



Note on Topological Indices of Hyaluronic Acid-Paclitaxel Conjugates

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Abstract: The design of drug compounds relies upon molecular structures, which contain all the information needed to determine their chemical, biological, and physical properties. A topological index is a graph theory descriptor tool that can be used to evaluate these characteristics. The topological indices of Hyaluronic Acid-Paclitaxel Conjugates were recently derived. We update their results by correcting their edge partition of Hyaluronic Acid-Paclitaxel Conjugates. Additionally, we compute M-polynomials for Hyaluronic Acid-paclitaxel conjugates and compute many degree-based topological indices via M-polynomials.

Keywords: topological indices; M-polynomial; hyaluronic acid-paclitaxel conjugate.

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1. Introduction

Developing drugs requires considerable research and time to establish their pharmacological, chemical, and biological properties. It is well established that there is a strong intrinsic correlation between drugs' chemical, pharmacological properties and their molecular structures. Due to this large amount of research has been carried out on the molecular descriptors, which play a fundamental role in chemistry and pharmaceutical sciences [1–3].

A topological index is a particular type of molecular descriptor that quantitates the molecular structure of a chemical compound. It plays a vital role in modeling many physicochemical properties in numerous quantitative structure-activity relationships (QSAR) and quantitative structure-property relationships (QSPR) studies. By doing so, researchers can find out more about the physical characteristics, chemical reactivity, and biological activity. Several applications of topological indices have been discovered in theoretical chemistry, including QSAR/QSPR research [4–6].

There are many kinds of topological indices such as degree-based, distance-based, spectral-based, counting-based; among them, degree-based topological indices have been extensively studied to determine the properties of compounds and drugs. Some of them are the Randić index, Zagreb indices, harmonic index, sum connectivity index, etc. [7–11].

Drugs are modeled as molecular graphs, consisting of each vertex representing an atom and each edge representing a chemical bond between the atoms. Let $G = (V, E)$ be a molecular graph in which $V(G)$ be a vertex set, $E(G)$ be an edge set, $|V(G)|$ be the number of vertices and

$|E(G)|$ be the number of edges, respectively. The number of vertices that are adjacent to a vertex $u \in V(G)$ is called by the degree of vertex $d(u)$ and an edge between u and v is denoted by $e = uv$, where $e \in E(G)$.

Wiener [12] introduced the topological index in QSPR, demonstrating that it was well aligned with the boiling temperatures of alkanes. In 1975, Randić proposed a structural descriptor called branching index [7] that later became a well-known Randić connectivity index (or connectivity index), one of the oldest, most popular, and most effectively used molecular descriptors in QSPR and QSAR among all other topological indices. For more on the Randić index, see [13–15].

For graph G , Randić index $R_{-1/2}(G)$ is defined as

$$R_{-1/2}(G) = \sum_{uv \in E(G)} (d(u)d(v))^{-1/2}$$

In [16] Bollabas and Erdos introduce general Randić index as

$$R_k(G) = \sum_{uv \in E} (d(u)d(v))^k, \quad k \text{ is a real number}$$

The inverse Randić index is defined as

$$RR_k(G) = \sum_{uv \in E(G)} \frac{1}{(d(u)d(v))^k}$$

Obviously $R_{-1/2}(G)$ is the particular case of $R_k(G)$ and $RR_k(G)$ when $k = -1/2$ and $k = 1/2$.

Recall that Zagreb indices are among the oldest topological indices proposed by Gutman and Trinajstić in 1972 [17]. The first and second Zagreb indices are defined as

$$M_1(G) = \sum_{uv \in E(G)} (d(u) + d(v)), \quad M_2(G) = \sum_{uv \in E(G)} d(u)d(v)$$

Later is modified in [18] as the second modified Zagreb index

$$mM_2 = \sum_{uv \in E(G)} \frac{1}{d(u)d(v)}$$

The third Zagreb index is defined as

$$M_3(G) = \sum_{uv \in E(G)} |d(u) - d(v)|$$

The F-index, or Forgotten index of a graph, was proposed by Gutman *et al.* [17] in 1972, and it was reexamined by Furtula and Gutman [19]. Redefined versions of Zagreb indices for graph G were defined by Ranjini *et al.* [20].

For comprehensive details of these indices, we refer the reader to [8,21,22].

