Proceedings of the Jangjeon Mathematical Society
26 (2023), No. 4, pp. 381 – 405
www.jangjeon.or.kr
http://dx.doi.org/10.17777/pjms2023.26.4.381

TOPOLOGICAL COINDICES OF PHYTOCHEMICALS EXAMINED FOR COVID-19 THERAPY

V. LOKESHA, A.S.MARAGADAM, SUVARNA, AND ISMAIL NACI CANGUL

Abstract. A molecular descriptor (or topological index) is a numerical value that is utilized in describing the molecular structure of a compound and has been widely used to study many physicochemical properties in several QSPR/QSAR studies. Researchers used the topological indices in drug designing to create a high-quality design of physical structure and bio-organic and chemical properties of the existing and new drugs. This article discovers and investigates the M-polynomials corresponding to topological coindices. Maple graphics are used to illustrate the three dimensional molecular structures in a different way and these illustrations are useful in structural chemistry. A few degree-based topological coindices are considered including the first and second Zagreb coindices, forgotten topological coindex, general Randic and inverse Randic coindices, symmetric division coindex, harmonic coindex, inverse sum indeg coindex and augmented zagreb coindex.

1. Introduction

A branch of modern science called as graph theory deals with the use of graphic parameters and tools accurately reveal the properties of the compound under investigation. Graph theory creates a link between mathematics and chemistry through a helpful tool called topological indices. They describe the topology of molecular structures. Topological indices play a vital role in the QSPR and QSAR models to predict various physiochemical properties and bioactivity that aid drug discovery, [8]. In chemical or molecular graph theory, we use the concepts of graph theory to describe the mathematical models of various chemical structures. Chemical graph theory is a sub-domain of mathematical chemistry which is very beneficial for the progression of computational analysis of chemical compounds. The most devastating pandemic has been plague, influence, cholera, etc. At present, the COVID-19 pandemic is disrupting human health and the economy around the world. In this work, some degree based topological indices are studied for the antiviral medications mentioned using the polynomial approach, [12, 24]. Graphical representations of the computed topological indices are also provided.

The molecular structure of a drug is expressed as a molecular graph in chemical graph theory, where one atom represents a vertex and a link between two atoms

[1]Corresponding author: IN Cangul
2010 *Mathematics Subject Classification.* 05C07, 05C09, 05C92.
Key words and phrases. Covid-19, M-polynomial, molecular graph, topological coindex.

represents chemical bond, [11, 22]. In this article, we continue our investigation further into antiviral drugs captured by COVID-19 patients and define M-polynomials corresponding to co-indices (CIMP) by taking into consideration the equivalent contributions from pairs of nonadjacent vertices [18, 19, 27]. This encapsulates and summarises a potential influence of distant pairs of vertices on the characteristics of the molecule.

Most degree-based topological indices take into account adjacent vertex pairs, [15, 28]. Coindices are degree-based topological indices that were created as a result of researchers starting to take nonadjacent pairing of vertices into account when computing some topological properties of networks over time, [6]. For graph notations and terminology, see [1, 2, 3, 13, 16].

Table 1. Definition of topological indices and corresponding topological coindices

TI	**Degree based index**	**Degree based coindex**
$M_1(G)$ [14]	$M_1(G) = \sum_{st\in E(G)} [d_s + d_t]$	$\overline{M_1}(G) = \sum_{st\notin E(G)} [d_s + d_t].$
$M_2(G)$ [14]	$M_2(G) = \sum_{st\in E(G)} [d_s.d_t]$	$\overline{M_2}(G) = \sum_{st\notin E(G)} [d_s.d_t].$
$mM_2(G)$ [20]	$mM_2(G) = \sum_{st\in E(G)} \left[\frac{1}{d_s.d_t}\right]$	$\overline{mM_2}(G) = \sum_{st\notin E(G)} \left[\frac{1}{d_s.d_t}\right].$
$ReZG_3(G)$ [23]	$ReZG_3(G) = \sum_{st\in E(G)} d_sd_t[d_s + d_t]$	$\overline{ReZG_3}(G) = \sum_{st\notin E(G)} d_sd_t[d_s + d_t]$
$F(G)$ [10]	$F(G) = \sum_{st\in E(G)} [d_s^2 + d_t^2]$	$\overline{F}(G) = \sum_{st\notin E(G)} [d_s^2 + d_t^2]$
$R_k(G)$ [5]	$R_k(G) = \sum_{st\in E(G)} [d_s.d_t]^k$	$\overline{R_k}(G) = \sum_{st\notin E(G)} [d_s.d_t]^k$
$RR_k(G)$ [13]	$RR_k(G) = \sum_{st\in E(G)} \frac{1}{[d_s.d_t]^k}$	$\overline{RR_k}(G) = \sum_{st\notin E(G)} \frac{1}{[d_s.d_t]^k}$
$SDD(G)$ [26]	$SDD(G) = \sum_{st\in E(G)} \left[\frac{d_s^2 + d_t^2}{d_s.d_t}\right]$	$\overline{SDD}(G) = \sum_{st\notin E(G)} \left[\frac{d_s^2 + d_t^2}{d_s.d_t}\right]$
$H(G)$ [29]	$H(G) = \sum_{st\in E(G)} \left[\frac{2}{d_s + d_t}\right]$	$\overline{H}(G) = \sum_{st\notin E(G)} \left[\frac{2}{d_s + d_t}\right]$
$I(G)$ [21]	$I(G) = \sum_{st\in E(G)} \left[\frac{d_s.d_t}{d_s + d_t}\right]$	$\overline{I}(G) = \sum_{st\notin E(G)} \left[\frac{d_s.d_t}{d_s + d_t}\right]$
$A(G)$ [9]	$A(G) = \sum_{st\in E(G)} \left[\frac{d_s.d_t}{d_s + d_t - 2}\right]^3$	$\overline{A}(G) = \sum_{st\notin E(G)} \left[\frac{d_s.d_t}{d_s + d_t - 2}\right]^3$

2. Preliminaries

Definition 2.1. [4] For a connected graph G of order n, we have

$$\overline{p}_{ij} = |\overline{E}_{ij}| = \begin{cases} \frac{q_i(q_i-1)}{2} - p_{ii}, & \text{for} \quad i = j \\ q_i qj - p_{ij}, & \text{for} \quad i < j \end{cases}$$

where $q_i = |V_i|$ for $V_i = \{v \in V(G) | \ d(v) = i\}$, $p_{ij} = |E_{ij}|$, $E_{ij} = \{st \in E(G) | \ d(s) = i \quad \text{and} \quad d(t) = j\}$ and $\overline{p_{ij}} = |\overline{E_{ij}}|$ for $\overline{E_{ij}} = \{st \in E(\overline{G}) | \ d(s) = i \quad \text{and} \quad d(t) = j\}$.

Motivated from the above work, we define $CIMP$ as an extension of the M-polynomial notion for nonadjacent pairs of vertices as follows:

$$CIMP(G; x, y) = \overline{P}(G; x, y) = \sum_{i \leq j} \overline{p}_{ij}(G) x^i y^j$$

where $\overline{p}_{ij}(G), i, j \geq 1$, be the number of edges $st \notin E(G)$ such that $\{(d(s), d(t)) = \{i, j\}\}$.

3. Phytochemicals in $3D$ graphs

In this section, we use combinatorial computations, edge partition techniques, vertex partition techniques and non-edge counting methods to obtain the $CIMP$ of molecular graphs of Isoflavone (ISO), Myricitrin (MN), Methyl Rosmarinate (MRT), 3, 5, 7, 30, 40, 50-hexahydroxy flavanone, 3-Obeta-Dglucopyranoside (FOD), 2S-Eriodictyol 7-O-(600-Ogalloyl)-beta-Dglucopyranoside (EBD), Calceolarioside-B (CAB), Myricetin-3-beta-Dglucopyranoside (MOD), Licoleafol (LFL), Amaranthin (AMT), Nelfinavir (NIR), Prulifloxacin (PEN) and Colistin (CLN). For the provided molecular graphs, we additionally derived numerous well-known topological coindices. We have shown graphics of $CIMP$ in three dimensions for a variety of phytochemicals in this section.

