due to its vast applicability, it has been utilised to construct formulas for degree-based topological indices in several studies [12].

Recently in 2021 Hanan et.al. [5], based on the concept of domination introduced the concept of domination degree of a vertex and studied different TIs of graphs. B. Sooryanarayana et.al. [10], based on the concepts of resolving sets in graphs introduced resolving TIs and studied for different graphs, and chemical structures. The resolving degree of a vertex a, denoted by $d_\beta(a)$, is defined as the minimum cardinality of a resolving set of G containing the vertex a. That is, $d_\beta(a) = min\{|S_a|\}$ where S_a is a resolving set containing the vertex a. The resolving polynomial of graph G is defined as: $R(G;\ x,\ y) = \sum_{i \leq j} m_{ij}(G) x^i y^j$ where, $m_{ij}(G),\ i,j \geq 1$, be the number of edges uv of G such that $\left\{d_\beta(u), d_\beta(v)\right\} = \{i,j\}$. For related work on indices, we refer to [8,9].

2. Some resolving polynomials and topological indices of graphs

We obtain the metric dimension and resolving polynomial of eight chemical compounds used in the treatment of COVID-19. Based on resolving polynomial, different degree-based indices of these chemical compounds are derived. The formula for different resolving TIs and functions to obtain their values using resolving polynomials are listed in Table 1.

Table 1. Resolving TI and functions to obtain their values from resolving polynomial.

Topological Indices	**Formula**	**Derivation from**
Resolving first Zagreb index: ${}_{\beta}M_1(G)$ [10]	$\sum_{uv\in E(G)} \left(d_\beta(u)+d_\beta(v)\right)$	$\left(D_x+D_y\right)(\mathcal{P}(x,y))_{x=y=1}$
Resolving second Zagreb index: ${}_{\beta}M_2(G)$ [10]	$\sum_{uv\in E(G)} d_\beta(u)\ d_\beta(v)$	$\left(D_xD_y\right)(\mathcal{P}(x,y))_{x=y=1}$
Resolving second modified Zagreb index: $m_\beta M_2(G)$	$\sum_{uv\in E(G)} \frac{1}{d_\beta(u)\ d_\beta(v)}$	$\left(S_xS_y\right)(\mathcal{P}(x,y))_{x=y=1}$
Resolving redefined third Zagreb index: $Re_\beta M_3(G)$	$\sum_{uv\in E(G)} d_\beta(u)\ d_\beta(v)\left(d_\beta(u)+d_\beta(v)\right)$	$\left(D_xD_y\right)\left(D_x+D_y\right)$ $(\mathcal{P}(x,y))_{x=y=1}$
Resolving forgotten topological index: $F_\beta(G)$	$\sum_{uv\in E(G)} \left(d_\beta^2(u)+d_\beta^2(v)\right)$	$\left(D_x^2+D_y^2\right)$ $(\mathcal{P}(x,y))_{x=y=1}$
Resolving Randic index: ${}_{\beta}R_k(G)$	$\sum_{uv\in E(G)} \left(d_\beta(u)\ d_\beta(v)\right)^k$	$\left(D_x^kD_y^k\right)(\mathcal{P}(x,y))_{x=y=1}$
Inverse resolving Randic index: $R_\beta R_k(G)$	$\sum_{uv\in E(G)} \frac{1}{\left(d_\beta(u)\ d_\beta(v)\right)^k}$	$\left(S_x^kS_y^k\right)(\mathcal{P}(x,y))_{x=y=1}$
Resolving Symmetric division index: ${}_{\beta}SDD(G)$	$\sum_{uv\in E(G)} \frac{d_\beta^2(u)+d_\beta^2(v)}{d_\beta(u)\ d_\beta(v)}$	$\left(D_xS_y+S_xD_y\right)$ $(\mathcal{P}(x,y))_{x=y=1}$
Resolving harmonic index: ${}_{\beta}H(G)$	$\sum_{uv\in E(G)} \frac{2}{d_\beta(u)\ d_\beta(v)}$	$(2S_xJ)(\mathcal{P}(x,y))_{x=1}$
Resolving inverse sum index: ${}_{\beta}I(G)$	$\sum_{uv\in E(G)} \frac{d_\beta(u)d_\beta(v)}{\left(d_\beta(u)+d_\beta(v)\right)}$	$\left(S_xJD_xD_y\right)(\mathcal{P}(x,y))_{x=1}$
Resolving augmented Zagreb index: ${}_{\beta}A(G)$	$\sum_{uv\in E(G)} \left\{\frac{d_\beta(u)d_\beta(v)}{d_\beta(u)+d_\beta(v)-2}\right\}^3$	$\left(S_x^3\ Q_{-2}\ J\ D_x^3\ D_y^3\right)$ $(\mathcal{P}(x,y))_{x=1}$

Where $S_x=\int_0^x \frac{\mathcal{P}(z,y)}{z}dz$, $S_y=\int_0^y \frac{\mathcal{P}(x,z)}{z}dz$, $J(\mathcal{P}(x,y))=\mathcal{P}(x,x)$, $Q_k(\mathcal{P}(x,y))=x^k\mathcal{P}(x,y)$, and $\mathcal{P}(x,y)=R(G;x,\ y)$.

Lemma 2.1. *[10] For every vertex v of a connected graph G, $\beta(G)\le d_\beta(v)\le \beta(G)+1$ and $\mathrm{d}_\beta(v)=\beta(G)$ if and only if there is a metric basis containing v.*

Theorem 2.2. *[11] For any graph G of order n, $\beta(G) = 1$ if and only if $G \cong P_n$.*

Lemma 2.3. *Let S be a metric basis of the graph G and $H \subseteq V(G)$. If $d(a, x) = d(b,x)$ and $d(a, y) = d(b,y)$ for every pair $a, b \in S - H$ and for some $x, y \in H$, then $S \cap H \neq \emptyset$.*

Remark 2.4. *For a given graph G, based on resolving degree, edge set can be partitioned as $E = E_1 \cup E_2 \cup E_3$, where $E_1 = \{uv : d_\beta(u) = \beta = d_\beta(v)\}$, $E_2 = \{uv : d_\beta(u) = \beta,\ d_\beta(v) = \beta + 1\}$ and $E_3 = \{uv : d_\beta(u) = \beta + 1,\ d_\beta(v) = \beta + 1\}$.*

Definition 2.5. *Let β be the metric dimension of the graph G. Then the polynomial $R(G : a, b) = |E_1|x^\beta y^\beta + |E_2|x^\beta y^{\beta+1} + |E_3|x^{\beta+1}y^{\beta+1}$ is called the resolving polynomial of G, where E_1, $E_2$and E_3 are the sets defined in Remark 2.4.*

3. Resolving polynomial and topological indices of Lopinavir

Throughout this section, $\mathcal{L}$ denotes the molecular graph of Lopinavir. Let H_1, H_2, H_3, H_4, and H_5 be the subgraphs of $\mathcal{L}$ induced by the sets $\{w, w_1, w_2, \ldots, w_5\}$, $\{u, u_1, u_2, \ldots, u_5, u_6\}$, $\{\eta, \eta_1, \eta_2, \ldots, \eta_5\}$, $\{\xi, \xi_1, \xi_2\}$ and $\{v, v_1, v_2, \ldots, v_6, v_7\}$ respectively. Also, $T_1 = \{u, u_1, u_2, u_6, v, v_7, w, w_5, \eta, \eta_5, \xi\}$.

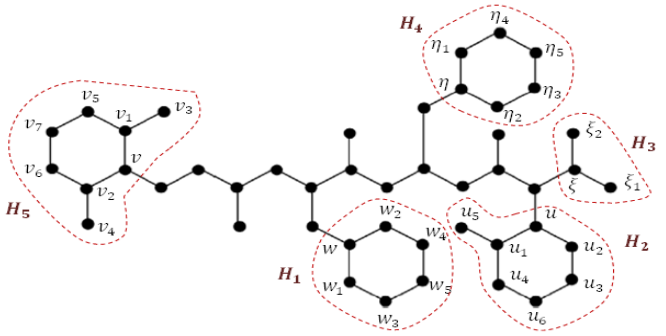

Figure 1. Molecular graph $\mathcal{L}$ of Lopinavir.