With motivation from the Randić index, Zhou and Trinajstić [9,10] introduced a novel variant of the connectivity index known as the sum-connectivity index and general sum connectivity index defined as

$$\chi(G) = \sum_{uv \in E(G)} (d(u) + d(v))^{-1/2}$$

and

$$\chi_k(G) = \sum_{uv \in E(G)} (d(u) + d(v))^k$$

Randić index and sum connectivity index are molecular descriptors that are high inter correlated quantities; for example, the correlation coefficient values 0.99088 for 136 trees representing the lower alkanes taken from Ivanciuc *et al.* [23].

Another variant of the Randić index, named the harmonic index is first appeared in [24] and was defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d(u) + d(v)}$$

For more on the harmonic index, we refer [11]. Yan *et al.* [25] implemented the general version of a harmonic index as the extension of the harmonic index for more applications and is defined as

$$H_k(G) = \sum_{uv \in E(G)} \left(\frac{2}{d(u) + d(v)} \right)^k$$

Eliasi and Iranmanesh [26] introduced the ordinary geometric-arithmetic index $OGA_k(G)$ as the extension of geometric arithmetic index $GA(G)$ given by Vukičević and Furtula in [27] where

$$OGA_k(G) = \sum_{uv \in E(G)} \left(\frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)} \right)^k, GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d(u)d(v)}}{d(u) + d(v)}$$

The generalized Zagreb index is defined by Azari and Iranmanesh [28] as follows

$$M_{t_1, t_2}(G) = \sum_{uv \in E(G)} (d(u)^{t_1} d(v))^{t_2} + (d(u)^{t_2} d(v))^{t_1}$$

t_1 and t_2 are arbitrary positive integers.

The symmetric division index (SDD), one of the significant discrete Adriatic indexes, is defined as [29,30].

$$SDD(G) = \sum_{uv \in E(G)} \left\{ \frac{\min(d(u), d(v))}{\max(d(u), d(v))} + \frac{\max(d(u), d(v))}{\min(d(u), d(v))} \right\} = \sum_{uv \in E(G)} \frac{d^2(u) + d^2(v)}{d(u)d(v)}$$

Another discrete Adriatic index, known as an inverse sum index [29] is denoted by $I(G)$ and is defined as

$$I(G) = \sum_{uv \in E(G)} \frac{d(u)d(v)}{d(u) + d(v)}$$

In [31], Furtula *et al.* defined the augmented Zagreb index as

$$A(G) = \sum_{uv \in E(G)} \left\{ \frac{d(u)d(v)}{d(u) + d(v) - 2} \right\}^3$$

Various graph polynomials have been introduced in the literature, and several of them emerged (transpired) to be applicable in chemical graph theory. For instance, the Hosoya polynomial [32] is the key polynomial in the area of distance-based topological indices. In 2015 Deutsch and Klavžar [33] presented a polynomial known as M-polynomial whose role for degree-based invariants is parallel to the Hosoya polynomial for distance-based invariants. The main advantage of M-polynomial is its information about closed formulas of degree-based topological indices. It is the most general polynomial developed to date. For more on M-polynomial reader is requested to refer [34–38].

The M-polynomial of graph G is defined as follows

$$M(G; x, y) = \sum_{\delta \leq i \leq j \leq \Delta} m_{ij}(G) x^i y^j$$

where

$\delta = \min\{d(u) : u \in V(G)\}$, $\Delta = \max\{d(v) : v \in V(G)\}$ and

$m_{ij}(G)$ is the edge $uv \in E(G)$ s. t. $\{d(u), d(v)\} = \{i, j\}$

Table 1 below relates topological indices with M-polynomial [33].

Table 1. Relation between topological indices and M-polynomial.

<i>Topological Index</i>	<i>Derivation from M(G; x, y)</i>
First Zagreb index : $M_1(G)$	$(D_x + D_y)(M(G; x, y))_{x=y=1}$
Second Zagreb index: $M_2(G)$	$(D_x D_y)(M(G; x, y))_{x=y=1}$
Second modified Zagreb index: $mM_2(G)$	$(S_x S_y)(M(G; x, y))_{x=y=1}$
Redefined third Zagreb index: $ReZG_3(G)$	$D_x D_y (D_x + D_y)(f(x, y))_{x=y=1}$
Forgotten topological index: $F(G)$	$(D_x^2 + D_y^2)(f(x, y))_{x=y=1}$
Randić index : $R_k(G)$	$(D_x^k D_y^k)(M(G; x, y))_{x=y=1}$
Inverse Randić index: $RR_k(G)$	$(S_x^k S_y^k)(M(G; x, y))_{x=y=1}$
Symmetric Division index: $SDD(G)$	$(D_x S_y + S_x D_y)(M(G; x, y))_{x=y=1}$
Harmonic Index: $H(G)$	$(2S_x J)(M(G; x, y))_{x=1}$
Inverse sum Index: $I(G)$	$(S_x J D_x D_y)(M(G; x, y))_{x=1}$
Augmented Zagreb Index: $A(G)$	$(S_x^3 Q_{-2} J D_x^3 D_y^3)(M(G; x, y))_{x=1}$

