

Retraction

Retracted: Topological Coindices and Quantitative Structure-Property Analysis of Antiviral Drugs Investigated in the Treatment of COVID-19

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This article has been retracted by Hindawi following an investigation undertaken by the publisher [1]. This investigation has uncovered evidence of one or more of the following indicators of systematic manipulation of the publication process:

- (1) Discrepancies in scope
- (2) Discrepancies in the description of the research reported
- (3) Discrepancies between the availability of data and the research described
- (4) Inappropriate citations
- (5) Incoherent, meaningless and/or irrelevant content included in the article
- (6) Manipulated or compromised peer review

The presence of these indicators undermines our confidence in the integrity of the article's content and we cannot, therefore, vouch for its reliability. Please note that this notice is intended solely to alert readers that the content of this article is unreliable. We have not investigated whether authors were aware of or involved in the systematic manipulation of the publication process.

Wiley and Hindawi regrets that the usual quality checks did not identify these issues before publication and have since put additional measures in place to safeguard research integrity.

We wish to credit our own Research Integrity and Research Publishing teams and anonymous and named external researchers and research integrity experts for contributing to this investigation.

The corresponding author, as the representative of all authors, has been given the opportunity to register their agreement or disagreement to this retraction. We have kept a record of any response received.

References

- [1] S. A. K. Kirmani, P. Ali, and J. Ahmad, "Topological Coindices and Quantitative Structure-Property Analysis of Antiviral Drugs Investigated in the Treatment of COVID-19," *Journal of Chemistry*, vol. 2022, Article ID 3036655, 15 pages, 2022.

Research Article

Topological Coindices and Quantitative Structure-Property Analysis of Antiviral Drugs Investigated in the Treatment of COVID-19

Syed Ajaz K. Kirmani ¹, Parvez Ali ², and Jawed Ahmad ³

¹Department of Electrical Engineering, College of Engineering, Qassim University, Unaizah, Saudi Arabia

²Department of Mechanical Engineering, College of Engineering, Qassim University, Unaizah, Saudi Arabia

³Department of Agricultural Engineering, Mai-Nefhi College of Engineering and Technology, Asmara, Eritrea

Correspondence should be addressed to Jawed Ahmad; jawed77asmarauni@gmail.com

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SARS-CoV-2 is a new strain of coronavirus family that has never been previously detected in humans. This has grown into a huge public health issue that has affected people all around the world. Presently, there is no specific antiviral treatment for COVID-19. To tackle the outbreak, a number of drugs are being explored or have been utilized based on past experience. A molecular descriptor (or topological index) is a numerical value that describes a compound's molecular structure and has been successfully employed in many QSPR/QSAR investigations to represent several physicochemical attributes. In order to determine topological characteristics of graphs, coindices (topological) take nonadjacent pair of vertices into account. In this study, we introduced CoM-polynomial and numerous degree-based topological coindices for several antiviral medicines such as lopinavir, ritonavir, remdesivir, hydroxychloroquine, chloroquine, theaflavin, thalidomide, and arbidol which were studied using the CoM-polynomial approach. In the QSPR model, the linear regression approach is used to analyze the relationships between physicochemical properties and topological coindices. The findings show that the topological coindices under investigation have a substantial relationship with the physicochemical properties of possible antiviral medicines in question. As a result, topological coindices may be effective tools for studying antiviral drugs in the future for QSPR analyses.

1. Introduction

COVID-19 is a disease caused by severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2), which is a positive single-stranded RNA virus containing proteins that belong to the beta-coronavirus family. Beta-coronavirus can change its tissue tropism, host selection, and toxicity dramatically [1–3]. Some of the symptoms observed in patients who have been infected with SARS-CoV-2 include fever, cough, sore throat, rhinorrhea, severe pneumonia, bilateral lung opacities, and septic shock [4].

COVID-19 is still untreatable with effective antiviral treatments despite the availability of several vaccinations to lower its severity. However, in order to combat the outbreak, many drugs are being evaluated or employed on prior

studies. Lopinavir, ritonavir, chloroquine, hydroxychloroquine, azithromycin, remdesivir, arbidol, favipiravir, theaflavin, thalidomide, ribavirin, and others are among the medications used to combat the pandemic [5]. However, there is no consensus on their efficacy in treating COVID-19 infection. Many investigations are being conducted on these medications and their derivatives in order to employ them in the treatment of COVID-19 disease and to develop novel COVID-19 disease drugs [6–10].

The process of drug discovery is multifaceted, costly, and time-consuming, and the use of computer-based approaches for design, synthesis, and biological screening of compounds provides an alternative to the old hit-or-miss strategy [11, 12]. Particularly, quantitative structure-property and activity relationship (QSPR/QSAR) modeling links a

molecule's physicochemical properties to its molecular structure.

A descriptor provides numerical value to illustrate a compound's molecular structure and molecular features. Although there are many other types of descriptors, topological descriptors, also known as topological indices, are frequently used in development of new drugs as they are data-rich, rapid to calculate, and have strong inclination towards prediction. The topological index, a graph invariant, is a numerical descriptor that encodes the topology of molecules represented as molecular graph [13, 14].

Chemical compounds can be converted into molecular graphs by turning them into graphs with atoms as vertices and bonds as edges. In a molecular graph, $G = (V, E)$, $V(G)$, and $E(G)$ are vertex and edge set, while $|V(G)|$ and $|E(G)|$ represent the number of vertices and edges in G . A degree of vertex is defined as the number of vertices that are adjacent to $u \in V(G)$ and is denoted by $d(u)$. The simple graph with the same vertex set $V(G)$ is called complement of a graph G , denoted by \overline{G} , such that any two vertices $uv \in E(\overline{G})$ if and only if $uv \notin E(G)$ [15].

Wiener was the first to apply topological indexes in QSPR, demonstrating that his index, dubbed the Wiener index after him, was closely aligned with alkane boiling points [16]. The Wiener index has been used to describe a range of chemical and physical properties of molecules, as well as to associate a molecule's structure with its biological activity [17]. Since 1947, there have been hundreds of topological indexes constructed nonetheless, in chemical and mathematical literature, the Wiener index, Randic index, Zagreb indices, and its variant, are the most extensively utilized [16, 18–28]. Symmetric division index (SDD), inverse sum index, F-index, harmonic index, augmented Zagreb index, and redefined versions of Zagreb indices are among the indices regularly encountered in the literature [23, 29–34].

A majority of degree-based topological indices take adjacent vertex pairs into consideration. However, over time, researchers have begun to incorporate nonadjacent pairing of vertices into consideration when computing some topological features of graphs, resulting in degree-based topological indices known as coindices.

To enhance our ability to quantify the contributions of nonadjacent vertices to various aspects of molecules, Doslic [35] formalized the first and second Zagreb coindices of graph G as follows:

$$\begin{aligned}\overline{M}_1(G) &= \sum_{uv \notin E(G)} (d(u) + d(v)), \\ \overline{M}_2(G) &= \sum_{uv \notin E(G)} d(u)d(v).\end{aligned}\quad (1)$$

It is worth noting that Zagreb coindices of G are not the same as Zagreb indices of \overline{G} . The degrees are with respect to G , whereas the defining sums are over $E(\overline{G})$.

Xu et al. [36] defined the multiplicative versions of Zagreb coindices described as follows:

$$\prod_1(G) = \prod_{uv \notin E(G)} (d(u) + d(v)), \quad \prod_2(G) = \prod_{uv \notin E(G)} d(u)d(v).\quad (2)$$

De et al. [37] demonstrated that the logarithm of the octanol-water partition coefficient ($\log(P)$) and the associated F -coindex values of octane isomers have a strong relationship ($r = 0.96$), leading to the introducing the F -coindex (\overline{F}) of G as follows:

$$\overline{F}(G) = \sum_{uv \notin E(G)} (d^2(u) + d^2(v)).\quad (3)$$

Recently Berhe et al. [38] computed various coindices of $C_4C_8(S)$ nanotubes, nanotorus and graphene sheets. For more literature on the topological coindices, readers might refer to [39–44].