4. Derivation of Topological $CIMP$ and its Molecular graphs

The results demonstrate a significant link between the physicochemical characteristics of potential antiviral drugs in use and the topological coindices under examination. Topological coindices could therefore be useful tools for QSPR analysis in the future to explore antiviral medicines, [25]. The medications considered in this work for a few phytochemicals are depicted in Fig. 1 as 3D structures, and their matching molecular structures are provided below in Fig. 2.

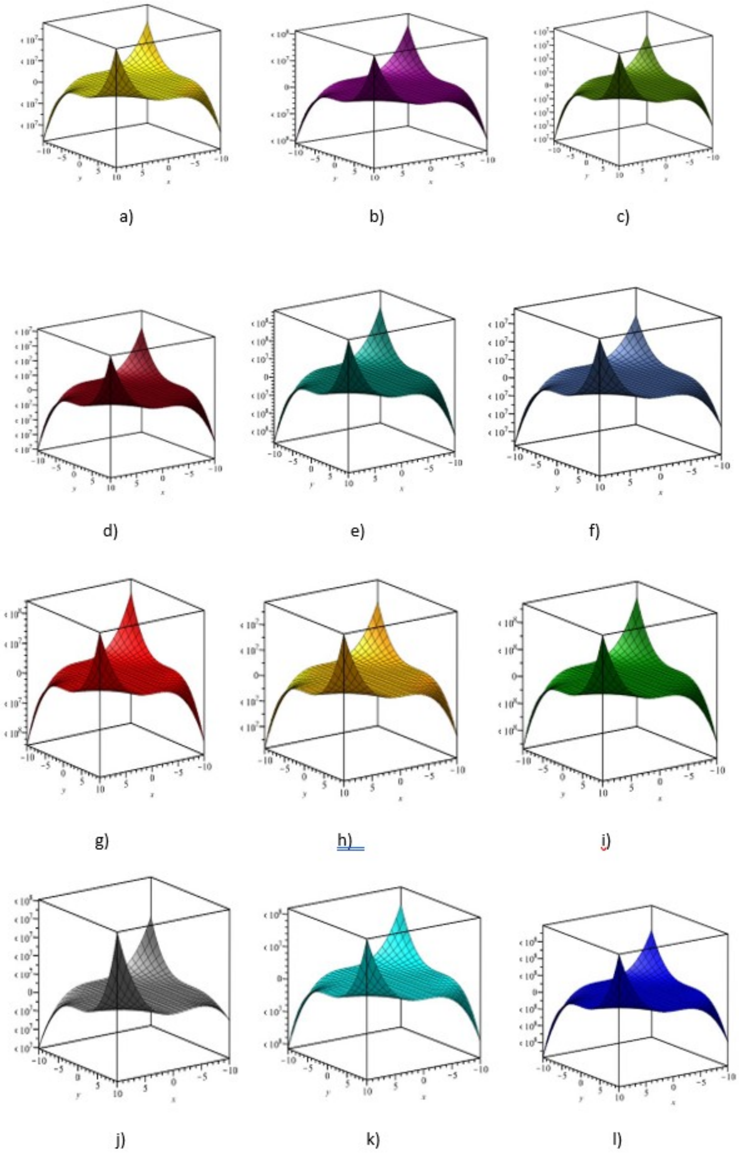

FIGURE 1. 3D graphs of $CIMP$ of a)ISO, b)MN, c)MRT, d)FOD, e)EBD, f)CAB,, g)MOD, h)LFL, i)AMT, J)NIR, k)PFN, l)CLN

Topological coindex	Derivation from $f(x,y) = CIMP(G:x,y)$
First Zagreb coindex: $\overline{M_1}(G)$	$(D_x + D_y)(f(x,y))_{x=y=1}$
Second Zagreb coindex: $\overline{M_2}(G)$	$(D_x D_y)(f(x,y))_{x=y=1}$
Second modified Zagreb coindex: $\overline{mM_2}(G)$	$(S_x S_y)(f(x,y))_{x=y=1}$
Redefined third Zagreb coindex: $\overline{ReZG_3}(G)$	$D_x D_y (D_x + D_y)(f(x,y))_{x=y=1}$
Forgotten topological coindex: $\overline{F}(G)$	$(D_x^2 + D_y^2)(f(x,y))_{x=y=1}$
Randic coindex: $\overline{R_k}(G)$	$(D_x^k D_y^k)(f(x,y))_{x=y=1}$
Inverse Randic coindex: $\overline{RR_k}(G)$	$(S_x^k S_y^k)(f(x,y))_{x=y=1}$
Symmetric division coindex: $\overline{SDD}(G)$	$(D_x S_y + S_x D_y)(f(x,y))_{x=y=1}$
Harmonic coindex: $\overline{H}(G)$	$(2S_x J)(f(x,y))_{x=y=1}$
Inverse sum indeg coindex: $\overline{I}(G)$	$(S_x j D_x D_y)(f(x,y))_{x=y=1}$
Augmented zagreb coindex: $\overline{A}(G)$	$(S_x^3 Q_{-2} J D_x^3 D_y^3)(f(x,y))_{x=y=1}$

Table 2. Derivation of few degree based topological coindices.

Table 2 is related to some of the most prominent degree-based topological coindices with M-polynomial, [7, 17], and the following fixed notations.

$$D_x = x\frac{\partial(f(x,y))}{\partial x},\ D_y = y\frac{\partial(f(x,y))}{\partial y},\ S_x = \int_0^x \frac{f(t,y)}{t}dt,\ S_y = \int_0^y \frac{f(x,t)}{t}dt\ ,$$
$$J(f(x,y)) = f(x,x),\ Q_\phi(f(x,y)) = x^\phi f(x,y).$$

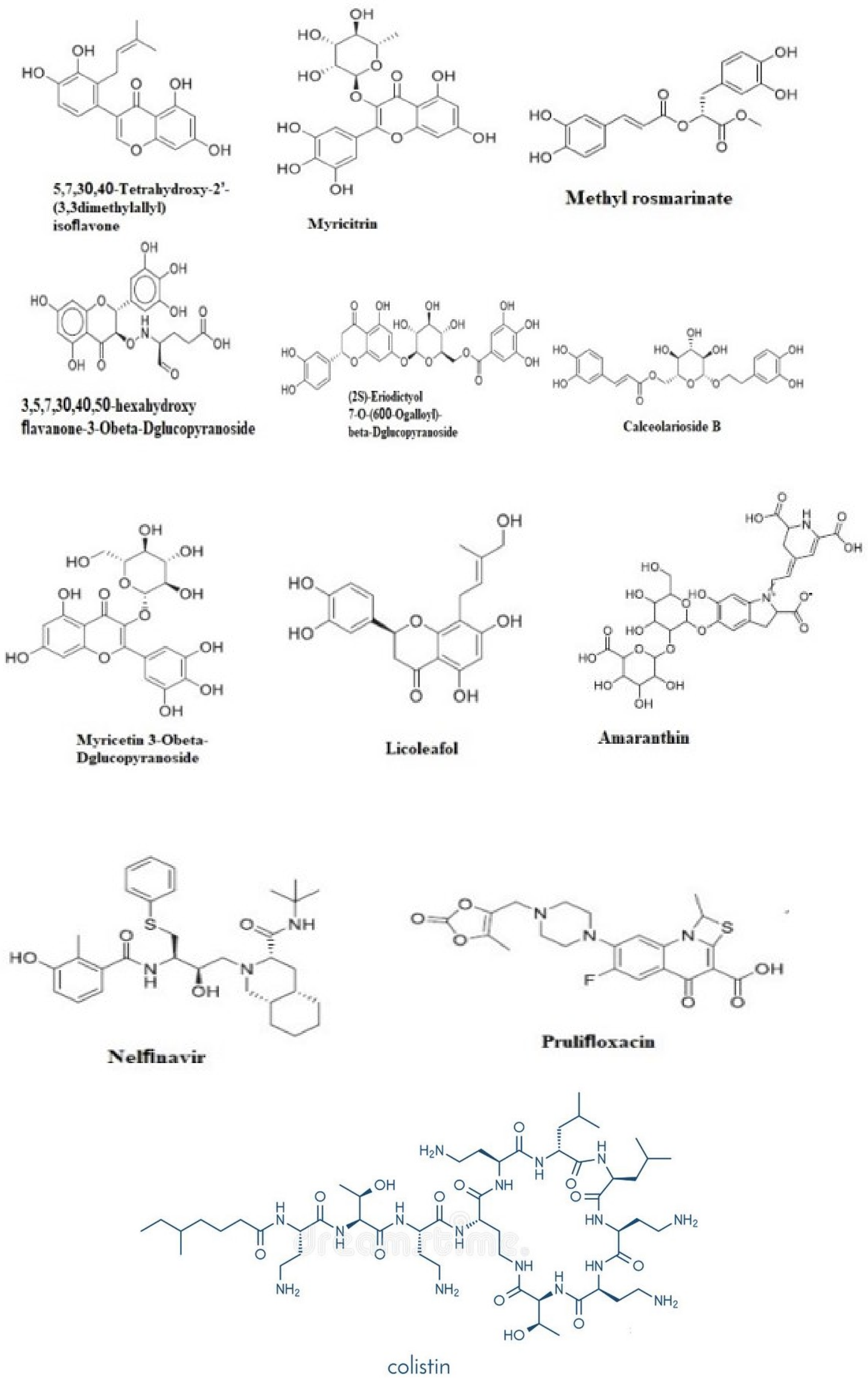

FIGURE 2. 3D graphs of $CIMP$ of a)ISO, b)MN, c)MRT, d)FOD, e)EBD, f)CAB,, g)MOD, h)LFL, i)AMT, j)NIR, k)PFN, l)CLN

