Molecular structure investigation of anticancer drug by topological indices

M.C. Shanmukha
Department of Mathematics
Jain Institute of Technology
Davanagere-577003
India
mcshanmukha@gmail.com

N.S. Basavarajappa*
Department of Mathematics
Bapuji Institute of Engineering and Technology
Davanagere-577004
India
dr.nsbasavaraj@gmail.com

K.N. Anil Kumar
Department of Mathematics
Bapuji Institute of Engineering and Technology
Davanagere-577004
India
kn.anil5340@gmail.com

A. Usha
Department of Mathematics
Alliance College of Engineering and Design
Alliance University
Bangalore-562106
India
usha.arcot@alliance.edu.in

Abstract. The various medical observations represent that the properties of the drugs have an adjacent relation to its molecular structures. Drug properties will be determined by analysing and investigating the corresponding molecular structures of the drug. In chemical graph theory, topological index is one of the significant tools which is applied to understand the properties of a chemical compound. Topological indices defined on these chemical molecular structures can help researchers to better understand the physical features, chemical re-activities and biological activities. This work is to demonstrate various topological indices on anticancer drug, Hyaluronic acid (HA) used in the manufacturing of anticancer drugs.

Keywords: atom bond connectivity (ABC) indices, symmetric division index (SDD), F−indices, multiplicative F−indices, F−polynomial indices, anticancer drug.

∗. Corresponding author

1. Introduction

In today's scenario, one of the main ailments that is alarming and fatal is cancer. As improved the pharmaceutical technology improved in several countries, new tremendous anticancer drugs are synthesized in the laboratory. They are tested and released in the market for public. Earlier many examinations were needed to analyse the new drugs to determine the biological characteristic, percentage of toxicity and side-effects on the human anatomy. Consequently, there was more work-load in the laboratories which resulted in various problems in the countries having least financial and worst laboratory situations.

The graph theory offers experts with the powerful tool, i.e. topological indices. In the early chemical experiments, experts compared a vast quantity of experimented results with the compound structure. It was concluded that the atom structure ordering of a compound had inherent relationship with the properties it exhibited. Based on these facts, using the interpretation of the topological indices on the compounds and the respective characteristics, the compounds were used in the drug design in medicine and pharmaceutical science fields. In the computation model, atoms are denoted as vertices and also link between each atom is represented as an edge between two vertices. A graph derived from a chemical compound is called a molecular graph.

This is an attempt to the application of graph theory in anticancer drugs. In this work, the drugs are taken and using the degree based calculations, few topological indices are computed.

Here, anticancer drug considered is Hyaluronic acid(HA), in which paclitaxel conjugate molecular structure is studied. The compound which is available naturally is HA. HA is also called as hyaluronan. It is very unique form in the plasma membrane instead of the Golgi Apparatus. HA contributes most importantly to cell multiplication and relocation. It helps in the development of fewer malignant tumours [8]. HA is a robust anticancer drug because of its distinct, biodegradable, bio-compatible, non-toxic, hydro-philic and non-immutable characters. Also, HA present in organs are experimented using expression on many of the tumour cells. Because of the fast improving competition, the main goal is to manufacture drugs containing HA for cancer treatments [15]. HA is an efficient drug bearer. The constructive drugs which are mostly used in various categories of cancers like ovarian, breast, lung and bladder is Paclitaxel (PTX). PTX has its own disadvantages, they are less soluble and has side effects. Ringsdorf introduced the concept of developing polymeric conjugate, outlined to provide small hydrophobic drug molecules to their sites of action. The important benefits of Hyaluronic acid-Paclitaxel (HA-PTX) conjugate are in the water solubility and recovery of anti tumour efficiently.

The topological index is described as a non-empirical numerical measure, which represent molecular structures and its branching pattern. And also at this end, topological indices will map each molecule structure to a real number and used as a descriptor of a molecule under testing. Various important indices are

applicable in chemical-engineering (e.g., QSPR/QSAR study) for establishing relationship between the molecular structures and the physical and chemical characters (see, [1, 5, 15, 18, 21]).

Usually, the chemical compound is modelled as a graph by considering the atoms as the vertex set and the links connecting them as the edge set (see, [16, 19, 20, 22]). In a similar fashion, these anticancer drugs under this study are considered as chemical compounds and the said topological indices (TI's) are determined.