Lemma 3.1. *Let S be a metric basis of the molecular graph $\mathcal{L}$. Then $|S \cap V(H_5)| \geq 2$ and $|S \cap V(H_i)| \geq 1$ for each $1 \leq i \leq 4$.*

Proof. We first see that for each $a, b \in S - V(H_i)$ (for some i), $d(a,x) = d(b,x)$ for some $x \in V(H_i)$. Hence, by Lemma 2.3, $S \cap V(H_i) \neq \emptyset$ (as $|V(H_i)| \geq 2$). This shows that $|S \cap V(H_i)| \geq 1$ for each $1 \leq i \leq 5$. Let $S' = S - V(H_5)$ and $V' = \{v_3, v_4, v_5, v_6\}$. Then for each $s \in S'$, $d(v_i, s) = d\left(v_j, s\right)$ for every $v_i, v_j \in V'$. Thus, the vertices in V' would be resolved by, only the vertices in $S \cap V(H_5)$. Further, the graph $\mathcal{L}$ is a bipartite and induced graph H_5 is isometric with diameter 4. Hence, $d(v_i, x) \in \{0, 1, 2, 3, 4\}$ for each $x \in S - S'$ and $v_i \in V'$. But each pair of vertices in V' are at an even distance and hence V' is a subset of one of the bi-partition of $\mathcal{L}$. Thus, for any $x \in S - S'$ either $d(v_i, x) \in \{0, 2, 4\}$ or $d(v_i, x) \in \{1, 3\}$. This shows that x is not unique (since $|V'| = 4$ and S is a resolving set). That is, $|S \cap V(H_5)| > 1$. □

Lemma 3.2. *Let $\mathcal{L}$ be the molecular graph of Lopinavir. Then $\beta(\mathcal{L}) = 6$.*

Proof. Let S be a metric basis of the graph $\mathcal{L}$. Then, by Lemma 3.1, $|S| \geq \sum_{i=1}^{5} |S \cap H_i| = \sum_{i=1}^{4} |S \cap H_i| + |S \cap H_5| = 4 + 2 = 6$. Thus, $\beta(\mathcal{L}) = |S| \geq 6$. The

reverse inequality follows by noting the distinct codes generated by the 6-element set $\{\xi_1,\ w_1,\ \eta_1,\ u_3,\ v_3, v_7\}$ as in Figure 1. □

Theorem 3.3. *Let $\mathcal{L}$ be the molecular graph of Lopinavir and $\alpha \in V(\mathcal{L})$. Then $d_\beta(\alpha) = \beta$ if and only if $\alpha \in V(H_i) - T_1$ for some $1 \le i \le 4$.*

Proof. Let S be a resolving set containing a vertex α. Suppose $\alpha \notin V(H_i)$, clearly by the proof of Lemma 3.2, $|S| > 6$ implies that S is not a metric basis and $\deg_\beta(\alpha) \neq \beta$. Suppose $\alpha \in T_1$, the vertices adjacent to α in H_i receives the same code with respect to S if $|S \cap V(H_i)| < 2$ for $i \in \{1,2,3,4\}$ and $|S \cap V(H_5)| < 3$. Thus, if $\alpha \in T_1$ then $|S \cap V(H_i)| \ge 2$ for $i \in \{1,2,3,4\}$ and $|S \cap V(H_5)| \ge 3$. This implies that $|S| > 6$, and hence $d_\beta(\alpha) \neq \beta$. To prove the reverse inequality, define a set $S = \{\alpha_1, \alpha_2, \beta_1, \gamma_1,\ \delta_1, \epsilon_1\}$, for some $\{\alpha_1,\ \alpha_2\} \subseteq \{v_3, v_4, v_5, v_6, v_7\}$ or $\{\alpha_1,\ \alpha_2\} = \{v_1,\ v_7\}$ or $\{\alpha_1,\ \alpha_2\} = \{v_2, v_7\}$, $\beta_1 \in \{w_1, w_2, w_3, w_4\}$, $\gamma_1 \in \{\eta_1, \eta_2, \eta_3, \eta_4\}$, $\delta_1 = \{\xi_1, \xi_2\}$ and $\epsilon_1 = \{u_2, u_3, u_4, u_5\}$. It is easy to observe that for each pair $y,\ z$ of vertices in $V(\mathcal{L}) - \bigcup_{i=1}^{5} V(H_i)$ with $d(y, \alpha_1) = d(z, \alpha_1)$ either y is in the $z\delta_1$-path or z is in the $y\delta_1$-path (since $2 \le deg(y), deg(z) \le 3$) and hence δ_1 will resolve such a pair. Any other pair of vertices $y,\ z$ is resolved by the set $\{\delta_1\} \cup (V(H_i) \cap S)$. Now let $\alpha \in V(H_i) - T_1$ then set $S_a = S \cup \{\alpha\}$ contains a vertex from each of the subgraph $H_i (1 \le i \le 4)$ and two vertices from H_5. The possible combination of two vertices of H_5 are v_i, v_j such that

- if $i \in \{1,2\}$ then $j = 7$
- if $i \in \{3,4,5,6\}$ then $j \neq i \in \{3,4,5,6,7\}$
- if $i = 7$ then $j \in \{1,2,3,4,5,6\}$.

Then, S_α is a metric basis containing α, hence $d_\beta(\alpha) = \beta$.

□

Theorem 3.4. *For the molecular graph $\mathcal{L}$ of Lopinavir, resolving polynomial $R(\mathcal{L}; x,\ y) = 10x^6y^6 + 15y^7 + 24x^7y^7$ and hence*

(1) ${}_\beta M_1(\mathcal{L}) = 651$
(2) ${}_\beta M_2(\mathcal{L}) = 2166$
(3) ${}_\beta mM_2(\mathcal{L}) = 1.1247$
(4) ${}_\beta ReM_2(\mathcal{L}) = 28974$
(5) ${}_\beta F(\mathcal{L}) = 4347$
(6) ${}_\beta R_k(\mathcal{L}) = 10 \times 6^{2k} + 15 \times 42^k + 24 \times 7^{2k}$
(7) ${}_\beta RR_k(\mathcal{L}) = \frac{10}{6^{2k}} + \frac{15}{42^k} + \frac{24}{7^{2k}}$
(8) ${}_\beta SDD(\mathcal{L}) = 98.35714$
(9) ${}_\beta H(\mathcal{L}) = 7.40293$
(10) ${}_\beta I(\mathcal{L}) = 162.4615$
(11) ${}_\beta A(\mathcal{L}) = 2935.525$

Proof. Let $H = \left(\bigcup_{i=1}^{5} H_i\right) - T_1$. From Theorem 3.3, $E_1 = \{ v_1v_3,\ v_1v_5,\ v_2v_4,\ v_2v_6,\ v_5v_7,\ v_6v_7,\ w_1w_3,\ w_2w_4,\ \eta_1\eta_4,\ \eta_2\eta_3\}$ and $E_2 = \{vv_1,\ vv_2,\ u_1u_5,\ u_2u_3,\ u_3u_5,\ ww_1,\ ww_2,\ w_3w_5,\ w_4w_5,\ \xi\xi_1,\ \xi\xi_2,\ \eta\eta_1,\ \eta\eta_2,\ \eta_3\eta_5,\ \eta_4\eta_5\}$ and remaining all the edges are in E_3 having $|E_1| = 10$, $|E_2| = 15$ and $|E_3| = |E(\mathcal{L})| - |E_1| - |E_2| = 49 - 10 - 15 = 24$. Therefore, $RM(\mathcal{L}; a,\ b) = |E_1|x^6y^6 + |E_2|x^6y^7 + |E_3|x^7y^7 = 10x^6y^6 + 15x^6y^7 + 24\ x^7y^7$.

(1) $${}_{\beta}M_1(\mathcal{L}) = \left[\left(D_x + D_y\right)RM(\mathcal{L};a,\ b)\right]_{(1,1)} = \left[x\frac{\partial f}{\partial x} + y\frac{\partial f}{\partial y}\right]_{(1,1)}$$
$$= 60x^6y^6 + 90x^6y^7 + 168x^7y^7 + 60x^6y^6 + 105x^6y^7 + 168x^7y^7$$
$$= 120x^6y^6 + 195x^6y^7 + 336x^7y^7 = 651.$$

(2) $${}_{\beta}M_2(\mathcal{L}) = \left[\left(D_xD_y\right)RM(\mathcal{L};a,\ b)\right]_{(1,1)} = \left[x\frac{\partial}{\partial x}\left(y\frac{\partial f}{\partial y}\right)\right]_{(1,1)}$$
$$= \left[360x^6y^6 + 630x^6y^7 + 1176x^7y^7\right]_{(1,1)} = 2166.$$

(3) $${}_{\beta}mM_2(\mathcal{L}) = \left[\left(S_xS_y\right)RM(\mathcal{L};a,\ b)\right]_{(1,1)} = \left[\left(S_xS_y\right)RM(\mathcal{L};a,\ b)\right]_{(1,1)}$$
$$= \left[S_x\int_0^y \frac{f(x,t)}{t}dt\right]_{(1,1)} = \left[S_x\left(\tfrac{11}{6}x^6y^6 + \tfrac{17}{7}x^6y^7 + \tfrac{21}{7}x^7y^7\right)\right]_{(1,1)}$$
$$= \left[\tfrac{10}{36}x^6y^6 + \tfrac{15}{42}x^6y^7 + \tfrac{24}{49}x^7y^7\right]_{(1,1)} = 1.1247.$$

(4) $${}_{\beta}ReM_2(\mathcal{L}) = \left[\left(D_xD_y\right)\left(D_x + D_y\right)RM(\mathcal{L};a,\ b)\right]_{(1,1)}$$
$$= \left[\left(D_xD_y\right)\left(120x^6y^6 + 195x^6y^7 + 336x^7y^7\ \right)\right]_{(1,1)}$$
$$= \left[D_x\left(792x^6y^6 + 1326x^6y^7 + 2058x^7y^7\right)\right]_{(1,1)}$$
$$= \left[4320x^6y^6 + 8190x^6y^7 + 16464x^7y^7\right]_{(1,1)} = 28974.$$