5. Discussion and Main Results

We studied the expression of the CIMP for eleven topological coindices in this paper and the formulae for these topological indices are presented in Table 2. First, we determine the CIMP result for Isoflavone (ISO).

Theorem 5.1. *The coindex M-polynomial for ISO is given by*

$$CIMP(ISO; x, y) = 70xy^3 + 25x^2y^2 + 78x^2y^3 + 47x^3y^3.$$

Proof. It is clear from Fig. 2(a) that $|V(ISO)| = 26$ and $|E(ISO)| = 28$. In addition, the ISO edge set can be divided into four groups based on the number of vertices as well as $p_{13} = |E_{13}| = 7$, $p_{22} = |E_{22}| = 3$, $p_{23} = |E_{23}| = 10$ and $p_{33} = |E_{33}| = 8$. Similarly to this, V(ISO) can be divided into three classes according to the degree they possess:

$q_i = \|V_i\|$	q_1	q_2	q_3
number	7	8	11

Using Definition 1, we have

$$\overline{p}_{13} = q_1q_3 - p_{13} = 70$$

$$\overline{p}_{22} = \frac{q_2(q_2-1)}{2} - p_{22} = 25$$

Similarly, $\overline{p}_{23} = 78$, $\overline{p}_{33} = 47$ and by the definition of $CIMP$, we have

$$CIMP(G; x, y) = \overline{P}(G; x, y) = \sum_{i \leq j} \overline{p}_{ij}(G)x^iy^j$$

where $\overline{p}_{ij}(G), i, j \geq 1$ is the number of edges $st \in E(G)$ such that $(d(s), d(t)) = \{i, j\}$. Let

$$\begin{aligned} CIMP(ISO; x, y) &= \sum_{i \leq j} \overline{p}_{ij}(G)x^iy^j \\ &= \sum_{1 \leq 3} \overline{p}_{13}(G)x^1y^3 + \sum_{2 \leq 2} \overline{p}_{22}(G)x^2y^2 + \sum_{2 \leq 3} \overline{p}_{23}(G)x^2y^3 \\ &+ \sum_{3 \leq 3} \overline{p}_{33}(G)x^3y^3. \\ &= 70xy^3 + 25x^2y^2 + 78x^2y^3 + 47x^3y^3. \end{aligned}$$

□

We extract some degree-based topological coindices of the ISO in the following assertion using Thm. 5.1 and Table 2.

Proposition 5.2. *For ISO, the topological coindices are delivered by*

1. $\overline{M}_1(ISO) = 1052.$
2. $\overline{M}_2(ISO) = 1201.$
3. $\overline{mM}_2(ISO) = 47.8.$
4. $\overline{ReZG}_3(ISO) = 6118.$
5. $\overline{F}(ISO) = 2760.$
6. $\overline{R}_k(ISO) = 70(3^k) + 25(4^k) + 78(6^k) + 47(9^k).$
7. $\overline{RR}_k(ISO) = \frac{70}{3^k} + \frac{25}{4^k} + \frac{78}{6^k} + \frac{47}{9^k}.$
8. $\overline{SDD}(ISO) = 546.33.$
9. $\overline{H}(ISO) = 94.36.$
10. $\overline{I}(ISO) = 241.6.$
11. $\overline{A}(ISO) = 1595.609.$

Proof. Let

$$f(x,y) = CIMP(G;x,y) = \overline{P}(G;x,y) = \sum_{i\leq j} \overline{p}_{ij}(G)x^i y^j$$

Then

$f(x,y) = 70xy^3 + 25x^2y^2 + 78x^2y^3 + 47x^3y^3.$
$D_x f(x,y) = 70xy^3 + 50x^2y^2 + 156x^2y^3 + 141x^3y^3.$
$D_y(f(x,y)) = 210xy^3 + 50x^2y^2 + 234x^2y^3 + 141x^3y^3.$
$D_x + D_y(f(x,y)) = 280xy^3 + 100x^2y^2 + 390x^2y^3 + 282x^3y^3.$
$D_xD_y(f(x,y)) = 20xy^3 + 100x^2y^2 + 468x^2y^3 + 423x^3y^3.$
$D_y + D_x(f(x,y)) = 210xy^3 + 100x^2y^2 + 468x^2y^3 + 423x^3y^3.$
$(D_x^2 + D_y^2)(f(x,y)) = 700xy^3 + 200x^2y^2 + 1014x^2y^3 + 846x^3y^3.$
$(D_x^k + D_y^k)(f(x,y)) = 70(3^k)xy^3 + 25(2^{2k})x^2y^2 + 78(6^k)x^2y^3 + 47(3^{2k})x^3y^3.$
$D_xD_y(D_x + D_y)(f(x,y)) = 840xy^3 + 400x^2y^2 + 2340x^2y^3 + 2538x^3y^3.$
$S_xS_y(f(x,y)) = \frac{70}{3}xy^3 + \frac{25}{4}x^2y^2 + \frac{78}{6}x^2y^3 + \frac{47}{9}x^3y^3.$
$S_x^kS_y^k(f(x,y)) = \frac{70}{3^k}xy^3 + \frac{25}{4^k}x^2y^2 + \frac{78}{6^k}x^2y^3 + \frac{47}{9^k}x^3y^3.$
$(S_yD_x + S_xD_y)(f(x,y)) = \frac{700}{3}xy^3 + 50x^2y^2 + 169x^2y^3 + 94x^3y^3.$
$S_xJ(f(x,y)) = \frac{70}{4}x^4 + \frac{25}{4}x^4 + \frac{78}{5}x^5 + \frac{47}{6}x^6.$
$S_xJD_yD_x(f(x,y)) = \frac{70}{12}x^4 + \frac{50}{8}x^4 + \frac{156}{15}x^5 + \frac{141}{18}x^6.$
$S_x^3Q_{-2}JD_x^3D_y^3(f(x,y)) = 236.25x^2 + 200x^2 + 624x^3 + 535.35x^4.$

Table 2 allows us to determine the following:

$$\overline{M}_1(ISO) = (D_x + D_y)(f(x,y))_{x=y=1} = 1052.$$
$$\overline{M}_2(ISO) = (D_x D_y)(f(x,y))_{x=y=1} = 1201.$$
$$\overline{mM}_2(ISO) = (S_x S_y)(f(x,y))_{x=y=1} = 47.8.$$
$$\overline{ReZG}_3(ISO) = D_x D_y (D_x + D_y)(f(x,y))_{x=y=1} = 6118.$$
$$\overline{F}(ISO) = (D_x^2 + D_y^2)(f(x,y))_{x=y=1} = 2760.$$
$$\overline{R}_k(ISO) = (D_x^k D_y^k)(f(x,y))_{x=y=1} = 70(3^k) + 25(4^k) + 78(6^k) + 47(9^k).$$
$$\overline{RR}_k(ISO) = (S_x^k S_y^k)(f(x,y))_{x=y=1} = \tfrac{70}{3^k} + \tfrac{25}{4^k} + \tfrac{78}{6^k} + \tfrac{47}{9^k}.$$
$$\overline{SDD}(ISO) = (D_x S_y + S_x D_y)(f(x,y))_{x=y=1} = 546.33.$$
$$\overline{H}(ISO) = (2S_x J)(f(x,y))_{x=y=1} = 94.36.$$
$$\overline{I}(ISO) = (S_x j D_x D_y)(f(x,y))_{x=y=1} = 241.6.$$
$$\overline{A}(ISO) = (S_x^3 Q_{-2} J D_x^3 D_y^3)(f(x,y))_{x=y=1} = 1595.609.$$

□

The CIMP for the Myricitrin molecular graph (MN) are as follows:

Theorem 5.3. *The coindex M-polynomial for MN is given by*

$$CIMP(MN; x, y) = 126xy^3 + 27x^2y^2 + 106x^2y^3 + 94x^3y^3.$$

Proof. It is clear from Fig. 2(b) that $|V(MN)| = 32$ and $|E(MN)| = 35$. In addition, the edge set of MN can be divided into four groups based on the number of vertices as well as $p_{13} = |E_{13}| = 9$, $p_{22} = |E_{22}| = 1$, $p_{23} = |E_{23}| = 14$ and $p_{33} = |E_{33}| = 11$.

