

A Computational Approach on Acetaminophen Drug using Degree-Based Topological Indices and M-Polynomials

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Abstract: Topological index is a numerical representation of a chemical structure. Based on these indices, physicochemical properties, thermodynamic behavior, chemical reactivity, and biological activity of chemical compounds are calculated. Acetaminophen is an essential drug to prevent/treat various types of viral fever, including malaria, flu, dengue, SARS, and even COVID-19. This paper computes the sum and multiplicative version of various topological indices such as General Zagreb, General Randić, General OGA, AG, ISI, SDD, Forgotten indices M-polynomials of Acetaminophen. To the best of our knowledge, for the Acetaminophen drugs, these indices have not been computed previously.

Keywords: topological index; chemical graph; Acetaminophen; M-polynomial; Zagreb; COVID-19.

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1. Introduction

In this article, all molecular (chemical) graphs are finite, loopless, connected, and with no multiple edges. The graph $G = (V, E)$ with vertex set V and edge set E . The degree of a vertex $u \in V(G)$ is denoted d_u as explained in graph theory [1,2].

1.1. A brief overview on topological indices.

Topological indices (TIs) are molecular descriptors that characterize the structure of the chemical compounds and can be used to predict some physical, chemical, and biological properties such as stability, vaporization enthalpy, boiling point, toxicity, and so on. A molecular graph is a graph-theoretic representation of a chemical compound's structural formula, where vertices represent atoms and edges represent chemical bonds [3]. Wiener proposed the notion of TIs in chemical graph theory (CGT) in 1947 to predict certain physicochemical properties of alkanes [4]. For predicting the total π electron energy of molecules, Gutman *et al.* [5] developed a pair of TIs called the first Zagreb ($M_1(G)$) and second Zagreb ($M_2(G)$) indices. A comprehensive discussion on different TIs was given in [6–13].

1.2. Significance of Acetaminophen drug.

The most prominent drug for treating fever and pain is acetaminophen, often known as paracetamol or APAP. Many ailments are treated with acetaminophen, including muscular

pains, headaches, toothaches, arthritis, fevers, and colds [14]. Fever, along with persistent cough and shortness of breath, are some of the symptoms of COVID-19 [15]. Fever is particularly unpleasant because it is frequently accompanied by shivers, nausea, headaches, and stomach distress. A fever can be brought down by taking an anti-inflammatory medication, especially acetaminophen, along with antivirals and antiretrovirals, which reduce some of the fever molecules [16]. Acetaminophen can be taken with or without food and is harmless for pregnant or breastfeeding women [17,18].

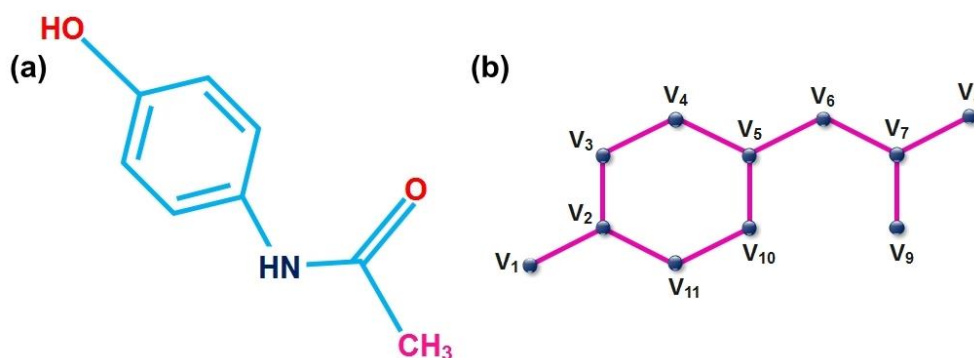


Figure 1. Chemical structure (a) and Chemical graph (b) of Acetaminophen drug.

