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A Computational Approach on Fenofibrate Drug Using Degree-Based Topological Indices and M-polynomials

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Authors' contributions

This work was carried out in collaboration between both authors. Both authors read and approved the final manuscript.

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ABSTRACT

Fenofibrate is a drug approved by FDA Food and Drugs Administration used to treat patients with Hypertrigly ceridemia primary hypercholesterolemia or mixed dyslipidemia. It reduces low-density lipoprotein cholesterol (LDL-c), total cholesterol, triglycerides, and apolipoprotein B and increases high -density lipoprotein cholesterol (HDL-C) in adults. The sum and multiplicative versions of several topological indices such as General Zagreb, General Randic, Arithmetic Geometric Index, Inverse sum (Indeg) Index, Symmetric Division (Deg) Index, Forgotten Indices M-polynomials of Fenofibrate are computed in this article.

Keywords: Topological indices; fenofibrate; m-polynomial; chemical graph.

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1. INTRODUCTION

All molecular graphs in this paper are finite, loopless, connected, and do not have numerous edges. $A = (V, E)$ graph having vertex set V and edge set E.

In Mathematical chemistry the analytical and structural properties of topological indices have been studied in depth over the last years. The Theoretical and practical interest of topological indices lies in the fact that they have become an important tool for the study of multiple practical problems in Computer science, Physics, Ecology, among others countless applications of topological indices have been reported, most of them concerned with exploring medicinal and pharmacological issues. A molecular graph is a graph-theoretic representation of the structural formula of a chemical molecule, with edges standing in for chemical bonds and vertices for atoms. Topological indices based on end-vertex degrees of edges have been used over 50 years. Among them, several indices are recognized to be useful tools in chemical researches. Probably the best known such descriptor is the Randic connectivity index. In 1972, Trinajstic and Gutman obtained a formula concerning the total energy of π electrons of molecules [1-3].

Fenofibrate was first synthesized in 1974, as a derivative of clofibrate, and was initially offered in France. It was initially known as procetofen, and was later renamed Fenofibrate to comply with World Health Organization international Nanoproprietary Name guidelines. It is developed by Groupe Fournier SA of France. Fenofibrate comes as a capsule, a delayed - release (long -acting) capsule, and a tablet to take by mouth. It is usually take once a day. Some Fenofibrate products (Fenoglide, Lipofen and Lofibra) should be taken with a meal. Other brands (Antara, Fibricor, Tricor, Triglide and Trilipix) may be taken with or without food. Its molecular formula is $C_{20}H_{21}CIO_4$ [4].

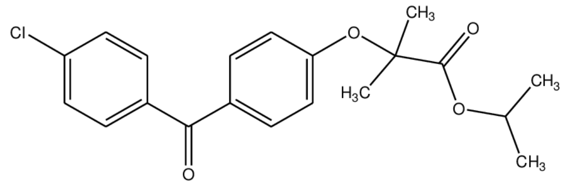

Fig. 1. Chemical structure of Fenofibrate

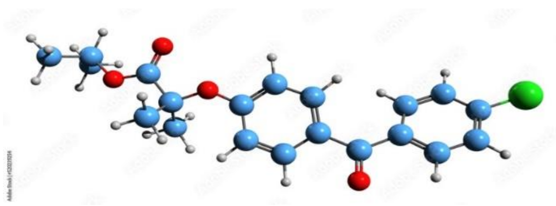

Fig. 2. Molecular graph of Fenofibrate

2. MATERIALS AND METHODS

2.1 Additive Degree-based Topological Indices

Topological indices are classified into different categories such as entropy-based, eigenvalue-based, spectrum-based, symmetry-based, distance-based and vertex-degree-based. Among these categories, *degree-based indices* have an outstanding position.

Assuming that the edge connecting vertices r and s is denoted by r s, the additive degree-based In mathematical chemistry, topological indices have a general form.

$$TI = TI(A) = \sum_{rs \in E(A)} F(d_r, d_s)$$

Table 1. Topological indices of a graph with additive degree basis

S. No.	Topological index	Notation	Formula of Topological index
1	First Zagreb Index	$M_1(A)$	$\sum_{rs \in E(A)} (d_r + d_{sv})$
2	Second Zagreb Index	$M_2(A)$	$\sum_{rs \in E(A)} (d_r \cdot d_s)$
3	Third Zagreb Index	$M_3(A)$	$\sum_{rs \in E(A)} \lvert d_r - d_s \rvert$
4	Modified First Zagreb Index	$M_1^*(A)$	$\sum_{s \in V(A)} (d_s)^2$