Other degree-based topological coindices mentioned in this article can be defined in the same way as their classical degree counterparts:

$$\text{Second modified Zagreb coindex: } m\overline{M}_2(G) = \sum_{uv \notin E(G)} 1/(d(u)d(v))$$

$$\text{Redefined third Zagreb coindex: } \overline{ReZG}_3(G) = \sum_{uv \notin E(G)} d(u)d(v)(d(u) + d(v))$$

$$\text{Randić coindex: } \overline{R}_k(G) = \sum_{uv \notin E(G)} (d(u)d(v))^k$$

$$\text{Inverse Randić coindex: } \overline{RR}_k(G) = \sum_{uv \notin E(G)} 1/(d(u)d(v))^k$$

$$\text{Symmetric division coindex: } \overline{SDD}(G) = \sum_{uv \notin E(G)} (d^2(u) + d^2(v))/(d(u)d(v))$$

$$\text{Harmonic coindex: } \overline{H}(G) = \sum_{uv \notin E(G)} 2/(d(u) + d(v))$$

$$\text{Inverse sum indeg coindex: } \overline{I}(G) = \sum_{uv \notin E(G)} (d(u)d(v))/(d(u) + d(v))$$

$$\text{Augmented Zagreb coindex: } \overline{A}(G) = \sum_{uv \notin E(G)} \{(d(u)d(v))/(d(u) + d(v) - 2)\}^3$$

In the literature, many distance-based graph polynomials have been proposed to accelerate the computation of certain graph indices [45–48]. Similarly, Deutsch and Klavzar [49] proposed the M -polynomial, a degree-based polynomial, which can be used to construct a number of indices. Because of its broad adaptability, it has been utilized in a number of articles to obtain topological indices [50–57]. Mondal et al. [58] recently examined four antiviral medicines for COVID-19 patients: remdesivir, chloroquine, hydroxychloroquine, and theaflavin. Kirmani et al. [59] studied eight antiviral drugs including lopinavir, ritonavir, arbidol, and thalidomide via M -polynomial and NM -polynomials and performed QSPR and QSAR to predict the strength of these topological indices. For recent topological results and QSPR/QSAR on drugs being used in COVID-19 treatment, refer [60–63]. Very recently, Yang et al. [64] consider nonadjacent vertices of molecular graph of COVID-19 drugs to investigate various topological coindices such as F -coindex, first Zagreb coindex, first multiplicative Zagreb coindex, second Zagreb coindex, and second multiplicative Zagreb coindex of hydroxyethyl starch

conjugated with hydroxychloroquine used for COVID-19 treatment.

As the M-polynomial takes into account the contributions of pairs of adjacent vertices, a polynomial that takes into account nonadjacent pairs of vertices is required which plays parallel role “to what M-polynomial does” to compute various types of graph coindices. This encourages us to cultivate polynomials based on nonadjacent pairs of vertices of chemical compounds. Therefore, in this article, we continue our investigation of antiviral drugs used in COVID-19 patients and define a CoM-polynomial by considering equivalent contributions from pairs of nonadjacent vertices, which capture and quantify a potential influence of distant pairs of vertices on the molecule’s attributes. The true strength of the CoM-polynomial is its comprehensiveness, which includes useful information on degree-based graph invariants. Many degree-based topological coindices that link chemical features of the material under research are produced in closed forms by the CoM-polynomial using elementary calculus.

Some physicochemical features of the drugs are used to test the predictive strength of these coindices. Using the linear regression models, we see that these coindices are found to have high correlation with the physicochemical properties except for polar surface area and surface tension. Additionally, Figure 1 shows the surface representation of CoM-polynomials for these drugs that shows different behaviors by varying the parameters x and y . Figure 2 depicts the chemical structure of these chemical compounds.

2. Preliminaries

Let us use the following notation for the rest of paper

$$\begin{aligned} n_i &= |V_i| \text{ for } V_i = \{v \in V(G) | d(v) = i\} \\ m_{ij} &= |E_{ij}| \text{ for } E_{ij} = \{uv \in E(G) | d(u) = i \text{ and } d(v) = j\} \\ \bar{m}_{ij} &= |\bar{E}_{ij}| \text{ for } \bar{E}_{ij} = \{uv \in E(\bar{G}) | d(u) = i \text{ and } d(v) = j\} \end{aligned}$$

We extend the concept of M-polynomial for nonadjacent pair of vertices and define CoM-polynomial as follows:

$$\text{CoM}(G; x, y) = \bar{M}(G; x, y) = \sum_{i \leq j} \bar{m}_{ij}(G) x^i y^j, \quad (4)$$

where $\bar{m}_{ij}(G)$, $i, j \geq 1$, be the number of edges $uv \notin E(G)$ such that $\{d(u), d(v)\} = \{i, j\}$.

Various topological coindices derived from CoM-polynomial are listed in Table 1.

The following lemma is due to Berhe [38].

Lemma 1. For a connected graph G of order n , we have

$$\bar{m}_{ij} = |\bar{E}_{ij}| = \begin{cases} \frac{n_i(n_i - 1)}{2} - m_{ii} & \text{for } i = j \\ n_i n_j - m_{ij} & \text{for } i < j \end{cases}. \quad (5)$$

where n_i , m_{ij} , and \bar{m}_{ij} are defined above.

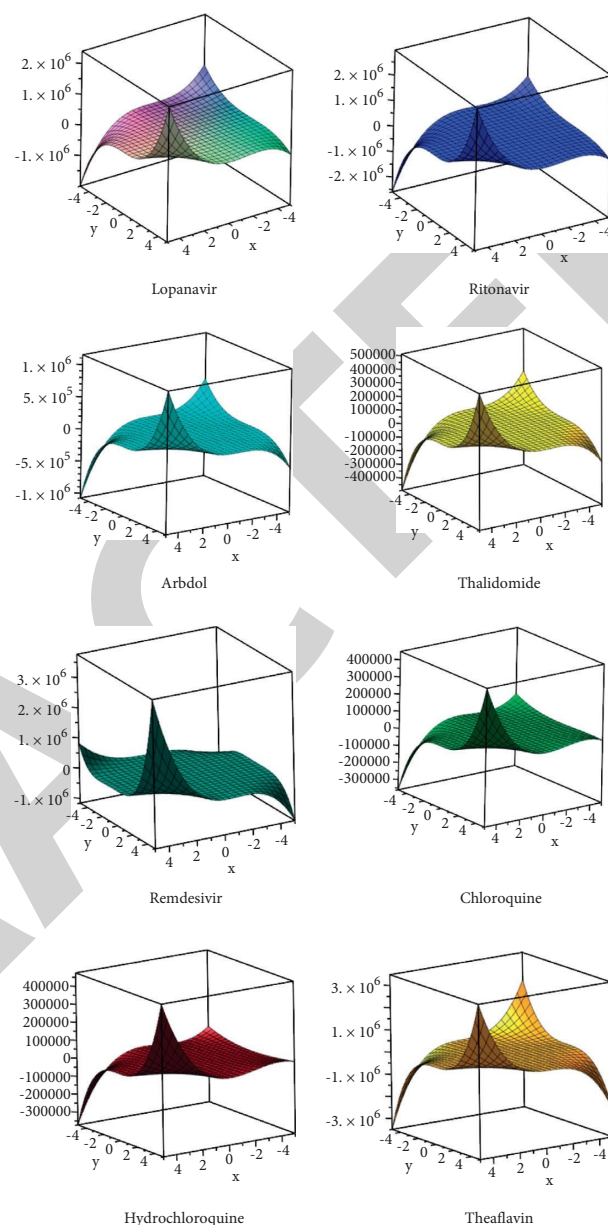


FIGURE 1: Plot of CoM-polynomials for various antiviral drugs.