Similarly to this, $V(MN)$ can be divided into three classes according to the degree they possess.

$q_i = \|V_i\|$	q_1	q_2	q_3
number	9	8	15

Using Definition 1, we have

$$\overline{p}_{13} = q_1 q_3 - p_{13} = 126$$
$$\overline{p}_{22} = \frac{q_2(q_2 - 1)}{2} - p_{22} = 27$$

Similarly, $\overline{p}_{23} = 106$, $\overline{p}_{33} = 94$. Let

$$\begin{aligned} CIMP(MN; x, y) &= \sum_{i \le j} \overline{p}_{ij}(G) x^i y^j \\ &= \sum_{1 \le 3} \overline{p}_{13}(G) x^1 y^3 + \sum_{2 \le 2} \overline{p}_{22}(G) x^2 y^2 + \sum_{2 \le 3} \overline{p}_{23}(G) x^2 y^3 \\ &+ \sum_{3 \le 3} \overline{p}_{33}(G) x^3 y^3. \end{aligned}$$

$$= 126xy^3 + 27x^2y^2 + 106x^2y^3 + 94x^3y^3.$$

Hence, the proof. □

In the next Proposition, we can extract various topological coindices for MN by using the same steps as in Proposition 5.1.

Proposition 5.4. *For MN, the topological coindices are delivered by*

1. $\overline{M}_1(MN) = 1706$.
2. $\overline{M}_2(MN) = 1968$.
3. $\overline{mM}_2(MN) = 76.85$.
4. $\overline{ReZG}_3(MN) = 10200$.
5. $\overline{F}(MN) = 4546$.
6. $\overline{R}_k(MN) = 126(3^k) + 27(4^k) + 106(6^k) + 94(9^k)$.
7. $\overline{RR}_k(MN) = \frac{126}{3^k} + \frac{27}{4^k} + \frac{106}{6^k} + \frac{94}{9^k}$.
8. $\overline{SDD}(MN) = 891.65$.
9. $\overline{H}(MN) = 150.22$.
10. $\overline{I}(MN) = 389.7$.
11. $\overline{A}(MN) = 2559.96$.

The expression for $CIMP$ of Methyl Rosmarinate (MRT) is derived in the following theorem.

Theorem 5.5. *The coindex M-polynomial for MRT is given by*

$$CIMP(MRT; x, y) = 76xy^2 + 57xy^3 + 52x^2y^2 + 84x^2y^3 + 33x^3y^3.$$

Proof. It is clear from Fig. 2(c) that $|V(MRT)| = 27$ and $|E(MRT)| = 28$. In addition, the edge set of MRT can be divided into five groups based on the number of vertices as well as $p_{12} = |E_{12}| = 1$, $p_{13} = |E_{13}| = 6$, $p_{22} = |E_{22}| = 3$,$p_{23} = |E_{23}| = 15$ and $p_{33} = |E_{33}| = 3$.

Similarly to this, $V(MRT)$ can be divided into three classes according to the degree they possess.

$q_i = \|V_i\|$	q_1	q_2	q_3
number	7	11	9

Using Definition 1, we have

$$\overline{p}_{12} = q_1q_2 - p_{12} = 76$$

$$\overline{p}_{22} = \frac{q_2(q_2-1)}{2} - p_{22} = 52$$

Similarly, $\overline{p}_{13} = 57$,$\overline{p}_{23} = 84$ and $\overline{p}_{33} = 33$. Let

$$\begin{aligned} CIMP(MRT; x, y) &= \sum_{i \leq j} \overline{p}_{ij}(G) x^i y^j \\ &= \sum_{1 \leq 2} \overline{p}_{12}(G) x^1 y^2 + \sum_{1 \leq 3} \overline{p}_{13}(G) x^1 y^3 + \sum_{2 \leq 2} \overline{p}_{22}(G) x^2 y^2 \\ &+ \sum_{2 \leq 3} \overline{p}_{23}(G) x^2 y^3 + \sum_{3 \leq 3} \overline{p}_{33}(G) x^3 y^3. \\ &= 76xy^2 + 57xy^3 + 52x^2y^2 + 84x^2y^3 + 33x^3y^3. \end{aligned}$$

Hence, the result. □

Using the aforementioned theorem, the following preposition can be computed instantly.

Proposition 5.6. *For MRT, the topological coindices are*

1. $\overline{M}_1(MRT) = 1282$.
2. $\overline{M}_2(MRT) = 1332$.
3. $\overline{mM}_2(MRT) = 87.66$.
4. $\overline{ReZG}_3(MRT) = 6274$.
5. $\overline{F}(MRT) = 3052$.
6. $\overline{R}_k(MRT) = 76(2^k) + 57(3^k) + 52(4^k) + 84(6^k) + 33(9^k)$.
7. $\overline{RR}_k(MRT) = \frac{76}{2^k} + \frac{57}{3^k} + \frac{52}{4^k} + \frac{84}{6^k} + \frac{33}{9^k}$.
8. $\overline{SDD}(MRT) = 732$.
9. $\overline{H}(MRT) = 149.76$.
10. $\overline{I}(MRT) = 295.71$.
11. $\overline{A}(MRT) = 2264.26$.

The CIMP of the molecular graph 3,5,7,30,40,50-hexahydroxy flavanone-3-Obeta-Dgluc-opyranoside(FOD) is calculated using the following theorem:

Theorem 5.7. *The coindex M-polynomial for FOD is given by*

$$CIMP(FOD; x, y) = 89xy^2 + 109xy^3 + 43x^2y^2 + 115x^2y^3 + 70x^3y^3.$$

Proof. It is clear from Fig. 2(d) that $|V(EBD)| = 43$ and $|E(EBD)| = 47$. In addition, the EBD edge set can be divided into four groups based on the number of vertices as well as $p_{13} = |E_{13}| = 11$, $p_{22} = |E_{22}| = 2$,$p_{23} = |E_{23}| = 22$ and $p_{33} = |E_{33}| = 12$.

Similarly, $V(EBD)$ can be divided into three classes according to the degree they possess:

$q_i = \|V_i\|$	q_1	q_2	q_3
number	11	13	19

Using Definition 1, we have

$$\overline{p}_{13} = q_1 q_3 - p_{13} = 198$$
$$\overline{p}_{22} = \frac{q_2(q_2-1)}{2} - p_{22} = 76$$

Similarly, $\overline{p}_{23} = 225$ and $\overline{p}_{33} = 159$

$$\begin{aligned} Let, CIMP(EBD; x, y) &= \sum_{i \leq j} \overline{p}_{ij}(G) x^i y^j \\ &= \sum_{1\leq 3} \overline{p}_{13}(G) x^1 y^3 + \sum_{2\leq 2} \overline{p}_{22}(G) x^2 y^2 \\ &+ \sum_{2\leq 3} \overline{p}_{23}(G) x^2 y^3 + \sum_{3\leq 3} \overline{p}_{33}(G) x^3 y^3. \\ &= 198xy^3 + 76x^2y^2 + 225x^2y^3 + 159x^3y^3. \end{aligned}$$

□

Now, with the above outcome, we obtain the following result:

Proposition 5.8. *For EBD, the topological coindices are*

1. $\overline{M}_1(EBD) = 3175.$
2. $\overline{M}_2(EBD) = 3679.$
3. $\overline{mM}_2(EBD) = 140.16.$
4. $\overline{ReZG}_3(EBD) = 18928.$
5. $\overline{F}(EBD) = 8375.$
6. $\overline{R}_k(EBD) = 198(3^k) + 76(4^k) + 225(6^k) + 159(9^k).$
7. $\overline{RR}_k(EBD) = \frac{198}{3^k} + \frac{76}{4^k} + \frac{225}{6^k} + \frac{159}{9^k}.$
8. $\overline{SDD}(EBD) = 1617.5.$
9. $\overline{H}(EBD) = 280.$
10. $\overline{I}(EBD) = 733.$
11. $\overline{A}(EBD) = 4887.35.$

Theorem 5.9. *The coindex M-polynomial for EBD is given by*

$$CIMP(EBD; x, y) = 198xy^3 + 76x^2y^2 + 225x^2y^3 + 159x^3y^3.$$

Proof. It is clear from Fig. 2(e) that $|V(FOD)| = 32$ and $|E(FOD)| = 34$. In addition, the FOD edge set can be divided into four subsets based on the number of vertices as well as $p_{12} = |E_{12}| = 1$, $p_{13} = |E_{13}| = 8$, $p_{22} = |E_{22}| = 2$,$p_{23} = |E_{23}| = 15$ and $p_{33} = |E_{33}| = 8$.

Similar to this, $V(FOD)$ can be divided into three classes according to the degree they possess.

$q_i = \|V_i\|$	q_1	q_2	q_3
number	9	10	13

Using Definition 1, we have

$$\overline{p}_{12} = q_1 q_2 - p_{12} = 89$$
$$\overline{p}_{22} = \frac{q_2(q_2-1)}{2} - p_{22} = 43$$

Similarly, $\overline{p}_{13} = 109$,$\overline{p}_{23} = 115$ and $\overline{p}_{33} = 70$. Let

$$\begin{aligned}
CIMP(FOD; x, y) &= \sum_{i \le j} \overline{p}_{ij}(G) x^i y^j \\
&= \sum_{1 \le 2} \overline{p}_{12}(G) x^1 y^2 + \sum_{1 \le 3} \overline{p}_{13}(G) x^1 y^3 + \sum_{2 \le 2} \overline{p}_{22}(G) x^2 y^2 \\
&+ \sum_{2 \le 3} \overline{p}_{23}(G) x^2 y^3 + \sum_{3 \le 3} \overline{p}_{33}(G) x^3 y^3. \\
&= 89xy^2 + 109xy^3 + 43x^2y^2 + 115x^2y^3 + 70x^3y^3.
\end{aligned}$$

This concludes the proof. □

The following outcomes are obtained in the light of Theorem 5.5:

Proposition 5.10. *For FOD, the topological coindices are*

1. $\overline{M}_1(FOD) = 1870.$
2. $\overline{M}_2(FOD) = 1997.$
3. $\overline{mM_2}(FOD) = 118.52.$
4. $\overline{ReZG_3}(FOD) = 9760.$
5. $\overline{F}(FOD) = 4634.$
6. $\overline{R}_k(FOD) = 89(2^k) + 109(3^k) + 43(4^k) + 115(6^k) + 70(9^k).$
7. $\overline{RR}_k(FOD) = \frac{89}{2^k} + \frac{109}{3^k} + \frac{43}{4^k} + \frac{115}{6^k} + \frac{70}{9^k}.$
8. $\overline{SDD}(FOD) = 1060.98.$
9. $\overline{H}(FOD) = 204.55.$
10. $\overline{I}(FOD) = 427.08.$
11. $\overline{A}(FOD) = 3141.21.$

Theorem 5.11. *The coindex M-polynomial for CAB is given by*

$$CIMP(CAB; x, y) = 88xy^3 + 85x^2y^2 + 152x^2y^3 + 60x^3y^3.$$

Proof. It is clear from Fig. 2(f) that $|V(CAB)| = 34$ and $|E(CAB)| = 36$. In addition, the CAB edge set can be divided into four subsets based on the number of vertices as well as $p_{13} = |E_{13}| = 8$, $p_{22} = |E_{22}| = 6$,$p_{23} = |E_{23}| = 16$ and $p_{33} = |E_{33}| = 6$.

Similarly, $V(CAB)$ can be divided into three classes according to the degree they possess.

$q_i = \|V_i\|$	q_1	q_2	q_3
number	8	14	12

Using Definition 1, we have

$$\overline{p}_{13} = q_1 q_3 - p_{13} = 88$$
$$\overline{p}_{22} = \frac{q_2(q_2-1)}{2} - p_{22} = 85$$

Similarly, $\overline{p}_{23} = 152$ and $\overline{p}_{33} = 60$. Let

$$\begin{aligned} CIMP(CAB;x,y) &= \sum_{i\leq j} \overline{p}_{ij}(G)x^i y^j \\ &= \sum_{1\leq 3} \overline{p}_{13}(G)x^1y^3 + \sum_{2\leq 2} \overline{p}_{22}(G)x^2y^2 \\ &+ \sum_{2\leq 3} \overline{p}_{23}(G)x^2y^3 + \sum_{3\leq 3} \overline{p}_{33}(G)x^3y^3. \\ &= 88xy^3 + 85x^2y^2 + 152x^2y^3 + 60x^3y^3. \end{aligned}$$

The proof is now complete. □

Proposition 5.12. *For CAB, the topological coindices are*

1. $\overline{M}_1(CAB) = 1812.$
2. $\overline{M}_2(CAB) = 2056.$
3. $\overline{mM}_2(CAB) = 82.57.$
4. $\overline{ReZG}_3(CAB) = 10216.$
5. $\overline{F}(CAB) = 4616.$
6. $\overline{R}_k(CAB) = 88(3^k) + 85(4^k) + 152(6^k) + 60(9^k).$
7. $\overline{RR}_k(CAB) = \frac{83}{3^k} + \frac{85}{4^k} + \frac{152}{6^k} + \frac{60}{9^k}.$
8. $\overline{SDD}(CAB) = 912.65.$
9. $\overline{H}(CAB) = 167.3.$
10. $\overline{I}(CAB) = 423.4.$
11. $\overline{A}(CAB) = 2876.43.$

Theorem 5.13. *The coindex M-polynomial for MOD is given by*

$$CIMP(MOD;x,y) = 79xy^2 + 155x^1y^3 + 113x^2y^3 + 108x^3y^3.$$

Proof. It is clear from Fig. 2(g) that $|V(MOD)| = 34$ and $|E(MOD)| = 37$. In addition, the MOD edge set can be divided into four groups based on the number of vertices as well as $p_{12} = |E_{12}| = 1$, $p_{13} = |E_{13}| = 9$,$p_{23} = |E_{23}| = 15$ and $p_{33} = |E_{33}| = 12$.

Similarly, $V(MOD)$ can be divided into three classes according to the degree they possess.

$q_i = \|V_i\|$	q_1	q_2	q_3
number	10	8	16

Using Definition 1, we have

$$\overline{p}_{12} = q_1 q_2 - p_{12} = 79$$

$$\overline{p}_{33} = \frac{q_3(q_3-1)}{2} - p_{33} = 108$$

Similarly, $\overline{p}_{13} = 151$ and $\overline{p}_{23} = 113$. Let

$$\begin{aligned} CIMP(MOD; x, y) &= \sum_{i\leq j} \overline{p}_{ij}(G) x^i y^j \\ &= \sum_{1\leq 2} \overline{p}_{12}(G)x^1y^2 + \sum_{1\leq 3} \overline{p}_{13}(G)x^1y^3 + \sum_{2\leq 3} \overline{p}_{23}(G)x^2y^3 \\ &+ \sum_{3\leq 3} \overline{p}_{33}(G)x^3y^3. \\ &= 79xy^2 + 151x^1y^3 + 113x^2y^3 + 108x^3y^3. \end{aligned}$$

□

Proposition 5.14. *For MOD, the topological coindices are*

1. $\overline{M}_1(MOD) = 2054$.
2. $\overline{M}_2(MOD) = 2261$.
3. $\overline{mM}_2(MOD) = 12.66$.
4. $\overline{ReZG}_3(MOD) = 11508$.
5. $\overline{F}(MOD) = 5318$.
6. $\overline{R}_k(MOD) = 79(2^k) + 51(3^k) + 113(6^k) + 108(9^k)$.
7. $\overline{RR}_k(MOD) = \frac{79}{2^k} + \frac{51}{3^k} + \frac{113}{6^k} + \frac{108}{9^k}$.
8. $\overline{SDD}(MOD) = 1161.66$.
9. $\overline{H}(MOD) = 209.36$.
10. $\overline{I}(MOD) = 463.51$.
11. $\overline{A}(MOD) = 2774.14$.