Where,

$$D_x = x \left(\frac{\partial(f(x, y))}{\partial x} \right), \quad D_y = y \left(\frac{\partial(f(x, y))}{\partial y} \right),$$

$$S_x = \int_0^x \frac{f(t, y)}{t} dt, \quad S_y = \int_0^y \frac{f(x, t)}{t} dt,$$

$$J(f(x, y)) = f(x, x), \quad Q_k(f(x, y)) = x^k f(x, y)$$

Hyaluronic acid (HA) is a polyanionic polysaccharide that exists naturally in the body. It is a linear polymer composed of repeating units of β-1,4-D-glucuronic acid and β-1,3-N-acetylglucosamine. Its ability to selectively bind specific receptors on disease-related cells such as cancer cells and activated macrophages makes HA extensively useful in developing target carriers to deliver therapeutic and imaging agents [39–41]. Paclitaxel (PTX) is an important drug prescribed for several types many cancers[42].

HA combined with small molecular drugs such as paclitaxel (PTX), doxorubicin (DOX), curcumin, etc., increases their aqueous solubility, targetability and could be used as targeted drug delivery to enhance anti-tumor effectiveness [43–46].

For more on various Hyaluronic Acid (HA)-drugs conjugates or other conjugated anticancer drugs and their topological properties, we encourage the reader to refer [47–54].

Recently, L Zheng *et al.* [55] have investigated several topological indices of Hyaluronic Acid and Paclitaxel conjugates(HA-PTX). Figure 1 depicts the molecular structure of the HA-PTX combination. In their paper, they use incorrect topological indices expression for HA-PTX.

The next section discusses the method employed to obtain our results. In the subsequent section of this note, we update the results reported by L Zheng *et al.* [55]. We obtain the expression for M-polynomials for HA-PTX and then apply fundamental mathematics on M-polynomials to compute various degree-based indices of HA-PTX.

2. Materials and Methods

We digitally capture all of the data and materials we need for our work. The major goal of this work is to improve on the hyaluronic acid-paclitaxel conjugates results reported by L. Zheng *et al.*[55] for HA-PTX conjugates. M-polynomial for hyaluronic acid-paclitaxel conjugates is obtained afterward, and M-polynomial is used to develop various degree-based topological indices for hyaluronic acid-paclitaxel conjugates. To obtain our conclusions, we first determine the degree of each graph's vertices; then, we partition the graph's edges, which follow the same property.

3. Results and Discussion

In this note, Let G_n indicate the linear iteration of the molecular graph of HA-PTX conjugates with n units. Figures 2 and 3 show the related molecular graphs G_1 and G_3 of HA-PTX conjugates for $n = 1$ and $n = 3$, respectively. Let $E_{ij} = \{uv \in E(G_n) | d(u) = i, d(v) = j\}$

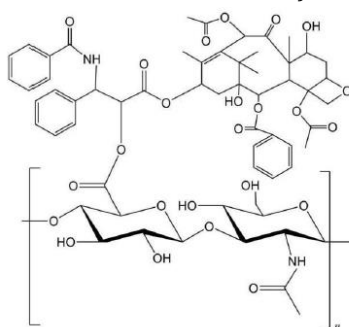


Figure 1. The chemical structure of Hyaluronic Acid-Paclitaxel Conjugates (HA-PTX).

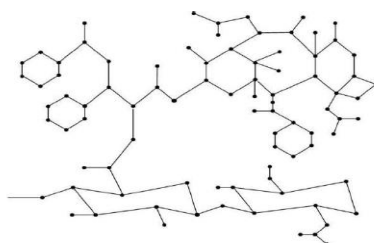


Figure 2. Corresponding molecular graph of HA-PTX G_1 ; $n = 1$.