S. No.	Topological index	Notation	Formula of Topological index
5	Randic Index	$R(A)$	$\sum_{rs\in E(A)} \frac{1}{\sqrt{d_r \cdot d_s}}$
6	First Hyper Zagreb Index	$HM_1(A)$	$\sum_{rs\in E(A)} (d_r + d_s)^2$
7	Second Hyper Zagreb Index	$HM_2(A)$	$\sum_{rs\in E(A)} (d_r \cdot d_s)^2$
8	General First Zagreb Index	$M_1^{\alpha}(A)$	$\sum_{rs\in E(A)} (d_r + d_s)^{\alpha}$
9	General SecondZagreb Index	$M_2^{\alpha}(A)$	$\sum_{rs\in E(A)} (d_r \cdot d_s)^{\alpha}$
10	Reduced Second Zagreb Index	$RM_2(A)$	$\sum_{rs\in E(A)} (d_r - 1)(d_s - 1)$
11	Redefined First Zagreb Index	$\operatorname{Re} M_1(A)$	$\sum_{rs\in E(A)} \frac{(d_r + d_s)}{(d_r \cdot d_s)}$
12	Redefined Second Zagreb Index	$\operatorname{Re} M_2(A)$	$\sum_{rs\in E(A)} \frac{(d_r \cdot d_s)}{(d_r + d_s)}$
13	Redefined Third Zagreb Index	$\operatorname{Re} M_3(A)$	$\sum_{rs\in E(A)} (d_r . d_s)(d_r + d_s)$
14	Modified Second Zagreb Index	${}^{m}M_2(A)$	$\sum_{rs\in E(A)} \frac{1}{d_r \cdot d_s}$
15	Nano - Zagreb Index	$N_z(A)$	$\sum_{s\in V(A)} \left[(d_r)^2 - (d_s)^2\right]$
16	Sum Nano - Zagreb Index	$x_{\frac{1}{2}} N_z(A)$	$\sum_{rs\in E(A)} (d_r^2 - d_s^2)^{\frac{1}{2}}$
17	Zeroth order Randić Index	$R_{\frac{-1}{2}}^{0}(A)$	$\sum_{s\in V(A)} (d_s)^{\frac{-1}{2}}$
18	Zeroth Order General Randić Index	$R_{\alpha}^{0}(A)$	$\sum_{s\in V(A)} (d_s)^{\alpha}$
19	Reciprocal Randić Index	$RR(A)$	$\sum_{rs\in E(A)} \sqrt{d_r \cdot d_s}$
20	Reduced Reciprocal Randić Index	$RRR(A)$	$\sum_{rs\in E(A)} \sqrt{(d_r - 1) \cdot (d_s - 1)}$
21	Inverse Randić Index	$RR_{\alpha}(A)$	$\sum_{rs\in E(A)} \frac{1}{(d_r \cdot d_s)^{\alpha}}$
22	Modified Randić Index	$R'(A)$	$\sum_{rs\in E(A)} \frac{1}{\max\{d_r \cdot d_s\}}$
23	Sum onnectivity Index	$SCI(A)$	$\sum_{rs\in E(A)} \frac{1}{\sqrt{d_r + d_s}}$
24	Arithmetic Geometric Index	$AG(A)$	$\sum_{rs\in E(A)} \frac{d_r + d_s}{2\sqrt{d_r \cdot d_s}}$

S. No.	Topological index	Notation	Formula of Topological index
25	Variable Sum Index	$SEI_{\alpha}(A)$	$\sum_{s\in V(A)} d_s(\alpha)^{d_s}$
26	Harmonic Index	$H(A)$	$\sum_{rs\in E(A)} \frac{2}{d_r+d_s}$
27	General Harmonic Index	$H_k(A)$	$\sum_{rs\in E(A)} \left(\frac{2}{d_r+d_s}\right)^k$
28	General Ordinary Geometric Arithmetic Index	$OGA_k(A)$	$\sum_{rs\in E(A)} \left(\frac{2\sqrt{d_r\cdot d_s}}{d_r+d_s}\right)^k$
29	Ordinary Geometric Arithmetic Index	$OGA(A)$	$\sum_{rs\in E(A)} \frac{2\sqrt{d_r\cdot d_s}}{d_r+d_s}$
30	SK Index	$SK(A)$	$\sum_{rs\in E(A)} \frac{d_r+d_s}{2}$
31	SK1 Index	$SK_1(A)$	$\sum_{rs\in E(A)} \frac{d_r\cdot d_s}{2}$
32	SK2 Index	$SK_2(A)$	$\sum_{rs\in E(A)} \left(\frac{d_r+d_s}{2}\right)^2$
33	Forgotten Index	$F(A)$	$\sum_{rs\in E(A)} \left[(d_r)^2+(d_s)^2\right]$
34	Inverse sum (Indeg) Index	$ISI(A)$	$\sum_{rs\in E(A)} \frac{d_r.\ d_s}{d_r+d_s}$
35	Symmetric Division (Deg) Index	$SDD(A)$	$\sum_{rs\in E(A)} \left[\frac{\min\{d_r.\ d_s\}}{\max\{d_r\cdot d_s\}}+\frac{\max\{d_r.\ d_s\}}{\min\{d_r\cdot d_s\}}\right]$
36	IRM Index	$IRM\,(A)$	$\sum_{rs\in E(A)} (d_r-d_s)^2$
37	Augmented Zagreb Index	$AZI(A)$	$\sum_{rs\in E(A)} \left(\frac{d_r.\ d_s}{d_r+d_s-2}\right)^3$
38	Albertson Index	$A(A)$	$\sum_{rs\in E(A)} \lvert d_r-d_s \rvert$
39	Atomic Bond Connectivity Index	$ABC(A)$	$\sum_{rs\in E(A)} \sqrt{\frac{d_r+d_s-2}{d_r\cdot d_s}}$
40	Bell Index	$B(A)$	$\sum_{s\in V(A)} \left(d_s-\frac{2q}{p}\right)^2$
41	First Entire Zagreb Index	$M_1^{\varepsilon}(A)$	$\sum_{s\in V(A)\cup E(A)} (d_s)^2$
42	Sombor Index	$SO(A)$	$\sum_{rs\in E(A)} \sqrt{(d_r)^2+(d_s)^2}$