Applications of graph theory are QSAR, QSPR and QSTR where chemists or pharmacists are welcome to use this data for further research study. There are several degree based indices introduced to test the properties of compounds and drugs, which are used in the manufacture of anticancer drugs.

All the graphs used in this paper are simple graphs, i.e. cycle free and not directed ([5]).

Let $G = (V(G), E(G))$ be a molecular graph, where $V(G)$ and $E(G)$ are vertices and edges which corresponds to atoms set and chemical bonds set.

Definition 1.1. For a graph G, the first $F-index$ and second $F-$index [4, 12], are defined respectively as

$$F_1(G) = \sum_{e=uv\in E(G)} \big[(d_G(u))^2 + (d_G(v))^2\big],$$
$$F_2(G) = \sum_{e=uv\in E(G)} \big[(d_G(u))^2 \times (d_G(v))^2\big].$$

Definition 1.2. The multiplicative first $F-$index was introduced by Bhanumathi [2] and Ghobadi [6], is defined as

$$F_1II(G) = \prod_{e=uv\in E(G)} \big[(d_G(u))^2 + (d_G(v))^2\big].$$

Definition 1.3. For a graph G, the second multiplicative F-index [12] is defined as

$$F_2II(G) = \prod_{e=uv\in E(G)} \big[(d_G(u))^2 \times (d_G(v))^2\big].$$

Definition 1.4. The multiplicative first and second hyper F-index [11, 12] for a graph G are

$$HF_1II(G) = \prod_{e=uv\in E(G)} \big[(d_G(u))^2 + (d_G(v))^2\big]^2,$$
$$HF_2II(G) = \prod_{e=uv\in E(G)} \big[(d_G(u))^2 \times (d_G(v))^2\big]^2.$$

Definition 1.5. For a graph G, both multiplicative sum connectivity and multiplicative product connectivity F-indices [12] are

$$SFII(G) = \prod_{e=uv\in E(G)} \frac{1}{\sqrt{(d_G(u))^2 + (d_G(v))^2}},$$
$$PFII(G) = \prod_{e=uv\in E(G)} \frac{1}{\sqrt{(d_G(u))^2 \times (d_G(v))^2}}.$$

Definition 1.6. For a graph G, general multiplicative first and second F-indices are stated [12, 13] as

$$F_1^k II(G) = \prod_{e=uv\in E(G)} \left[(d_G(u))^2 + (d_G(v))^2\right]^k,$$
$$F_2^k II(G) = \prod_{e=uv\in E(G)} \left[(d_G(u))^2 \times (d_G(v))^2\right]^k.$$

Definition 1.7. The multiplicative atom bond connectivity F-index [12, 14] for a graph G is

$$ABCFII(G) = \prod_{e=uv\in E(G)} \sqrt{\frac{(d_G(u))^2 + (d_G(v))^2 - 2}{(d_G(u))^2 \times (d_G(v))^2}}.$$

Definition 1.8. For a graph G, multiplicative geometric arithmetic F-index [12] can be defined as

$$GAFII(G) = \prod_{e=uv\in E(G)} \frac{2\sqrt{(d_G(u))^2 \times (d_G(v))^2}}{(d_G(u))^2 + (d_G(v))^2}.$$

Definition 1.9. Ghobadi et al., defined the first F- polynomial [6] of a graph as

$$F_1(G,x) = \sum_{e=uv\in E(G)} x^{(d_G(u))^2+(d_G(v))^2}.$$

Definition 1.10. The second F-polynomial, the first and second hyper F-polynomial [6, 13] of a graph are stated as

$$F_2(G,x) = \sum_{e=uv\in E(G)} x^{(d_G(u))^2\times(d_G(v))^2},$$
$$HF_1(G,x) = \sum_{e=uv\in E(G)} x^{\left[(d_G(u))^2+(d_G(v))^2\right]^2},$$
$$HF_2(G,x) = \sum_{e=uv\in E(G)} x^{\left[(d_G(u))^2\times(d_G(v))^2\right]^2}.$$