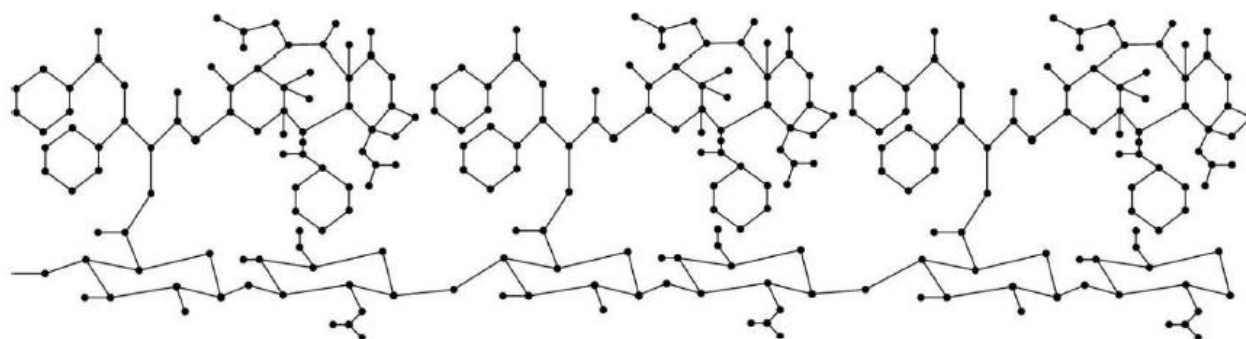


Figure 3. Corresponding molecular graph of HA-PTX G_3 ; $n = 3$.

3.1. Modification of results.

In [55] L. Zheng *et al.* obtained the following results for $R_k(G_n)$ and $\chi_k(G_n)$.

Theorem 1 [55]: For the molecular graph G_n , we have

$$R_k(G_n) = 2^k \cdot 2n + 3^k \cdot 16n + 4^k \cdot (17n + 1) + 6^k \cdot (33n - 1) + 8^k \cdot 3n + 9^k \cdot (19n - 1) + 12^k \cdot 7n + 16^k \cdot 2n.$$

$$\chi_k(G_n) = 3^k \cdot 2n + 4^k \cdot (29n + 1) + 5^k \cdot (37n - 1) + 6^k \cdot (22n - 1) + 7^k \cdot 7n + 8^k \cdot 2n.$$

To prove their theorem, they used the following edge partition of G_n

$$|E_{12}| = 2n, |E_{13}| = 16n, |E_{22}| = 13n + 1, |E_{14}| = 4n, |E_{23}| = 33n - 1, |E_{24}| = 3n; \\ |E_{33}| = 19n - 1, |E_{34}| = 7n, |E_{44}| = 2n.$$

Unfortunately, the expression in Theorem 1 is not correct. By using the above partition, $|E(G_n)| = 99n - 1$ which contradicts the claim made in the same paper that $|E(G_n)| = 96n$. Let's take an example for $n = 1$; from Figure 2, it is easy to see $|E(G_1)| = 96$, but by using the above partition $|E(G_1)| = 98$, which is a contradiction.

Now we modify the edge partition of G_n . By means of structural analysis, the edge set of G_n can be divided into nine classes as follows

$$E_{12} = \{uv \in E(G_n) | d(u) = 1, d(v) = 2\}; \\ E_{13} = \{uv \in E(G_n) | d(u) = 1, d(v) = 3\}; \\ E_{22} = \{uv \in E(G_n) | d(u) = 2, d(v) = 2\}; \\ E_{14} = \{uv \in E(G_n) | d(u) = 1, d(v) = 4\}; \\ E_{23} = \{uv \in E(G_n) | d(u) = 2, d(v) = 3\}; \\ E_{24} = \{uv \in E(G_n) | d(u) = 2, d(v) = 4\}; \\ E_{33} = \{uv \in E(G_n) | d(u) = 3, d(v) = 3\}; \\ E_{34} = \{uv \in E(G_n) | d(u) = 3, d(v) = 4\}; \\ E_{44} = \{uv \in E(G_n) | d(u) = 4, d(v) = 4\}.$$

From the molecular graph of HA-PTX (figure2 and figure 3), we obtained the following

$$|E_{12}| = n + 1, |E_{13}| = 16n, |E_{22}| = 13n + 1, |E_{14}| = 4n, |E_{23}| = 32n - 1, |E_{24}| = 3n, \\ |E_{33}| = 19n - 1, |E_{34}| = 7n, |E_{44}| = n.$$

We also have $|V(G_n)| = 87n$ and $|E(G_n)| = 96n$.