Theorem 5.15. *The coindex M-polynomial for LFL is given by*

$$CIMP(LFL; x, y) = 62xy^2 + 71x^1y^3 + 34x^2y^2 + 86x^2y^3 + 48x^3y^3.$$

Proof. It is clear from Fig. 2(h) that $|V(LFL)| = 27$ and $|E(LFL)| = 29$. In addition, the LFL edge set can be divided into five groups based on the number of vertices as well as $p_{12} = |E_{12}| = 1$, $p_{13} = |E_{13}| = 6$,$p_{22} = |E_{22}| = 2$,$p_{23} = |E_{23}| = 13$ and $p_{33} = |E_{33}| = 7$.

In a similar manner, $V(LFL)$ can be divided into three classes according to the degree they possess.

$q_i = \|V_i\|$	q_1	q_2	q_3
number	7	9	11

Using Definition 1, we have

$$\overline{p}_{12} = q_1 q_2 - p_{12} = 62$$

$$\overline{p}_{33} = \frac{q_3(q_3-1)}{2} - p_{33} = 48$$

Similarly, $\overline{p}_{13} = 71$, $\overline{p}_{22} = 34$ and $\overline{p}_{23} = 86$. Let

$$\begin{aligned} CIMP(LFL; x, y) &= \sum_{i \leq j} \overline{p}_{ij}(G) x^i y^j \\ &= \sum_{1 \leq 2} \overline{p}_{12}(G) x^1 y^2 + \sum_{1 \leq 3} \overline{p}_{13}(G) x^1 y^3 + \sum_{2 \leq 2} \overline{p}_{22}(G) x^2 y^2 \\ &+ \sum_{2 \leq 3} \overline{p}_{23}(G) x^2 y^3 + \sum_{3 \leq 3} \overline{p}_{33}(G) x^3 y^3 \\ &= 62xy^2 + 71x^1y^3 + 34x^2y^2 + 86x^2y^3 + 48x^3y^3. \end{aligned}$$

□

Proposition 5.16. *For LFL, the topological coindices are*

1. $\overline{M}_1(LFL) = 1324$.
2. $\overline{M}_2(LFL) = 1421$.
3. $\overline{mM}_2(LFL) = 82.82$.
4. $\overline{ReZG}_3(LFL) = 6940$.
5. $\overline{F}(LFL) = 3274$.
6. $\overline{R}_k(LFL) = 62(2^k) + 71(3^k) + 34(4^k) + 86(6^k) + 48(9^k)$.
7. $\overline{RR}_k(LFL) = \frac{62}{2^k} + \frac{71}{3^k} + \frac{34}{4^k} + \frac{86}{6^k} + \frac{48}{9^k}$.
8. $\overline{SDD}(LFL) = 741.99$.
9. $\overline{H}(LFL) = 144.23$.
10. $\overline{I}(LFL) = 303.78$.
11. $\overline{A}(LFL) = 2242.37$.

Theorem 5.17. *The coindex M-polynomial for AMT is given by*

$$CIMP(AMT; x, y) = 195xy^2 + 309x^1y^3 + 90x^2y^2 + 298x^2y^3 + 237x^3y^3.$$

Proof. It is clear from Fig. 2(i) that $|V(AMT)| = 51$ and $|E(AMT)| = 55$. In addition, the AMT edge set can be divided into five groups based on the number of vertices as well as $p_{12} = |E_{12}| = 1$, $p_{13} = |E_{13}| = 13$,$p_{22} = |E_{22}| = 1$,$p_{23} = |E_{23}| = 24$ and $p_{33} = |E_{33}| = 16$.

Similarly, $V(AMT)$ can be divided into three classes according to the degree they possess.

$q_i = \|V_i\|$	q_1	q_2	q_3
number	14	14	23

Using Definition 1, we have

$$\overline{p}_{12} = q_1 q_2 - p_{12} = 195$$
$$\overline{p}_{33} = \frac{q_3(q_3-1)}{2} - p_{33} = 237$$

.

Similarly, $\overline{p}_{13} = 309$, $\overline{p}_{22} = 90$ and $\overline{p}_{23} = 298$. Let

$$\begin{aligned} CIMP(AMT; x, y) &= \sum_{i \leq j} \overline{p}_{ij}(G) x^i y^j \\ &= \sum_{1 \leq 2} \overline{p}_{12}(G) x^1 y^2 + \sum_{1 \leq 3} \overline{p}_{13}(G) x^1 y^3 + \sum_{2 \leq 2} \overline{p}_{22}(G) x^2 y^2 \\ &+ \sum_{2 \leq 3} \overline{p}_{23}(G) x^2 y^3 + \sum_{3 \leq 3} \overline{p}_{33}(G) x^3 y^3 \\ &= 195xy^2 + 309x^1y^3 + 90x^2y^2 + 298x^2y^3 + 237x^3y^3. \end{aligned}$$

□

Proposition 5.18. *For AMT, the topological coindices are*

1. $\overline{M}_1(AMT) = 5093$.
2. $\overline{M}_2(AMT) = 5598$.
3. $\overline{mM}_2(AMT) = 298.99$.
4. $\overline{ReZG}_3(AMT) = 28056$.
5. $\overline{F}(AMT) = 12925$.
6. $\overline{R}_k(AMT) = 195(2^k) + 309(3^k) + 90(4^k) + 298(6^k) + 237(9^k)$.
7. $\overline{RR}_k(AMT) = \frac{195}{2^k} + \frac{309}{3^k} + \frac{90}{4^k} + \frac{298}{6^k} + \frac{237}{9^k}$.
8. $\overline{SDD}(AMT) = 2817.16$.
9. $\overline{H}(AMT) = 527.7$.
10. $\overline{I}(AMT) = 1164.85$.
11. $\overline{A}(AMT) = 8406.44$.

Theorem 5.19. *The coindex M-polynomial for NIR is given by*

$$CIMP(NIR;x,y) = 91xy^3 + 5x^1y^4 + 161x^2y^2 + 18x^2y^4 + 211x^2y^3 + 59x^3y^3.$$

Proof. It is clear from Fig. 2(j) that $|V(NIR)| = 40$ and $|E(NIR)| = 43$. In addition, the NIR edge set can be divided into six groups based on the number of vertices as well as $p_{13} = |E_{13}| = 5$, $p_{14} = |E_{14}| = 3$,$p_{22} = |E_{22}| = 10$,$p_{24} = |E_{24}| = 1$,$p_{23} = |E_{23}| = 17$ and $p_{33} = |E_{33}| = 7$.

Similarly, $V(NIR)$ can be divided into four classes according to the degree they possess.

$q_i = \|V_i\|$	q_1	q_2	q_3	q_4
number	8	19	12	1

Using Definition 1, we have

$$\overline{p}_{13} = q_1q_3 - p_{13} = 91$$
$$\overline{p}_{33} = \frac{q_3(q_3-1)}{2} - p_{33} = 59$$

. Similarly, $\overline{p}_{14} = 5$, $\overline{p}_{22} = 161$, $\overline{p}_{24} = 18$ and $\overline{p}_{23} = 211$. Let

$$\begin{aligned} CIMP(NIR;x,y) &= \sum_{i\leq j} \overline{p}_{ij}(G)x^iy^j \\ &= \sum_{1\leq 3} \overline{p}_{13}(G)x^1y^3 + \sum_{1\leq 4} \overline{p}_{14}(G)x^1y^4 + \sum_{2\leq 2} \overline{p}_{22}(G)x^2y^2 \\ &+ \sum_{2\leq 4} \overline{p}_{24}(G)x^2y^4 + \sum_{2\leq 3} \overline{p}_{23}(G)x^2y^3 + \sum_{3\leq 3} \overline{p}_{33}(G)x^3y^3 \\ &= 91xy^3 + 5x^1y^4 + 161x^2y^2 + 18x^2y^4 + 211x^2y^3 + 59x^3y^3. \end{aligned}$$

□

Proposition 5.20. *For NIR, the topological coindices are*

1. $\overline{M}_1(NIR) = 2550$.
2. $\overline{M}_2(NIR) = 2878$.
3. $\overline{mM}_2(NIR) = 115.79$.
4. $\overline{ReZG}_3(NIR) = 14148$.
5. $\overline{F}(NIR) = 6448$.
6. $\overline{R}_k(NIR) = 91(3^k) + 5(4^k) + 161(4^k) + 18(8^k) + 211(6^k) + 59(9^k)$.
7. $\overline{RR}_k(NIR) = \frac{91}{3^k} + \frac{5}{4^k} + \frac{161}{4^k} + \frac{18}{8^k} + \frac{211}{6^k} + \frac{59}{9^k}$.
8. $\overline{SDD}(NIR) = 1266.72$.
9. $\overline{H}(NIR) = 238.06$.
10. $\overline{I}(NIR) = 598.95$.
11. $\overline{A}(NIR) = 4111.01$.