Acetaminophen was invented in 1877 [19] and is featured on the WHO's list of essential drugs, which includes the most efficient and safe medicines that are required for constructing a well-being community. It has a benzene ring core replaced by one hydroxyl group and the nitrogen atom of an amide group in the para (1,4) pattern [19]. Its molecular formula is $C_8H_9NO_2$. The hydroxyl oxygen lone pair, the nitrogen lone pair, the benzene pi cloud, the carbonyl oxygen lone pair, and the p orbital on the carbonyl carbon are all conjugated in the structure. The benzene ring is also highly reactive towards electrophilic aromatic substitution due to the existence of two activating groups. Figure 1 depicts the chemical structure and molecular graph of the Acetaminophen drug.

1.3. Proposed work and organization.

This paper primarily focuses on computing various vertex degree-based sum and product connectivity TIs of Acetaminophen drugs. This paper is constructed as follows. The fundamental notions are presented in Section 1. In Section 2, vertex degree-based TIs and M-polynomials are tabulated. In Section 3, we compute certain indices and polynomials of acetaminophen using its molecular graph. In Section 4, there is a conclusion.

2. Materials and Methods

2.1. Additive degree-based Tis.

In 1975, Milan Randić invented the branching index (later known as the Randić index), which is symbolized by $\chi(G)$ and has proven to be a good parameter for quantitative assessment of molecular branching QSAR, and QSPR research [20]. To date, several important additive degree-based TIs have been reported, some of which are enumerated in Table 1. For more insight on these indices, we offer [21-26] for ambitious readers.

Suppose uw is the edge that connects the vertices u and w , then the additive degree-based TIs in mathematical chemistry have the general form $TI = TI(G) = \sum_{uw \in E(G)} F(d_u, d_w)$.

Table 1. Additive degree-based TIs of a graph G .

S.No	TI	Notation	Formula of TI
1.	First Zagreb Index [5]	$M_1(G)$	$\sum_{uw \in E(G)} (d_u + d_w)$
2.	Modified First Zagreb Index [5]	$M_1^*(G)$	$\sum_{w \in V(G)} (d_w)^2$
3.	Second Zagreb Index [5]	$M_2(G)$	$\sum_{uw \in E(G)} (d_u \cdot d_w)$
4.	Randić Index [20]	$R(G)$	$\sum_{uw \in E(G)} \frac{1}{\sqrt{d_u \cdot d_w}}$
5.	Third Zagreb Index [25]	$M_3(G)$	$\sum_{uw \in E(G)} d_u - d_w $
6.	First Hyper Zagreb Index [26]	$HM_1(G)$	$\sum_{uw \in E(G)} (d_u + d_w)^2$
7.	Second Hyper Zagreb Index [26]	$HM_2(G)$	$\sum_{uw \in E(G)} (d_u \cdot d_w)^2$
8.	General First Zagreb Index [26] (or) General Sum Connectivity Index [38]	$M_1^\alpha(G)$	$\sum_{uw \in E(G)} (d_u + d_w)^\alpha$
9.	General Second Zagreb Index [26]	$M_2^\alpha(G)$	$\sum_{uw \in E(G)} (d_u \cdot d_w)^\alpha$
10.	Reduced Second Zagreb Index [27]	$RM_2(G)$	$\sum_{uw \in E(G)} (d_u - 1) \cdot (d_w - 1)$
11.	Redefined First Zagreb Index [28]	$Re M_1(G)$	$\sum_{uw \in E(G)} \left(\frac{d_u + d_w}{d_u \cdot d_w} \right)$
12.	Redefined Second Zagreb Index [28]	$Re M_2(G)$	$\sum_{uw \in EG} \frac{d_u \cdot d_w}{d_u + d_w}$
13.	Redefined Third Zagreb Index [28]	$Re M_3(G)$	$\sum_{uw \in EG} (d_u \cdot d_w) (d_u + d_w)$
14.	Modified Second Zagreb Index [29]	${}^m M_2(G)$	$\sum_{uw \in E(G)} \frac{1}{d_u \cdot d_w}$
15.	Nano - Zagreb Index [30]	$N_Z(G)$	$\sum_{uw \in E(G)} \left[(d_u)^2 - (d_w)^2 \right]$
16.	Sum Nano - Zagreb Index [31]	$\chi_{\frac{1}{2}}^{N_Z}(G)$	$\sum_{uw \in E(G)} \left(d_u^2 - d_w^2 \right)^{\frac{1}{2}}$
17.	Zeroth order Randić Index [32]	$\frac{R_{-1}^0(G)}{2}$	$\sum_{w \in V(G)} (d_w)^{-\frac{1}{2}}$
18.	Zeroth Order General Randić Index [33]	$R_\alpha^0(G)$	$\sum_{w \in V(G)} (d_w)^\alpha$
19.	Reciprocal Randić Index [34]	$RR(G)$	$\sum_{uw \in E(G)} \sqrt{d_u \cdot d_w}$
20.	Reduced Reciprocal Randić Index [34]	$RRR(G)$	$\sum_{uw \in E(G)} \sqrt{(d_u - 1) \cdot (d_w - 1)}$
21.	Inverse Randić Index [35]	$RR_\alpha(G)$	$\sum_{uw \in E(G)} \frac{1}{(d_u \cdot d_w)^\alpha}$