Now we have the following modified version of theorem 1

Theorem 1A: For the molecular graph G_n , we have

$$R_k(G_n) = 2^k(n + 1) + 3^k 16n + 4^k(17n + 1) + 6^k(32n - 1) + 8^k 3n + 9^k(19n - 1) + 12^k 7n + n16^k.$$

$$\chi_k(G_n) = 3^k(n + 1) + 4^k(29n + 1) + 5^k(36n - 1) + 6^k(22n - 1) + n \cdot 7^{k+1} + n8^k.$$

Proof: By the definition of the Randić index, we have

$$R_k(G_n) = \sum_{uv \in E} (d(u)d(v))^k \\ = (1.2)^k(n + 1) + (1.3)^k 16n + (2.2)^k(13n + 1) + (1.4)^k 4n + (2.3)^k(32n - 1) + \\ (2.4)^k 3n + (3.3)^k(19n - 1) + (3.4)^k 7n + (4.4)^k n \\ = 2^k(n + 1) + 3^k 16n + 4^k(17n + 1) + 6^k(32n - 1) + 8^k 3n + 9^k(19n - 1) + \\ 12^k 7n + n16^k.$$

Sum connectivity index is defined as

$$\chi_k(G_n) = \sum_{uv \in E} (d(u) + d(v))^k \\ = 3^k(n + 1) + 4^k 16n + 4^k(13n + 1) + 5^k 4n + 5^k(32n - 1) + 6^k 3n + 6^k(19n - \\ 1) + 7^k 7n + 8^k n. \\ = 3^k(n + 1) + 4^k(29n + 1) + 5^k(36n - 1) + 6^k(22n - 1) + n \cdot 7^{k+1} + n8^k.$$

The following expression for $H_k(G_n)$ also reported in [55].

Theorem 2 [55]: The general harmonic index of G_n is

$$H_k(G_n) = \left(\frac{2}{3}\right)^k \cdot 2n + \left(\frac{1}{2}\right)^k \cdot (29n + 1) + \left(\frac{2}{5}\right)^k \cdot (37n - 1) + \left(\frac{1}{3}\right)^k \cdot (22n - 1) + \left(\frac{2}{7}\right)^k \cdot 7n + \left(\frac{1}{4}\right)^k \cdot 2n.$$

The following theorem gives the modified expression of theorem 2

Theorem 2A: For the molecular graph G_n , we have

$$H_k(G_n) = \left(\frac{2}{3}\right)^k (n + 1) + \left(\frac{2}{4}\right)^k (29n + 1) + \left(\frac{2}{5}\right)^k (36n - 1) + \left(\frac{2}{6}\right)^k (22n - 1) + \left(\frac{2}{7}\right)^k \cdot 7n + \left(\frac{2}{8}\right)^k n.$$

Proof: From the definition of H_k , we have

$$\begin{aligned} H_k(G_n) &= \sum_{uv \in E} \left(\frac{2}{d(u) + d(v)}\right)^k \\ &= \left(\frac{2}{3}\right)^k (n + 1) + \left(\frac{2}{4}\right)^k 16n + \left(\frac{2}{4}\right)^k (13n + 1) + \left(\frac{2}{5}\right)^k 4n + \left(\frac{2}{5}\right)^k (32n - 1) \\ &\quad + \left(\frac{2}{6}\right)^k 3n + \left(\frac{2}{6}\right)^k (19n - 1) + \left(\frac{2}{7}\right)^k 7n + \left(\frac{2}{8}\right)^k n. \\ &= \left(\frac{2}{3}\right)^k (n + 1) + \left(\frac{2}{4}\right)^k (29n + 1) + \left(\frac{2}{5}\right)^k (36n - 1) + \left(\frac{2}{6}\right)^k (22n - 1) + \left(\frac{2}{7}\right)^k 7n + \left(\frac{2}{8}\right)^k n. \end{aligned}$$

Corollary 3:

For $k = 1$, Harmonic index

$$H(G_n) = \sum_{uv \in E} \frac{2}{d(u) + d(v)} = \frac{783}{20}n - \frac{13}{30}.$$

In a similar fashion, we present correct expressions for $OGA_k(G_n)$, $M_{t_1, t_2}(G_n)$ and $M_3(G_n)$ as follows

