

DEGREE-BASED TOPOLOGICAL INDICES OF DOX-LOADED PEG-PASP POLYMER

By

M. C. Shanmukha¹, N. S. Basavarajappa², K. N. Anil Kumar³ and A. Usha⁴

¹Department of Mathematics,

Jain Institute of Technology, Davanagere-577003, Karnataka, India
and affiliated to Visvesvaraya Technological University, Belagavi, Karnataka, India

Email:mcshanmukha@gmail.com

^{2,3}Department of Mathematics,

Bapuji Institute of Engineering and Technology, Davanagere-577004, Karnataka, India
and affiliated to Visvesvaraya Technological University, Belagavi, Karnataka, India

Email:dr.nsbasavaraj@gmail.com, kn.anil5340@gmail.com

⁴Department of Mathematics,

Alliance College of Engineering and Design, Alliance University,
Anekal-Chandapura Road, Bangalore-562106, Karnataka, India

Email:usha.arcot@alliance.edu.in

(Received : February 13, 2020 ; Revised: May 02, 2020)

DOI: <https://doi.org/10.58250/jnanabha.2020.50111>

Abstract

The drugs which are effective for malignant disease are anticancer drugs. They are also called antineoplastic. Anti cancer drugs are classified into several classes which include alkylating agents, hormones and anti metabolites. Studies reveal the fact that, there will be an intrinsic relationship with the properties of alkanes and also drugs(e.g., Boiling Point-BP and Melting Point-MP) with its chemical structure. In this paper, various topological indices are defined on the drug to assist the researchers for better understanding of physical properties and chemical reactions. Here the topological indices are defined and computed for an anticancer drug .

2010 Mathematics Subject Classifications: 05C05, 05C12, 05C35.

Keywords and phrases: Atom Bond Connectivity (ABC) indices, Symmetric division index(SDD), *F*-indices, Multiplicative *F*-indices, *F*-polynomial indices, Anticancer drug.

1 Introduction and Terminologies

One of the main disease that lead to death in the world is Cancer. The proportion of death increases as increase of deaths caused by breast, stomach, lungs and colon cancers. When cells divide uncontrollably and invasively it causes cancer. It also invades the surrounding tissues there by causing damage to it. Cell division is a normal process in a human body. When cells get harmful or grow old, new cells take their place and old once die. This ordered process broke down as cancer grows. When cells became more harm, older or damage cells survive when they should die and new cells survive when those were not in need. All these extra cells divide without stopping and causes tumour. Tumours are malignant when they roll out into surrounding tissues. Unlike malignant tumours do not invade the neighbouring tissues. This dangerous disease can be cured by several treatments like surgery, radiotherapy, chemotherapy, hormone therapy, targeted therapy and more. Surgery of cancer includes some terms and conditions specified for the disease. Further this consist of not only taking away the tumour but also organism involvement. In various cases,

the simple excision with extended resection beyond the tumour margin won't resolve the issue of recurrence and metastasis. Surgery is the first treatment for oncology, even though we have various limitations and constraints named adenopathies, metastases, etc. This solution will be very effective one, easy to perform and economical. Contradictions will get generate for some cases like multi centric cancer(leukosis), cancer with special locations, mesenteric lymph node tumour, facial, spinal, pelvic osteosarcomas, cancer characterized by important local extensions, tonsillar epidermoid carcinoma, bilateral thyroid adenocarcinoma, disseminated pancreatic insulinomas.

The therapeutic method will consist of satisfied defined plans: In the first-stage, for each patient this should be separated and particularized. Then it should consist of parallel treatment of metastases, para-neoplastic syndrome and its side effects also. The general condition of the patients are essentially evaluated and continuously maintained over the total duration of treatment being needed. The option to make use few anticancer drugs relies on many of the considerations like the type and location of the cancer, its gravity state, surgery or radiation therapy needed or not, and also considers the side effects of the drugs. Maximum of the drugs will be given intravenously where as few are taken orally and some others are given within the spinal cord.

This is an attempt to the application of graph theory in anticancer drugs. In this work, the drug is taken and using the degree based calculations few topological indices are determined. In this work the drug considered is dox-loaded micelle consisting of PEG-PAsp copolymer. First polymeric micelle developed was filled with anti cancer drug doxorubicin(DOX). Here DOX was covalently conjugated to side chains of the poly(aspartate)(PAsp)segmeny by an amide bond between the carboxylic group of the glycosidyl residue in DOX [17, 18].

The molecular structure topological index is described as a non-empirical numerical measure, which represents the molecular structures and their branching pattern. Also at this end, topological indices will map each molecule structure to a real number and used as a descriptor of the molecule under testing. Various important indices applicable in chemical-engineering (e.g., QSPR/QSAR study) for establishing the relationship within the molecular structures and the physico-chemical properties [4].

Usually, chemical compounds are modelled as a graph[16, 20] considering the atoms as the vertices and the links connecting them as the edges. In a similar fashion, the anti cancer drug under this study is considered as chemical compound and the said topological indices 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.