S.No	TI	Notation	Formula of TI
22.	Modified Randić Index [36]	$R'(G)$	$\sum_{u w \in E(G)} \frac{1}{\max\{d_u, d_w\}}$
23.	Sum Connectivity Index [37]	$SCI(G)$ $\chi(G)$	$\sum_{u w \in E(G)} \frac{1}{\sqrt{d_u + d_w}}$
24.	Arithmetic Geometric Index [39]	$AG(G)$	$\sum_{u w \in E(G)} \frac{d_u + d_w}{2\sqrt{d_u \cdot d_w}}$
25.	Variable Sum exdeg Index [40,41]	$SEI_\alpha(G)$	$\sum_{w \in V(G)} d_w (\alpha)^{d_w}$, and $\alpha \neq 1$
26.	Harmonic Index [42,43]	$H(G)$	$\sum_{u w \in E(G)} \frac{2}{d_u + d_w}$
27.	General Harmonic Index [44]	$H_k(G)$	$\sum_{u w \in E(G)} \left(\frac{2}{d_u + d_w}\right)^k$
28.	General Ordinary Geometric Arithmetic Index [45]	$OGA_k(G)$	$\sum_{u w \in E(G)} \left(\frac{2\sqrt{d_u \cdot d_w}}{d_u + d_w}\right)^k$
29.	Ordinary Geometric Arithmetic Index [45]	$OGA(G)$	$\sum_{u w \in E(G)} \frac{2\sqrt{d_u \cdot d_w}}{d_u + d_w}$
30.	SK Index [46]	$SK(G)$	$\sum_{u w \in E(G)} \frac{d_u + d_w}{2}$
31.	SK ₁ Index [46]	$SK_1(G)$	$\sum_{u w \in E(G)} \frac{d_u \cdot d_w}{2}$
32.	SK ₂ Index [46]	$SK_2(G)$	$\sum_{u w \in E(G)} \left(\frac{d_u + d_w}{2}\right)^2$
33.	Forgotten Index [47]	$F(G)$	$\sum_{u w \in E(G)} \left[(d_u)^2 + (d_w)^2 \right]$
34.	Inverse sum (Indeg) Index [48]	$ISI(G)$	$\sum_{u w \in EG} \frac{d_u \cdot d_w}{d_u + d_w}$
35.	Symmetric Division (Deg) Index [49]	$SDD(G)$	$\sum_{u w \in E(G)} \left[\frac{\min\{d_u, d_w\} + \max\{d_u, d_w\}}{\max\{d_u, d_w\} + \min\{d_u, d_w\}} \right]$
36.	IRM Index [49]	$IRM(G)$	$\sum_{u w \in E(G)} (d_u - d_w)^2$
37.	Augmented Zagreb Index [50]	$AZI(G)$	$\sum_{u w \in E(G)} \left(\frac{d_u \cdot d_w}{d_u + d_w - 2}\right)^3$
38.	Albertson Index [51,52]	$A(G)$	$\sum_{u w \in E(G)} d_u - d_w $
39.	Atomic Bond Connectivity Index [53]	$ABC(G)$	$\sum_{u w \in E(G)} \sqrt{\frac{d_u + d_w - 2}{d_u \cdot d_w}}$
40.	Bell Index[54]	$B(G)$	$\sum_{w \in V(G)} \left(d_w - \frac{2q}{p}\right)^2$
41.	First Entire Zagreb Index[55]	$M_1^E(G)$	$\sum_{w \in V(G) \cup E(G)} (d_w)^2$
42.	Sombor Index [56 – 64]	$SO(G)$	$\sum_{u w \in E(G)} \sqrt{(d_u)^2 + (d_w)^2}$