Definition 1.11. Consider a molecular graph $G = (V, E)$, $d_G(u)$ is the vertex degree of u and $d_G(v)$ is the vertex degree of v then ABC index [7] can be stated as

$$ABC(G) = \sum_{e=uv \in E(G)} \left[\sqrt{\frac{(d_G(u) + d_G(v) - 2)}{(d_G(u)) \times (d_G(v))}} \right].$$

Definition 1.12. In chemical graph theory field, there are some new degree based graph types, which plays an important role. These topological indices are required for finding total surface area and heat-formation of various chemical compounds. These graphs types are as follow symmetric division index [9],

$$SSD(G) = \sum_{e=uv \in E(G)} \left[\frac{P}{Q} + \frac{Q}{P} \right],$$

where $P = \min [d_G(u), d_G(v)]$ and $Q = \max [d_G(u), d_G(v)]$.

In section 2, main results obtained are highlighted with detail proofs and the calculations of topological indices on the family of molecular graphs.

2. Results and discussions

In this segment, our goal is to represent few topological indices of HA-paclitaxel conjugates. The important method used here separates links which results the molecular structure graph in to few parts. In the below discussions, consider G_n as the molecular graph of HA-PTX conjugates with n units of linear iteration. In Figure 2 and 3 denotes their equivalent molecular graphs G_1 and G_3 with $n = 1$ and $n = 3$.

By considering the graph representation and computation, the vertex set and the edge set are respectively $|V(G_n)|$=87n and $|E(G_n)|$=96n.

If δ and Δ are the lowest and highest degrees of the graph G_n, respectively describes:

(i) $E_i = \{e = uv \in E(G_n)/d_G(u) + d_G(v) = i\}$, for every i with $2\delta \leq i \leq 2\Delta$;

(ii) $E_j^* = \{e = uv \in E(G_n)/d_G(u) \times d_G(v) = j\}$, for every j with $\delta^2 \leq j \leq \Delta^2$.

In specific, the sets E_i and E_j^* might be non-empty. Now with Δ= 4 and $\delta \geq 1$, we notice that the G_n sides can be degraded with the following subsets according to E_i and E_j^* definitions:

(i) $E_3 = E_2^* : d_G(u) = 1$ and $d_G(v) = 2$;

(ii) $E_{4,1} = E_3^* : d_G(u) = 1$ and $d_G(v) = 3$;

(iii) $E_{5,1} = E_{4,1}^* : d_G(u) = 1$ and $d_G(v) = 4$;

(iv) $E_{4,2} = E_{4,2}^* : d_G(u) = 2$ and $d_G(v) = 2$;

(v) $E_{5,2} = E_6^* : d_G(u) = 2$ and $d_G(v) = 3$;

(vi) $E_{6,1} = E_8^* : d_G(u) = 2$ and $d_G(v) = 4$;

(vii) $E_{6,2} = E_9^* : d_G(u) = d_G(v) = 3$;

(viii) $E_7 = E_{12}^* : d_G(u) = 3$ and $d_G(v) = 4$;

(ix) $E_8 = E_{16}^* : d_G(u) = d_G(v) = 4$.

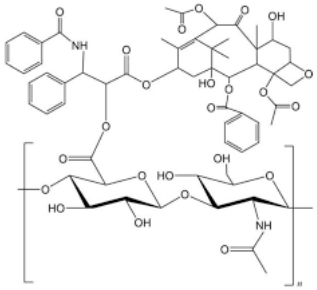

Figure 1: The HA-PTX conjugate molecular structure.

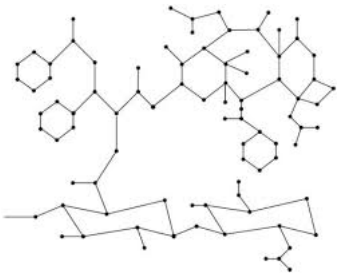

Figure 2: The corresponding molecular graph G_1: n = 1.

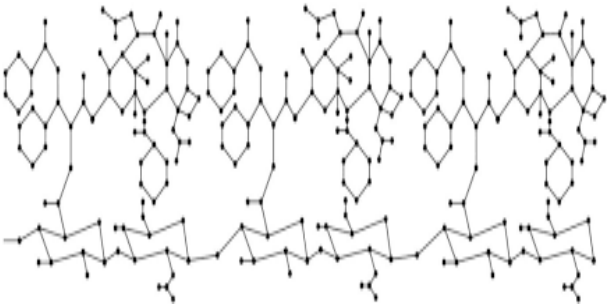

Figure 3: The corresponding molecular graph G_3: n = 3.