3. Discussion and Main Results

This section uses combinatorial computation, edge partition technique, vertex partition technique, and nonedge counting method to obtain CoM-polynomials of molecular graphs of lopinavir (LOP), ritonavir (RIT), arbidol (ARD), thalidomide (THD), remdesivir (REM), Chloroquine (CLO), hydroxychloroquine (HYC), and theaflavin (THF). We also deduce many well-known topological coindices for the given molecular graphs.

The expression of the CoM-polynomial for lopinavir is established first.

Theorem 1. The CoM-polynomial for LOP is given by

$$\text{CoM}(\text{LOP}; x, y) = 104x^3 + 262x^2y^3 + 316x^2y^2 + 84x^3y^3. \quad (6)$$

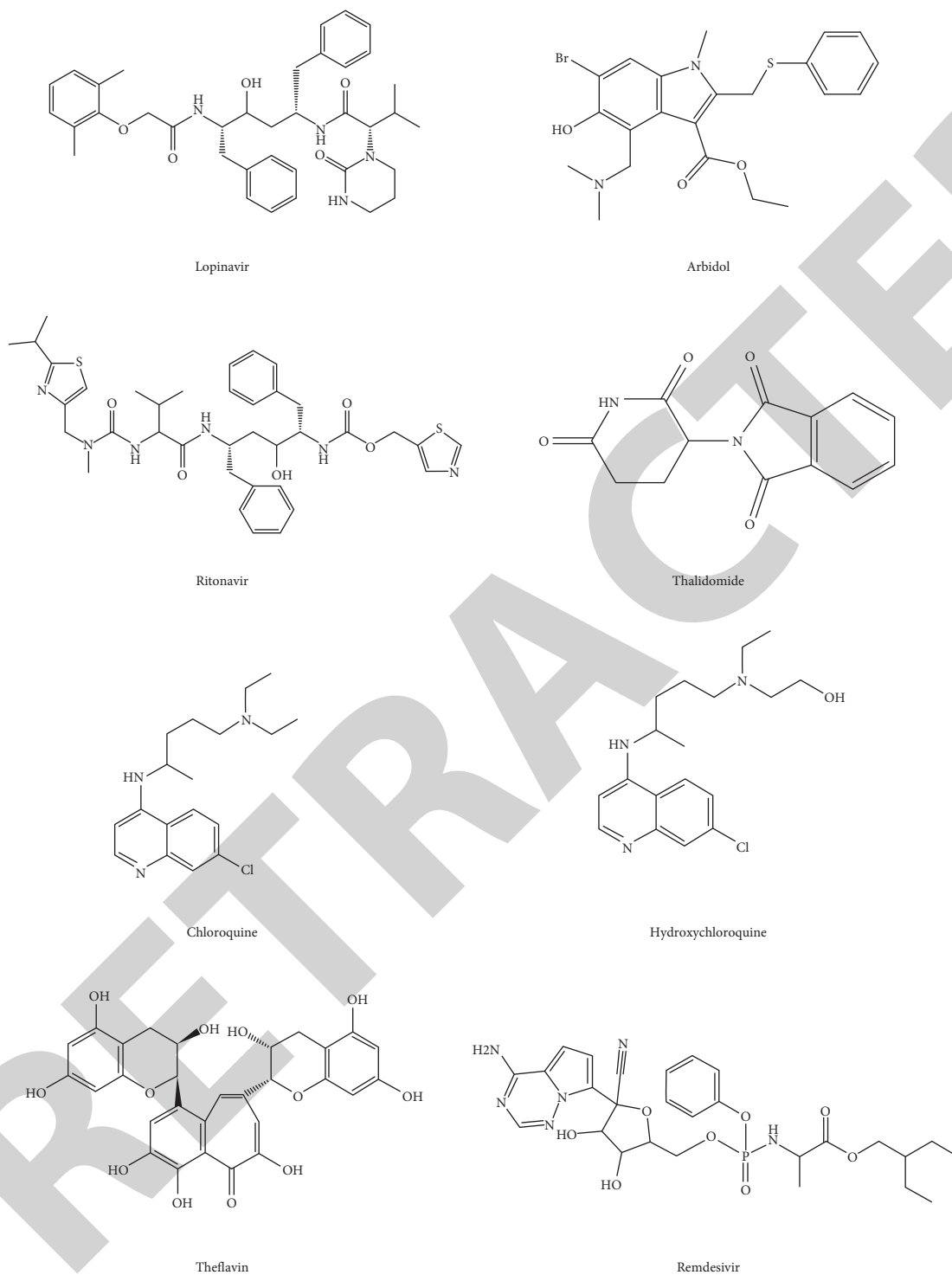


FIGURE 2: Antiviral drugs and their molecular structure.

TABLE 1: Topological coindices and its derivation from CoM-polynomial.

Topological coindex	Formula $\phi(d(u), d(v))$	Derivation from $f(x, y) = \text{CoM}(G, x, y)$
First Zagreb coindex: $\overline{M}_1(G)$	$\sum_{uv \notin E(G)} (d(u) + d(v))$	$(D_x + D_y)(f(x, y))_{x=y=1}$
Second Zagreb coindex: $\overline{M}_2(G)$	$\sum_{uv \notin E(G)} d(u)d(v)$	$(D_x D_y)(f(x, y))_{x=y=1}$
Second modified Zagreb coindex: $m\overline{M}_2(G)$	$\sum_{uv \notin E(G)} 1/(d(u)d(v))$	$(S_x S_y)(f(x, y))_{x=y=1}$
Redefined third Zagreb coindex: $\overline{\text{ReZG}}_3(G)$	$\sum_{uv \notin E(G)} d(u)d(v)(d(u) + d(v))$	$D_x D_y (D_x + D_y)(f(x, y))_{x=y=1}$
Forgotten topological coindex: $\overline{F}(G)$	$\sum_{uv \notin E(G)} (d^2(u) + d^2(v))$	$(D_x^2 + D_y^2)(f(x, y))_{x=y=1}$
Randić coindex: $\overline{R}_k(G)$	$\sum_{uv \notin E(G)} (d(u)d(v))^k$	$(D_x^k D_y^k)(f(x, y))_{x=y=1}$
Inverse Randić coindex: $\overline{RR}_k(G)$	$\sum_{uv \notin E(G)} 1/(d(u)d(v))^k$	$(S_x^k S_y^k)(f(x, y))_{x=y=1}$
Symmetric division coindex: $\overline{SDD}(G)$	$\sum_{uv \notin E(G)} (\chi^2(u) + \chi^2(v))/(d(u)d(v))$	$(D_x S_y + S_x D_y)(f(x, y))_{x=y=1}$
Harmonic coindex: $\overline{H}(G)$	$\sum_{uv \notin E(G)} 2/(d(u) + d(v))$	$(2S_x J)(f(x, y))_{x=1}$
Inverse sum indeg coindex: $\overline{I}(G)$	$\sum_{uv \notin E(G)} (d(u)d(v))/(d(u) + d(v))$	$(S_x J D_x D_y)(f(x, y))_{x=1}$
Augmented Zagreb coindex: $\overline{A}(G)$	$\sum_{uv \notin E(G)} \{(d(u)d(v))/(d(u) + d(v) - 2)\}^3$	$(S_x^3 Q_{-2} J D_x^3 D_y^3)(f(x, y))_{x=1}$

Where

$D_x = x(\partial(f(x, y))/\partial x)$, $D_y = y(\partial(f(x, y))/\partial y)$, $S_x = \int_0^x f(t, y)/tdt$, $S_y = \int_0^y f(x, t)/tdt$, $J(f(x, y)) = f(x, x)$, $Q_k(f(x, y)) = x^k f(x, y)$

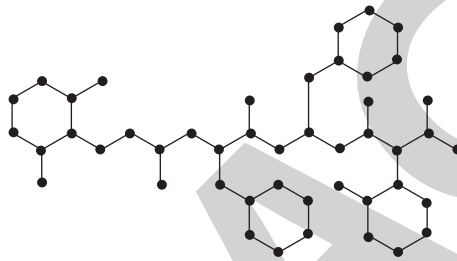


FIGURE 3: Molecular graph of lopinavir.