(5) $${}_{\beta}F(\mathcal{L}) = \left[\left(D_x^2 + D_y^2\right)RM(\mathcal{L};a,\ b)\right]_{(1,1)}$$
$$= \left[\left(D_x\left(x\frac{\partial}{\partial x}\right) + D_y\left(y\frac{\partial}{\partial y}\right)\right)\left(10x^6y^6 + 15x^6y^7 + 24x^7y^7\right)\right]_{(1,1)}$$
$$= \left[D_x\left(60x^6y^6 + 90x^6y^7 + 168x^7y^7\right) + D_y\left(60x^6y^6 + 90x^6y^7 + 168x^7y^7\right)\right]_{(1,1)}$$
$$= \left[360x^6y^6 + 540x^6y^7 + 1176x^7y^7 + 360x^6y^6 + 735x^6y^7 + 1176x^7y^7\right]_{(1,1)}$$
$$= 4347.$$

(6) $${}_{\beta}R_k(\mathcal{L}) = \left(D_x^kD_y^k\right)(RM(\mathcal{L};a,\ b))_{(1,1)}$$
$$= \left[{D_x}^k\left(y\frac{\partial}{\partial y}\right)^k\left(10x^6y^6 + 15x^6y^7 + 24x^7y^7\right)\right]_{(1,1)}$$
$$= \left[{D_x}^k\left(10\times6^k\ x^6y^6 + 15\times7^k\ x^6y^7 + 24\times7^k\ x^7y^7\right)\right]_{(1,1)}$$
$$= \left[10\times6^{2k}\ x^6y^6 + 15\times6^k\ 7^kx^6y^7 + 24\times7^{2k}\ x^7y^7\right]_{(1,1)}$$
$$= 10\times6^{2k}\ + 15\times42^k\ + 24\times7^{2k}$$

(7) $${}_{\beta}RR_k(\mathcal{L}) = \left(\left({S_x}^k\ {S_y}^k\right)(RM(\mathcal{L};a,\ b))\right)_{(1,1)}$$
$$= \left[{S_x}^k\left(\tfrac{10}{6^k}x^6y^6 + \tfrac{15}{7^k}x^6y^7 + \tfrac{24}{7^k}x^7y^7\right)\right]_{(1,1)}$$
$$= \left[\tfrac{10}{6^{2k}}x^6y^6 + \tfrac{15}{42^k}x^6y^7 + \tfrac{24}{7^{2k}}x^7y^7\right]_{(1,1)} = \tfrac{10}{6^{2k}} + \tfrac{15}{42^k} + \tfrac{24}{7^{2k}}$$

(8) $${}_{\beta}SDD(\mathcal{L}) = \left[\left(D_xS_y + D_yS_x\right)RM(\mathcal{L};a,\ b)\right]_{(1,1)}$$
$$= \left[D_x\left(\tfrac{10}{6}x^6y^6 + \tfrac{15}{7}x^6y^7 + \tfrac{24}{7}x^7y^7\right) + D_y\left(\tfrac{10}{6}x^6y^6 + \tfrac{15}{6}x^6y^7 + \tfrac{24}{7}x^7y^7\right)\right]_{(1,1)}$$
$$= \left[\tfrac{10\times6}{6}x^6y^6 + \tfrac{15\times6}{7}x^6y^7 + \tfrac{24\times7}{7}x^7y^7 + \tfrac{10\times6}{6}x^6y^6 + \tfrac{15\times7}{6}x^6y^7 + \tfrac{24\times7}{7}x^7y^7\right]_{(1,1)}$$
$$= 98.35714.$$

(9) $${}_{\beta}H(\mathcal{L}) = \left[(2S_xJ)(RM(\mathcal{L};a,\ b))\right]_{x=1} = \left[2S_x\left(10x^{12} + 15x^{13} + 24x^{14}\right)\right]_{x=1}$$
$$= \left[2\left(\tfrac{10}{12}x^{12} + \tfrac{15}{13}x^{13} + \tfrac{24}{14}x^{14}\right)\right]_{x=1} = 7.40293.$$

$$
\begin{aligned}
(10)\quad {}_{\beta}I(\mathcal{L}) &= \left[\left(S_x J D_x D_y\right) RM(\mathcal{L};a,\ b)\right]_{x=1} \\
&= \left[(S_x J D_x)\left(66x^6y^6 + 105x^6y^7 + 168x^7y^7\right)\right]_{x=1} \\
&= \left[(S_x J)\left(360x^6y^6 + 630x^6y^7 + 1176x^7y^7\right)\right]_{x=1} \\
&= \left[S_x\left(360x^{12} + 630x^{13} + 1176x^{14}\right)\right]_{x=1} \\
&= \left[\tfrac{360}{12}x^{12} + \tfrac{630}{13}x^{13} + \tfrac{1176}{14}x^{14}\right]_{x=1} = 161.4231. \\
(11)\quad {}_{\beta}A(\mathcal{L}) &= \left[\left(S_x{}^3 Q_{-2} J D_x{}^3 D_y{}^3\right) RM(\mathcal{L};a,\ b)\right]_{x=1} \\
&= \left[S_x{}^3 Q_{-2} J\left(10\times 6^6 x^6y^6 + 15\times(6\times 7)^3\ x^6y^7 + 24\times 7^6 x^7y^7\right)\right]_{x=1} \\
&= \left[S_x{}^3\left(x^{-2}\left(10\times 6^6 x^{12} + 15\times 42^3\ x^{13} + 24\times 7^6 x^{14}\right)\right)\right]_{x=1} \\
&= \left[S_x{}^3\left(10\times 6^6 x^{10} + 15\times 42^3\ x^{11} + 24\times 7^6 x^{12}\right)\right]_{x=1} \\
&= \left[\tfrac{10\times 6^6}{10\times 10\times 10}x^{10} + \tfrac{15\times 42^3}{11\times 11\times 11}\ x^{11} + \tfrac{24\times 7^6}{12\times 12\times 12}x^{12}\right]_{x=1} = 2935.525
\end{aligned}
$$

□

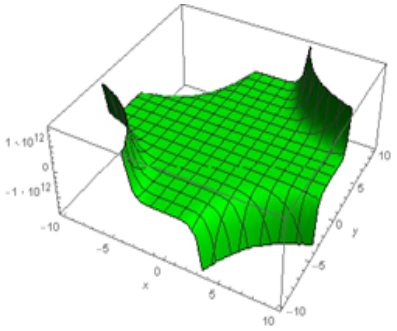

Figure 2.(a) Plot of Resolving Polynomial of Lopinavir

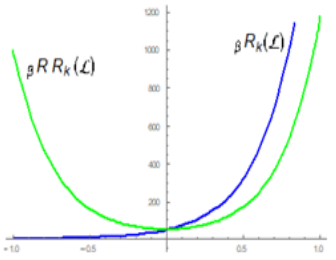

Figure 2.(b) ${}_{\beta}R_k(\mathcal{L})$ and ${}_{\beta}RR_k(\mathcal{L})$ for $(-10 \le k \le 10)$

4. Resolving polynomial and topological indices of Arbidol

Throughout this section, $\mathcal{A}$ denotes the Molecular graph of Arbidol. Let H_1, H_2 and H_3 be the subgraphs of $\mathcal{A}$ induced by the sets $\{a, a_1, a_2\}$, $\{b,\ b_1, b_2, b_3, b_4\}$ and $\{c,\ c_1, c_2, \ldots,\ c_5\}$ respectively. Also, $T_1 = \{a, b, c,\ c_5\}$.

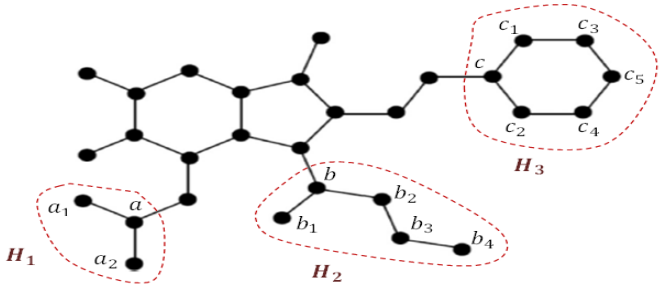

Figure 3. Molecular graph $\mathcal{A}$ of Arbidol.

Lemma 4.1. *Let S be a metric basis of the molecular graph $\mathcal{A}$. Then $|S \cap V(H_i)| \ge 1$ for each $1 \le i \le 3$.*

Proof. We first see that for each $u, v \in S - V(H_i)$ (for some i), $d(u,x) = d(v,x)$ for some $x \in V(H_i)$. Hence, by Lemma 2.3, $S \cap V(H_i) \neq \emptyset$ (as $|V(H_i)| \geq 2$). This shows that $|S \cap V(H_i)| \geq 1$ for each $1 \leq i \leq 3$.