Theorem 2.1. *The general multiplicative first F-index of HA-PTX conjugates with n units linear iteration, denoted by molecular graph G_n, is given by*

$$F_1^K II(G_n) = 5^{k(35n)} \times 2^{k(90n+2)} \times 9^{k(19n-1)} \times 13^{k(33n-1)} \times 17^{k(4n)}.$$

Proof. Using the graph representation studies and observations, it is easy to define $|E_3| = |E_2^*| = 2n$, $|E_{4,1} \cap E_3^*| = 16n$, $|E_{5,1} \cap E_{4,1}^*| = 4n$, $|E_{4,2}| = |E_{4,2}^*| = 13n + 1$, $|E_{5,2}| = |E_6^*| = 33n - 1$, $|E_{6,1} \cap E_8^*| = 3n$, $|E_{6,2} \cap E_9^*| = 19n - 1$, $|E_7 \cap E_{12}^*| = 7n$ and $|E_8| = |E_{16}^*| = 2n$. For a graph G_n, the general multiplicative first F- index is

$$\begin{aligned}
F_1^k II(G_n) &= \prod_{e=uv \in E(G)} \left[(d_G(u))^2 + (d_G(v))^2\right]^k \\
&= \prod_{uv \in E_3} \left[(1)^2 + (2)^2\right]^k \times \prod_{uv \in E_3^*} \left[(1)^2 + (3)^2\right]^k \times \prod_{uv \in E_{4,1}^*} \left[(1)^2 + (4)^2\right]^k \\
&\quad \times \prod_{uv \in E_{4,2}} \left[(2)^2 + (2)^2\right]^k \times \prod_{uv \in E_6^*} \left[(2)^2 + (3)^2\right]^k \times \prod_{uv \in E_8^*} \left[(2)^2 + (4)^2\right]^k \\
&\quad \times \prod_{uv \in E_9^*} \left[(3)^2 + (3)^2\right]^k \times \prod_{uv \in E_{12}^*} \left[(3)^2 + (4)^2\right]^k \times \prod_{uv \in E_{16}^*} \left[(4)^2 + (4)^2\right]^k \\
&= 5^{k(35n)} \times 2^{k(90n+2)} \times 9^{k(19n-1)} \times 13^{k(33n-1)} \times 17^{k(4n)}.
\end{aligned}$$

□

We get the following results by using Theorem 2.1.

Corollary 2.1. *The multiplicative first F- index of a graph G_n is*

$$F_1 II(G_n) = 5^{(35n)} \times 2^{(90n+2)} \times 9^{(19n-1)} \times 13^{(33n-1)} \times 17^{(4n)}.$$

Proof. Put $k = 1$ in Theorem 2.1, we obtain the desired result. □

Corollary 2.2. *The multiplicative first hyper F- index of a graph G_n is*

$$HF_1 II(G_n) = 5^{(70n)} \times 2^{(180n+4)} \times 9^{(38n-2)} \times 13^{(66n-2)} \times 17^{(8n)}.$$

Proof. Put $k = 2$ in Theorem 2.1, we obtain the desired result. □

Corollary 2.3. *The multiplicative sum connectivity F- index of a graph G_n is*

$$SFII(G_n) = \left(\frac{1}{\sqrt{5}}\right)^{35n} \times \left(\frac{1}{\sqrt{2}}\right)^{90n+2} \times \left(\frac{1}{\sqrt{9}}\right)^{19n-1} \times \left(\frac{1}{\sqrt{13}}\right)^{33n-1} \times \left(\frac{1}{\sqrt{17}}\right)^{4n}.$$

Proof. Put $k = \frac{-1}{2}$ in Theorem 2.1, we get the desired result. □

Theorem 2.2. *The general multiplicative second F- index of a graph G_n is*

$$F_2^K II(G_n) = 4^{k(100n-1)} \times 9^{k(78n-3)}$$

Proof.