Proof. From the Figure 3, it is easy to conclude that $|V(\text{LOP})| = 46$ and $|E(\text{LOP})| = 49$. Also, the edge set of LOP may be categorized into five categories based on the degree of vertices:

$$\begin{aligned}
 E_{13} &= \{uv \in E(\text{LOP}) | d(u) = 1, d(v) = 3\}, \\
 E_{23} &= \{uv \in E(\text{LOP}) | d(u) = 2, d(v) = 3\}, \\
 E_{22} &= \{uv \in E(\text{LOP}) | d(u) = 2, d(v) = 2\}, \\
 E_{33} &= \{uv \in E(\text{LOP}) | d(u) = 3, d(v) = 3\},
 \end{aligned} \tag{7}$$

such that $m_{13} = |E_{13}| = 8$, $|E_{22}| = 14$, $|E_{23}| = 20$, and $|E_{33}| = 7$.

Similarly, $V(\text{LOP})$ can also be split into three classes based on the degree they have.

$$\begin{aligned}
 n_1 &= |V_1| = 8, \\
 n_2 &= |V_2| = 24, \\
 n_3 &= |V_3| = 14.
 \end{aligned} \tag{8}$$

Using Lemma 1, we have

$$\begin{aligned}
 \overline{m}_{13} &= n_1 n_3 - m_{13} = 8 * 14 - 8 = 104, \\
 \overline{m}_{22} &= \frac{n_2(n_2 - 1)}{2} - m_{22} = \frac{24 * 23}{2} - 14 = 262.
 \end{aligned} \tag{9}$$

Similarly, $\overline{m}_{23} = |\overline{E}_{23}| = 316$ and $\overline{m}_{33} = |\overline{E}_{33}| = 84$
By definition of CoM-polynomial,

$$\text{CoM}(G; x, y) = \overline{M}(G; x, y) = \sum_{i \leq j} \overline{m}_{ij}(G) x^i y^j, \tag{10}$$

where $\overline{m}_{ij}(G)$, $i, j \geq 1$, be the number of edges $uv \notin E(G)$ such that $\{(d(u), d(v)) = \{i, j\}\}$.

$$\begin{aligned}
 \text{CoM}(\text{LOP}; x, y) &= \sum_{1 \leq 3} \overline{m}_{13} x y^3 + \sum_{2 \leq 2} \overline{m}_{22} x^2 y^2 + \sum_{2 \leq 3} \overline{m}_{23} x^2 y^3 + \sum_{3 \leq 3} \overline{m}_{33} x^3 y^3 \\
 &= 104 x y^3 + 262 x^2 y^2 + 316 x^2 y^3 + 84 x^3 y^3.
 \end{aligned} \tag{11}$$

Hence, the result.

Using Theorem 1 and Table 1, we recover some degree-based topological coindices (DBTCI) of the LOP in the following proposition. \square

Proposition 1. *The topological coindices for LOP are given by*

$$\begin{aligned}\overline{M}_1(LOP) &= 3548 \\ \overline{M}_2(LOP) &= 4012 \\ m\overline{M}_2(LOP) &= 162.1667 \\ \overline{ReZG}_3(LOP) &= 19456 \\ \overline{F}(LOP) &= 8756\end{aligned}$$

$$\begin{aligned}\overline{R}_k(LOP) &= 104.3^k + 262.2^{2k} + 316.2^k 3^k + 84.3^{2k} \\ \overline{RR}_k(LOP) &= (104/3^k) + (262/2^{2k}) + (316/2^k 3^k) + (84/3^{2k}) \\ \overline{SDD}(LOP) &= 1723.33 \\ \overline{H}(LOP) &= 337.4 \\ \overline{I}(LOP) &= 845.2 \\ \overline{A}(LOP) &= 5931.8125\end{aligned}$$

Proof. Let,

$$f(x, y) = \text{CoM}(LOP; x, y) = 104xy^3 + 262x^2y^3 + 316x^2y^2 + 84x^3y^3. \quad (12)$$

Then,

$$\begin{aligned}D_x f(x, y) &= 104xy^3 + 524x^2y^2 + 632x^2y^3 + 252x^3y^3, \\ D_y f(x, y) &= 312xy^3 + 524x^2y^2 + 948x^2y^3 + 252x^3y^3, \\ (D_x + D_y)(f(x, y)) &= 416xy^3 + 1048x^2y^2 + 1580x^2y^3 + 504x^3y^3, \\ D_y D_x(f(x, y)) &= 312xy^3 + 1048x^2y^2 + 1896x^2y^3 + 756x^3y^3, \\ (D_x^2 + D_y^2)(f(x, y)) &= 1040xy^3 + 2096x^2y^2 + 4108x^2y^3 + 1512x^3y^3, \\ D_x^k D_y^k(f(x, y)) &= (3^k)104xy^3 + (2^{2k})262x^2y^2 + (2^k 3^k)316x^2y^3 + (3^{2k})84x^3y^3, \\ D_x D_y(D_x + D_y)(f(x, y)) &= 1248xy^3 + 4192x^2y^2 + 9480x^2y^3 + 4536x^3y^3, \\ S_x S_y(f(x, y)) &= \frac{104xy^3}{3} + \frac{131x^2y^2}{2} + \frac{158x^2y^3}{3} + \frac{28x^3y^3}{3}, \\ S_x^k S_y^k(f(x, y)) &= \frac{104xy^3}{3^k} + \frac{262x^2y^2}{2^{2k}} + \frac{316x^2y^3}{2^k 3^k} + \frac{84x^3y^3}{3^{2k}}, \\ (S_y D_x + S_x D_y)(f(x, y)) &= \frac{1040}{3}xy^3 + 524x^2y^2 + \frac{2054}{3}x^2y^3 + 168x^3y^3, \\ S_x J(f(x, y)) &= \frac{366x^4}{4} + \frac{316x^5}{5} + \frac{84x^6}{6}, \\ S_x J D_y D_x(f(x, y)) &= 340x^4 + \frac{1896x^5}{5} + 126x^6, \\ S_x^3 Q_{-2} J D_x^3 D_y^3(f(x, y)) &= 2447x^2 + 2528x^3 + \frac{9^3 \cdot 21}{16}x^4.\end{aligned} \quad (15)$$

With the help of Table 1, we get the following:

$$\begin{aligned}\overline{M}_1(LOP) &= (D_x + D_y)f(x, y)|_{x=y=1} = 3548 \\ \overline{M}_2(LOP) &= D_x D_y f(x, y)|_{x=y=1} = 4012 \\ m\overline{M}_2(LOP) &= S_x S_y f(x, y)|_{x=y=1} = 162.1667\end{aligned}$$

$$\begin{aligned}\overline{ReZG}_3(LOP) &= D_x D_y (D_x + D_y)f(x, y)|_{x=y=1} = 19456 \\ \overline{F}(LOP) &= (D_x^2 + D_y^2)(f(x, y))|_{x=y=1} = 8756 \\ \overline{R}_k(LOP) &= D_x^k D_y^k f(x, y)|_{x=y=1} = 104.3^k + 262.2^{2k} + 316.2^k 3^k + 84.3^{2k}\end{aligned}$$

$$\begin{aligned}\overline{RR}_k(\text{LOP}) &= S_x^k S_y^k f(x, y)|_{x=y=1} = (104/3^k) + \\ & (262/2^{2k}) + (316/2^k 3^k) + (84/3^{2k}) \\ \overline{SDD}(\text{LOP}) &= (S_y D_x + S_x D_y) f(x, y)|_{x=y=1} = 1723.33 \\ \overline{H}(\text{LOP}) &= 2S_x J f(x, y)|_{x=y=1} = 337.4 \\ \overline{I}(\text{LOP}) &= S_x J D_x D_y f(x, y)|_{x=y=1} = 845.2 \\ \overline{A}(\text{LOP}) &= S_x^3 Q_{-2} J D_x^3 D_y^3 f(x, y)|_{x=y=1} = 5931.8125\end{aligned}$$

The CoM-polynomial for Ritonavir's molecular graph (RIT) is obtained in the following theorem. \square

Theorem 2. The CoM-polynomial for RIT is given by

$$\text{CoM}(\text{RIT}; x, y) = 126x^3y^3 + 312x^2y^2 + 364x^2y^3 + 100x^3y^3. \quad (16)$$

Proof. We have $|V(\text{RIT})| = 50$ and $|E(\text{RIT})| = 53$ from the graph shown in Figure 4.