□

Lemma 4.2. *Let $\mathcal{A}$ be the molecular graph of Arbidol. Then $\beta(\mathcal{A}) = 3$.*

Proof. Let S be a metric basis of the graph $\mathcal{A}$. Then, by Lemma 4.1, $|S| \geq \sum_{i=1}^{3} |S \cap H_i| = 3$. Thus, $\beta(\mathcal{A}) = |S| \geq 3$. The reverse inequality follows by noting the distinct codes generated by the 3-element set $\{a_1, b_1, c_1\}$ as in Figure 3. □

Theorem 4.3. *Let $\mathcal{A}$ be the molecular graph of Arbidol and $\alpha \in V(\mathcal{A})$. Then $d_\beta(\alpha) = \beta$ if and only if $\alpha \in V(H_i) - T_1$ for some $1 \leq i \leq 3$.*

Proof. Let S be any resolving set containing a vertex α. If $\alpha \notin V(H_i)$, then clearly by the proof of Lemma 4.2, $|S| > 3$ and hence S is not a metric basis. Hence $\deg_\beta(\alpha) \neq \beta$. If $\alpha \in T_1$, then $\alpha \in H_i$ for some $1 \leq i \leq 3$. The vertices adjacent to α in H_i receive the same code with respect to S This implies that $|S| > 3$, and hence $d_\beta(\alpha) \neq \beta$. To prove the reverse inequality, define a set $S = \{\alpha_1, \beta_1, \gamma_1\}$, for some $\alpha_1 \in \{a_1, a_2\}$, $\beta_1 \in \{b_1, b_2, b_3, b_4\}$ and $\gamma_1 \in \{c_1, c_2, c_3, c_4\}$. It is easy to observe that for each pair y, z of vertices in $V(\mathcal{A}) - \bigcup_{i=1}^{3} V(H_i)$ with $d(y, \beta_1) = d(z, \beta_1)$ either y is in the $z\alpha_1$-path or z is in the $y\alpha_1$-path (since $2 \leq deg(y), deg(z) \leq 3$) and hence α_1 will resolve such a pair. Any other pair of vertices y, z is resolved by the set $\{\alpha_1\} \cup (V(H_i) \cap S)$. Now for $\alpha \in V(H_i) - T_1$. Let $S_\alpha = S \cup \{\alpha\} - S \cap V(H_i)$ for $1 \leq i \leq 3$. □

Theorem 4.4. *For the molecular graph $\mathcal{A}$ of Arbidol, resolving polynomial $RM(\mathcal{A}; x, y) = 4x^3y^3 + 8x^3y^4 + 19x^4y^4$ and hence*

(1) ${}_\beta M_1^*(\mathcal{A}) = 232$
(2) ${}_\beta M_2(\mathcal{A}) = 436$
(3) ${}_\beta mM_2(\mathcal{A}) = 2.2986$
(4) ${}_\beta ReM_2(\mathcal{A}) = 3320$
(5) ${}_\beta F(\mathcal{A}) = 880$
(6) ${}_\beta R_k(\mathcal{A}) = 4 \times 3^{2k} + 8 \times 12^k + 19 \times 4^{2k}$
(7) ${}_\beta RR_k(A) = \frac{4}{3^{2k}} + \frac{8}{12^k} + \frac{19}{4^{2k}}$
(8) ${}_\beta SDD(\mathcal{A}) = 60$
(9) ${}_\beta H(\mathcal{A}) = 8.36904$
(10) ${}_\beta I(A) = 57.7142$
(11) ${}_\beta A(\mathcal{A}) = 516.4508$

Proof. Let $H = \left(\bigcup_{i=1}^{3} H_i\right) - T_1$. From Theorem 4.3, $E_1 = \{b_2b_3, b_3b_4, c_1c_3, c_2c_4\}$ and $E_2 = \{aa_1, aa_2, bb_1, bb_2, cc_1, cc_2, c_3c_5, c_4c_5\}$ and remaining all the edges are in E_3 having $|E_1| = 4$, $|E_2| = 8$ and $|E_3| = |E(\mathcal{A})| - |E_1| - |E_2| = 31 - 4 - 8 = 19$. Therefore,
$(\mathcal{L}; a, b) = |E_1|x^3y^3 + |E_2|x^3y^4 + |E_3|x^4y^4 = 4x^3y^3 + 8x^3y^4 + 19x^4y^4$.

$$(1)\quad {}_\beta M_1(\mathcal{A}) = \left[\left(D_x + D_y\right) RM(\mathcal{A}; a, b)\right]_{(1,1)} = \left[x\frac{\partial f}{\partial x} + y\frac{\partial f}{\partial y}\right]_{(1,1)}$$
$$= \left[12x^3y^3 + 24x^3y^4 + 76x^4y^4 + 12x^3y^3 + 32x^3y^4 + 76x^4y^4\right]_{(1,1)}$$
$$= \left[24x^3y^3 + 56x^3y^4 + 152x^4y^4\right]_{(1,1)} = 232$$

$$(2)\quad {}_{\beta}M_2(\mathcal{A}) = \left[\left(D_xD_y\right)RM(\mathcal{A};a,\ b)\right]_{(1,1)} = \left[x\frac{\partial}{\partial x}\left(y\frac{\partial f}{\partial y}\right)\right]_{(1,1)}$$
$$= \left[36x^3y^3 + 96x^3y^4 + 304x^4y^4\right]_{(1,1)} = 436.$$
$$(3)\quad {}_{\beta}mM_2(\mathcal{A}) = \left[\left(S_xS_y\right)RM(\mathcal{A};a,\ b)\right]_{(1,1)} = \left[\left(S_xS_y\right)RM(\mathcal{A};a,\ b)\right]_{(1,1)}$$
$$= \left[S_x\int_0^y \frac{f(x,t)}{t}dt\right]_{(1,1)} = \left[S_x\left(\tfrac{4}{3}x^3y^3 + \tfrac{8}{4}x^3y^4 + \tfrac{19}{4}x^4y^4\right)\right]_{(1,1)}$$
$$= \left[\tfrac{4}{9}x^3y^3 + \tfrac{8}{12}x^3y^4 + \tfrac{19}{16}x^4y^4\right]_{(1,1)} = 2.2986.$$
$$(4)\quad {}_{\beta}ReM_2(\mathcal{A}) = \left[\left(D_xD_y\right)\left(D_x + D_y\right)RM(\mathcal{A};a,\ b)\right]_{(1,1)}$$
$$= \left[\left(D_xD_y\right)\left(24x^3y^3 + 56x^3y^4 + 152x^4y^4\ \right)\right]_{(1,1)}$$
$$= \left[D_x\left(72x^3y^3 + 224x^3y^4 + 608x^4y^4\right)\right]_{(1,1)}$$
$$= \left[216x^3y^3 + 672x^3y^4 + 2432x^4y^4\right]_{(1,1)} = 3320.$$
$$(5)\quad {}_{\beta}F(\mathcal{A}) = \left[\left(D_x^2 + D_y^2\right)RM(\mathcal{A};a,\ b)\right]_{(1,1)}$$
$$= \left[\left(D_x\left(x\frac{\partial}{\partial x}\right) + D_y\left(y\frac{\partial}{\partial y}\right)\right)\left(4x^3y^3 + 8x^3y^4 + 19x^4y^4\right)\right]_{(1,1)}$$
$$= \left[D_x\left(12x^3y^3 + 24x^3y^4 + 76x^4y^4\right) + \ D_y\left(12x^3y^3 + 32x^3y^4 + 76x^4y^4\right)\right]_{(1,1)}$$
$$= \left[36x^3y^3 + 72x^3y^4 + 304x^4y^4 + 36x^3y^3 + 128x^3y^4 + 304x^4y^4\right]_{(1,1)}$$
$$= \left[72x^3y^3 + 200x^3y^4 + 608x^4y^4\right]_{(1,1)} = 880.$$
$$(6)\quad {}_{\beta}R_k(\mathcal{A}) = \left(D_x^kD_y^k\right)(RM(\mathcal{A};a,\ b))_{(1,1)}$$
$$= \left[{D_x}^k\left(y\frac{\partial}{\partial y}\right)^k\left(4x^3y^3 + 8x^3y^4 + 19x^4y^4\right)\right]_{(1,1)}$$
$$= \left[{D_x}^k\left(4\times3^k\ x^3y^3 + 8\times4^k\ x^3y^4 + 19\times4^k\ x^4y^4\right)\right]_{(1,1)}$$
$$= \left[4\times3^{2k}\ x^3y^3 + 8\times4^k\times3^k\ x^3y^4 + 19\times4^{2k}\ x^4y^4\right]_{(1,1)}$$
$$= 4\times3^{2k} + 8\times4^k\times3^k\ + 19\times4^{2k}$$
$$(7)\quad {}_{\beta}RR_k(\mathcal{A}) = \left(\left({S_x}^k\ {S_y}^k\right)(RM(\mathcal{A};a,\ b))\right)_{(1,1)}$$
$$= \left[{S_x}^k\left(\tfrac{4}{3^k}x^3y^3 + \tfrac{8}{4^k}x^3y^4 + \tfrac{19}{4^k}x^4y^4\right)\right]_{(1,1)}$$
$$= \left[\tfrac{4}{3^{2k}}x^3y^3 + \tfrac{8}{12^k}x^3y^4 + \tfrac{19}{4^{2k}}x^4y^4\right]_{(1,1)} = \tfrac{4}{3^{2k}} + \tfrac{8}{12^k} + \tfrac{19}{4^{2k}}$$
$$(8)\quad {}_{\beta}SDD(\mathcal{A}) = \left[\left(D_xS_y + D_yS_x\right)RM(\mathcal{A};a,\ b)\right]_{(1,1)}$$
$$= \left[D_x\left(\tfrac{4}{3}x^3y^3 + \tfrac{8}{4}x^3y^4 + \tfrac{19}{4}x^4y^4\right) + D_y\left(\tfrac{4}{3}x^3y^3 + \tfrac{8}{3}x^3y^4 + \tfrac{19}{4}x^4y^4\right)\right]_{(1,1)}$$
$$= \left[4x^3y^3 + 6x^3y^4 + 19x^4y^4 + 4x^3y^3 + 8x^3y^4 + 19x^4y^4\right]_{(1,1)}$$
$$= \left[8x^3y^3 + 14x^3y^4 + 38x^4y^4\right]_{(1,1)} = 60.$$
$$(9)\quad {}_{\beta}H(\mathcal{A}) = \left[(2S_xJ)(RM(\mathcal{A};a,\ b))\right]_{x=1} = \left[2S_x\left(4x^6 + 8x^7 + 19x^8\right)\right]_{x=1}$$
$$= \left[2\left(\tfrac{4}{6}x^6 + \tfrac{8}{7}x^7 + \tfrac{19}{8}x^8\right)\right]_{x=1} = 8.36904.$$