$$\begin{aligned}
F_2^k II(G_n) &= \prod_{e=uv\in E(G)} \left[(d_G(u))^2 \times (d_G(v))^2\right]^k \\
&= \prod_{uv\in E_3} \left[(1)^2(2)^2\right]^k \times \prod_{uv\in E_3^*} \left[(1)^2(3)^2\right]^k \times \prod_{uv\in 4,1^*} \left[(1)^2(4)^2\right]^k \\
&\quad \times \prod_{uv\in E_{4,2}} \left[(2)^2(2)^2\right]^k \times \prod_{uv\in E_6^*} \left[(2)^2(3)^2\right]^k \times \prod_{uv\in E_8^*} \left[(2)^2(4)^2\right]^k \\
&\quad \times \prod_{uv\in E_9^*} \left[(3)^2(3)^2\right]^k \times \prod_{uv\in E_{12}^*} \left[(3)^2(4)^2\right]^k \times \prod_{uv\in E_{16}^*} \left[(4)^2(4)^2\right]^k \\
&= 4^{k(100n-1)} \times 9^{k(78n-3)}.
\end{aligned}$$

□

The following results are obtained by using Theorem 2.2.

Corollary 2.4. *The multiplicative second F- index of a graph G_n is*

$$F_2 II(G_n) = 4^{(100n-1)} \times 9^{(78n-3)}.$$

Proof. Put $k = 1$ in Theorem 2.2, we get the required result. □

Corollary 2.5. *The multiplicative second hyper F- index of a graph G_n is*

$$HF_2 II(G_n) = 4^{(200n-2)} \times 9^{(156n-6)}.$$

Proof. Put $k = 2$ in Theorem 2.2, we get the required result. □

Corollary 2.6. *The multiplicative product connectivity F- index of a graph G_n is*

$$PFII(G_n) = \left(\frac{1}{\sqrt{4}}\right)^{100n-1} \times \left(\frac{1}{\sqrt{9}}\right)^{78n-3}.$$

Proof. Put $k = \frac{-1}{2}$in Theorem 2.2, we get the required result. □

Theorem 2.3. *The multiplicative atom bond connectivity F- index of a graph G_n is*

$$\begin{aligned}
ABCFII(G_n) &= \left(\sqrt{\frac{3}{4}}\right)^{2n} \times \left(\sqrt{\frac{8}{9}}\right)^{16n} \times \left(\sqrt{\frac{15}{16}}\right)^{4n} \\
&\quad \times \left(\sqrt{\frac{6}{16}}\right)^{13n+1} \times \left(\sqrt{\frac{11}{36}}\right)^{33n-1} \\
&\quad \times \left(\sqrt{\frac{18}{64}}\right)^{3n} \times \left(\sqrt{\frac{16}{81}}\right)^{19n-1} \times \left(\sqrt{\frac{23}{144}}\right)^{7n} \times \left(\sqrt{\frac{30}{256}}\right)^{2n}.
\end{aligned}$$

Proof.

$$ABCFII(G_n) = \prod_{e=uv\in E(G)} \left[\sqrt{\frac{(d_G(u))^2+(d_G(v))^2-2}{(d_G(u))^2\times(d_G(v))^2}}\right]$$
$$= \left(\sqrt{\frac{(1)^2+(2)^2-2}{(1)^2(2)^2}}\right)^{2n} \times \left(\sqrt{\frac{(1)^2+(3)^2-2}{(1)^2(3)^2}}\right)^{16n} \times \left(\sqrt{\frac{(1)^2+(4)^2-2}{(1)^2(4)^2}}\right)^{4n}$$
$$\times\left(\sqrt{\frac{(2)^2+(2)^2-2}{(2)^2(2)^2}}\right)^{13n+1} \times\left(\sqrt{\frac{(2)^2+(3)^2-2}{(2)^2(3)^2}}\right)^{33n-1} \times\left(\sqrt{\frac{(2)^2+(4)^2-2}{(2)^2(4)^2}}\right)^{3n}$$
$$\times \left(\sqrt{\frac{(3)^2+(3)^2-2}{(3)^2(3)^2}}\right)^{19n-1} \times \left(\sqrt{\frac{(3)^2+(4)^2-2}{(3)^2(4)^2}}\right)^{7n} \times \left(\sqrt{\frac{(4)^2+(4)^2-2}{(4)^2(4)^2}}\right)^{2n}$$
$$=\left(\sqrt{\frac{3}{4}}\right)^{2n} \times\left(\sqrt{\frac{8}{9}}\right)^{16n} \times\left(\sqrt{\frac{15}{16}}\right)^{4n} \times\left(\sqrt{\frac{6}{16}}\right)^{13n+1} \times\left(\sqrt{\frac{11}{36}}\right)^{33n-1} \times\left(\sqrt{\frac{18}{64}}\right)^{3n}$$
$$\times \left(\sqrt{\frac{16}{81}}\right)^{19n-1} \times \left(\sqrt{\frac{23}{144}}\right)^{7n} \times \left(\sqrt{\frac{30}{256}}\right)^{2n}.$$