All the graphs used in this work are simple graphs, i.e. cycle free and undirected [4].

Consider $G=(V(G), E(G))$ will be a molecular graph, where $V(G)$ and $E(G)$ are vertex and edge respectively, which maps to atoms set and chemical bond set.

Definition 1.1. For a graph G , the First F – index and Second F –index [3, 14] are defined respectively as

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

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

Definition 1.2. The multiplicative first F -index is defined as follows [1, 5]

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

Definition 1.3. For a graph G , the second multiplicative F -index [14] can be defined as

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

Definition 1.4. The multiplicative First and Second hyper F -index [10] for a graph G are

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

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

Definition 1.5. For a graph G , both Multiplicative Sum Connectivity and Multiplicative Product Connectivity F -indices [14] 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. Again to the graph G , general multiplicative First and Second F -indices are stated [12, 14] as

$$F_1^kII(G) = \prod_{e=uv \in E(G)} [(d_G(u))^2 + (d_G(v))^2]^k.$$

$$F_2^kII(G) = \prod_{e=uv \in E(G)} [(d_G(u))^2 \times (d_G(v))^2]^k.$$

Definition 1.7. The multiplicative atom bond connectivity F -index [8, 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 [14] 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 [5] 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 [5, 15] of a graph are stated as

$$F_2(G, x) = \sum_{e=uv \in E(G)} x^{(d_G(u))^2 \times (d_G(v))^2}.$$

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

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

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 first index ABC of G [6] 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 [7, 19],

$$SSD(G) = \sum_{e=uv \in E(G)} \left[\frac{A}{B} + \frac{B}{A} \right].$$

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

In Section 2 we highlight main results obtained, in detail proofs and the calculations of topological indices of molecular graphs family.

2 Results and Discussions

Dox-loaded micelle consisting of $PEG - PAsp$ block polymer and copolymers with chemically conjugated Dox $SP[n]$ is considered in this study, as shown in **Figure 1**. The integer number n is step of growth in these form of polymers. Here **Figure 2** represents $SP[1]$, **Figure 3** represents $SP[2]$ and **Figure 4** represents $SP[3]$. And also for $n = 1, 2$ and 3 (consider the **Figures 2, 3** and **4** respectively) are determined.

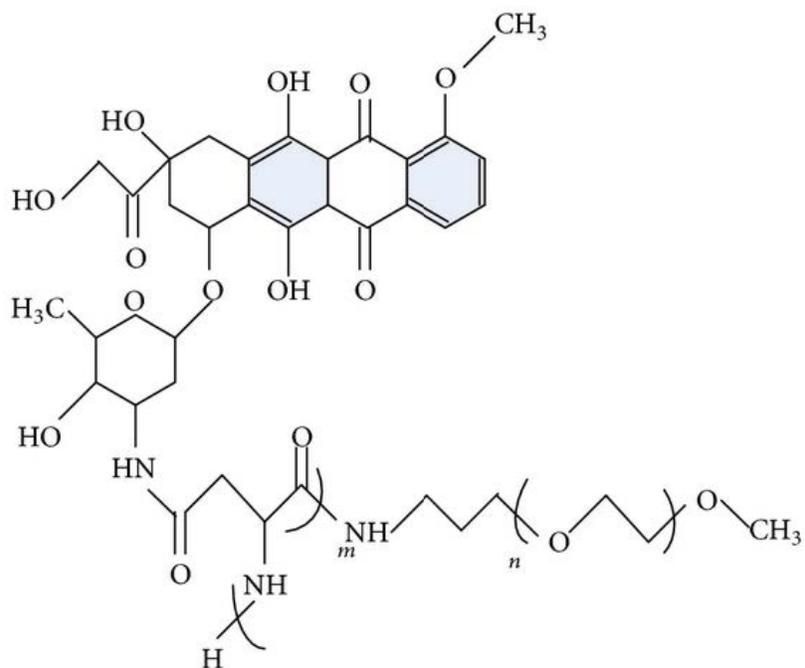


Figure 2.1: Dox-loaded micelle consisting PEG-PAsp block copolymer with chemically conjugated Dox SP[n]