Theorem 4: The generalized ordinary geometric-arithmetic index, generalized Zagreb index, and third Zagreb index of G_n is

$$\begin{aligned} OGA_k(G_n) &= \left(\frac{2\sqrt{2}}{3}\right)^k (4n + 1) + \left(\frac{\sqrt{3}}{2}\right)^k 16n + \left(\frac{4}{5}\right)^k 4n + \left(\frac{2\sqrt{6}}{5}\right)^k (32n - 1) + \left(\frac{4\sqrt{3}}{7}\right)^k 7n + 33n. \\ M_{t_1, t_2}(G_n) &= (n + 1)(2^{t_1} + 2^{t_2}) + 16n(3^{t_1} + 3^{t_2}) + 4n(4^{t_1} + 4^{t_2}) + (13n + 1) \cdot 2^{t_1+t_2+1} \\ &\quad + (32n - 1)(2^{t_1} \cdot 3^{t_2} + 2^{t_2} \cdot 3^{t_1}) + 3n(2^{t_1+2t_2} + 2^{2t_1+t_2}) + 2(19n - 1)3^{t_1+t_2} \\ &\quad + 7n(3^{t_1} \cdot 4^{t_2} + 3^{t_2} \cdot 4^{t_1}) + 2n4^{t_1+t_2}. \end{aligned}$$

$$M_3(G_n) = \sum_{uv \in E} |d(u) - d(v)| = 90n.$$

We intentionally left the results for the first, second, and third Zagreb polynomials discussed in [55] as these can easily be obtained in a similar way.

3.2. Obtaining M-polynomial and derivation of degree-based topological indices.

We compute M-polynomial for the HA-PTX in the theorem that follows

Theorem 5: For the molecular graph G_n , we have

$$M(G_n; x, y) = (n + 1)xy^2 + 16nxy^3 + (13n + 1)x^2y^2 + 4nxy^4 + (32n - 1)x^2y^3 + 3nx^2y^4 + (19n - 1)x^3y^3 + 7nx^3y^4 + nx^4y^4.$$

Proof: By definition of M-polynomial

$$\begin{aligned} M(G_n; x, y) &= \sum_{\delta \leq i \leq j \leq \Delta} m_{ij}(G)x^i y^j \\ M(G_n; x, y) &= \sum_{1 \leq 2} m_{12} xy^2 + \sum_{1 \leq 3} m_{13} xy^3 + \sum_{2 \leq 2} m_{22} x^2 y^2 + \sum_{1 \leq 4} m_{14} xy^4 + \sum_{2 \leq 3} m_{23} x^2 y^3 \\ &\quad + \sum_{2 \leq 4} m_{24} x^2 y^4 + \sum_{3 \leq 3} m_{33} x^3 y^3 + \sum_{3 \leq 4} m_{34} x^3 y^4 + \sum_{4 \leq 4} m_{44} x^4 y^4. \\ &= (n + 1)xy^2 + 16nxy^3 + (13n + 1)x^2y^2 + 4nxy^4 + (32n - 1)x^2y^3 + 3nx^2y^4 \\ &\quad + (19n - 1)x^3y^3 + 7nx^3y^4 + nx^4y^4. \end{aligned}$$

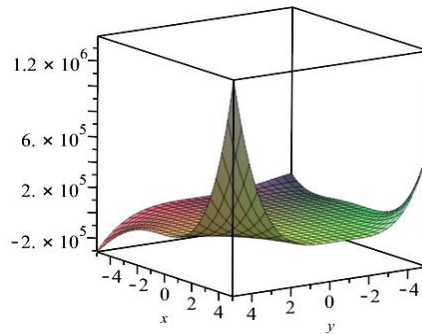


Figure 4. Plot of M-polynomial of HA-PTX [n = 1].

Using the M-polynomial for HA-PTX, we can now construct formulas for various degree-based topological indices. Expression for $R_k(G_n)$ and $H(G_n)$ can be verified from theorem 1A and corollary 3.

Proposition 6: For G_n we have

1. $M_1(G_n) = 488n - 4.$
2. $M_2(G_n) = 605n - 9.$
3. $mM_2(G_n) = 2563n - 68.$
4. $ReZG_3(G) = 3332n - 62$
5. $F(G) = 1362n - 18.$
6. $R_k(G_n) = 2^k(n + 1) + 3^k 16n + 4^k(17n + 1) + 6^k(32n - 1) + 8^k 3n + 9^k(19n - 1) + 12^k 7n + 16^k n.$
7. $RR_k(G_n) = \frac{n + 1}{2^k} + \frac{16n}{3^k} + \frac{(17n + 1)}{4^k} + \frac{(32n - 1)}{6^k} + \frac{3n}{8^k} + \frac{(19n - 1)}{9^k} + \frac{7n}{12^k} + \frac{n}{16^k}.$
8. $SDD(G_n) = \frac{973n}{4} + \frac{4}{3}.$
9. $H(G_n) = \frac{783}{20}n - \frac{13}{30}.$
10. $I(G_n) = \frac{3413n}{30} - \frac{31}{30}.$
11. $A(G_n) = 787.63n + 19.39.$