□

Theorem 2.4. *The multiplicative geometric-arithmetic F- index of a graph G_n is*

$$\left(\frac{24}{25}\right)^{2n} \times \left(\frac{12}{13}\right)^{16n} \times \left(\frac{4}{5}\right)^{4n} \times \left(\frac{3}{5}\right)^{33n-1} \times \left(\frac{8}{17}\right)^{3n}.$$

Proof.

$$GAFII(G_n) = \prod_{e=uv\in E(G)} \frac{2\sqrt{(d_G(u))^2\times(d_G(v))^2}}{(d_G(u))^2+(d_G(v))^2}$$
$$= \left(\frac{2\sqrt{(1)^2(2)^2}}{(1)^2+(2)^2}\right)^{2n} \times \left(\frac{2\sqrt{(1)^2(3)^2}}{(1)^2+(3)^2}\right)^{16n} \times \left(\frac{2\sqrt{(1)^2(4)^2}}{(1)^2+(4)^2}\right)^{4n}$$
$$\times \left(\frac{2\sqrt{(2)^2(2)^2}}{(2)^2+(2)^2}\right)^{13n+1} \times \left(\frac{2\sqrt{(2)^2(3)^2}}{(2)^2+(3)^2}\right)^{33n-1} \times \left(\frac{2\sqrt{(2)^2(4)^2}}{(2)^2+(4)^2}\right)^{3n}$$
$$\times \left(\frac{2\sqrt{(3)^2(3)^2}}{(3)^2+(3)^2}\right)^{19n-1} \times \left(\frac{2\sqrt{(3)^2(4)^2}}{(3)^2+(4)^2}\right)^{7n} \times \left(\frac{2\sqrt{(4)^2(4)^2}}{(4)^2+(4)^2}\right)^{2n}$$
$$= \left(\frac{24}{25}\right)^{2n} \times \left(\frac{12}{13}\right)^{16n} \times \left(\frac{4}{5}\right)^{4n} \times \left(\frac{3}{5}\right)^{33n-1} \times \left(\frac{8}{17}\right)^{3n}.$$

□

Theorem 2.5. *For the graph G_n, the first F- polynomial is*

$$(2n)x^5 + (16n)x^{10} + (4n)x^{17} + (13n+1)x^8 + (33n-1)x^{13} + (3n)x^{20} + (19n-1)x^{18} + (7n)x^{25} + (2n)x^{32}.$$

Proof.

$$\begin{aligned}
F_1(G_n, x) &= \sum_{e=uv\in E(G)} x^{(d_G(u))^2+(d_G(v))^2} \\
&= (2n)\left[x^{(1+4)}\right] + (16n)\left[x^{(1+9)}\right] + (4n)\left[x^{(1+16)}\right] + (13n+1)\left[x^{(4+4)}\right] \\
&+ (33n-1)\left[x^{(4+9)}\right] + (3n)\left[x^{(4+16)}\right] + (19n-1)\left[x^{(9+9)}\right] + (7n)\left[x^{(9+16)}\right] \\
&+ (2n)\left[x^{(16+16)}\right] \\
&= (2n)x^5 + (16n)x^{10} + (4n)x^{17} + (13n+1)x^8 + (33n-1)x^{13} + (3n)x^{20} \\
&+ (19n-1)x^{18} + (7n)x^{25} + (2n)x^{32}.
\end{aligned}$$

□

Theorem 2.6. *For the graph G_n, the second F- polynomial is*

$$(2n)x^4 + (16n)x^9 + (17n+1)x^{16} + (33n-1)x^{36} + (3n)x^{64} + (19n-1)x^{81} + (7n)x^{144} + (2n)x^{256}.$$