Theorem 5.21. *The coindex M-polynomial for PFN is given by*

$$CIMP(PFN; x, y) = 98xy^3 + 88x^2y^2 + 134x^2y^3 + 94x^3y^3.$$

Proof. It is clear from Fig. 2(k) that $|V(PFN)| = 32$ and $|E(PFN)| = 36$. In addition, the PFN edge set can be divided into four groups based on the number of vertices as well as $p_{13} = |E_{13}| = 7$, $p_{22} = |E_{22}| = 2$,$p_{23} = |E_{23}| = 16$ and $p_{33} = |E_{33}| = 11$.

Similarly, $V(PFN)$ can be divided into three classes according to the degree they possess.

$q_i = \lvert V_i \rvert$	q_1	q_2	q_3
number	7	10	15

Using Definition 1, we have

$$\overline{p}_{13} = q_1q_3 - p_{13} = 98$$

$$\overline{p}_{22} = \frac{q_2(q_2-1)}{2} - p_{22} = 88$$

. Similarly, $\overline{p}_{23} = 134$ and $\overline{p}_{33} = 94$. Let

$$\begin{aligned} CIMP(PFN; x, y) &= \sum_{i \le j} \overline{p}_{ij}(G)x^iy^j \\ &= \sum_{1\le 3} \overline{p}_{13}(G)x^1y^3 + \sum_{2\le 2} \overline{p}_{22}(G)x^2y^2 + \sum_{2\le 3} \overline{p}_{23}(G)x^2y^3 \\ &+ \sum_{3\le 3} \overline{p}_{33}(G)x^3y^3. \\ &= 98xy^3 + 88x^2y^2 + 134x^2y^3 + 94x^3y^3. \end{aligned}$$

□

Proposition 5.22. *For PFN, the topological coindices are*

1. $\overline{M}_1(PFN) = 1978.$
2. $\overline{M}_2(PFN) = 2296.$
3. $\overline{mM}_2(PFN) = 87.43.$
4. $\overline{ReZG}_3(PFN) = 11680.$
5. $\overline{F}(PFN) = 5118.$
6. $\overline{R}_k(PFN) = 98(3^k) + 88(4^k) + 134(6^k) + 94(9^k).$
7. $\overline{RR}_k(PFN) = \frac{98}{3^k} + \frac{88}{4^k} + \frac{134}{6^k} + \frac{94}{9^k}.$
8. $\overline{SDD}(PFN) = 980.97.$
9. $\overline{H}(PFN) = 177.93$
10. $\overline{I}(PFN) = 463.3.$
11. $\overline{A}(PFN) = 3177.46.$

Theorem 5.23. *The coindex M-polynomial for CLN is given by*

$$CIMP(CLN; x, y) = 670xy^2 + 656x^1y^3 + 397x^2y^2 + 720x^2y^3 + 314x^3y^3.$$

Proof. It is clear from Fig. 2(l) that $|V(CLN)| = 81$ and $|E(CLN)| = 80$. In addition, the CLN edge set can be divided into five groups based on the number of vertices as well as $p_{12} = |E_{12}| = 6$, $p_{13} = |E_{13}| = 20$,$p_{22} = |E_{22}| = 9$,$p_{23} = |E_{23}| = 34$ and $p_{33} = |E_{33}| = 11$. Similarly, $V(CLN)$ can be divided into three classes according to the degree they possess.

$q_i = \lvert V_i \rvert$	q_1	q_2	q_3
number	26	29	26

Using Definition 1, we have

$$\overline{p}_{12} = q_1q_2 - p_{12} = 670$$

$$\overline{p}_{33} = \frac{q_3(q_3-1)}{2} - p_{33} = 314$$

Similarly, $\overline{p}_{13} = 656$, $\overline{p}_{22} = 397$ and $\overline{p}_{23} = 720$

$$\begin{aligned} Let, CIMP(CLN; x, y) &= \sum_{i\leq j} \overline{p}_{ij}(G)x^iy^j \\ &= \sum_{1\leq 2} \overline{p}_{12}(G)x^1y^2 + \sum_{1\leq 3} \overline{p}_{13}(G)x^1y^3 + \sum_{2\leq 2} \overline{p}_{22}(G)x^2y^2 \\ &+ \sum_{2\leq 3} \overline{p}_{23}(G)x^2y^3 + \sum_{3\leq 3} \overline{p}_{33}(G)x^3y^3 \\ &= 670xy^2 + 656x^1y^3 + 397x^2y^2 + 720x^2y^3 + 314x^3y^3. \end{aligned}$$

□

Proposition 5.24. *For CLN, the topological coindices are*

1. $\overline{M}_1(CLN) = 11706$.
2. $\overline{M}_2(CLN) = 12034$.
3. $\overline{mM}_2(CLN) = 807.79$.
4. $\overline{ReZG}_3(CLN) = 56800$.
5. $\overline{F}(CLN) = 28098$.
6. $\overline{R}_k(CLN) = 670(2^k) + 656(3^k) + 397(4^k) + 720(6^k) + 314(9^k)$.
7. $\overline{RR}_k(CLN) = \frac{670}{2^k} + \frac{656}{3^k} + \frac{397}{4^k} + \frac{720}{6^k} + \frac{314}{9^k}$.
8. $\overline{SDD}(CLN) = 6843.66$.
9. $\overline{H}(CLN) = 1365.82$.
10. $\overline{I}(CLN) = 2670.66$.
11. $\overline{A}(CLN) = 20086.656$.

6. Conclusion

Structural features of chemical molecules are critical for the development of innovative pharmaceutical products and they can be discovered using molecular descriptors known as topological indices and topological coindices. The degree-based topological coindices that correlate the chemical properties of the substance under study can be created in closed forms by the CIMP explained in this article. In order to verify the CIMP for these medicines, we explore a number of potential COVID-19 remedies in this work and examine their structural details. Then, a variety of degree-based topological coindices are produced using these polynomials. Our findings may aid life science researchers in their research for anticovid-19 drugs. Moreover, Fig. 1 displays the CIMP's surface representation for these drugs which displays various behaviours by varying the x and y parameters. The chemical structures of these chemical compounds are shown in Fig. 2. The many calculated topological coindices have demonstrated strong predictive power for the characteristics of these potential COVID-19 treatments.