Partition of the $E(\text{RIT})$ can be calculated based on the degree of vertices as follows:

$$\begin{aligned}E_{13} &= \{uv \in E(\text{RIT}) | d(u) = 1, d(v) = 3\}, \\ E_{23} &= \{uv \in E(\text{RIT}) | d(u) = 2, d(v) = 3\}, \\ E_{22} &= \{uv \in E(\text{RIT}) | d(u) = 2, d(v) = 2\}, \\ E_{33} &= \{uv \in E(\text{RIT}) | d(u) = 3, d(v) = 3\}.\end{aligned} \quad (17)$$

$$\begin{aligned}\text{CoM}(\text{RIT}; x, y) &= \sum_{1 \leq 3} \overline{m}_{13} x y^3 + \sum_{2 \leq 2} \overline{m}_{22} x^2 y^2 + \sum_{2 \leq 3} \overline{m}_{23} x^2 y^3 + \sum_{3 \leq 3} \overline{m}_{33} x^3 y^3 \\ &= 126x^3y^3 + 312x^2y^2 + 364x^2y^3 + 100x^3y^3.\end{aligned} \quad (20)$$

Hence, the theorem.

Now, using the same procedure as in Proposition 1, we may extract several topological coindices for RIT in the following proposition. \square

Proposition 2. The topological coindices for RIT are given by

$$\begin{aligned}\overline{M}_1(\text{RIT}) &= 4172 \\ \overline{M}_2(\text{RIT}) &= 4170 \\ m\overline{M}_2(\text{RIT}) &= 191,778 \\ \overline{\text{ReZG}}_3(\text{RIT}) &= 22824 \\ \overline{F}(\text{RIT}) &= 10288 \\ \overline{R}_k(\text{RIT}) &= 126 \cdot 3^k + 312 \cdot 2^{2k} + 364 \cdot 2^k 3^k + 100 \cdot 3^{2k}\end{aligned}$$

such that $m_{13} = |E_{13}| = 9, m_{22} = |E_{22}| = 13, m_{23} = |E_{23}| = 26, m_{33} = |E_{33}| = 5$.

Likewise, $V(\text{RIT})$ can be classified into three groups based on their degrees.

$$\begin{aligned}n_1 &= |V_1| = 9, \\ n_2 &= |V_2| = 26, \\ n_3 &= |V_3| = 15.\end{aligned} \quad (18)$$

Using Lemma 1, we have

$$\begin{aligned}\overline{m}_{13} &= n_1 n_3 - m_{13} = 9 * 15 - 9 = 126, \\ \overline{m}_{22} &= \frac{n_2(n_2 - 1)}{2} - m_{22} = \frac{26 * 25}{2} - 13 = 312.\end{aligned} \quad (19)$$

Similarly, $\overline{m}_{23} = |E_{23}| = 364$ and $\overline{m}_{33} = |E_{33}| = 100$. We have CoM-polynomial according to the definition:

$$\begin{aligned}\overline{RR}_k(\text{RIT}) &= (126/3^k) + (312/2^{2k}) + (364/2^k 3^k) + \\ & (100/3^{2k}) \\ \overline{SDD}(\text{RIT}) &= 2032.667 \\ \overline{H}(\text{RIT}) &= 397.933 \\ \overline{I}(\text{RIT}) &= 993.3 \\ \overline{A}(\text{RIT}) &= 6972.313\end{aligned}$$

In the following theorem, expression for CoM-polynomial of Arbidol (ARD) is derived.

Theorem 3. The CoM-polynomial for ARD is given by

$$\text{CoM}(\text{ARD}; x, y) = 76x^2y^2 + 71x^3y^3 + 49x^2y^2 + 112x^2y^3 + 46x^3y^3. \quad (21)$$

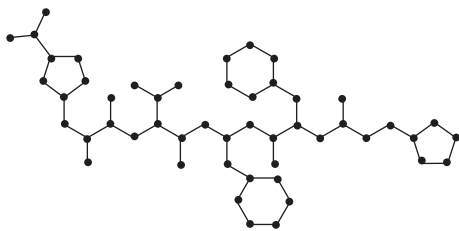


FIGURE 4: Molecular graph of Ritonavir.

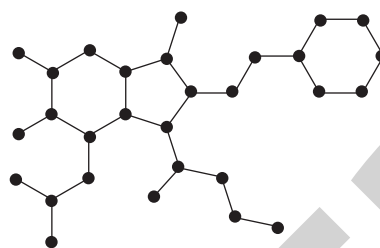


FIGURE 5: Molecular graph of arbidol.

Proof. We have $|V(\text{ARD})| = 29$ and $|E(\text{ARD})| = 31$ from Figure 5.

$E(\text{ARD})$ and $V(\text{ARD})$ can be grouped in following way:

$$\begin{aligned} m_{12} = |E_{12}| = 1, |m_{13} = E_{13}| = 6, m_{22} = |E_{22}| = 6, m_{23} = |E_{23}| = 9, \\ m_{33} = |E_{33}| = 9, n_1 = |V_1| = 7, n_2 = |V_2| = 11, n_3 = |V_3| = 11. \end{aligned} \quad (22)$$

From Lemma 1, we get

$$\bar{m}_{12} = |\bar{E}_{12}| = 76, \bar{m}_{13} = |\bar{E}_{13}| = 71, \bar{m}_{22} = |\bar{E}_{22}| = 49, \bar{m}_{23} = |\bar{E}_{23}| = 112, \bar{m}_{33} = |\bar{E}_{33}| = 46. \quad (23)$$

Now, $\text{CoM}(\text{ARD}; x, y)$ can easily be obtained:

$$\text{CoM}(\text{ARD}; x, y) = 76xy^2 + 71xy^3 + 49x^2y^2 + 112x^2y^3 + 46x^3y^3. \quad (24)$$

The following preposition may be computed instantaneously using the aforementioned theorem. \square

Proposition 3. The topological coindices for **ARD** are calculated as

$$\bar{M}_1(\text{ARD}) = 1544$$

$$\bar{M}_2(\text{ARD}) = 1647$$

$$m\bar{M}_2(\text{ARD}) = 97.694$$

$$\overline{\text{ReZG}}_3(\text{ARD}) = 7936$$

$$\bar{F}(\text{ARD}) = 3766$$

$$\bar{R}_k(\text{ARD}) = 76 \cdot 2^k + 71 \cdot 3^k + 49 \cdot 2^{2k} + 112 \cdot 2^k 3^k + 46 \cdot 3^{2k}$$

$$\overline{RR}_k(\text{ARD}) = (76/2^k) + (71/3^k) + (49/2^{2k}) + (112/2^k 3^k) + (46/3^{2k})$$

$$\overline{SDD}(\text{ARD}) = 859.33$$

$$\bar{H}(\text{ARD}) = 85.4$$

$$\bar{I}(\text{ARD}) = 356.317$$

$$\bar{A}(\text{ARD}) = 2659.594$$

The following theorem calculates the CoM-polynomial of the molecular graph (**THD**) of thalidomide.