Proof.

$$\begin{aligned}
F_2(G_n, x) &= \sum_{e=uv\in E(G)} x^{(d_G(u))^2\times(d_G(v))^2} \\
&= (2n)\left[x^{(1)(4)}\right] + (16n)\left[x^{(1)(9)}\right] + (4n)\left[x^{(1)(16)}\right] + (13n+1)\left[x^{(4)(4)}\right] \\
&+ (33n-1)\left[x^{(4)(9)}\right] + (3n)\left[x^{(4)(16)}\right] + (19n-1)\left[x^{(9)(9)}\right] + (7n)\left[x^{(9)(16)}\right] \\
&+ (2n)\left[x^{(16)(16)}\right] \\
&= (2n)x^4 + (16n)x^9 + (17n+1)x^{16} + (33n-1)x^{36} + (3n)x^{64} \\
&+ (19n-1)x^{81} + (7n)x^{144} + (2n)x^{256}.
\end{aligned}$$

□

Theorem 2.7. *For the graph G_n, the first hyper F- polynomial is*

$$(2n)x^{10} + (16n)x^{20} + 4n(x^{34}) + (13n+1)x^{16} + (33n-1)x^{26} + (3n)x^{40} + (19n-1)x^{36} + (7n)x^{50} + (2n)x^{64}.$$

Proof.

$$HF_1(G_n, x) = \sum_{e=uv\in E(G)} x^{\left[(d_G(u))^2+(d_G(v))^2\right]^2}$$
$$= (2n)\left[x^{(1+4)^2}\right] + (16n)\left[x^{(1+9)^2}\right] + (4n)\left[x^{(1+16)^2}\right] + (13n+1)\left[x^{(4+4)^2}\right]$$
$$+ (33n-1)\left[x^{(4+9)^2}\right] + (3n)\left[x^{(4+16)^2}\right] + (19n-1)\left[x^{(9+9)^2}\right] + (7n)\left[x^{(9+16)^2}\right]$$
$$+ (2n)\left[x^{(16+16)^2}\right]$$
$$= (2n)x^{10} + (16n)x^{20} + 4n(x^{34}) + (13n+1)x^{16} + (33n-1)x^{26} + (3n)x^{40}$$
$$+ (19n-1)x^{36} + (7n)x^{50} + (2n)x^{64}.$$

□

Theorem 2.8. *For the graph, G_n the second hyper F- polynomial is*

$$(2n)x^8 + (16n)x^{18} + (17n+1)x^{32} + (33n-1)x^{72} + (3n)x^{128} + (19n-1)x^{162}$$
$$+ (7n)x^{288} + (2n)x^{512}.$$

Proof.

$$HF_2(G_n, x) = \sum_{e=uv\in E(G)} x^{\left[(d_G(u))^2\times(d_G(v))^2\right]^2}$$
$$= (2n)\left[x^{(1)(4)}\right]^2 + (16n)\left[x^{(1)(9)}\right]^2 + (4n)\left[x^{(1)(16)}\right]^2 + (13n+1)\left[x^{(4)(4)}\right]^2$$
$$+ (33n-1)\left[x^{(4)(9)}\right]^2 + (3n)\left[x^{(4)(16)}\right]^2 + (19n-1)\left[x^{(9)(9)}\right]^2 + (7n)\left[x^{(9)(16)}\right]^2$$
$$+ (2n)\left[x^{(16)(16)}\right]^2$$
$$= (2n)x^8 + (16n)x^{18} + (17n+1)x^{32} + (33n-1)x^{72} + (3n)x^{128} + (19n-1)x^{162}$$
$$+ (7n)x^{288} + (2n)x^{512}.$$

□

Theorem 2.9. *For a graph G_n, The ABC index will be*

$$ABC(G_n) = 38n - \frac{18}{27}.$$

Proof.