2.2. Multiplicative degree-based Tis.

This subsection tabulated some significant multiplicative degree-based TIs, that can be used to develop our primary results. Narumi and Katayama [65] proposed a multiplicative TI, known as $NK(G)$. After, Wang *et al.* redefined $NK(G)$ as a general multiplicative index [66]. Kulli *et al.* have established the multiplicative sum connectivity $SCII(G)$ and multiplicative product connectivity $PCII(G)$ indices to further study of TIs [67]. For more about multiplicative degree-based TIs the following literature [65-76] can be quite helpful.

According to CGT, the generalized form of multiplicative TIs is given below [66],

$$MTI = MTI(G) = \prod_{uw \in E(G)} F(d_u, d_w)$$

Table 2. Multiplicative degree-based TIs of a graph G.

S.No	TI	Notation	Formula of TI
1.	Narumi – Katayama Index [65]	$NK(G)$	$\prod_{w \in V(G)} (d_w)$
2.	First Multiplicative Zagreb Index [68]	$II_1(G)$	$\prod_{w \in V(G)} (d_w)^2$
3.	General Multiplicative Index [66]	$W_1^\alpha(G)$	$\prod_{w \in V(G)} (d_w)^\alpha$
4.	First Multiplicative Generalized Zagreb Index [69]	$MZ_1^\alpha(G)$	$\prod_{uw \in E(G)} (d_u + d_w)^\alpha$
5.	Second Multiplicative Generalized Zagreb Index [69]	$MZ_2^\alpha(G)$	$\prod_{uw \in E(G)} (d_u \cdot d_w)^\alpha$
6.	Multiplicative version of First Zagreb Index [70]	$II_1^*(G)$	$\prod_{uw \in E(G)} (d_u + d_w)$
7.	Second Multiplicative Zagreb Index [68]	$II_2(G)$	$\prod_{uw \in E(G)} (d_u \cdot d_w)$
8.	Multiplicative First Hyper Zagreb Index [71]	$HII_1(G)$	$\prod_{uw \in E(G)} (d_u + d_w)^2$
9.	Multiplicative Second Hyper Zagreb Index [71]	$HII_2(G)$	$\prod_{uw \in E(G)} (d_u \cdot d_w)^2$
10.	Multiplicative Sum Connectivity Index [67]	$SCII(G)$	$\prod_{uw \in E(G)} \frac{1}{\sqrt{d_u + d_w}}$
11.	Multiplicative Product Connectivity Index (or) Multiplicative Randić Index [67]	$PCII(G)$ (or) $RII(G)$	$\prod_{uw \in E(G)} \frac{1}{\sqrt{d_u \cdot d_w}}$
12.	Multiplicative Sum Connectivity F –Index [71]	$SFII(G)$	$\prod_{uw \in E(G)} \frac{1}{\sqrt{d_u^2 + d_w^2}}$
13.	Multiplicative Product Connectivity F –Index [71]	$PFII(G)$	$\prod_{uw \in E(G)} \frac{1}{\sqrt{d_u^2 \cdot d_w^2}}$
14.	Multiplicative First F –Index [72]	$F_1II(G)$	$\prod_{uw \in E(G)} [(d_u)^2 + (d_w)^2]$
15.	Multiplicative Second F –Index [73]	$F_2II(G)$	$\prod_{uw \in E(G)} [(d_u)^2 \cdot (d_w)^2]$