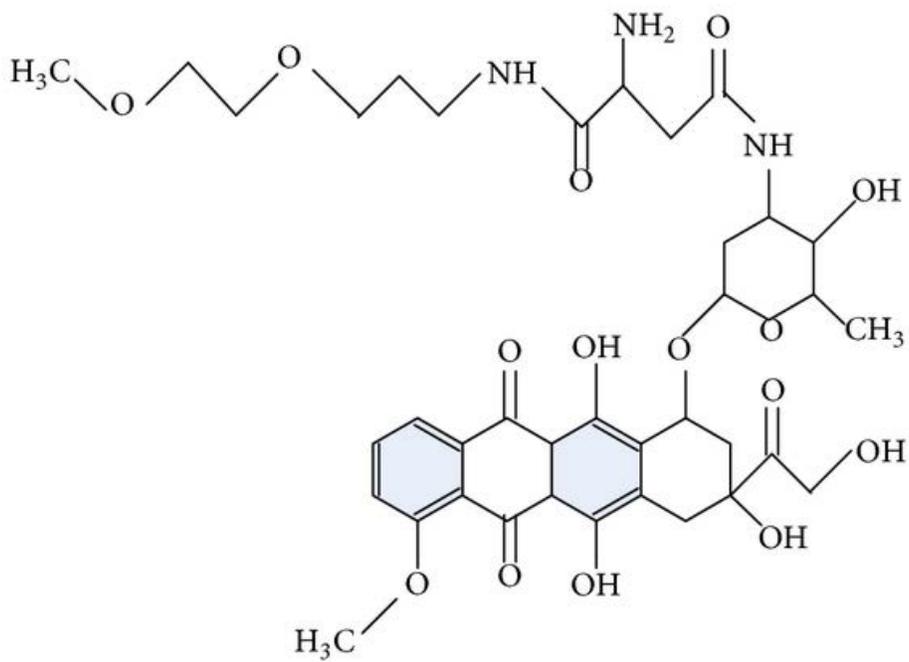


Figure 2.2: The molecular structure of SP[1]

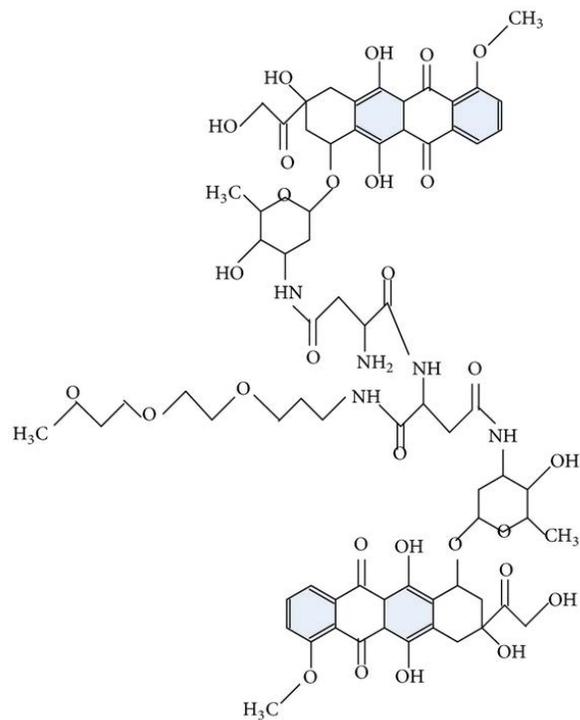


Figure 2.3: The molecular structure of SP[2]

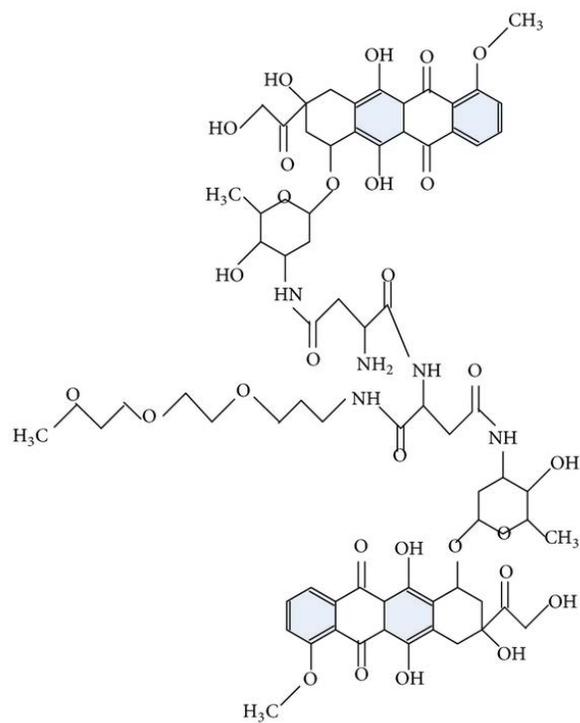


Figure 2.4: The molecular structure of SP[3]

Theorem 2.1. *The Dox-loaded micelle consisting PEG-PAsp block copolymer with chemically conjugated Dox SP[n], One has*

$$SP[n] = F_1^k II(G) = 5^{k(18n+2)} \times 2^{k(44n+13)} \times 9^{k(16n)} \times 13^{k(18n-1)} \times 17^{k(n)}.$$

Proof. Let the lowest and highest degree of $SP[n]$ respectively are δ and Δ . Suppose the edge set $E(SP[n])$ can categorised as various divisions:

- (i) $E_3(or E_2^*) : d_G(u) = 1 \text{ and } d_G(v) = 2;$
- (ii) $E_3^* : d_G(u) = 1 \text{ and } d_G(v) = 3;$
- (iii) $E_5 \cap E_4^* : d_G(u) = 1 \text{ and } d_G(v) = 4;$
- (iv) $E_4 \cap E_4^* : d_G(u) = 2 \text{ and } d_G(v) = 2;$
- (v) $E_6^* : d_G(u) = 2 \text{ and } d_G(v) = 3;$
- (vi) $E_8^* : d_G(u) = 2 \text{ and } d_G(v) = 4;$
- (vii) $E_9^* : d_G(u) = d_G(v) = 3;$
- (viii) $E_7(or E_{12}^*) : d_G(u) = 3 \text{ and } d_G(v) = 4.$

Again Calculating in terms, we observe that $|V(SP[n])| = 49n + 6$ and $|E(SP[n])| = 54n + 5$. In specific, we define

$$\begin{aligned} |E_3| = |E_2^*| = 2n + 1, |E_3^*| = 9n + 1, |E_5 \cap E_4^*| = |E_7| = |E_{12}^*| = n, \\ |E_4 \cap E_4^*| = 5n + 4, |E_6^*| = 18n - 1, |E_8^*| = 2n \text{ and } |E_9^*| = 16n. \end{aligned}$$

\therefore The general multiplicative first F - index of a graph $SP[n]$ is

$$\begin{aligned} F_1^k II(G) &= \prod_{e=uv \in E(G)} [(d_G(u))^2 + (d_G(v))^2]^k \\ &= \prod_{uv \in E_3} [(1)^2 + (2)^2]^k \times \prod_{uv \in E_3^*} [(1)^2 + (3)^2]^k \times \prod_{uv \in E_5 \cap E_4^*} [(1)^2 + (4)^2]^k \\ &\quad \times \prod_{uv \in E_4 \cap E_4^*} [(2)^2 + (2)^2]^k \times \prod_{uv \in E_6^*} [(2)^2 + (3)^2]^k \times \prod_{uv \in E_8^*} [(2)^2 + (4)^2]^k \\ &\quad \times \prod_{uv \in E_9^*} [(3)^2 + (3)^2]^k \times \prod_{uv \in E_7} [(3)^2 + (4)^2]^k \\ &= 5^{k(18n+2)} \times 2^{k(44n+13)} \times 9^{k(16n)} \times 13^{k(18n-1)} \times 17^{k(n)}. \end{aligned}$$

We get the below results by using **Theorem 2.1**.

Corollary 2.1. *The multiplicative first F - index of a graph $SP[n]$ is*

$$F_1 II(G) = 5^{(18n+2)} \times 2^{(44n+13)} \times 9^{(16n)} \times 13^{(18n-1)} \times 17^{(n)}.$$

Proof. Put $k = 1$ in **Theorem 2.1**, we gain the required result.

Corollary 2.2. *The multiplicative first hyper F - index of a graph $SP[n]$ is*

$$HF_1 II(G) = 5^{(36n+4)} \times 2^{(88n+26)} \times 9^{(32n)} \times 13^{(36n-2)} \times 17^{(2n)}.$$

Proof. Put $k = 2$ in **Theorem 2.1**, we gain the required result.

Corollary 2.3. The multiplicative sum connectivity F - index of a graph $SP[n]$ will be

$$SFII(G) = \left(\frac{1}{\sqrt{5}}\right)^{18n+2} \times \left(\frac{1}{\sqrt{2}}\right)^{44n+13} \times \left(\frac{1}{\sqrt{9}}\right)^{16n} \times \left(\frac{1}{\sqrt{13}}\right)^{18n-1} \times \left(\frac{1}{\sqrt{17}}\right)^n.$$

Proof. Put $k = \frac{-1}{2}$ in **Theorem 2.1**, we gain the desired result. We now determine the general multiplicative second F - index of $SP[n]$.

Theorem 2.2. The general multiplicative second F - index of a graph $SP[n]$ is

$$F_2^K II(G) = 4^{k(20n+4)} \times 9^{k(30n)}.$$

Proof.

$$\begin{aligned} F_2^k II(G) &= \prod_{e=uv \in E(G)} [(d_G(u))^2 \cdot (d_G(v))^2]^k \\ &= \prod_{uv \in E_3} [(1)^2(2)^2]^k \times \prod_{uv \in E_3^*} [(1)^2(3)^2]^k \times \prod_{uv \in E_5 \cap 4^*} [(1)^2(4)^2]^k \\ &\quad \times \prod_{uv \in E_4 \cap 4^*} [(2)^2(2)^2]^k \times \prod_{uv \in E_6^*} [(2)^2(3)^2]^k \times \prod_{uv \in E_8^*} [(2)^2(4)^2]^k \\ &\quad \times \prod_{uv \in E_9^*} [(3)^2(3)^2]^k \times \prod_{uv \in E_7} [(3)^2(4)^2]^k \\ &= 4^{k(20n+4)} \times 9^{k(30n)}. \end{aligned}$$

The following results are obtained by using **Theorem 2.5**.

Corollary 2.4. The multiplicative second F - index of a graph $SP[n]$ is

$$F_2 II(G) = 4^{(20n+4)} \times 9^{(30n)}.$$

Proof. Put $k = 1$ in **Theorem 2.5**, we gain the required results.