2.2 Multiplicative Degree-based Topological Indices

Several significant multiplicative degree-based Topological indices were outlined in this section. This can be used to provide our primary results [5,6]. $NK(A)$ is the Multiplicative Topological index that Narumi and Katayama suggested. Following that, $NK(A)$ was redefined by Wang et al. as a broad multiplicative index. In order to advance the study of Topological indices, Kulli.V R, devised the multiplicative sum connectivity index ($SCII(A)$) and multiplicative product connectivity index ($PCII(A)$) ratings. The generalized version of multiplicative Topological indices is given below, according to Chemical Graph Theory.

$$MTI = MTI(A) = \prod_{rs\in E(A)} F(d_r, d_s)$$

Table 2. Topological indices of a graph A based on multiplication of degrees

S. No.	Topological index	Notation	Formula of topological index
1	Narumi – Katayama Index	$NK(A)$	$\prod_{s\in V(A)}(d_s)$
2	First Multiplicative Zagreb Index	$\prod_1(A)$	$\prod_{s\in V(A)}(d_s)^2$
3	General Multiplicative Index	$W_1^{\alpha}(A)$	$\prod_{s\in V(A)}(d_s)^{\alpha}$
4	First Multiplicative Generalized Zagreb Index	$MZ_1^{\alpha}(A)$	$\prod_{uv\in E(G)}(d_u + d_v)^{\alpha}$
5	Second Multiplicative Generalized Zagreb Index	$MZ_2^{\alpha}(A)$	$\prod_{rs\in E(A)}(d_r \cdot d_s)^{\alpha}$
6	Multiplicative version of First Zagreb Index	$\prod_1^*(A)$	$\prod_{rs\in E(A)}(d_r + d_s)$
7	Second Multiplicative Zagreb Index	$\prod_2(A)$	$\prod_{rs\in E(A)}(d_r \cdot d_s)$
8	Multiplicative First Hyper Zagreb Index	$H\prod_1(A)$	$\prod_{rs\in E(A)}(d_r + d_s)^2$
9	Multiplicative Second Hyper Zagreb Index	$H\prod_2(A)$	$\prod_{rs\in E(A)}(d_r \cdot d_s)^2$
10	Multiplicative Sum Connectivity Index	$SC\prod(A)$	$\prod_{rs\in E(A)}\frac{1}{\sqrt{d_r + d_s}}$
11	Multiplicative Product Connectivity Index	$PC\prod(A)$ (or) $R\prod(A)$	$\prod_{rs\in E(A)}\frac{1}{\sqrt{d_r \cdot d_s}}$
12	Multiplicative Sum Connectivity F –Index	$SCF\prod(A)$	$\prod_{rs\in E(A)}\frac{1}{\sqrt{d_r^2 + d_s^2}}$
13	Multiplicative Product Connectivity F – Index	$PG\prod(A)$	$\prod_{rs\in E(A)}\frac{1}{\sqrt{d_r^2 \cdot d_s^2}}$
14	Multiplicative First F –Index	$F_1\prod(A)$	$\prod_{rs\in E(A)}\left[(d_r)^2 + (d_s)^2\right]$

S. No.	Topological index	Notation	Formula of topological index
15	Multiplicative Second F – Index	$F_2\prod(A)$	$\prod_{rs\in E(A)}\left[(d_r)^2\cdot(d_s)^2\right]$
16	Multiplicative Atomic Bond Connectivity Index	$ABC\prod(A)$	$\prod_{rs\in E(A)}\sqrt{\frac{d_r+d_s-2}{d_r\cdot d_s}}$
17	Multiplicative Harmonic Index	$H\prod(A)$	$\prod_{rs\in E(A)}\frac{2}{d_r+d_s}$
18	Multiplicative Geometric Arithmetic Index	$GA\prod(A)$	$\prod_{rs\in E(A)}\frac{2\sqrt{d_r\cdot d_s}}{d_r+d_s}$
19	General Multiplicative Geometric Arithmetic Index	$GA^{\alpha}\prod(A)$	$\prod_{rs\in E(A)}\left(\frac{2\sqrt{d_r\cdot d_s}}{d_r+d_s}\right)^{\alpha}$
20	Multiplicative Augmented Zagreb Index	$AZ\prod(A)$	$\prod_{rs\in E(A)}\left(\frac{d_r\cdot d_s}{d_r+d_s-2}\right)^3$

2.3 Zagreb, Forgotten, Harmonic, Inverse Degree Indices and M-Polynomials of a Graph

Fath-Tabar provided the definitions of the first, second, and third Zagreb polynomials. Harmonic polynomial are introduces by Iranmanesh et al. [7]. Shuxian [8] established the modifies first zagreb index. In 2015 [9], Deutsch and Klavzar created a number of new algebraic polynomials. By specifying the closed form of specific degree-based Topological indices, it serves a similar function. One of M-Polynomial's best features is the abundance of information it offers on molecular labels. A few polynomials of graph invariants are shown in Tables 3 and 4.