Theorem 4. The CoM-polynomial for **THD** is given by

$$\text{CoM}(\text{THD}; x, y) = 28xy^3 + 17x^2y^2 + 50x^2y^3 + 21x^3y^3. \quad (25)$$

Proof. Figure 6 depicts shows the molecular graph (**THD**) of thalidomide

We have $|V(\text{THD})| = 19$, $|E(\text{THD})| = 21$ such that $|E_{13}| = 4$, $|E_{22}| = 4$, $|E_{23}| = 6$, $|E_{33}| = 7$ and

$$n_1 = |V_1| = 4, n_2 = |V_2| = 7, n_3 = |V_3| = 8. \quad (26)$$

Lemma 1 gives

$$\bar{m}_{13} = |\bar{E}_{13}| = 28, \bar{m}_{22} = |\bar{E}_{22}| = 17, \bar{m}_{23} = |\bar{E}_{23}| = 50, \bar{m}_{33} = |\bar{E}_{33}| = 21. \quad (27)$$

Thus, $\text{CoM}(\text{THD}; x, y)$ can be calculated as

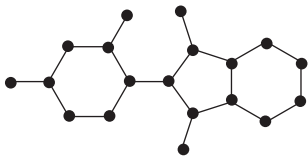


FIGURE 6: Molecular graph of thalidomide.

$$\text{CoM}(\text{THD}; x, y) = 28xy^3 + 17x^2y^2 + 50x^2y^3 + 21x^3y^3. \quad (28)$$

This completes the proof.

In the light of Theorem 4, the following results are yielded. \square

Proposition 4. *The topological coindices for THD are calculated as*

$$\overline{M}_1(\text{THD}) = 556$$

$$\overline{M}_2(\text{THD}) = 641$$

$$m\overline{M}_2(\text{THD}) = 24.25$$

$$\overline{\text{ReZG}}_3(\text{THD}) = 3242$$

$$\overline{F}(\text{THD}) = 1444$$

$$\overline{R}_k(\text{THD}) = 28.3^k + 17.2^{2k} + 50.2^k 3^k + 21.3^{2k}$$

$$\overline{\overline{R}}_k(\text{THD}) = (28/3^k) + (17/2^{2k}) + (50/2^k 3^k) + (21/3^{2k})$$

$$\begin{aligned} m_{12} = |E_{12}| = 2, m_{13} = |E_{13}| = 5, m_{14} = |E_{14}| = 2, m_{22} = |E_{22}| = 9, \\ m_{23} = |E_{23}| = 14, m_{24} = |E_{24}| = 4, m_{33} = |E_{33}| = 6, m_{34} = |E_{34}| = 2. \end{aligned} \quad (30)$$

Similarly for vertex set of REM

$$n_1 = |V_1| = 9, \quad n_2 = |V_2| = 20, \quad n_3 = |V_3| = 11, \quad \text{and} \\ n_4 = |V_4| = 2.$$

$$\begin{aligned} \overline{m}_{12} = |\overline{E}_{12}| = 177, \overline{m}_{13} = |\overline{E}_{13}| = 94, \overline{m}_{14} = |\overline{E}_{14}| = 17, \overline{m}_{22} = |\overline{E}_{22}| = 181, \\ \overline{m}_{23} = |\overline{E}_{23}| = 206, \overline{m}_{24} = |\overline{E}_{24}| = 35, \overline{m}_{33} = |\overline{E}_{33}| = 49, \overline{m}_{34} = |\overline{E}_{34}| = 20. \end{aligned} \quad (31)$$

Using above information, we can easily obtain

$$\begin{aligned} \text{CoM}(\text{REM}; x, y) = 177xy^2 + 94xy^3 + 17xy^4 + 181x^2y^2 \\ + 206x^2y^3 + 35x^2y^4 + 49x^3y^3 + 20x^3y^4. \end{aligned} \quad (32)$$

Now, using the aforementioned result, we get the Proposition 5. \square

Proposition 5. *The topological coindices for REM are given by*

$$\overline{M}_1(\text{REM}) = 3390$$

$$\overline{M}_2(\text{REM}) = 3625$$

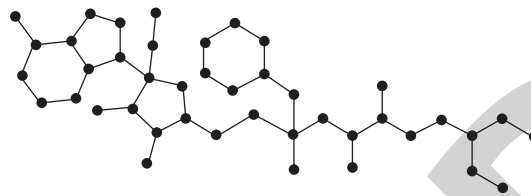


FIGURE 7: Molecular graph of remdesivir.

$$\overline{\overline{SDD}}(\text{THD}) = 277.667$$

$$\overline{H}(\text{THD}) = 49.5$$

$$\overline{I}(\text{THD}) = 129.5$$

$$\overline{A}(\text{THD}) = 782.203$$

Theorem 5. *The CoM-polynomial for REM is given by*

$$\begin{aligned} \text{CoM}(\text{REM}; x, y) = 177xy^2 + 94xy^3 + 17xy^4 + 181x^2y^2 \\ + 206x^2y^3 + 35x^2y^4 + 49x^3y^3 + 20x^3y^4. \end{aligned} \quad (29)$$

Proof. By analyzing the structure of the REM shown in Figure 7, we have

Also, Lemma 1 gives

$$m\overline{M}_2(\text{REM}) = 215.153$$

$$\overline{\text{ReZG}}_3(\text{REM}) = 17612$$

$$\overline{F}(\text{REM}) = 8322$$

$$\overline{R}_k(\text{REM}) = 177.2^k + 94.3^k + 17.4^k + 181.2^{2k} + 206.2^k 3^k + 35.2^{3k} + 49.3^{2k} + 20.3^k 4^k$$

$$\overline{\overline{R}}_k(\text{REM}) = (177/2^k) + (94/3^k) + (17/4^k) + (181/2^{2k}) + (206/2^k 3^k) + (35/2^{3k}) + (49/3^{2k}) + (20/3^k 4^k)$$

$$\overline{\overline{SDD}}(\text{REM}) = 1863.583$$

$$\overline{H}(\text{REM}) = 378.414$$

$$\overline{I}(\text{REM}) = 784.752$$

$$\overline{A}(\text{REM}) = 5984.167$$

Theorem 6. The CoM-polynomial for CLO is given by

$$\begin{aligned} \text{CoM}(\text{CLO}; x, y) = & 46xy^2 + 22xy^3 + 61x^2y^2 \\ & + 60x^2y^3 + 13x^3y^3. \end{aligned} \quad (33)$$

Proof. By means of structure analysis of molecular graph CLO depicted in Figure 8, we have $m_{12} = 2, m_{13} = 2, m_{22} = 5, m_{23} = 12,$ and $m_{33} = 2$ such that $|E(\text{CLO})| = 23$ and $n_1 = |V_1| = 4, n_2 = |V_2| = 12,$ and $n_3 = |V_3| = 6$ vertex set of CLO, i.e., $|V(\text{CLO})| = 22$.