Corollary 2.5. The multiplicative second hyper F - index of a graph $SP[n]$ will be

$$HF_2 II(G) = 4^{(40n+8)} \times 9^{(60n)}.$$

Proof. Put $k = 2$ in **Theorem 2.5**, we acquire the required result.

Corollary 2.6. The multiplicative product connectivity F - index of a graph $SP[n]$ will be

$$PFII(G) = \left(\frac{1}{4}\right)^{10n+2} \times \left(\frac{1}{9}\right)^{15n}.$$

Proof. Put $k = \frac{-1}{2}$ in **Theorem 2.5**, we obtained the required result. In the following theorems, we deduce the multiplicative atom bond connectivity F -index and multiplicative geometric-arithmetic F -index of $SP[n]$.

Theorem 2.3. The multiplicative atom bond connectivity F - index of $SP[n]$ will be

$$\begin{aligned} ABCFII(G) &= \left(\sqrt{\frac{3}{4}}\right)^{2n+1} \times \left(\sqrt{\frac{8}{9}}\right)^{9n+1} \times \left(\sqrt{\frac{15}{16}}\right)^n \times \left(\sqrt{\frac{6}{16}}\right)^{5n+4} \times \left(\sqrt{\frac{11}{36}}\right)^{18n-1} \\ &\quad \times \left(\sqrt{\frac{18}{64}}\right)^{2n} \times \left(\sqrt{\frac{16}{81}}\right)^{16n} \times \left(\sqrt{\frac{23}{144}}\right)^n. \end{aligned}$$

Proof.

$$\begin{aligned}
ABCFII(G) &= \prod_{e=uv \in E(G)} \left[\sqrt{\frac{(d_G(u))^2 + (d_G(v))^2 - 2}{(d_G(u))^2 \cdot (d_G(v))^2}} \right] \\
&= \left(\sqrt{\frac{(1)^2 + (2)^2 - 2}{(1)^2(2)^2}} \right)^{2n+1} \times \left(\sqrt{\frac{(1)^2 + (3)^2 - 2}{(1)^2(3)^2}} \right)^{9n+1} \times \left(\sqrt{\frac{(1)^2 + (4)^2 - 2}{(1)^2(4)^2}} \right)^n \\
&\quad \times \left(\sqrt{\frac{(2)^2 + (2)^2 - 2}{(2)^2(2)^2}} \right)^{5n+4} \times \left(\sqrt{\frac{(2)^2 + (3)^2 - 2}{(2)^2(3)^2}} \right)^{18n-1} \times \left(\sqrt{\frac{(2)^2 + (4)^2 - 2}{(2)^2(4)^2}} \right)^{2n} \\
&\quad \times \left(\sqrt{\frac{(3)^2 + (3)^2 - 2}{(3)^2(3)^2}} \right)^{16n} \times \left(\sqrt{\frac{(3)^2 + (4)^2 - 2}{(3)^2(4)^2}} \right)^n \\
&= \left(\sqrt{\frac{3}{4}} \right)^{2n+1} \times \left(\sqrt{\frac{8}{9}} \right)^{9n+1} \times \left(\sqrt{\frac{15}{16}} \right)^n \times \left(\sqrt{\frac{6}{16}} \right)^{5n+4} \times \left(\sqrt{\frac{11}{36}} \right)^{18n-1} \times \left(\sqrt{\frac{18}{64}} \right)^{2n} \\
&\quad \times \left(\sqrt{\frac{16}{81}} \right)^{16n} \times \left(\sqrt{\frac{23}{144}} \right)^n.
\end{aligned}$$

Theorem 2.4. The multiplicative geometric-airtmetic F - index of $SP[n]$ is

$$= \left(\frac{24}{25} \right)^{7n} \times \left(\frac{12}{13} \right)^{33n-1} \times \left(\frac{4}{5} \right)^{4n} \times \left(\frac{3}{5} \right)^{16n} \times \left(\frac{8}{17} \right)^{4n}.$$

Proof.

$$\begin{aligned}
GAFII(G) &= \prod_{e=uv \in E(G)} \frac{2\sqrt{(d_G(u))^2 \cdot (d_G(v))^2}}{(d_G(u))^2 + (d_G(v))^2} \\
&= \left(\frac{2\sqrt{(1)^2(2)^2}}{(1)^2 + (2)^2} \right)^{2n+1} \times \left(\frac{2\sqrt{(1)^2(3)^2}}{(1)^2 + (3)^2} \right)^{9n+1} \times \left(\frac{2\sqrt{(1)^2(4)^2}}{(1)^2 + (4)^2} \right)^n \\
&\quad \times \left(\frac{2\sqrt{(2)^2(2)^2}}{(2)^2 + (2)^2} \right)^{5n+4} \times \left(\frac{2\sqrt{(2)^2(3)^2}}{(2)^2 + (3)^2} \right)^{18n-1} \times \left(\frac{2\sqrt{(2)^2(4)^2}}{(2)^2 + (4)^2} \right)^{2n} \\
&\quad \times \left(\frac{2\sqrt{(3)^2(3)^2}}{(3)^2 + (3)^2} \right)^{16n} \times \left(\frac{2\sqrt{(3)^2(4)^2}}{(3)^2 + (4)^2} \right)^n \\
&= \left(\frac{24}{25} \right)^{7n} \times \left(\frac{12}{13} \right)^{33n-1} \times \left(\frac{4}{5} \right)^{4n} \times \left(\frac{3}{5} \right)^{16n} \times \left(\frac{8}{17} \right)^{4n}.
\end{aligned}$$