Table 3. Topological indices of a graph A depending on degree and their corresponding polynomials

S. No.	Topological index	Polynomial $P(A,a)$	Derivation from $P(A,a)$
1	First Zagreb	$M_1(\mathrm{A},a)=\sum_{rs\in E(A)}a^{d_r+d_s}$	$D_a(M_1(A;a))\|_{a=1}$
2	Second Zagreb	$M_2(A,a)=\sum_{rs\in E(A)}a^{d_r\cdot d_s}$	$D_a(M_2(A;a))\|_{a=1}$
3	Third Zagreb	$M_3(A,a)=\sum_{rs\in E(A)}a^{\|d_r-d_s\|}$	$D_a(M_3(A;a))\|_{a=1}$
4	Forgotten	$F(A,a)=\sum_{rs\in E(A)}a^{(d_r{}^2+d_s{}^2)}$	$D_a(F(A;a))\|_{a=1}$
5	Modified First Zagreb	$M_1^*(A,a)=\sum_{s\in V(A)}d_s\,a^{d_s}$	$D_a(M_1^*(A;a))\|_{a=1}$
6	Harmonic	$H(A,a)=\sum_{rs\in E(A)}a^{d_r+d_s-1}$	$2I_a(H(A;a))\|_{a=1}$
7	Modified Forgotten	$F^*(A,a)=\sum_{s\in V(A)}a^{d_s{}^3}$	$D_a(F^*(A;a))\|_{a=1}$
8	Inverse Degree	$ID(A,a)=\sum_{s\in V(A)}a^{d_s-1}$	$I_a(H(A;a))\|_{a=1}$

Theorem 2.1. [9] Assume that A is a simple connected graph.

(1) *If* $I(A)=\sum_{rs\in E(A)} f(dr\cdot ds)$, where $f(a,b)$ is a polynomial in a and b, then $I(A)=f(D_a,D_b)(M(A;a,b))|_{a=b=1}$.

(2) *If* $I(A)=\sum_{rs\in E(A)} f(dr\cdot ds)$, where, $I(A)$ can be obtained from $M(A;\ a,b)$ using the operators D_a, D_b, S_a, S_b.

(3) *If* $I(A)=\sum_{rs\in E(A)} f(dr\cdot ds)$, where $f(a,b)=\dfrac{a^i b^j}{(a+b+\alpha)^t}$, where a and b are variables, $i,j\geq 0,\ t\geq 1$, then $I(A)=S_a^t Q_\alpha J D_a^i D_b^j (M(A;a,b))|_{a=b=1}$.

The definition of a molecular graph's M-Polynomial [10-13] is

$M(A;a,b) = \sum_{\delta\leq i\leq j\Delta} m_{ij}(A)a^i b^j$ ---------(1)

Table 4. Degree–based Topological indices derived from M-Polynomial of a graph A

S. No	Topological index	$f(a,b)$	Derivation from $M(A;\ a,b)$
1	$M_1(A)$	$a+b$	$(D_a+D_b)(M(A;a))|_{a=b=1}$
2	$M_2(A)$	ab	$(D_aD_b)(M(A;a))|_{a=b=1}$
3	${}^mM_2(A)$	$\frac{1}{ab}$	$(S_aS_b)(M(A;a))|_{a=b=1}$
4	$SDD(A)$	$\frac{a^2+b^2}{ab}$	$(D_aS_b+D_bS_a)(M(A;a))|_{a=b=1}$
5	$H(A)$	$\frac{2}{a+b}$	$2S_aJ(M(A;a))|_{a=b=1}$
6	$ISI(A)$	$\frac{ab}{a+b}$	$S_aJD_aD_a(M(A;a))|_{a=b=1}$
7	$AZI(A)$	$\left(\frac{ab}{a+b-2}\right)^3$	$S_a^3Q_{-2}JD_a{}^3D_b{}^3(M(A;a))|_{a=b=1}$
8	$F(A)$	a^2+b^2	$(D_a{}^2+D_b{}^2)(M(A;a))|_{a=b=1}$
9	$\operatorname{Re}M_3(A)$	$ab(a+b)$	$(D_aD_b)(D_a+D_b)(M(A;a))|_{a=b=1}$
10	$ABC(A)$	$\sqrt{\frac{a+b-2}{a.b}}$	$S_a^{\frac{-1}{2}}Q_{-2}JD_b^{\frac{-1}{2}}(M(A;a))|_{a=b=1}$

To calculate the corresponding Topological indices of a graph A from the $M(A;a,b)$ as stated in Table 4. Table 2 lists the equations of derivations in terms of integral, derivative, or both integral and derivative. [9], where

$$D_a = a\frac{\partial(f(a,b))}{\partial a},\quad D_b = b\frac{\partial(f(a,b))}{\partial b},\ S_a=\int_0^a \frac{f(t,b)}{t}dt,\ S_b=\int_0^{ba}\frac{f(a,t)}{t}dt,$$

$$J(f(a,b)) = f(a,a)\ \ and\ \ Q_\alpha(f(a,b)) = x^\alpha f(a,b),\ \alpha\neq 0$$

2.4 Methodology

One of our main conclusions is that Tis of antiviral drug structures can be derived using algebraic polynomials. Fenofibrate molecular structure can be accessed at pubchem.ncbi.nlm.nih.gov. hydrogen suppressed molecular graph of a compound can be considered, since the vertices representing the hydrogen atoms do not contribute to graph isomorphism. We employ edge partitioning, degree counting, graph theoretical tools, combinatorial computation, and analytical techniques to arrive at our main findings. Using edge partitions and the formulas listed in Tables 1 and 2, expressions of additive and multiplicative degree-based Topological indices were calculated. likewise, Tables 3 and 4 are used to generate several closed versions of M-Polynomials, Zagreb, Forgotten, Harmonic, Inverse degree polynomials, and so on. To compare the numerical findings graphically, MATLAB 2017b was used to plot the polynomials on a surface.