$$(10)\quad {}_{\beta}I(\mathcal{A}) = \left[\left(S_x J D_x D_y\right) RM(\mathcal{A}; a, b)\right]_{x=1} = \left[(S_x J D_x)(4x^3y^3 + 8x^3y^4 + 19x^4y^4)\right]_{x=1}$$
$$= \left[(S_x J)\left(36x^3y^3 + 96x^3y^4 + 304x^4y^4\right)\right]_{x=1} = \left[S_x\left(36x^6 + 96x^7 + 304x^8\right)\right]_{x=1}$$
$$= \left[\tfrac{36}{6}x^6 + \tfrac{96}{7}x^7 + \tfrac{304}{8}x^8\right]_{x=1} = 57.7142.$$
$$(11)\quad {}_{\beta}A(\mathcal{A}) = \left[\left(S_x{}^3 Q_{-2} J D_x{}^3 D_y{}^3\right) RM(\mathcal{A}; a, b)\right]_{x=1}$$
$$= \left[S_x{}^3 Q_{-2} J\left(4\times 3^6 x^3y^3 + 8\times 4^3\times 3^3\, x^3y^4 + 19\times 4^6 x^3y^4\right)\right]_{x=1}$$
$$= \left[S_x{}^3\left(x^{-2}\left(4\times 3^6 x^6 + 8\times 4^3\times 3^3\, x^7 + 19\times 4^6 x^8\right)\right)\right]_{x=1}$$
$$= \left[S_x{}^3\left(4\times 3^6 x^4 + 8\times 4^3\times 3^3\, x^5 + 19\times 4^6 x^6\right)\right]_{x=1}$$
$$= \left[\tfrac{4\times 3^6}{4\times 4\times 4}x^4 + \tfrac{8\times 12^3}{5\times 5\times 5}\, x^5 + \tfrac{19\times 4^6}{6\times 6\times 6}x^6\right]_{x=1} = 516.4508.$$

□

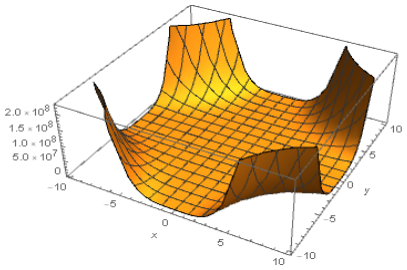

Figure 4.(a) Plot of Resolving Polynomial of Arbidol.

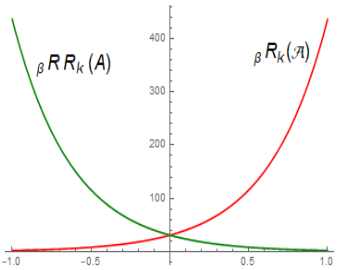

Figure 4.(b) ${}_{\beta}R_k(\mathcal{A})$ and ${}_{\beta}RR_k(\mathcal{A})$ for $(-10 \le k \le 10)$.

5. Resolving polynomial and topological indices of Thalidomide

Throughout this section, $\mathcal{T}$ denotes the molecular graph of Thalidomide. Let H_1 and H_2 be the subgraphs of $\mathcal{T}$ induced by the sets $\{a, a_1, a_2, \ldots, a_{10}\}$ and $\{b, b_1, b_2, \ldots, b_7\}$ respectively. Also, $T_1 = \{a, b, b_6, b_7\}$.

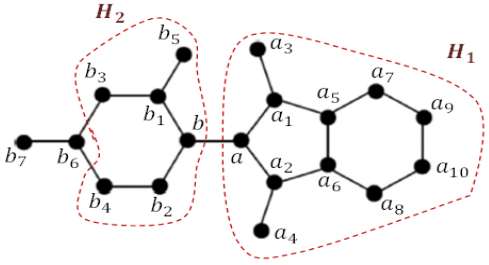

Figure 5 Molecular graph $\mathcal{T}$ of Thalidomide.

Lemma 5.1. *Let S be a metric basis of the molecular graph $\mathcal{T}$. Then $|S \cap V(H_i)| \ge 1$ for each $1 \le i \le 2$.*

Proof. We first see that for each $u, v \in S - V(H_i)$ (for some i), $d(u,x) = d(v,x)$ for some $x \in V(H_i)$. Hence, by Lemma 2.3, $S \cap V(H_i) \ne \emptyset$ (as $|V(H_i)| \ge 2$). This shows that $|S \cap V(H_i)| \ge 1$ for each $1 \le i \le 2$. □

Lemma 5.2. *Let $\mathcal{T}$ be the molecular graph of Thalidomide. Then $\beta(\mathcal{T}) = 2$.*

Proof. Let S be a metric basis of the graph $\mathcal{T}$. Then, by Lemma 5.1, $|S| \geq \sum_{i=1}^{2} |S \cap H_i| = 2$. Thus, $\beta(\mathcal{T}) = |S| \geq 2$. The reverse inequality follows by noting the distinct codes generated by the 2 -element set $\{a_1, b_1\}$ as in Figure 5. □

Theorem 5.3. *Let $\mathcal{T}$ be the molecular graph of Thalidomide and $\alpha \in V(\mathcal{T})$. Then $d_\beta(\alpha) = \beta$ if and only if $\alpha \in V(H_i) - T_1$ for some $1 \leq i \leq 2$.*

Proof. Let S be any resolving set containing a vertex α. If $\alpha \notin V(H_i)$, then clearly by the proof of Lemma 5.2, $|S| > 2$ and hence S is not a metric basis. Hence $\deg_\beta(\alpha) \neq \beta$. If $\alpha \in T_1$, then $\alpha \in H_i$ for some $1 \leq i \leq 2$. The vertices adjacent to α in H_i receive the same code with respect to S This implies that $|S| > 2$, and hence $d_\beta(\alpha) \neq \beta$. To prove the reverse inequality, define a set $S = \{\alpha_1, \beta_1\}$, for some $\alpha_1 \in \{a_i : 1 \leq i \leq 10\}$ and $\beta_1 \in \{b_1, b_2, b_3, b_4, b_5\}$. It is easy to observe that for each pair y, z of vertices in $V(\mathcal{T}) - \bigcup_{i=1}^{2} V(H_i)$ with $d(y, \alpha_1) = d(z, \alpha_1)$ either y is in the $z\beta_1$-path or z is in the $y\beta_1$-path (since $2 \leq deg(y), deg(z) \leq 3$) and hence β_1 will resolve such a pair. Any other pair of vertices y, z is resolved by the set $\{\beta_1\} \cup (V(H_i) \cap S)$.
Now for $\alpha \in V(H_i) - T_1$. Let $S_\alpha = S \cup \{\alpha\} - S \cap V(H_i)$ for $1 \leq i \leq 2$, Then, S_α is a metric basis containing α, hence $d_\beta(\alpha) = \beta$. □

Theorem 5.4. *For the molecular graph $\mathcal{T}$ of Thalidomide, resolving polynomial $RM(\mathcal{T}; x, y) = 7x^2y^2 + 7x^2y^3 + 7x^3y^3$ and hence*

(1) ${}_\beta M_1^*(\mathcal{T}) = 105$
(2) ${}_\beta M_2(\mathcal{T}) = 133$
(3) ${}_\beta mM_2(\mathcal{T}) = 3.69444$
(4) ${}_\beta ReM_2(\mathcal{T}) = 700$
(5) ${}_\beta F(\mathcal{T}) = 273$
(6) ${}_\beta R_k(\mathcal{T}) = 7 \times 2^{2k} + 7 \times 6^k + 7 \times 3^{2k}$
(7) ${}_\beta RR_k(\mathcal{T}) = \frac{7}{2^{2k}} + \frac{7}{6^k} + \frac{7}{3^{2k}}$
(8) ${}_\beta SDD(\mathcal{T}) = 43.16666$
(9) ${}_\beta H(\mathcal{T}) = 8.6333$
(10) ${}_\beta I(\mathcal{T}) = 25.9$
(11) ${}_\beta A(\mathcal{T}) = 191.7343$

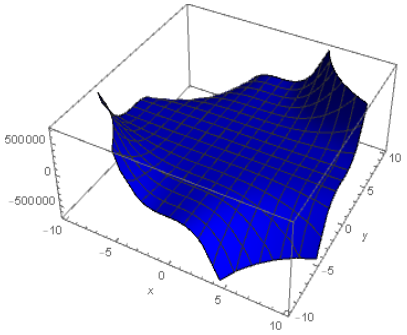

Figure 6.(a) Plot of Resolving Polynomial of Thalidomide.