S.No	TI	Notation	Formula of TI
16.	Multiplicative Atomic Bond Connectivity Index [74]	$ABCII(G)$	$\prod_{u w \in E(G)} \sqrt{\frac{d_u + d_w - 2}{d_u \cdot d_w}}$
17.	Multiplicative Harmonic Index [72]	$HII(G)$	$\prod_{u w \in E(G)} \frac{2}{d_u + d_w}$
18.	Multiplicative Geometric Arithmetic Index [74]	$GAII(G)$	$\prod_{u w \in E(G)} \frac{2\sqrt{d_u \cdot d_w}}{d_u + d_w}$
19.	General Multiplicative Geometric Arithmetic Index [75]	$GA^\alpha II(G)$	$\prod_{u w \in E(G)} \left(\frac{2\sqrt{d_u \cdot d_w}}{d_u + d_w}\right)^\alpha$
20.	Multiplicative Augmented Zagreb Index [76]	$AZII(G)$	$\prod_{u w \in E(G)} \left(\frac{d_u \cdot d_w}{d_u + d_w - 2}\right)^3$

2.3. Zagreb, Forgotten, Harmonic, Inverse degree, and M-polynomials of a graph.

The first, second, and third Zagreb polynomials were defined by Fath-Tabar [25]. Iranmanesh *et al.* [77] introduced harmonic polynomial. Shuxian [78] established the modified first Zagreb index. Numerous algebraic polynomials find potential applications in mathematical chemistry, such as Wiener polynomial [4] that would be used to calculate distance-based TIs. Amongst many other algebraic polynomials, M-polynomial was established in 2015 [79], which fulfills a similar role in defining the closed-form of several degree-based TIs. The valuable feature of M-polynomial is the abundance of information on molecular descriptors which it offers. We refer to the texts [77-84] for a more in-depth review of M-polynomials. Table 3 and Table 4 illustrate certain polynomials of graph invariants.

Table 3. Degree-based TIs with their polynomial of a graph G.

S.No.	TI	Polynomial P(G,x)	Derivation from P(G,x)
1.	First Zagreb [75]	$M_1(G, x) = \sum_{u w \in E(G)} x^{d_u + d_w}$	$D_x (M_1(G; x)) _{x=1}$
2.	Second Zagreb [75]	$M_2(G, x) = \sum_{u w \in E(G)} x^{d_u \cdot d_w}$	$D_x (M_2(G; x)) _{x=1}$
3.	Third Zagreb [75]	$M_3(G, x) = \sum_{u w \in E(G)} x^{ d_u - d_w }$	$D_x (M_3(G; x)) _{x=1}$
4.	Forgotten [47]	$F(G, x) = \sum_{u w \in E(G)} x^{(d_u^2 + d_w^2)}$	$D_x (F(G; x)) _{x=1}$
5.	Modified First Zagreb [78]	$M_1^*(G, x) = \sum_{w \in V(G)} d_w x^{d_w}$	$D_x (M_1^*(G; x)) _{x=1}$
6.	Harmonic [77]	$H(G, x) = \sum_{u w \in E(G)} x^{d_u + d_w - 1}$	$2I_x (H(G; x)) _{x=1}$
7.	Modified Forgotten [47]	$F^*(G, x) = \sum_{w \in V(G)} x^{d_w^3}$	$D_x (F^*(G; x)) _{x=1}$
8.	Inverse Degree [80]	$ID(G, x) = \sum_{w \in V(G)} x^{d_w - 1}$	$I_x (ID(G; x)) _{x=1}$

Where, $D_x = \frac{d(P(G, x))}{dx}$, $I_x = \int_0^x P(G, t) dt$.