3. RESULTS AND DISCUSSION

This section begins with the following derivation of the ID, Zagreb, Harmonic, and Forgotten polynomials.

Theorem 3.1. For a molecular graph Fenofibrate $(C_{20}H_{21}CIO_4)$ drug . Then we have

(1) $M_1(A,a) = a^7 + 3a^6 + 13a^5 + 9a^4$.

(2) $M_2(A,a) = a^{12} + 2a^9 + a^8 + 11a^6 + 6a^4 + 5a^3$.

(3) $M_3(A,a) = 2a^3 + 6a^2 + 12a + 6$

(4) $F(A,a) = a^{25} + a^{20} + 2a^{18} + 2a^{17} + 11a^{13} + 5a^{10} + 4a^8$.

(5) $H(A,a) = a^6 + 3a^5 + 13a^4 + 9a^3$.

(6) $M_1^*(A,a) = 4a^4 + 21a^3 + 20a^2 + 7a$.

(7) $F^*(A,a) = a^{64} + 7a^{27} + 10a^8 + 7a^3$.

(8) $D(A,a) = a^3 + 7a^2 + 10a + 7.$

Proof: Consider a molecular graph of Fenofibrate as A. There are 26 edges and 25 vertices in the graph A. Let J_m be the collection of the vertices with degree m, i.e., $J_m = \{s \in V(A) : d_s = m\}$. Let j_m be the number of vertices in J_m. Let $K_{n,m}$ be the set that has edges with vertices of degree n and m. i.e., $k_{n,m} = \{rs \in E(A) : d_r = n, d_s = m\}$. $k_{n,m}$ denotes the number of edges in. $j_1 = 7,\ j_2 = 10,\ j_3 = 7. j_4 = 1$

$d_r, d_s : rs \in E(A)$	**Number of edges**
(1,3)	5
(1,4)	2
(2,2)	4
(2,4)	1
(2,3)	11
(3,3)	2
(3,4)	1

Applying the polynomial formulas provided in Table 3, we obtain

(1) $M_1(A,a) = \sum_{rs \in E(A)} k_{n,m}\, a^{n+m}$

$= 5a^{(1+3)} + 11a^{(2+3)} + 4a^{(2+2)} + 2a^{(1+4)} + a^{(2+4)} + a^{(3+4)} + 2a^{(3+3)}$

$= a^7 + 3a^6 + 13a^5 + 9a^4$

(2) $M_2(A,a)=\sum_{rs\in E(A)} k_{n,m}\ a^{n.m}$

$=5a^{(1.3)}+11a^{(2.2)}+2a^{(1.4)}+a^{(2.4)}+a^{(3.4)}+2a^{(3.3)}$

$=a^{12}+2a^{9}+a^{8}+11a^{6}+6a^{4}+5a^{3}$

(3) $M_3(A,a)=\sum_{rs\in E(A)} k_{n,m}\ a^{|n-m|}$

$=5a^{|1-3|}+11a^{|2-3|}+4a^{|2-2|}+2a^{|1-4|}+a^{|2-4|}+a^{|3-4|}+2a^{|3-3|}$

$=2a^{3}+6a^{2}+12a+6$

(4) $F(A,a)=\sum_{rs\in E(A)} k_{n,m}\ a^{(n^2+m^2)}$

$=5a^{(1^2+3^2)}+11a^{(2^2+3^2)}+4a^{(2^2+2^2)}+2a^{(1^2+4^2)}+a^{(2^2+4^2)}+a^{(3^2+4^2)}+2a^{(3^2+3^2)}$

$=a^{25}+a^{20}+2a^{18}+2a^{17}+11a^{13}+5a^{10}+4a^{8}$

(5) $M_1^{*}(A,a)\ =\sum_{rs\in E(A)} m\ a^{m}$

$=j_1(1)a^1+j_2(2)a^2+j_3(3)a^3+j_4(4)a^4$

$=4a^4+21a^3+20a^2+7a$

(6) $H(A,a)\ =\sum_{rs\in E(A)} k_{n,m}\ a^{(n+m-1)}$

$=5a^{(1+3-1)}+11a^{(2+3-1)}+4a^{(2+2-1)}+2a^{(1+4-1)}+a^{(2+4-1)}+a^{(3+4-1)}+2a^{(3+3-1)}$

$=a^6+3a^5+13a^4+9a^3$

(7) $F^{*}(A,a)=\sum_{rs\in E(A)} k_{n,m}\ a^{m^3}$

$=j_1a^{(1)^3}+j_2a^{(2)^3}+j_3a^{(3)^3}+j_4a^{(4)^3}$

$=a^{64}+7a^{27}+10a^{8}+7a^{3}$

(8) $ID(A,a)=\sum_{rs\in E(A)} a^{m-1}$

$=j_1a^{1-1}+j_2a^{2-1}+j_3a^{3-1}+j_4a^{4-1}$

$=a^3+7a^2+10a+7.$

We obtain the relevant Topological indices using the polynomials mentioned below.