Now, applying Lemma 1, we have

$$\bar{m}_{12} = 46, \bar{m}_{13} = 22, \bar{m}_{22} = 61, \bar{m}_{23} = 60, \bar{m}_{33} = 13. \quad (34)$$

With the help of above information and definition of CoM-polynomial, it is easy to deduce

$$\begin{aligned} \text{CoM}(\text{CLO}; x, y) = & 46xy^2 + 22xy^3 + 61x^2y^2 \\ & + 60x^2y^3 + 13x^3y^3. \end{aligned} \quad (35)$$

□

Proposition 6. The topological coindices for CLO are given by

$$\bar{M}_1(\text{CLO}) = 848$$

$$\bar{M}_2(\text{CLO}) = 879$$

$$m\bar{M}_2(\text{CLO}) = 57.028$$

$$\overline{\text{ReZG}}_3(\text{CLO}) = 4066$$

$$\bar{F}(\text{CLO}) = 1952$$

$$\bar{R}_k(\text{CLO}) = 46.2^k + 22.3^k + 61.2^{2k} + 60.2^k3^k + 13.3^{2k}$$

$$\overline{\text{RR}}_k(\text{CLO}) = (46/2^k) + (22/3^k) + (61/2^{2k}) + (60/2^k3^k) + (13/3^{2k})$$

$$\overline{\text{SDD}}(\text{CLO}) = 466.333$$

$$\bar{H}(\text{CLO}) = 100.5$$

$$\bar{I}(\text{CLO}) = 219.167$$

$$\bar{A}(\text{CLO}) = 1558.328$$

Theorem 7. The CoM-polynomial for HYC is given by

$$\begin{aligned} \text{CoM}(\text{HYC}; x, y) = & 50xy^2 + 22xy^3 + 72x^2y^2 \\ & + 66x^2y^3 + 13x^3y^3. \end{aligned} \quad (36)$$

Proof. By means of analyzing Figure 9, we have $m_{12} = 2, m_{13} = 2, m_{22} = 6, m_{23} = 12,$ and $m_{33} = 2$ such that $|E(\text{HYC})| = 24,$ and for the vertex set of HYC, i.e., $|V(\text{HYC})| = 23,$ we have following groups $n_1 = |V_1| = 4, n_2 = |V_2| = 13,$ and $n_3 = |V_3| = 6$.

Using above information Lemma 1 gives

$$\bar{m}_{12} = 50, \bar{m}_{13} = 22, \bar{m}_{22} = 72, \bar{m}_{23} = 66, \bar{m}_{33} = 13. \quad (37)$$

With the help of above information and definition of CoM-polynomial, it is easy to deduce

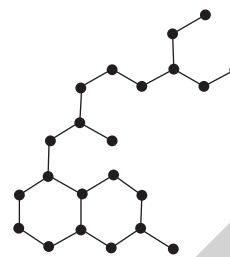


FIGURE 8: Molecular graph of chloroquine.

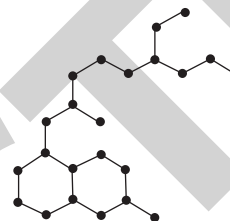


FIGURE 9: Molecular graph of hydroxychloroquine.

$$\begin{aligned} \text{CoM}(\text{HYC}; x, y) = & 50xy^2 + 22xy^3 + 72x^2y^2 \\ & + 66x^2y^3 + 13x^3y^3. \end{aligned} \quad (38)$$

□

Proposition 7. The topological coindices for HYC are given by

$$\bar{M}_1(\text{HYC}) = 634$$

$$\bar{M}_2(\text{HYC}) = 967$$

$$m\bar{M}_2(\text{HYC}) = 62.778$$

$$\overline{\text{ReZG}}_3(\text{HYC}) = 2598$$

$$\bar{F}(\text{HYC}) = 2138$$

$$\bar{R}_k(\text{HYC}) = 50.2^k + 22.3^k + 72.2^{2k} + 66.2^k3^k + 13.3^{2k}$$

$$\overline{\text{RR}}_k(\text{HYC}) = (50/2^k) + (22/3^k) + (72/2^{2k}) + (66/2^k3^k) + (13/3^{2k})$$

$$\overline{\text{SDD}}(\text{HYC}) = 511.333$$

$$\bar{H}(\text{HYC}) = 111.067$$

$$\bar{I}(\text{HYC}) = 220.533$$

$$\bar{A}(\text{HYC}) = 1726.328$$

Theorem 8. The CoM-polynomial for THF is given by

$$\text{CoM}(\text{THF}; x, y) = 190xy^3 + 198x^2y^3 + 176x^3y^3. \quad (39)$$

Proof. Let THF be the molecular graph of theaflavin (see Figure 10) having $|E(\text{THF})| = 46$ such that $m_{13} = 10, m_{23} = 22,$ and $m_{33} = 14$. Its vertex $|V(\text{THF})| = 41$ can be grouped into three classes on the basis of their degrees $n_1 = |V_1| = 10, n_2 = |V_2| = 11,$ and $n_3 = |V_3| = 20$.

Now, applying Lemma 1, we get

$$\bar{m}_{13} = 190, \bar{m}_{23} = 198, \bar{m}_{33} = 176. \quad (40)$$

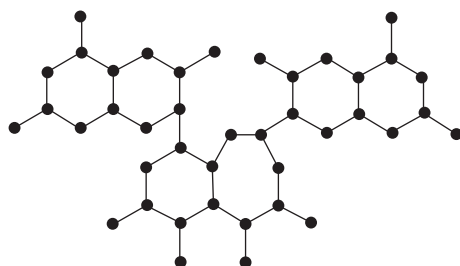


FIGURE 10: Molecular graph of theaflavin.

TABLE 2: COVID-19 drugs and their physicochemical properties.

Drugs	Boiling point (BP)	Enthalpy of vaporization: (E)	Flash point: (FP)	Molar refractivity (MR)	Polar surface area (PSA)	Polarizability (P)	Surface tension (T)	Molar volume (MV)
Lopinavir	924.2	140.8	512.7	179.2	120	71.0	49.5	540.5
Ritonavir	947.0	144.4	526.6	198.9	202	78.9	53.7	581.7
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
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
Remdesivir	—	—	—	149.5	213	59.3	62.3	409

Next, it is easy to plug these values in definition of CoM-polynomial to obtain

$$\text{CoM}(\text{THF}; x, y) = 190xy^3 + 198x^2y^3 + 176x^3y^3. \quad (41)$$

Proposition 8. The topological coindices for THF are given by

$$\overline{M}_1(\text{THF}) = 2806$$

$$\overline{M}_2(\text{THF}) = 3342$$

$$m\overline{M}_2(\text{THF}) = 115.889$$

$$\overline{\text{ReZG}}_3(\text{THF}) = 17724$$

$$\overline{F}(\text{THF}) = 7642$$

$$\overline{R}_k(\text{THF}) = 190 \cdot 3^k + 198 \cdot 2^k 3^k + 176 \cdot 3^{2k}$$

$$\overline{RR}_k(\text{THF}) = (190/3^k) + (198/2^k 3^k) + (176/3^{2k})$$

$$\overline{SDD}(\text{THF}) = 1414.333$$

$$\overline{H}(\text{THF}) = 232.867$$

$$\overline{I}(\text{THF}) = 644.1$$

$$\overline{A}(\text{THF}) = 4230$$

4. Quantitative Structure Analysis via Topological Coindices

The aim of this piece is to assess the efficiency of topological coindices and to develop a QSPR between the various topological coindices stated above and specific physicochemical aspects of the drugs being studied for COVID-19 treatment. For this, the benchmark set eight of physicochemical properties of these drugs are taken

from ChemSpider (<http://www.chemspider.com>) and presented in Table 2. However, some physicochemical properties like boiling point, enthalpy of vaporization, and flash point for remdesivir is not available in literature.

The values of the drugs' various topological coindices are reported in Table 3, while Table 4 contains the linear regression model's correlation coefficient (r) between coindices and properties of various COVID-19 drugs.

Table 4 demonstrates that \overline{I} has a strong positive association ($r=0.97$) with molar refractivity (MR) and polarizability (P), whereas \overline{A} has the significant correlation ($r=0.97$) with flash point (FP).

Among the linear regression models, the most suitable coindices for modeling the various for physicochemical properties are as follows:

- (1) The $\overline{\text{ReZG}}_3$ for BP, E , and PSA. However, $\overline{\text{ReZG}}_3$ does not predict PSA strongly.
- (2) The \overline{I} for MR and P.
- (3) The \overline{A} for FP and MV.