Theorem 2.1. ([79], Theorems 2.1 and 2.2). Let G be a simple connected graph.

(1) If $I(G) = \sum_{uv \in E(G)} f(d(u), d(v))$, where $f(x, y)$ is a polynomial in x and y , then

$$I(G) = f(D_x, D_y) (M(G; x, y))|_{x=y=1}$$

(2) If $I(G) = \sum_{uv \in E(G)} f(d(u), d(v))$, where $f(x, y) = \sum_{i, j \in \mathbb{N}} \alpha_{i, j} x^i y^j$, then $I(G)$ can be

obtained from $M(G; x, y)$ using the operators D_x, D_y, S_x, S_y .

(3) If $I(G) = \sum_{uv \in E(G)} f(d(u), d(v))$, where

$$f(x, y) = \frac{x^r y^s}{(x + y + \alpha)^t}$$

where x and y are variables, $r, s \geq 0, t \geq 1$ and $\alpha \in \mathbb{N}$, then

$$I(G) = S_x^t Q_\alpha J D_x^r D_y^s (M(G; x, y))|_{x=y=1}$$

M – Polynomial of a chemical graph is defined as

$$M(G; x, y) = \sum_{l \leq m} (\text{Number of every edges } uv \text{ such that } d_u = l, d_w = m) x^l y^m \text{ -----(1)}$$

Table 4. Degree-based TIs derived from M-Polynomial of a graph G.

S. No.	TI	f(x,y)	Derivation from (M(G;x,y))
1.	$M_1(G)$	$x + y$	$(D_x + D_y) (M(G; x, y)) _{x=y=1}$
2.	$M_2(G)$	xy	$(D_x D_y) (M(G; x, y)) _{x=y=1}$
3.	${}^m M_2(G)$	$\frac{1}{xy}$	$(S_x S_y) (M(G; x, y)) _{x=y=1}$
4.	$R_\alpha(G)$	$(xy)^\alpha$	$(D_x^\alpha D_y^\alpha) (M(G; x, y)) _{x=y=1}$
5.	$RR_\alpha(G)$	$\frac{1}{(xy)^\alpha}$	$(S_x^\alpha S_y^\alpha) (M(G; x, y)) _{x=y=1}$
6.	$SDD(G)$	$\frac{x^2 + y^2}{xy}$	$(D_x S_y + D_y S_x) (M(G; x, y)) _{x=y=1}$
7.	$H(G)$	$\frac{2}{x + y}$	$2 S_x J (M(G; x, y)) _{x=1}$
8.	$ISI(G)$	$\frac{xy}{x + y}$	$S_x J D_x D_y (M(G; x, y)) _{x=1}$
9.	$AZI(G)$	$\left(\frac{xy}{x + y - 2}\right)^3$	$S_x^3 Q_{-2} J D_x^3 D_y^3 (M(G; x, y)) _{x=1}$
10.	$F(G)$	$x^2 + y^2$	$(D_x^2 + D_y^2) (M(G; x, y)) _{x=y=1}$
11.	$Re M_3(G)$	$xy(x + y)$	$D_x D_y (D_x + D_y) (M(G; x, y)) _{x=y=1}$
12.	$ABC(G)$	$\sqrt{\frac{x+y-2}{x.y}}$	$S_x^{-\frac{1}{2}} Q_{-2} J D_x^{-\frac{1}{2}} D_y^{-\frac{1}{2}} (M(G; x, y)) _{x=1}$