Theorem 2.5. The $SP[n]$ for the first F - polynomial of a graph is

$$\begin{aligned}
&= (2n + 1)x^5 + (9n + 1)x^{10} + (n)x^{17} + (5n + 4)x^8 + (18n - 1)x^{13} + (2n)x^{20} \\
&\quad + (16n)x^{18} + (n)x^{25}.
\end{aligned}$$

Proof.

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

$$\begin{aligned}
&= (2n + 1) \left[x^{(1+4)} \right] + (9n + 1) \left[x^{(1+9)} \right] + (n) \left[x^{(1+16)} \right] + (5n + 4) \left[x^{(4+4)} \right] \\
&\quad + (18n - 1) \left[x^{(4+9)} \right] + (2n) \left[x^{(4+16)} \right] + (16n) \left[x^{(9+9)} \right] + (n) \left[x^{(9+16)} \right]. \\
&= (2n + 1)x^5 + (9n + 1)x^{10} + (n)x^{17} + (5n + 4)x^8 + (18n - 1)x^{13} + (2n)x^{20} \\
&\quad + (16n)x^{18} + (n)x^{25}.
\end{aligned}$$

Theorem 2.6. The $SP[n]$ for the second F - polynomial of a graph is

$$\begin{aligned}
&(2n + 1)x^4 + (9n + 1)x^9 + (6n + 4)x^{16} + (18n - 1)x^{36} + (2n)x^{64} + (16n)x^{81} \\
&\quad + (n)x^{144}.
\end{aligned}$$

Proof.

$$\begin{aligned}
F_2(G, x) &= \sum_{e=uv \in E(G)} x^{(d_G(u))^2 \cdot (d_G(v))^2}. \\
&= (2n + 1) \left[x^{(1)(4)} \right] + (9n + 1) \left[x^{(1)(9)} \right] + (n) \left[x^{(1)(16)} \right] + (5n + 4) \left[x^{(4)(4)} \right] \\
&\quad + (18n - 1) \left[x^{(4)(9)} \right] + (2n) \left[x^{(4)(16)} \right] + (16n) \left[x^{(9)(9)} \right] + (n) \left[x^{(9)(16)} \right]. \\
&= (2n + 1)x^4 + (9n + 1)x^9 + (6n + 4)x^{16} + (18n - 1)x^{36} + (2n)x^{64} + (16n)x^{81} \\
&\quad + (n)x^{144}.
\end{aligned}$$

Theorem 2.7. The $SP[n]$ for the first hyper F - polynomial of a graph is

$$\begin{aligned}
&(2n + 1)x^{10} + (9n + 1)x^{20} + n(x)^{34} + (5n + 4)x^{16} + (18n - 1)x^{26} + (2n)x^{40} + (16n)x^{36} \\
&\quad + (n)x^{50}.
\end{aligned}$$

Proof.

$$\begin{aligned}
HF_1(G, x) &= \sum_{e=uv \in E(G)} x^{[(d_G(u))^2 + (d_G(v))^2]^2}. \\
&= (2n + 1) \left[x^{(1+4)^2} \right] + (9n + 1) \left[x^{(1+9)^2} \right] + (n) \left[x^{(1+16)^2} \right] + (5n + 4) \left[x^{(4+4)^2} \right] \\
&\quad + (18n - 1) \left[x^{(4+9)^2} \right] + (2n) \left[x^{(4+16)^2} \right] + (16n) \left[x^{(9+9)^2} \right] + (n) \left[x^{(9+16)^2} \right]. \\
&= (2n + 1)x^{10} + (9n + 1)x^{20} + n(x)^{34} + (5n + 4)x^{16} + (18n - 1)x^{26} + (2n)x^{40} \\
&\quad + (16n)x^{36} + (n)x^{50}.
\end{aligned}$$

Theorem 2.8. The $SP[n]$ for the second hyper F - polynomial of a graph is

$$\begin{aligned}
&(2n + 1)x^8 + (9n + 1)x^{18} + (6n + 4)x^{32} + (18n - 1)x^{72} + (2n)x^{128} + (16n)x^{162} \\
&\quad + (n)x^{288}.
\end{aligned}$$

Proof.