Theorem 3.2 If A is a molecular graph of Fenofibrate $(C_{20}H_{21}ClO_4)$ drug then,

(i) $M_1(A)=126$

(ii) $M_2(A)=143$

(iii) $M_3(A)=30$

(iv) $F(A)=340$

(v) $M_1^{*}(A)=126$

(vi) $H(A)=7.74$

(vii) $F^{*}(A)=354$

(viii) $ID(A)=14.55$

Proof: We derive using Table 3 and Theorem 3.1,

$$(i)\quad M_1(A,a) = D_a(M_1(A;a))|_{a=1} = \frac{d}{da}\left(a^7 + 3a^6 + 13a^5 + 9a^4\right)$$
$$= 7a^6 + 18a^5 + 65a^4 + 36a^3 = 126$$

$$(ii)\quad M_2(A,a) = D_a(M_2(A;a))|_{a=1} = \frac{d}{da}\left(a^{12} + 2a^9 + a^8 + 11a^6 + 6a^4 + 5a^3\right)$$
$$= 12a^{11} + 18a^8 + 8a^7 + 66a^5 + 24a^3 + 15a^2 = 143$$

$$(iii)\quad M_3(A,a) = D_a(M_3(A;a))|_{a=1} = \frac{d}{da}\left(2a^3 + 6a^2 + 12a + 6\right)$$
$$= 6a^2 + 12a + 12 = 30$$

$$(iv)\quad F(A,a) = D_a(F(A;a))|_{a=1} = \frac{d}{da}\left(a^{25} + a^{20} + 2a^{18} + 2a^{17} + 11a^{13} + 5a^{10} + 4a^8\right)$$
$$= 25a^{24} + 20a^{19} + 36a^{17} + 34a^{16} + 143a^{12} + 50a^9 + 32a^7 = 340$$

$$(v)\quad M_1^*(A,a) = D_a(M_1^*(A;a))|_{a=1} = \frac{d}{da}\left(4a^4 + 21a^3 + 20a^2 + 7a\right)$$
$$= 16a^3 + 63a^2 + 40a + 7 = 126$$

$$(vi)\quad H(A,a) = 2I_a(H(A;a))|_{a=1} = 2\int_0^a \left(a^6 + 3a^5 + 13a^4 + 9a^3\right) d_a$$
$$= 2\left(\frac{a^7}{7} + \frac{3a^6}{6} + \frac{13a^5}{5} + \frac{9a^4}{4}\right)_{a=1} = 7.74$$

$$(vii)\quad F^*(A,a) = D_a(F^*(A;a))|_{a=1} = \frac{d}{da}\left(a^{64} + 7a^{27} + 10a^8 + 7a^3\right)$$
$$= 64a^{63} + 189a^{26} + 80a^7 + 21a^2 = 354$$

$$(viii)\quad ID(A,a) = I_a(ID(A;a))|_{a=1} = \int_0^a \left(a^3 + 7a^2 + 10a + 7\right) d_a$$
$$= \left(\frac{a^4}{4} + \frac{7a^3}{3} + \frac{13a^2}{2} + 7a\right)_{a=1} = 14.55$$

Theorem 3.3. If A is a molecular graph of Fenofibrate ($C_{20}H_{21}ClO_4$) drug then,

$$M(A;a,b) = 5ab^3 + 2ab^4 + 4a^2b^2 + 11a^2b^3 + a^2b^4 + 2a^3b^3 + a^3b^4.$$

Proof: The M -Polynomials of A are obtained as follows from equation (1).

$$M(A;a,b) = \sum_{n\le m} k_{n,m}a^n b^m,\ where\ \ n,m \in \{1,2,3,4\}$$
$$= k_{1,3}a^1b^3 + k_{1,4}a^1b^4 + k_{2,2}a^2b^2 + k_{2,4}a^2b^4 + k_{2,3}a^2b^3 + k_{3,3}a^3b^3 + k_{3,4}a^3b^4$$
$$= 5ab^3 + 2ab^4 + 4a^2b^2 + 11a^2b^3 + a^2b^4 + 2a^3b^3 + a^3b^4$$

The polynomials obtained in the previous theorem are now used to evaluate a few indices for the drug's molecular graph.

Theorem 3.4. Let A be the fenofibrate molecular graph $(C_{20}H_{21}ClO_4)$. Then we have,

i. $M_1(A)=126$
ii. $M_2(A)=143$
iii. ${}^mM_2(A)=5.415$
iv. $H(A)=5.492$
v. $ISI(A)=28.264$
vi. $AZI(A)=186.22$
vii. $F(A)=626$
viii. $\operatorname{Re}M_3(A)=886$