To evaluate the concerned TIs (as given in Table 4) of a graph G from the $M(G; x; y)$, the formulae of derivations in terms of derivative or integral (or both integral and derivative) are listed in Table 2 [79], where

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

$$J(f(x, y)) = f(x, x) \text{ and } Q_\alpha(f(x, y)) = x^\alpha f(x, y), \alpha \neq 0$$

2.4. Methodology.

The use of algebraic polynomials to derive TIs of antiviral medication structure is one of our primary findings. Acetaminophen's chemical structure can be accessed at pubchem.ncbi.nlm.nih.gov. Since the vertices depicting hydrogen atoms have no contribution to graph isomorphism, consider a hydrogen suppressed molecular graph of a compound. To arrive at our main results, we use graph-theoretical tools, combinatorial computation, analytical techniques, edge partition, and degree counting methods. The degree of end vertices is used to generate patterns of edge partitions of the hydrogen deleted molecular graph of the compound above. Expressions of additive and multiplicative degree-based TIs were computed using those partitions along with the formulae presented in Table 1 and Table 2. Similarly, certain closed forms of Zagreb, Forgotten, Harmonic, inverse-degree polynomials, and M-polynomials are derived using Table 3 and Table 4. The surface plotting of the polynomials is done by using GNU-OCTAVE 5.2.0. MATLAB 2017 was employed to compare the numerical results graphically.

3. Results and Discussion

In this section, primary computational results are obtained. Zagreb, Harmonic, ID, and Forgotten polynomials were established as follows.

Theorem 3.1. If G is a chemical graph of acetaminophen ($C_8H_9NO_2$) drug then,

- (i) $M_1(G, x) = 6x^5 + 5x^4.$
- (ii) $M_2(G, x) = 6x^6 + 2x^4 + 3x^3.$
- (iii) $M_3(G, x) = 3x^2 + 6x + 2.$
- (iv) $F(G, x) = 6x^{13} + 3x^{10} + 2x^8.$
- (v) $M_1^*(G, x) = 9x^3 + 10x^2 + 3x.$
- (vi) $H(G, x) = 6x^4 + 5x^3.$
- (vii) $F^*(G, x) = 3x^{27} + 5x^8 + 3x.$
- (viii) $ID(G, x) = 3x^2 + 5x + 3.$

Proof: Consider a chemical graph of acetaminophen ($C_8H_9NO_2$) as G (see Figure 1(b)). G has 11 number of vertices and that of edges. Let J_m , the set containing the vertices with given degree m , i.e., $J_m = \{w \in V(G) : d_w = m\}$. Let j_m be the number of vertices in J_m . Let $K_{l, m}$, the set containing the edges with degrees of terminal vertices l, m , i.e., $K_{l, m} = \{u w \in E(G) : d_u = l, d_w = m\}$. $k_{l, m}$ denotes the number of edges in $K_{l, m}$. As seen from

Figure 1(b), acetaminophen contains edges of the type $K_{1,3}$, $K_{2,2}$ and $K_{2,3}$. It is observed that, $k_{1,3}=3$, $k_{2,2}=2$, $k_{2,3}=6$, $j_1=3$, $j_2=5$, $j_3=3$.