$$\begin{aligned}
HF_2(G, x) &= \sum_{e=uv \in E(G)} x^{[(d_G(u))^2 \cdot (d_G(v))^2]^2}. \\
&= (2n + 1) \left[x^{(1)(4)} \right]^2 + (9n + 1) \left[x^{(1)(9)} \right]^2 + (n) \left[x^{(1)(16)} \right]^2 + (5n + 4) \left[x^{(4)(4)} \right]^2 \\
&\quad + (18n - 1) \left[x^{(4)(9)} \right]^2 + (2n) \left[x^{(4)(16)} \right]^2 + (16n) \left[x^{(9)(9)} \right]^2 + (n) \left[x^{(9)(16)} \right]^2. \\
&= (2n + 1)x^8 + (9n + 1)x^{18} + (6n + 4)x^{32} + (18n - 1)x^{72} + (2n)x^{128} + (16n)x^{162} \\
&\quad + (n)x^{288}.
\end{aligned}$$

Theorem 2.9. For a graph G , The ABC index of $SP[n]$ will be

$$ABC(G) = \frac{194n}{5} + \frac{18}{5}.$$

Proof. By the definition, the ABC index of a graph $SP[n]$ is

$$\begin{aligned} ABC(G) &= \sum_{e=uv \in E(G)} \left[\sqrt{\frac{(d_G(u) + d_G(v) - 2)}{(d_G(u))(d_G(v))}} \right]. \\ &= \sum_{uv \in E_3} \left[\sqrt{\frac{(1+2-2)}{(1)(2)}} \right] + \sum_{uv \in E_3^*} \left[\sqrt{\frac{(1+3-2)}{(1)(3)}} \right] + \sum_{uv \in E_5 \cap E_4^*} \left[\sqrt{\frac{(1+4-2)}{(1)(4)}} \right] \\ &\quad + \sum_{uv \in E_4 \cap E_4^*} \left[\sqrt{\frac{(2+2-2)}{(2)(2)}} \right] + \sum_{uv \in E_6^*} \left[\sqrt{\frac{(2+3-2)}{(2)(3)}} \right] + \sum_{uv \in E_8^*} \left[\sqrt{\frac{(2+4-2)}{(2)(4)}} \right] \\ &\quad + \sum_{uv \in E_9^*} \left[\sqrt{\frac{(3+3-2)}{(3)(3)}} \right] + \sum_{uv \in E_7} \left[\sqrt{\frac{(3+4-2)}{(3)(4)}} \right]. \\ &= (25n + 4) \left(\sqrt{\frac{1}{2}} \right) + (9n + 1) \left(\sqrt{\frac{2}{3}} \right) + n \left(\sqrt{\frac{3}{4}} \right) + 2n \left(\sqrt{\frac{5}{8}} \right) + 16n \left(\sqrt{\frac{4}{9}} \right) \\ &\quad + n \left(\sqrt{\frac{5}{12}} \right). \\ ABC(G) &= \frac{194n}{5} + \frac{18}{5}. \end{aligned}$$

Theorem 2.10. The Symmetric division index of a graph $SP[n]$ is

$$SDD(G) = \frac{1273n}{10} + \frac{117}{10}.$$

Proof.

$$\begin{aligned} SSD(G) &= \sum_{e=uv \in E(G)} \left[\frac{A(d_G(u), d_G(v))}{B(d_G(u), d_G(v))} + \frac{B(d_G(u), d_G(v))}{A(d_G(u), d_G(v))} \right]. \\ &= \sum_{uv \in E_3} \left[\frac{A(1, 2)}{B(1, 2)} + \frac{B(1, 2)}{A(1, 2)} \right] + \sum_{uv \in E_3^*} \left[\frac{A(1, 3)}{B(1, 3)} + \frac{B(1, 3)}{A(1, 3)} \right] \\ &\quad + \sum_{uv \in E_5 \cap E_4^*} \left[\frac{A(1, 4)}{B(1, 4)} + \frac{B(1, 4)}{A(1, 4)} \right] + \sum_{uv \in E_4 \cap E_4^*} \left[\frac{A(2, 2)}{B(2, 2)} + \frac{B(2, 2)}{A(2, 2)} \right] \\ &\quad + \sum_{uv \in E_6^*} \left[\frac{A(2, 3)}{B(2, 3)} + \frac{B(2, 3)}{A(2, 3)} \right] + \sum_{uv \in E_8^*} \left[\frac{A(2, 4)}{B(2, 4)} + \frac{B(2, 4)}{A(2, 4)} \right] \\ &\quad + \sum_{uv \in E_9^*} \left[\frac{A(3, 3)}{B(3, 3)} + \frac{B(3, 3)}{A(3, 3)} \right] + \sum_{uv \in E_7} \left[\frac{A(3, 4)}{B(3, 4)} + \frac{B(3, 4)}{A(3, 4)} \right]. \end{aligned}$$

$$\begin{aligned}
&= (2n + 1) \binom{5}{2} + (9n + 1) \binom{10}{3} + n \binom{17}{4} + (5n + 4)(2) + (18n - 1) \binom{13}{6} + 2n \binom{20}{8} \\
&\quad + 16n(2) + n \binom{25}{12}. \\
&= \frac{1273n}{10} + \frac{117}{10}.
\end{aligned}$$

3 Conclusion

In this work, various topological indices are obtained with the values inspired by Dox-loaded micelle consisting of PEG-PAsp block copolymer for an anti cancer drug. By means of which the exact expressions are denoted for several important indices. These formulae help in correlating chemical structure of polymers with the physical properties. The outcome obtained in this work demonstrate the optimistic applications in chemical and pharmaceutical engineering field.