Proof: Let $M(A;a,b)=5ab^3+2ab^4+4a^2b^2+11a^2b^3+a^2b^4+2a^3b^3+a^3b^4$

Using Table 4 we obtained the following results

$$(i)\quad M_1(A)=(D_a+D_b)M(A;a,b)|_{a=b=1}$$
$$=20ab^3+10ab^4+16a^2b^2+55a^2b^3+6a^2b^4+12a^3b^3+7a^3b^4\,|_{a=b=1}$$
$$=126$$

$$(ii)\quad M_2(A)=(D_aD_b)M(A;a,b)|_{a=b=1}$$
$$=15ab^3+8ab^4+16a^2b^2+66a^2b^3+8a^2b^4+18a^3b^3+12a^3b^4\,|_{a=b=1}$$
$$=143$$

$$(iii)\quad {}^mM_2(A)=(S_aS_b)M(A;a,b)|_{a=b=1}$$
$$=\frac{5ab^3}{3}+\frac{2ab^4}{4}+\frac{4a^2b^2}{4}+\frac{11a^2b^3}{6}+\frac{a^2b^4}{8}+\frac{2a^3b^3}{9}+\frac{a^3b^4}{12}\,|_{a=b=1}$$
$$=5.415$$

$$(iv)\quad H(A)=2S_aJ(M(A;a,b))|_{a=1}$$
$$J(f(a,b))=a^7+3a^6+13a^5+9a^4$$
$$2S_aJ(M(A;a,b)=2\int_0^a\frac{a^7+3a^6+13a^5+9a^4}{x}d_a$$
$$=2\left(\frac{a^7}{7}+\frac{3a^6}{6}+\frac{13a^5}{5}+\frac{9a^4}{4}\right)_{a=1}=2(5.492)=10.984$$

$$(v)\quad ISI(A)=S_aJ(D_aD_b)M(A;a,b)|_{a=b=1}$$
$$=15ab^3+8ab^4+16a^2b^2+66a^2b^3+8a^2b^4+18a^3b^3+12a^3b^4\,|_{a=b=1}$$
$$=15a^4+8a^5+16a^4+66a^5+8a^6+18a^6+12a^7$$
$$=\left(\frac{12a^7}{7}+\frac{26a^7}{6}+\frac{74a^5}{5}+\frac{31a^4}{4}\right)_{a=1}$$
$$=28.594$$

$(vi)\quad AZI(A) = S_a^{\,3} Q_{-2} J(D_a^{\,3} D_b^{\,3}) M(A;a,b)|_{a=b=1}$

$(D_a^{\,3} D_b^{\,3}) M(A;a,b) = 135ab^3 + 128ab^4 + 256a^2b^2 + 2376a^2b^3 + 512a^2b^4 + 1458a^3b^3 + 1728a^3b^4$

$= 1728a^7 + 1970b^6 + 2504b^5 + 391b^4$

$Q_{-2} J(D_a^{\,3} D_b^{\,3}) M(A;a,b) = 1728a^5 + 1970a^4 + 2504a^3 + 391a^2$

$$= \left(\frac{1728a^5}{125} + \frac{1970a^4}{64} + \frac{2504a^3}{27} + \frac{391a^2}{8} \right)_{a=1}$$

$AZI(A) = 186.22$

$(vii)\quad F(A) = (D_a^{\,2} + D_b^{\,2}) M(A;a,b)|_{a=b=1}$

$= 80ab^3 + 50ab^4 + 64a^2b^2 + 275a^2b^3 + 36a^2b^4 + 72a^3b^3 + 49a^3b^4 |_{a=b=1}$

$= 626$

$(viii)\quad \operatorname{Re} M_3(A) = (D_a + D_b)(D_a D_b) M(A;a,b)|_{a=b=1}$

$= 60ab^3 + 40ab^4 + 216a^2b^2 + 330a^2b^3 + 48a^2b^4 + 108a^3b^3 + 84a^3b^4 |_{a=b=1}$

$= 886$

The multiplicative Topological indices of fenofibrate are obtained in the following manner

Theorem 3.5. For a chemical graph of Fenofibrate $(C_{20}H_{21}ClO_4)$ drug A, we obtain,

(i) $NK(A) = 52$
(ii) $\prod_1(A) = 126$
(iii) $\prod_1^*(A) = 126$
(iv) $H\prod_1(A) = 626$
(v) $H\prod_2(A) = 907$
(vi) $SC\prod(A) = 0.089$
(vii) $PC\prod(A) = 0.083$
(viii) $SF\prod(A) = 7.423$
(ix) $PF\prod(A) = 5.418$
(x) $F_1\prod(A) = 340$
(xi) $F_2\prod(A) = 907$
(xii) $ABC\prod(A) = 12.726$
(xiii) $H(A) = 0.015$
(xiv) $GAII(A) = 0.189$

Proof: By using the degrees of the vertices d_r, d_s of vertices r and s and the values $j_1 = 7,\ j_2 = 10,\ j_3 = 7. j_4 = 1\ k_{1,3} = 5,\ k_{1,4} = 2,\ k_{2,2} = 4,\ k_{2,3} = 11,\ k_{3,3} = 2,\ k_{2,4} = 1,\ k_{3,4} = 1,$

We are able to compute multiplicative Topological indices using the formulas shown in Table 2.

The graph in Fig. 3 illustrates the different Fenofibrate drug polynomials, which are mostly self-explanatory. In Fig. 4, the M-polynomial of the medication is plotted in three dimensions.