$$ABC(G_n) = \sum_{e=uv\in E(G)} \left[\sqrt{\frac{(d_G(u)+d_G(v)-2)}{(d_G(u))(d_G(v))}}\right]$$
$$= \sum_{uv\in E_3} \left[\sqrt{\frac{(1+2-2)}{(1)(2)}}\right] + \sum_{uv\in E_3^*} \left[\sqrt{\frac{(1+3-2)}{(1)(3)}}\right] + \sum_{uv\in E_{4,1}^*} \left[\sqrt{\frac{(1+4-2)}{(1)(4)}}\right]$$

$$+\sum_{uv\in E_{4,2}}\left[\sqrt{\frac{(2+2-2)}{(2)(2)}}\right]+\sum_{uv\in E_6^*}\left[\sqrt{\frac{(2+3-2)}{(2)(3)}}\right]+\sum_{uv\in E_8^*}\left[\sqrt{\frac{(2+4-2)}{(2)(4)}}\right]$$
$$+\sum_{uv\in E_9^*}\left[\sqrt{\frac{(3+3-2)}{(3)(3)}}\right]+\sum_{uv\in E_{12}^*}\left[\sqrt{\frac{(3+4-2)}{(3)(4)}}\right]+\sum_{uv\in E_{16}^*}\left[\sqrt{\frac{(4+4-2)}{(4)(4)}}\right]$$
$$=51n\left(\sqrt{\frac{1}{2}}\right)+16n\left(\sqrt{\frac{2}{3}}\right)+4n\left(\sqrt{\frac{3}{4}}\right)+(19n-1)\left(\sqrt{\frac{4}{9}}\right)+(7n)\left(\sqrt{\frac{5}{12}}\right)$$
$$+(2n)\left(\sqrt{\frac{6}{16}}\right)$$
$$ABC(G_n)=38n-\frac{18}{27}.$$

□

Theorem 2.10. *The symmetric division index for a graph G_n is $SDD(G_n)=\frac{2369n}{10}-\frac{21}{10}$.*

Proof.

$$SSD(G_n)=\sum_{e=uv\in E(G)}\left[\frac{P(d_G(u),d_G(v))}{Q(d_G(u),d_G(v))}+\frac{Q(d_G(u),d_G(v))}{P(d_G(u),d_G(v))}\right]$$
$$=\sum_{uv\in E_3}\left[\frac{P(1,2)}{Q(1,2)}+\frac{Q(1,2)}{P(1,2)}\right]+\sum_{uv\in E_3^*}\left[\frac{P(1,3)}{Q(1,3)}+\frac{Q(1,3)}{P(1,3)}\right]$$
$$+\sum_{uv\in E_{4,1}^*}\left[\frac{P(1,4)}{Q(1,4)}+\frac{Q(1,4)}{P(1,4)}\right]+\sum_{uv\in E_{4,2}}\left[\frac{P(2,2)}{Q(2,2)}+\frac{Q(2,2)}{P(2,2)}\right]$$
$$+\sum_{uv\in E_6^*}\left[\frac{P(2,3)}{Q(2,3)}+\frac{Q(2,3)}{P(2,3)}\right]+\sum_{uv\in E_8^*}\left[\frac{P(2,4)}{Q(2,4)}+\frac{Q(2,4)}{P(2,4)}\right]$$
$$+\sum_{uv\in E_9^*}\left[\frac{P(3,3)}{Q(3,3)}+\frac{Q(3,3)}{P(3,3)}\right]+\sum_{uv\in E_{12}*}\left[\frac{P(3,4)}{Q(3,4)}+\frac{Q(3,4)}{P(3,4)}\right]$$
$$+\sum_{uv\in E_{16}*}\left[\frac{P(4,4)}{Q(4,4)}+\frac{Q(4,4)}{P(4,4)}\right]$$
$$=2n\left(\frac{5}{2}\right)+16n\left(\frac{10}{3}\right)+4n\left(\frac{17}{4}\right)+(13n+1)(2)$$
$$+(33n-1)\left(\frac{13}{6}\right)+3n\left(\frac{20}{8}\right)$$
$$+(19n-1)(2)+7n\left(\frac{25}{12}\right)+2n(2)=\frac{2369n}{10}-\frac{21}{10}.$$

□

3. Conclusion

The main goal of this work is to demonstrate various topological indices on HA-PTX, an anticancer drug using molecular structure analysis and computations. Various indices are represented as expressions to link the chemical structure of drugs with the physical characteristics. The results obtained here helps the experts to decide the characteristics of the drugs used in the treatment of threatening ailment cancer. Experimental set up is not required as the topological indices help to determine physico-chemical properties of anticancer drugs. Topological indices have many advantages over conducting the experiments.

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