Acknowledgement

The authors would like to express their grateful thanks to the referee and Editor for their kind suggestions and corrections that helped to improve the original manuscript .

References

- [1] M. Bhanumathi and K. Easu Julia Rani, On multiplicative harmonic index, multi-plicative ISI index and multiplicative F-index of TUC4C8[m; n] and TUC4[m; n] nanotubes, *International J. on Recent Trends in Life Science and Mathematics*, **4(9)**(2017), 1-88.
- [2] M. Eliasi, A. Iranmanesh and I. Gutman, Multiplicative versions of first Zagreb index, *MATCH Commun. Math. Comput. Chem*, **68**(2012), 217- 230.
- [3] B. Furtula and I. Gutman, A forgotten topological index, *J. Math. Chem.*, **53**(2015), 1184-1190.
- [4] W. Gao, W. F. Wang and M. R. Farahani, Topological indices study of molecular structure in anticancer drugs, *J.Chem.*, **10**(2016), 1-8, DOI:10.1155/2016/3216327.
- [5] S. Ghobadi and M. Ghorbaninejad, On F-polynomial, Multiple and hyper F-index of sum molecular graphs, *Bulletin of Mathematical Sciences and Applications*, **20**(2018), 36-43.
- [6] M. Ghorbani and M. A. Hosseinzateh, Computing ABC_4 index of Nanostar dendrimers, *Optoelectron.Adv.Mater-Rapid Commun.*, **4(9)**(2010), 419-1422.
- [7] M. Javaid, A. Raheem, M. Abbas and J. Cao, M-polynomial method for topological indices of 3-Layered probabilistic neural networks, *TWMS J.APP.Eng.Math.*, **9**(2019), 864-875.
- [8] V.R. Kulli, Edge version of multiplicative atom bond connectivity index of certain nanotubes and nanotorus, *International Journal of Mathematics And its Applications*, **6(1-E)**(2018), 977-982.
- [9] V. R. Kulli, Edge version of F-index, General sum connectivity index of certain nan-otubes, *Annals of Pure and Applied Mathematics*, **14(3)**(2017), 449-455.
- [10] V. R. Kulli, Multiplicative hyper-Zagreb indices and coindices of graphs, *International Journal of Pure Algebra*, **67**(2016), 342-347.
- [11] V. R. Kulli, Branden Stone and Bing Wei, Generalized multiplicative indices of poly-cyclic aromatic hydrocarbons and benzenoid systems, *Zeitschrift fur Naturforschung*, **72(6)**(2017), 573-576.

- [12] V. R. Kulli, Multiplicative connectivity indices of certain nano-tubes, *Annals of Pure and Applied Mathematics*, **12(2)**(2016), 169-176.
- [13] V. R. Kulli, Multiplicative Connectivity Indices of Nano-structures, *Journal of Ultra Scientist of Physical Sciences*, **29(1)**(2017), 1-10.
- [14] V. R. Kulli, On multiplicative F -indices and multiplicative connectivity F -indices of chemical networks, *International Journal of current research in Science and Technology*, **5(2)**(2019), 1-10.
- [15] V. R. Kulli, F -indices of chemical networks, *International Journal of Mathematical Archieve*, **10(3)**(2019), 21-30.
- [16] V. Lokesha and P. S. Ranjini, Eccentric Connectivity index, Hyper and reverse-Wiener indices of the subdivision Graph, *General Mathematics Notes*, **2(2)**(2011), 34-46.
- [17] N. Nishiyama, K. Kataoka, Polymeric micelle drug carrier systems: PEG-PAsp(Dox) and second generation of micellar drugs, in Polymer Drugs in the Clinical Stage. *Advances in Experimental Medicine and Biology*, **519**(2003), 155-177.
- [18] K. Osada, R. J. Christie and K. Kataoka, Polymeric micelles from poly(ethyleneglycol)-poly(amino acid) block copolymer, *Journal of the Royal Society Interface*, **6(3)**(2019), 325-339.
- [19] H.L. Parashivamurthy, M. R. Rajesh Kanna and R. Jagdeesh, *Topological Indices of Nicotine*, **6(3)**(2019), 20-28.
- [20] P. S. Ranjini, V. Lokesha and M. A. Rajan, On Wiener Polynomial of the Subdivision Graphs, *Chinese Journal of Engineering Mathematics*, **3**(2011), 411-418.