Proof: we have

$$M(G_n; x, y) = f(x, y) \\ = (n + 1)xy^2 + 16nxy^3 + (13n + 1)x^2y^2 + 4nxy^4 + (32n - 1)x^2y^3 \\ + 3nx^2y^4 + (19n - 1)x^3y^3 + 7nx^3y^4 + nx^4y^4.$$

Then

$$D_x f(x, y) = (n + 1)xy^2 + 16nxy^3 + 2(13n + 1)x^2y^2 + 4nxy^4 + 2(32n - 1)x^2y^3 \\ + 6nx^2y^4 + 3(19n - 1)x^3y^3 + 21nx^3y^4 + 4nx^4y^4.$$

$$D_y f(x, y) = 2(n + 1)xy^2 + 48nxy^3 + 2(13n + 1)x^2y^2 + 16nxy^4 + 3(32n - 1)x^2y^3 \\ + 12nx^2y^4 + 3(19n - 1)x^3y^3 + 28nx^3y^4 + 4nx^4y^4.$$

$$D_y D_x f(x, y) = 2(n + 1)xy^2 + 48nxy^3 + 4(13n + 1)x^2y^2 + 16nxy^4 + 6(32n - 1)x^2y^3 \\ + 24nx^2y^4 + 9(19n - 1)x^3y^3 + 84nx^3y^4 + 16nx^4y^4.$$

$$(D_x^2 + D_y^2)f(x, y) \\ = 5(n + 1)xy^2 + 160nxy^3 + 8(13n + 1)x^2y^2 + 68nxy^4 \\ + 13(32n - 1)x^2y^3 + 60nx^2y^4 + 18(19n - 1)x^3y^3 + 175nx^3y^4 \\ + 32nx^4y^4.$$

$$D_y D_x (D_y + D_x)f(x, y) \\ = 6(n + 1)xy^2 + 192nxy^3 + 16(13n + 1)x^2y^2 + 80nxy^4 \\ + 30(32n - 1)x^2y^3 + 144nx^2y^4 + 54(19n - 1)x^3y^3 + 588nx^3y^4 \\ + 128nx^4y^4.$$

$$D_x^k D_y^k f(x, y) \\ = 2^k(n + 1)xy^2 + 3^k 16nxy^3 + 2^{2k}(13n + 1)x^2y^2 + 4^{k+1}nxy^4 \\ + 2^k 3^k(32n - 1)x^2y^3 + 2^k 4^k 3nx^2y^4 + 3^{2k}(19n - 1)x^3y^3 + 3^k 4^k 7nx^3y^4 \\ + 4^{2k}nx^4y^4.$$

$$S_x S_y f(x, y) = (n + 1)x \frac{y^2}{2} + 16nx \frac{y^3}{3} + (13n + 1) \frac{x^2 y^2}{2 \cdot 2} + 4nx \frac{y^4}{4} + (32n - 1) \frac{x^2 y^3}{2 \cdot 3} \\ + 3n \frac{x^2 y^4}{2 \cdot 4} + (19n - 1) \frac{x^3 y^3}{3 \cdot 3} + 7n \frac{x^3 y^4}{3 \cdot 4} + n \frac{x^4 y^4}{4 \cdot 4}.$$

$$S_x^k S_y^k f(x, y) = (n + 1)x \frac{y^2}{2^k} + 16nx \frac{y^3}{3^k} + (13n + 1) \frac{x^2 y^2}{2^k 2^k} + 4nx \frac{y^4}{4^k} + (32n - 1) \frac{x^2 y^3}{2^k 3^k} \\ + 3n \frac{x^2 y^4}{2^k 4^k} + (19n - 1) \frac{x^3 y^3}{3^k 3^k} + 7n \frac{x^3 y^4}{3^k 4^k} + n \frac{x^4 y^4}{4^k 4^k}.$$

$$S_x D_y f(x, y) = 2(n + 1)xy^2 + 48nxy^3 + 2(13n + 1) \frac{x^2}{2} y^2 + 16nxy^4 + 3(32n - 1) \frac{x^2}{2} y^3 \\ + 12 \frac{x^2}{2} y^4 + 3(19n - 1) \frac{x^3}{3} y^3 + 28n \frac{x^3}{3} y^4 + 4n \frac{x^4}{4} y^4.$$