Table 3: Topological coindices computed for the molecular graph of covid-19 drugs

$Sl.No$	$Drugs$	$\overline{M_1}$	$\overline{M_2}$	$\overline{mM_2}$	$\overline{ReZG_3}$	$\overline{F}$	$\overline{SDD}$	$\overline{H}$	$\overline{I}$	$\overline{A}$
1	ISO	1052	1201	47.8	6118	2760	546.33	94.36	241.6	1595.60
2	MN	1706	1968	76.85	10200	4546	891.65	150.22	389.7	2559.96
3	MRT	1282	1332	87.66	6274	3052	732	149.76	295.71	2264.26
4	FOD	1870	1997	118.52	9760	4634	1060.98	204.55	427.08	3141.21
5	EBD	3175	3679	140.16	18928	8375	1617.5	280	733	4887.35
6	CAB	1812	2056	82.57	10216	4616	912.65	167.3	423.4	2876.43
7	MOD	2054	2261	120.66	11508	5318	1161.66	209.36	463.51	2774.14
8	LFL	1324	1421	82.82	6940	3274	741.99	144.23	303.78	2242.37
9	AMT	5093	5598	298.99	28056	12925	2817.16	527.7	1164.85	8406.44
10	NIR	2550	2878	115.79	14148	6448	1266.72	238.06	598.95	4111.01
11	PFN	1978	2296	87.43	11680	5118	980.97	177.93	463.3	3177.46
12	CLN	11706	12034	807.79	56800	28098	6843.66	1365.82	2670.66	20086.65

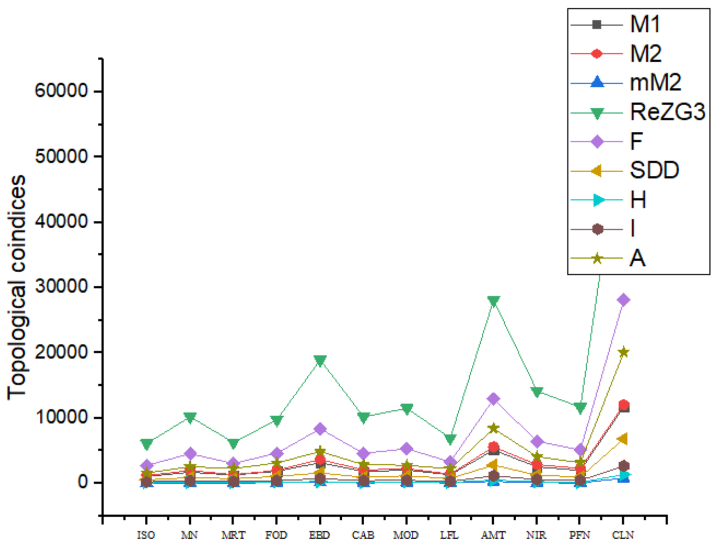

FIGURE 3. Topological coindices plot for the calculated values in table 3.

7. Conclusion

In this paper, we discovered and investigated M-polynomials corresponding to topological coindices. Maple grapichs are used to illustrate the three dimensional molecular structures in a new and different way, and these illustrations are useful in structural chemistry. We discussed a few degree-based topological coindices including the first and second Zagreb coindices, forgotten topological coindex, general Randic and inverse Randic coindices, symmetric division coindex, harmonic coindex, inverse sum indeg coindex and augmented Zagreb coindex.

Conflict of Interest. The authors hereby declare that there is no potential conflict of interest.

Acknowledgement. The last author is supported by Bursa Uludağ University Research Fund (Project No: FGA-2022-1049).

References

[1] A. R. Ashrafi, T. Doslic, A. Hamzeh, *The Zagreb coindices of graph operations*, Discrete Applied Mathematics, **158(15)** (2010), 1571–1578.

[2] B. Basavanagoud, I. Gutman, C. S. Gali, *On second Zagreb index and coindex of some derived graphs*, Kragujevac Journal of Science, **37** (2015), 113–121.

[3] B. Basavanagoud, S. Patil, *Multiplicative Zagreb indices and coindices of some derived graphs*, Opuscula Mathematica, **36(3)** (2016), 287–299.

[4] M. Berhe, C. Wang, *Computation of certain topological coindices of graphene sheet and C 4 C 8(S) nanotubes and nanotorus*, Applied Mathematics and Nonlinear Sciences, **4(2)** (2019), 455–468.

[5] B. Bollobas, P. Erdos, *Graphs of extremal weights*, Ars Comb, **50** (1998), 225–233.

[6] T. Doslic, *Vertex-weighted wiener polynomials for composite graphs*, Ars Mathematica Contemporanea, **1(1)** (2008), 66–80.

[7] E. Deutsch, S. Klavzar, *M-Polynomial, and degree-based topological indices*, Iran. J. Math. Chem., **6** (2015), 93–102.

[8] J. Devillers, A. T. Balaban, *Topological Indices and Related Descriptors in QSAR and QSPR*, Gordon and Breach, Amsterdam, (1999).

[9] B. Furtula, A. Graovac, D. Vukicević, *Augmented Zagreb index*, Journal of Mathematical Chemistry, **48(2)** (2010), 370-380.

[10] B. Furtula, I. Gutman, *A forgotten topological index*, Journal of Mathematical Chemistry, **53(4)** (2015), 1184–1190.

[11] C. K. Gupta, V. Lokesha, S. Shetty, P. S. Ranjini, *Graph Operations On The Symmetric Division Deg Index of Graphs*, Palestine Journal of Mathematics, **6(1)** (2017), 280-286.

[12] I. Gutman, *Geometric approach to degree based topological indices*, MATCH Communications in Mathematical and in Computer Chemistry, **86(1)** (2021), 11-16.

[13] I. Gutman, B. Furtula, Z. Vukicević, G. Popivoda, *On Zagreb indices and coindices*, Match, **74** (2015), 5–16.

[14] I. Gutman, N. Trinajstic, *Graph theory and molecular orbitals. Total π − electron energy of alternant hydrocarbons*, Chemical Physics Letters, **17(4)** (1972), 535-538.

[15] Harisha, P. S. Ranjini, V. Lokesha, S. Kumar, *The K. Banhatti Indices Of Certain Graphs*, Southeast Asian Bulletin Of Mathematics, **46(4)** (2022), 453-466.

[16] H. Hua, A. R. Ashrafi, L. Zhang, *More on Zagreb coindices of graphs* Filomat, **26(6)** (2012), 1215–1225.

[17] V. Lokesha, J. Sushmitha, A. S. Maragadam, *M-polynomials for subdivision graphs of antiviral drugs using in treatment of covid-19*, International Asian congress on Contemporary Sciences-V, Azerbaijan Nakhchivan State University-İksad Publications, (2021), 1005-1018.

[18] M. Manjunath, V. Lokesha, *The degree sequences of s-corona graphs*, Int. J. of Advance and innovative Research, **6(2)** (2019), 191-196.

[19] M. Manjunath, V. Lokesha, *S-corona operations of standard graphs in terms of degree sequences*, Proc. Of the Jangjeon Mathematical society, **23(2)** (2020), 149-157.

[20] A. Milicevic, S. Nikolic, N. Trinajstic, *On reformulated Zagreb indices*, **8** (2004), 393–399.

[21] K. Pattabiraman, *Inverse sum indeg index of graphs*, AKCE International Journal of Graphs and Combinatorics, **15(2)** (2018), 155-167.

[22] M. Randić, *Characterization of molecular branching*, Journal of the American Chemical Society, **97(23)** (1975), 6609–6615.

[23] P. S. Ranjini, V. Lokesha, A. Usha, *Relation between phenylene and hexagonal squeez using harmonic index*, Int J Graph Theory, **1** (2013), 116–21.

[24] P. S. Ranjini, V. Lokesha, A. Usha, T. Deepika, *Harmonic Index, Redefined Zagreb Indices of Dragon Graph with Complete Graph*, Asian Journal of Mathematics and Computer Research, **9(2)** (2016), 161-166.

[25] K. Roy, *Topological descriptors in drug design and modeling studies*, Molecular Diversity, **8(4)** (2004), 321–323.

[26] D. Vukicevic, *Bond Additive Modeling 2 Mathematical Properties of Max-Min Rodeg Index*, Croatica Chemica Acta, **54(3)** (2010), 261-273.

[27] J. Wei, M. Cancan, A. U. Rehman et al., *On topological indices of remdesivir compound used in treatment of corona virus (COVID 19)*, Polycyclic Aromatic Compounds, **45** (2021), 1–19.

[28] H. Wiener, *Correlation of heats of isomerization, and differences in heats of vaporization of isomers, among the paraffin hydrocarbons*, Journal of the American Chemical Society, **69(11)** (1947), 2636–2638.

[29] L. Zhong, *The harmonic index for graphs*, Applied Mathematics Letters, **25(3)** (2012), 561-566.

Department of Studies in Mathematics, Vijayanagara Sri Krishnadevaraya University, Ballari, Karnataka, INDIA.
Email address: v.lokesha@gmail.com

Department of Studies in Mathematics, Vijayanagara Sri Krishnadevaraya University, Ballari, Karnataka, INDIA.
Email address: maragadamvijay@gmail.com

Department of Studies in Mathematics, Vijayanagara Sri Krishnadevaraya University, Ballari, Karnataka, INDIA.
Email address: suvarnasalimath17@gmail.com

Department of Mathematics, Bursa Uludag University, Bursa 16059 Bursa-Turkey
Email address: cangul@uludag.edu.tr