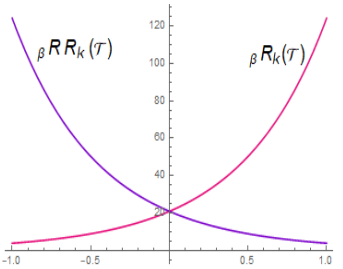

Figure 6.(b) ${}_\beta R_k(\mathcal{T})$ and ${}_\beta RR_k(\mathcal{T})$ for $(-10 \leq k \leq 10)$.

6. Resolving polynomial and topological indices of Ritonavir

Throughout this section, $\mathcal{R}t$ denotes the molecular graph of Ritonavir. Let H_1, H_2, H_3, H_4 and H_5 be the subgraphs of $\mathcal{R}t$, induced by the sets $\{a, a_1, a_2,$

$a_3, a_4, a_5\}$, $\{b, b_1, b_2, b_3, b_4, b_5\}$, $\{c, c_1, c_2\}$, $\{d, d_1, d_2, d_3, d_4, d_5\}$ and $\{e, e_1, e_2\}$ respectively. Also, $T_1 = \{a, a_5, b, b_5, c, d, e\}$.

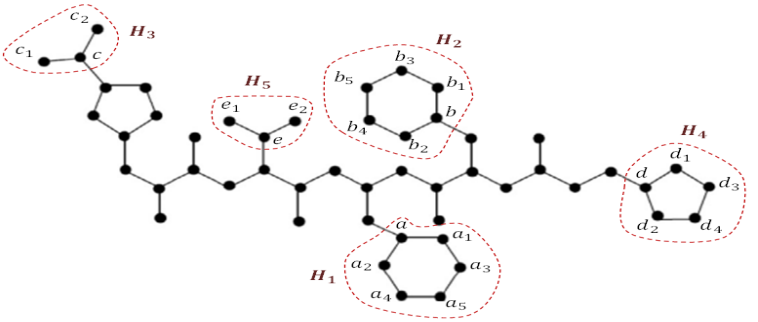

Figure 7. Molecular graph $\mathcal{R}t$ of Ritonavir.

Lemma 6.1. *Let S be a metric basis of the molecular graph $\mathcal{R}t$. Then $|S \cap V(H_i)| \geq 1$ for each $1 \leq i \leq 5$.*

Proof. We first see that for each $u, v \in S - V(H_i)$ (for some i), $d(u,x) = d(v,x)$ for some $x \in V(H_i)$. Hence, by Lemma 2.3, $S \cap V(H_i) \neq \emptyset$ (as $|V(H_i)| \geq 2$). This shows that $|S \cap V(H_i)| \geq 1$ for each $1 \leq i \leq 5$. □

Lemma 6.2. *Let $\mathcal{R}t$ be the molecular graph of Ritonavir. Then $\beta(\mathcal{R}t) = 5$.*

Proof. Let S be a metric basis of the graph $\mathcal{R}t$. Then, by Lemma 6.1, $|S| \geq \sum_{i=1}^{6} |S \cap H_i| = 5$. Thus, $\beta(\mathcal{R}t) = |S| \geq 5$. The reverse inequality follows by noting the distinct codes generated by the 3-element set $\{a_1, b_1, c_1\}$ as in Figure 7. □

Theorem 6.3. *Let $\mathcal{R}t$ be the molecular graph of Ritonavir and $\alpha \in V(\mathcal{R}t)$. Then $d_\beta(\alpha) = \beta$ if and only if $\alpha \in V(H_i) - T_1$ for some $1 \leq i \leq 5$.*

Proof. Let S be any resolving set containing a vertex α. If $\alpha \notin V(H_i)$, then clearly by the proof of Lemma 6.2, $|S| > 5$ and hence S is not a metric basis. Hence $\deg_\beta(\alpha) \neq \beta$. If $\alpha \in T_1$, then $\alpha \in H_i$ for some $1 \leq i \leq 5$. The vertices adjacent to α in H_i receive the same code with respect to S This implies that $|S| > 5$, and hence $d_\beta(\alpha) \neq \beta$. To prove the reverse inequality, define a set $S = \{\alpha_1, \beta_1, \gamma_1, \delta_1, \epsilon_1\}$, for some $\{\alpha_1\} \in \{a_1, a_2, a_3, a_4\}$, $\beta_1 \in \{b_1, b_2, b_3, b_4\}$, $\gamma_1 \in \{c_1, c_2\}$, $\delta_1 \in \{d_1, d_2, d_3, d_4\}$ and $\epsilon_1 \in \{e_1, e_2\}$. It is easy to observe that for each pair y, z of vertices in $V(\mathcal{L}) - \bigcup_{i=1}^{5} V(H_i)$ with $d(y, \alpha_1) = d(z, \alpha_1)$ either y is in the $z\delta_1$-path or z is in the $y\delta_1$-path (since $2 \leq deg(y), deg(z) \leq 3$) and hence δ_1 will resolve such a pair. Any other pair of vertices y, z is resolved by the set $\{\delta_1\} \cup (V(H_i) \cap S)$. Now for $\alpha \in V(H_i) - T_1$. Let $S_\alpha = S \cup \{\alpha\} - S \cap V(H_i)$ for $1 \leq i \leq 5$, Then, S_α is a metric basis containing α, hence $d_\beta(\alpha) = \beta$. □

Theorem 6.4. *For the molecular graph $\mathcal{R}t$, of Ritonavir, resolving polynomial $RM(\mathcal{R}t; x, y) = 7x^5y^5 + 14x^5y^6 + 32x^6y^6$ and hence*

(1) ${}_{\beta}M_1(\mathcal{R}t) = 608$
(2) ${}_{\beta}M_2(\mathcal{R}t) = 1747$
(3) ${}_{\beta}mM_2(\mathcal{R}t) = 1.63555$
(4) ${}_{\beta}ReM_2(\mathcal{R}t) = 20194$
(5) ${}_{\beta}F(\mathcal{R}t) = 3508$
(6) ${}_{\beta}R_k(\mathcal{R}t) = 7\times 5^{2k} + 14\times 30^{k} + 32\times 6^{2k}$
(7) ${}_{\beta}RR_k(\mathcal{R}t) = \frac{7}{5^{2k}} + \frac{14}{30^{k}} + \frac{32}{6^{2k}}$
(8) ${}_{\beta}SDD(\mathcal{R}t) = 106.46667$
(9) ${}_{\beta}H(\mathcal{R}t) = 9.27878$
(10) ${}_{\beta}I(\mathcal{R}t) = 151.6818$
(11) ${}_{\beta}A(\mathcal{R}t) = 2225.1333$

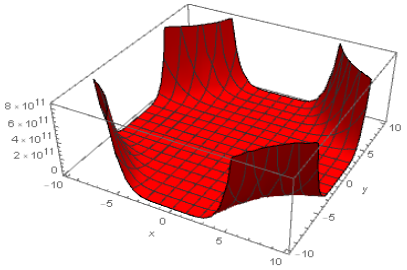

Figure 8.(a) Plot of Resolving Polynomial of Ritonavir.

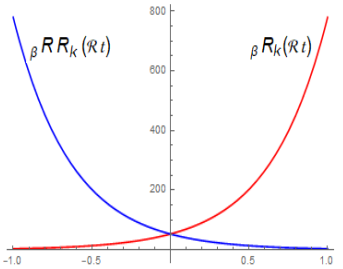

Figure 8.(b) ${}_{\beta}R_k(\mathcal{R}t)$ and ${}_{\beta}RR_k(\mathcal{R}t)$ for $(-10 \le k \le 10)$.

7. Resolving polynomial and topological indices of Remdesivir

Throughout this section, $\mathcal{R}m$ denotes the molecular graph of Remdesivir. Let H_1, H_2 and H_3 be the subgraphs of $\mathcal{R}m$ induced by the sets $\{a, a_1, a_2, a_3, a_4\}$, $\{b, b_1, b_2, b_3, b_4, b_5\}$ and $\{c, c_1, c_2, \ldots, c_9\}$ respectively. Also, $T_1 = \{a, b, b_5, c, c_1, c_2, c_3, c_4, c_6, c_9\}$

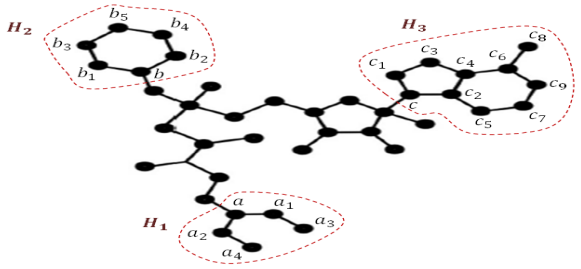

Figure 9 Molecular graph $\mathcal{R}m$ of Remdesivir.