$$S_y D_x f(x, y) = (n + 1)x \frac{y^2}{2} + 16nx \frac{y^3}{3} + 2(13n + 1)x^2 \frac{y^2}{2} + 4nx \frac{y^4}{4} + 2(32n - 1)x^2 \frac{y^3}{3} \\ + 6nx^2 \frac{y^4}{4} + 3(19n - 1)x^3 \frac{y^3}{3} + 21nx^3 \frac{y^4}{4} + 4nx^4 \frac{y^4}{4}.$$

$$S_x J f(x, y) = (n + 1) \frac{x^3}{3} + (29n + 1) \frac{x^4}{4} + (36n - 1) \frac{x^5}{5} + (22n - 1) \frac{x^6}{6} + 7n \frac{x^7}{7} + n \frac{x^8}{8}.$$

$$S_x J D_y D_x f(x, y) \\ = (2n + 1) \frac{x^3}{3} + (100n + 4) \frac{x^4}{4} + (208n - 6) \frac{x^5}{5} + (195n - 9) \frac{x^6}{6} \\ + 84n \frac{x^7}{7} + 16n \frac{x^8}{8}.$$

$$S_x^3 Q_{-2} J D_x^3 D_y^3 f(x, y)$$

$$= 2^3(n+1)x + 16 \cdot 3^3 n \frac{x^2}{2^3} + 2^6(13n+1) \frac{x^3}{2^3} + 4^4 n \frac{x^3}{3^3} + 6^3(32n-1) \frac{x^3}{3^3}$$

$$+ 2^9 3n \frac{x^4}{4^3} + 3^6(19n-1) \frac{x^4}{4^3} + 12^3 7n \frac{x^5}{5^3} + 4^6 n \frac{x^6}{6^3}.$$

1. $M_1(G_n) = (D_x + D_y)f(x, y)|_{x=y=1} = 488n - 4.$
2. $M_2(G_n) = D_x D_y f(x, y)|_{x=y=1} = 605n - 9.$
3. $mM_2(G_n) = S_x S_y f(x, y)|_{x=y=1} = 2563n - 68.$
4. $ReZG_3(G_n) = D_x D_y (D_x + D_y)(f(x, y))|_{x=y=1} = 3332n - 62$
5. $F(G_n) = (D_x^2 + D_y^2)(f(x, y))|_{x=y=1} = 1362n - 18$
6. $R_k(G_n) = D_x^k D_y^k f(x, y)|_{x=y=1} = 2^k(n+1) + 3^k 16n + 4^k(17n+1) + 6^k(32n-1) + 8^k 3n + 9^k(19n-1) + 12^k 7n + n 16^k.$
7. $RR_k(G_n) = S_x^k S_y^k f(x, y)|_{x=y=1} = \frac{n+1}{2^k} + \frac{16n}{3^k} + \frac{(17n+1)}{4^k} + \frac{(32n-1)}{6^k} + \frac{3n}{8^k} + \frac{(19n-1)}{9^k} + \frac{7n}{12^k} + \frac{n}{16^k}.$
8. $SDD(G_n) = (S_y D_x + S_x D_y)f(x, y)|_{x=y=1} = \frac{973n}{4} + \frac{4}{3}.$
9. $H(G_n) = 2S_x J f(x, y)|_{x=y=1} = \frac{783}{20}n - \frac{13}{30}.$
10. $I(G_n) = S_x J D_x D_y f(x, y)|_{x=y=1} = \frac{3413n}{30} - \frac{31}{30}.$
11. $A(G_n) = S_x^3 Q_{-2} J D_x^3 D_y^3 f(x, y)|_{x=y=1} = 787.63n + 19.39.$

4. Conclusions

In this note, we have given the correct expression for several topological indices of HA-PTX. We also computed M-polynomials of HA-PTX from which we recovered eleven degree-based topological indices First and second Zagreb index, second modified Zagreb index, redefined third Zagreb index, forgotten topological index, Randić index, Inverse Randić index, Symmetric Division index, Harmonic Index, Inverse sum Index, Augmented Zagreb Index. These topological indices help us predict many properties like biological activities, chemical reactivity, and physical characteristics of the understudy HA-PTX making our results determine the significance of HA-PTX in pharmacy and industry.

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Conflicts of Interest

The authors declare that they have no conflict of interest.

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