Among the linear regression models, there is no topological coindices that can predict surface tension (T) well. The best compatible fitting and predictive linear regression models for $\overline{\text{ReZG}}_3$ (Co- $\overline{\text{ReZG}}_3$), \overline{I} (Co- \overline{I}), and \overline{A} (Co- \overline{A}) with physicochemical attributes of the drugs are plotted in Figure 11.

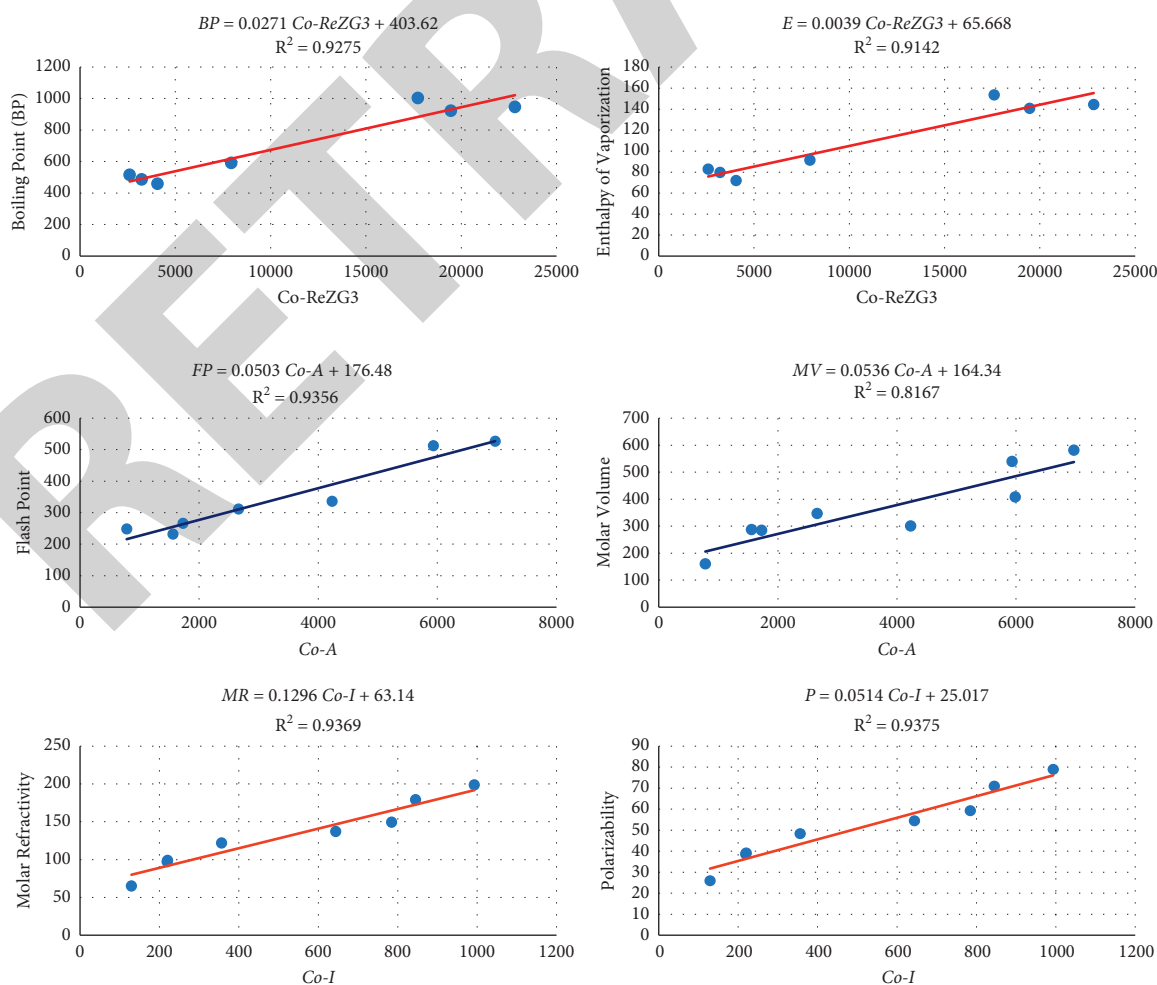
These findings suggest that topological coindices can predict the properties of the drugs in question. Therefore, topological coindices could be a useful tool for QSPR analysis in antiviral therapy.

TABLE 3: The values of topological coincides for molecular graph of COVID-19 Drugs.

Drugs	\overline{M}_1	\overline{M}_2	$m\overline{M}_2$	\overline{ReZG}_3	\overline{F}	\overline{SDD}	\overline{H}	\overline{I}	\overline{A}
Lopinavir	3548	4012	162.167	19456	8756	1723.333	337.4	845.2	5931.8123
Ritonavir	4172	4710	191.778	22824	10288	2032.667	397.933	993.3	6972.313
Arbidol	1544	1647	97.694	7936	3766	859.333	85.4	356.317	2659.594
Thalidomide	556	641	24.25	3242	1444	277.667	49.5	129.5	782.203
Chloroquine	848	879	57.028	4066	1952	466.333	100.5	219.167	1558.328
Hydroxychloroquine	634	967	62.778	2598	2138	511.333	111.067	220.533	1726.328
Theaflavin	2806	3342	115.889	17724	7642	1414.333	232.867	644.1	4230
Remdesivir	3390	3625	215.153	17612	8322	1863.583	378.414	784.752	5984.167

TABLE 4: The linear regression model's correlation coefficient (r) between topological coincides and physicochemical features of various medications for COVID-19 patients

Coindex	Boiling point (BP)	Enthalpy of vaporization (E)	Flash point: (FP)	Molar refractivity (MR)	Polar surface area (PSA)	Polarizability (P)	Surface tension (T)	Molar volume (MV)
\overline{M}_1	0.932	0.924	0.949	0.955	0.829	0.956	0.164	0.874
\overline{M}_2	0.948	0.942	0.943	0.958	0.834	0.958	0.204	0.869
$m\overline{M}_2$	0.861	0.849	0.954	0.895	0.775	0.896	-0.003	0.843
\overline{ReZG}_3	0.963	0.957	0.914	0.934	0.861	0.934	0.274	0.828
\overline{F}	0.957	0.951	0.933	0.949	0.852	0.949	0.228	0.853
\overline{SDD}	0.933	0.926	0.946	0.947	0.839	0.947	0.148	0.865
\overline{H}	0.881	0.876	0.950	0.912	0.790	0.912	0.074	0.855
\overline{I}	0.922	0.915	0.959	0.968	0.807	0.968	0.131	0.896
\overline{A}	0.900	0.892	0.967	0.964	0.794	0.965	0.072	0.904

FIGURE 11: Plot of the most compatible fitting and predictive linear regression models for the different coincides with physicochemical properties of the drugs ($r \geq 0.9$).

5. Conclusion

The structural features of chemical molecules are critical for the development of innovative products in pharmaceutical sciences, and they can be discovered using molecular descriptors known as topological indices and topological coindices.

The CoM-polynomial described in this article is capable of creating closed forms of a large number of degree-based topological coindices that correlate chemical properties of the substance under investigation. As a result, in this study, we examine a variety of prospective COVID-19 therapies and analyze their structure to determine the CoM-polynomial for these treatments. Then, these polynomials are also used to generate a number of degree-based topological coindices. Linear models are investigated using eight descriptors and eleven topological coindices in the QSPR study. The numerous topological coindices calculated have shown to have good prediction ability for the properties of these prospective COVID-19 therapies. In particular the best predictive topological coindices are as follows: \bar{I} showing strong positive correlation value with MR and P and \bar{A} which predicts FP strongly among all correlations. Because the quantitative structure-activity relationship model (QSAR) was not included in this study, it could be used in future studies for antiviral medications that treat COVID-19.

Data Availability

The data used to support the findings of this study are included within the article.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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