Lemma 7.1. *Let S be a metric basis of the molecular graph $\mathcal{R}m$. Then $|S \cap V(H_i)| \ge 1$ for each $1 \le i \le 3$.*

Proof. We first see that for each $u, v \in S - V(H_i)$ (for some i), $d(u,x) = d(v,x)$ for some $x \in V(H_i)$. Hence, by Lemma 2.3, $S \cap V(H_i) \ne \emptyset$ (as $|V(H_i)| \ge 2$). This shows that $|S \cap V(H_i)| \ge 1$ for each $1 \le i \le 3$. □

Lemma 7.2. *Let $\mathcal{R}m$ be the molecular graph of Remdesivir. Then $\beta(\mathcal{R}m) = 3$.*

Proof. Let S be a metric basis of the graph $\mathcal{R}m$. Then, by Lemma 7.1, $|S| \ge \sum_{i=1}^{3} |S \cap H_i| = 3$. Thus, $\beta(\mathcal{R}m) = |S| \ge 3$. The reverse inequality follows by noting the distinct codes generated by the 3-element set $\{a_1, b_1, c_5\}$ as in Figure 9. □

Theorem 7.3. *Let $\mathcal{R}m$ be the molecular graph of Remdesivir and $\alpha \in V(\mathcal{R}m)$. Then $d_\beta(\alpha) = \beta$ if and only if $\alpha \in V(H_i) - T_1$ for some $1 \le i \le 3$.*

Proof. Let S be any resolving set containing a vertex α. If $\alpha \notin V(H_i)$, then clearly by the proof of Lemma 7.2, $|S| > 3$ and hence S is not a metric basis. Hence $\deg_\beta(\alpha) \neq \beta$. If $\alpha \in T_1$, then $\alpha \in H_i$ for some $1 \le i \le 3$. The vertices adjacent to α in H_i receive the same code with respect to S This implies that $|S| > 5$, and hence $d_\beta(\alpha) \neq \beta$. To prove the reverse inequality, define a set $S = \{\alpha_1, \beta_1, \gamma_1\}$, for some $\{\alpha_1\} \in \{a_1, a_2, a_3, a_4\}$, $\beta_1 \in \{b_1, b_2, b_3, b_4\}$ and $\gamma_1 \in \{c_5, c_7, c_8\}$, . It is easy to observe that for each pair y, z of vertices in $V(\mathcal{R}m) - \bigcup_{i=1}^{3} V(H_i)$ with $d(y, \beta_1) = d(z, \beta_1)$ either y is in the $z\alpha_1$-path or z is in the $y\alpha_1$-path (since $2 \le deg(y), deg(z) \le 4$) and hence α_1 will resolve such a pair. Any other pair of vertices y, z is resolved by the set $\{\alpha_1\} \cup (V(H_i) \cap S)$. Now for $\alpha \in V(H_i) - T_1$. Let $S_\alpha = S \cup \{\alpha\} - S \cap V(H_i)$ for $1 \le i \le 3$, Then, S_α is a metric basis containing α, hence $d_\beta(\alpha) = \beta$. □

Theorem 7.4. *For the molecular graph $\mathcal{R}m$ of Remdesivir, resolving polynomial $RM(\mathcal{R}t; x, y) = 5x^3y^3 + 9x^3y^4 + 30x^4y^4$ and hence*

(1) ${}_\beta M_1(\mathcal{R}m) = 333$
(2) ${}_\beta M_2(\mathcal{R}m) = 633$
(3) ${}_\beta mM_2(\mathcal{R}m) = 3.1806$
(4) ${}_\beta ReM_2(\mathcal{R}m) = 4866$
(5) ${}_\beta F(\mathcal{R}m) = 1275$
(6) ${}_\beta R_k(\mathcal{R}m) = 5 \times 3^{2k} + 9 \times 12^k + 30 \times 4^{2k}$
(7) ${}_\beta RR_k(\mathcal{R}m) = \frac{5}{3^{2k}} + \frac{9}{12^k} + \frac{30}{4^{2k}}$
(8) ${}_\beta SDD(\mathcal{R}m) = 88.75$
(9) ${}_\beta H(\mathcal{R}m) = 11.7381$
(10) ${}_\beta I(\mathcal{R}m) = 82.9286$
(11) ${}_\beta A(\mathcal{R}m) = 750.2580$

8. Resolving polynomial and topological indices of Chloroquine, Hydroxychloroquine and Theaflavin

Throughout this section, $\mathcal{C}$ denotes the molecular graph of Chloroquine.Let H_1 and H_2 be the subgraphs of $\mathcal{C}$, induced by the sets $\{a, a_1, a_2, a_3, a_4\}$ and $\{b, b_1, b_2, b_3, b_5\}$ respectively.Also, $T_1 = \{a, b, b_1, b_2, b_3, b_4, b_6, b_7, b_9, b_{10}\}$.

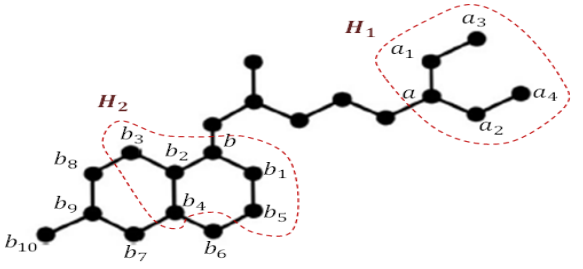

Figure 10 Molecular graph $\mathcal{C}$ of Chloroquine.

Lemma 8.1. *Let S be a metric basis of the molecular graph $\mathcal{C}$. Then $|S \cap V(H_i)| \ge 1$ for each $1 \le i \le 2$.*

Proof. We first see that for each $u, v \in S - V(H_i)$ (for some i), $d(u, x) = d(v, x)$ for some $x \in V(H_i)$. Hence, by Lemma 2.3, $S \cap V(H_i) \neq \emptyset$ (as $|V(H_i)| \ge 2$). This shows that $|S \cap V(H_i)| \ge 1$ for each $1 \le i \le 2$. □

Lemma 8.2. *Let $\mathcal{C}$ be the molecular graph of Chloroquine. Then $\beta(\mathcal{C}) = 3$.*

Proof. Let S be a metric basis of the graph $\mathcal{C}$. Then, by Lemma 7.1, $|S| \geq \sum_{i=1}^{2} |S \cap H_i| = 2$. Thus, $\beta(\mathcal{C}) = |S| \geq 2$. The reverse inequality follows by noting the distinct codes generated by the 3-element set $\{a_2, b_5\}$ as in Figure 11. □

Theorem 8.3. *Let $\mathcal{C}$ be the molecular graph of Chloroquine and $\alpha \in V(\mathcal{C})$. Then $d_\beta(\alpha) = \beta$ if and only if $\alpha \in V(H_i) - T_1$ for some $1 \leq i \leq 2$.*

The following Theorem is derived from Theorem 8.3 using the same proof technique as Theorems 3.4 and 4.4.

Theorem 8.4. *For the molecular graph $\mathcal{C}$ of Chloroquine, resolving polynomial $RM(\mathcal{C}; x, y) = 2x^2y^2 + 6x^2y^3 + 15x^3y^3$ and hence*

(1) ${}_\beta M_1(\mathcal{C}) = 128$
(2) ${}_\beta M_2(\mathcal{C}) = 179$
(3) ${}_\beta mM_2(\mathcal{C}) = 3.1667$
(4) ${}_\beta ReM_2(\mathcal{C}) = 1022$
(5) ${}_\beta F(\mathcal{C}) = 364$
(6) ${}_\beta R_k(\mathcal{C}) = 2 \times 2^{2k} + 6 \times 6^k + 15 \times 3^{2k}$
(7) ${}_\beta RR_k(\mathcal{C}) = \frac{2}{2^{2k}} + \frac{6}{6^k} + \frac{15}{3^{2k}}$
(8) ${}_\beta SDD(\mathcal{C}) = 47$
(9) ${}_\beta H(\mathcal{C}) = 8.4$
(10) ${}_\beta I(\mathcal{C}) = 31.7$
(11) ${}_\beta A(\mathcal{C}) = 234.8513$

Theorem 8.5. *Let $\mathcal{H}c$ be the molecular graph of hydroxychloroquine and $\alpha \in V(\mathcal{H}c)$. Then $d_\beta(\alpha) = \beta$ if and only if $\alpha \in V(H_i) - T_1$ for some $1 \leq i \leq 2$.*

Theorem 8.6. *For the molecular graph $\mathcal{H}c$ of hydroxychloroquine, resolving polynomial $RM(\mathcal{H}c; x, y) = R(\mathcal{H}c; x, y) = 3x^2y^2 + 6x^2y^3 + 15x^3y^3$ and hence*

(1) ${}_\beta M_1(\mathcal{H}c) = {}_\beta M_1(\mathcal{C}) + 4$
(2) ${}_\beta M_2(\mathcal{H}c) = {}_\beta M_2(\mathcal{C}) + 4$
(3) ${}_\beta mM_2(\mathcal{H}c) = {}_\beta mM_2(\mathcal{C}) + \frac{1}{4}$
(4) ${}_\beta ReM_2(\mathcal{H}c) = {}_\beta ReM_2(\mathcal{C}) + 16$
(5) ${}_\beta F(\mathcal{H}c) = {}_\beta F(\mathcal{C}) + 8$
(6) ${}_\beta R_k(\mathcal{H}c) = {}_\beta R_k(\mathcal{C}) + 2^{2k}$
(7) ${}_\beta RR_k(\mathcal{H}c) = {}_\beta RR_k(\mathcal{C}) + \frac{1}{2^{2k}}$
(8) ${}_\beta SDD(\mathcal{H}c) = {}_\beta SDD(\mathcal{C}) + 2$
(9) ${}_\beta H(\mathcal{H}c) = {}_\beta H(\mathcal{C}) + \frac{1}{2}$
(10) ${}_\beta I(\mathcal{H}c) = {}_\beta I(\mathcal{C}) + 1$
(11) ${}_\beta A(\mathcal{H}c) = {}_\beta A(\mathcal{C}) + 8$