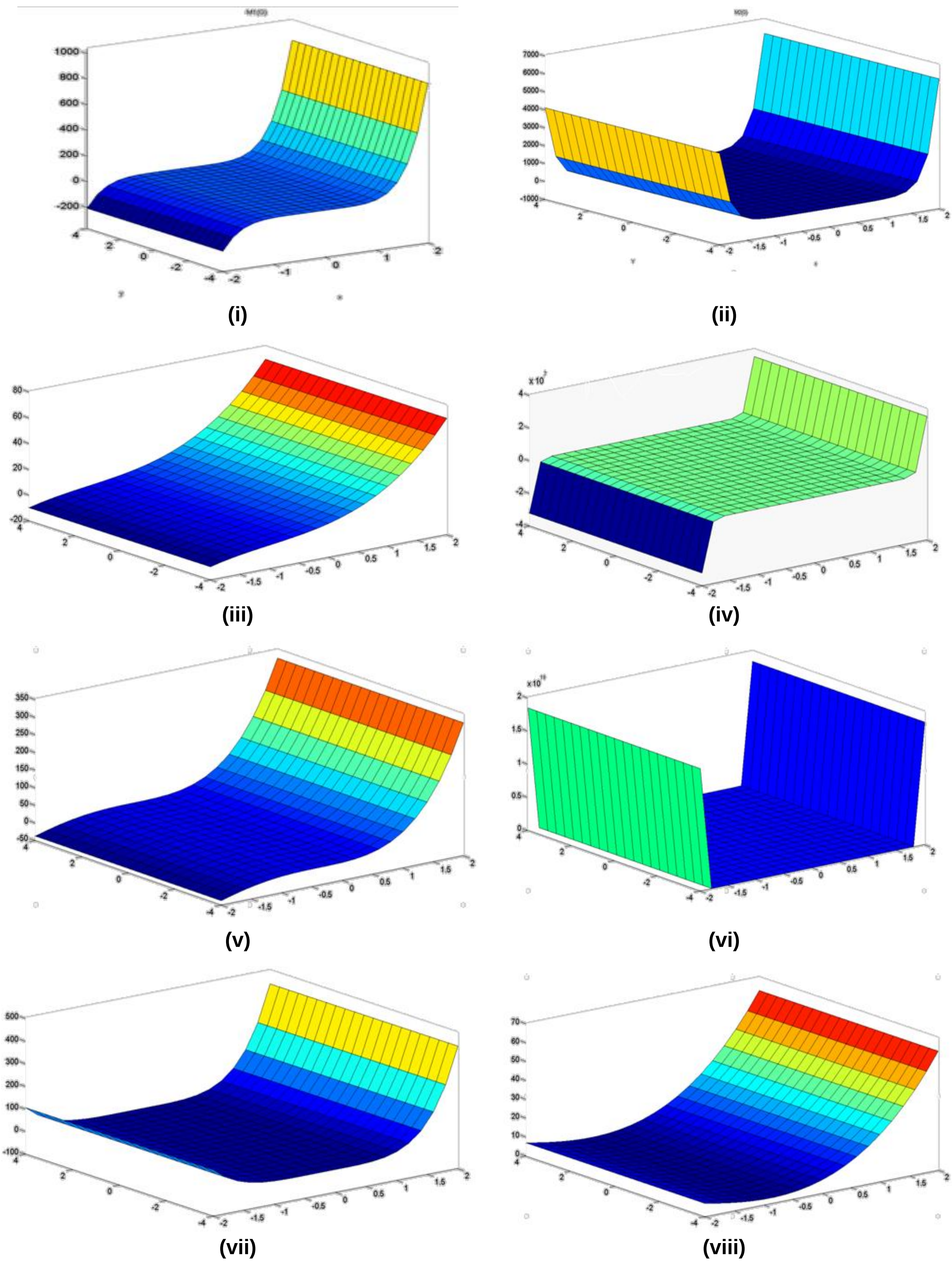

Fig. 3. Plotting (i) $M_1(A)$ **,(ii)** $M_2(A)$ **, (iii)** $M_3(A)$ **, (iv)** $F(A)$ **, (v)** $M_1 * (A)$ **(vi)** $F^* A)$ **, (vii)** $H(A)$ **(viii)** $ID(A)$

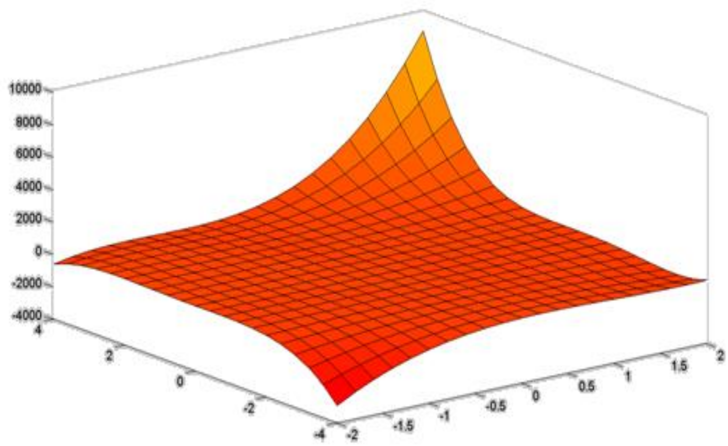

Fig. 4. M-Polynomial

4. CONCLUSION

Our analysis of many significant sums and the product connectivity topological index for the Fenofibrate drug's molecular graph is being provided numerically for the first time. Using graphical representations, the Zagreb, Harmonic, Forgotten, and Inverse degree polynomials were also calculated. Additionally, it was successful to commence the closed version of Fenofibrate's M-polynomials, and precise formulas were found. The calculated indices may have uses in the pharmaceutical sciences, including data mining, chemical documentation investigations, and the field of medication design.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

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