Theorem 8.7. *Let $\mathcal{T}f$ be the molecular graph of Theaflavin and $\alpha \in V(\mathcal{T}f)$. Then $d_\beta(\alpha) = \beta$ if and only if $\alpha \in V(H_i) - T_1$ for some $1 \leq i \leq 2$.*

Theorem 8.8. *For the molecular graph $\mathcal{T}f$ of Theaflavin, resolving polynomial $RM(\mathcal{T}f, ; x, y) = 2x^2y^3 + 44x^3y^3$ and hence*

(1) ${}_\beta M_1(\mathcal{T}f) = 274$
(2) ${}_\beta M_2(\mathcal{T}f) = 408$
(3) ${}_\beta mM_2(\mathcal{T}f) = 5.222$
(4) ${}_\beta ReM_2(\mathcal{T}f) = 2436$
(5) ${}_\beta F(\mathcal{T}f) = 818$
(6) ${}_\beta R_k(\mathcal{T}f) = 2 \times 6^k + 44 \times 3^{2k}$
(7) ${}_\beta RR_k(\mathcal{T}f) = \frac{2}{6^k} + \frac{44}{3^{2k}}$
(8) ${}_\beta SDD(\mathcal{T}f) = 92.3333$
(9) ${}_\beta H(\mathcal{T}f) = 10.4444$
(10) ${}_\beta I(\mathcal{T}f) = 68.4$
(11) ${}_\beta A(\mathcal{T}f) = 517.1875$

9. QSPR Analysis

The primary goal of this section is to determine the efficacy of the topological indices by establishing a quantitative structure–property/activity relationship (QSPR/QSAR) between some TIs and properties such as boiling point (BP), enthalpy of vaporization (E), flash point (FP), molar refraction (MR), polar surface area (PSA), polarizability (P), surface tension (T), and molar volume (MV) of chemical compounds. The chemical properties of eight compounds are shown in Table 2.

Table 2. Physicochemical Properties of Chemical Compounds used in COVID-19 drugs

Drugs	**BP**	**E**	**FP**	**MR**	**PSA**	**P**	**T**	**MV**
Lopinavir	924.2	140.8	512.7	179.2	120	71.0	49.5	540.5
Arbidol	591.8	91.5	311.7	121.9	80	48.3	45.3	347.3
Thalidomide	487.8	79.4	248.8	65.2	87	25.9	71.6	161
Ritonavir	947.0	144.4	526.6	198.9	202	78.9	53.7	581.7
Remdesivir	-	-	-	149.5	213	59.3	62.3	409
Chloroquine	460.6	72.1	232.3	97.4	28	38.6	44.0	287.9
Hydroxychloroquine	516.7	83.0	266.3	99.0	48	39.2	49.8	285.4
Theaflavin	1003.9	153.5	336.5	137.3	218	54.4	138.6	301.0

In Table 3, correlation between the resolving TIs and the chemical properties of compounds are given. It can be observed that, properties BP, E, MR, PSA and P are well correlated with ${}_{\beta}SDD$. FP is well correlated with all the given TIs except ${}_{\beta}mM_2$ and ${}_{\beta}H$ which are negatively correlated. T is not correlated with any of the TIs except ${}_{\beta}mM_2$. Estimation of the theoretical values of the properties of the compounds, with reference to ${}_{\beta}SDD$ are given in the Table 4 along with their practical values.

Table 3. Correlation of properties of chemical compounds with topological indices.

Indices	**BP**	**E**	**FP**	**MR**	**PSA**	**P**	**MV**
${}^{q}{}_{\beta}M_1$	0.7990	0.7905	0.9926	0.9438	0.5454	0.9439	0.9479
${}_{\beta}M_2$	0.7089	0.7006	0.9693	0.8741	0.3923	0.8740	0.9159
${}_{\beta}mM_2$	-0.1335	-0.1170	-0.6631	-0.5601	0.1215	-0.5602	-0.7413
${}_{\beta}ReM_2$	0.6609	0.6530	0.9419	0.8173	0.3032	0.8172	0.8752
${}_{\beta}F$	0.7081	0.6998	0.9691	0.8738	0.3917	0.8738	0.9159
${}_{\beta}SDD$	0.9714	0.9664	0.9174	0.9451	0.8433	0.9453	0.8403
${}_{\beta}H$	0.3420	0.3550	-0.1352	0.1295	0.7036	0.1303	-0.0380
${}_{\beta}I$	0.7998	0.7913	0.9926	0.9440	0.5460	0.9440	0.9478
${}_{\beta}A$	0.6991	0.6911	0.9596	0.8525	0.3630	0.8525	0.8977

TABLE 4. Comparison between practical and theoretical values of boiling point and enthalpy of chemical compounds with reference to ${}_{\beta}SDD$.

Drugs	**BP**			**E**		
	Practical	Theoretical	|O-T|	Practical	Theoretical	|O-T|
Lopinavir	924.2	942.3398	18.14	140.8	143.7318	2.93
Arbidol	591.8	610.1404	18.34	91.5	95.54539	4.05
Thalidomide	487.8	464.3514	23.45	79.4	74.3983	5
Ritonavir	947	1012.574	65.57	144.4	153.9195	9.52
Chloroquine	460.6	497.5513	36.95	72.1	79.21404	7.11
Hydroxychloroquine	516.7	514.8727	1.83	83.0	81.72655	1.27
Theaflavin	1003.9	890.1695	113.73	153.5	136.1644	17.34

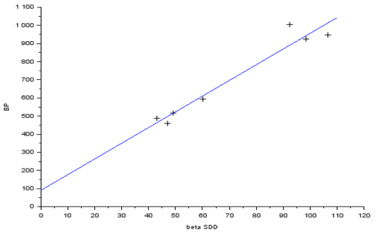

Figure 11. Correlation of BP with ${}_{\beta}SDD$.

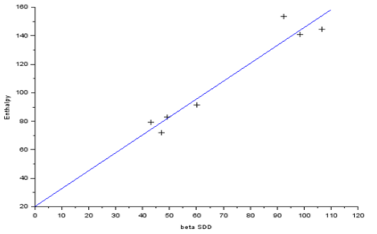

Figure 12. Correlation of Enthalpy(E) with ${}_{\beta}SDD$.

TABLE 5. Comparison between practical(O) and theoretical(T) values of MR and FP of chemical compounds with reference to ${}_{\beta}SDD$ and ${}_{\beta}M_1$ respectively.

Drugs	**MR**			**FP**		
	O	T	|O-T|	O	T	|O-T|
Lopinavir	179.2	172.0377	7.16	512.7	531.0079	18.31
Arbidol	121.9	109.7066	12.19	311.7	309.6552	2.04
Thalidomide	65.2	82.35199	17.15	248.8	242.5626	6.24
Ritonavir	198.9	185.216	13.68	526.6	508.2915	18.31
Remdesivir	149.5	156.426	6.93	-	-	-
Chloroquine	97.4	88.58135	8.82	232.3	254.7132	22.41
Hydroxychloroquine	99.0	91.83139	7.17	266.3	256.8263	9.47
Theaflavin	137.3	162.2489	24.95	336.5	331.8433	4.66

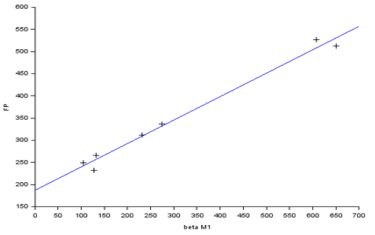

Figure 13. Correlation of FP with ${}_{\beta}M_1$.

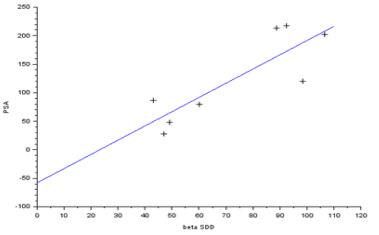

Figure 14. Correlation of PSA with ${}_{\beta}SDD$.

Conclusion

In this paper, eight chemical compounds used in the treatment of COVID-19 are studied, and eleven degree-based TI are calculated using a resolving polynomial. The correlation between these TIs and the physicochemical properties of Lopinavir, Arbidol, Thalidomide, Ritonavir, Chloroquine, Hydroxychloroquine, Theaflavin, and Remdesivir was then investigated. Our findings can aid in developing new drugs and vaccines for COVID-19 treatment because topological indices can predict several properties such as boiling point, entropy, acentric factor, and enthalpy.

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Department of Mathematics, Nitte Meenakshi Institute of Technology, Bengaluru, India
Email address: chandrakalasb14@gmail.com

Department of Mathematics, Dr. Ambedkar Institute of Technology, Bengaluru, Karnataka, India
Email address: dr_bsnrao@yahoo.co.in

Department of Mathematics, Nagarjuna College of Engineering and Technology, Bengaluru, India
Email address: gr.roshini@gmail.com

Department of Mathematics, Manipal Institute of Technology Bengaluru, Manipal Academy of Higher Education, Manipal, Karnataka, India
Email address: * poojary.prasanna@manipal.edu; poojaryprasanna34@gmail.com