Using the polynomial expressions given in Table 3, we have,

- (i) $M_1(G, x) = \sum_{u w \in E(G)} x^{l+m} = k_{1,3} x^{1+3} + k_{2,2} x^{2+2} + k_{2,3} x^{2+3} = 6x^5 + 5x^4.$
- (ii) $M_2(G, x) = \sum_{u w \in E(G)} x^{l.m} = k_{1,3} x^{1 \times 3} + k_{2,2} x^{2 \times 2} + k_{2,3} x^{2 \times 3} = 6x^6 + 2x^4 + 3x^3.$
- (iii) $M_3(G, x) = \sum_{u w \in E(G)} x^{|l-m|} = k_{1,3} x^{|1-3|} + k_{2,2} x^{|2-2|} + k_{2,3} x^{|2-3|} = 3x^2 + 6x + 2.$
- (iv) $F(G, x) = \sum_{u w \in E(G)} x^{(l^2+m^2)} = k_{1,3} x^{1^2+3^2} + k_{2,2} x^{2^2+2^2} + k_{2,3} x^{2^2+3^2} = 6x^{13} + 3x^{10} + 2x^8.$
- (v) $M_1^*(G, x) = \sum_{w \in V(G)} m x^m = j_1 (1)x^1 + j_2 (2)x^2 + j_3 (3)x^3 = 9x^3 + 10x^2 + 3x.$
- (vi) $H(G, x) = \sum_{u w \in E(G)} x^{l+m-1} = k_{1,3} x^{1+3-1} + k_{2,2} x^{2+2-1} + k_{2,3} x^{2+3-1} = 6x^4 + 5x^3.$
- (vii) $F^*(G, x) = \sum_{w \in V(G)} x^{m^3} = j_1 x^1 + j_2 x^8 + j_3 x^{27} = 3x^{27} + 5x^8 + 3x.$
- (viii) $ID(G, x) = \sum_{w \in V(G)} x^{m-1} = j_1 x^{1-1} + j_2 x^{2-1} + j_3 x^{3-1} = 3x^2 + 5x + 3.$

Using these polynomials, we compute the corresponding TIs as described below.

Theorem 3.2. If G is a chemical graph of acetaminophen ($C_8H_9NO_2$) drug then,

- (i) $M_1(G) = 50.$
- (ii) $M_2(G) = 53.$
- (iii) $M_3(G) = 12.$
- (iv) $F(G) = 124.$
- (v) $M_1^*(G) = 50.$
- (vi) $H(G) = 4.9.$
- (vii) $F^*(G) = 124.$
- (viii) $ID(G) = 6.5.$

Proof: Using Table 3 and theorem 3.1, we obtain,

- (i) $M_1(G) = D_x (M_1(G; x)) |_{x=1} = \frac{d}{dx} (6x^5 + 5x^4) = 30x^4 + 20x^3 |_{x=1} = 30 + 20 = 50.$
- (ii) $M_2(G) = D_x (M_2(G; x)) |_{x=1} = \frac{d}{dx} (6x^6 + 2x^4 + 3x^3) = 36x^5 + 8x^3 + 9x^2 |_{x=1} = 36 + 8 + 9 = 53.$
- (iii) $M_3(G) = D_x (M_3(G; x)) |_{x=1} = \frac{d}{dx} (3x^2 + 6x + 2) = 6x + 6 |_{x=1} = 6 + 6 = 12.$
- (iv) $F(G) = D_x (F(G; x)) |_{x=1} = \frac{d}{dx} (6x^{13} + 3x^{10} + 2x^8) = 78x^{12} + 30x^9 + 16x^7 |_{x=1} = 78 + 30 + 16 = 124.$
- (v) $M_1^*(G) = D_x (M_1^*(G; x)) |_{x=1} = \frac{d}{dx} (9x^3 + 10x^2 + 3x) = 27x^2 + 20x + 3 |_{x=1} = 27 + 20 + 3 = 50.$

$$(vi) \quad H(G) = 2I_x (H(G; x))|_{x=1} = 2 \int_0^x (6t^4 + 5t^3) dt = 2 \left(\frac{6}{5} x^5 + \frac{5}{4} x^4 \right) \Big|_{x=1} = \frac{6}{5} + \frac{5}{4} = 4.9.$$

$$(vii) \quad F^*(G) = D_x (F^*(G; x))|_{x=1} = \frac{d}{dx} (3x^{27} + 5x^8 + 3x) = 81x^{26} + 40x^7 + 3|_{x=1} = 81 + 40 + 3 = 124.$$

$$(viii) \quad ID(G) = I_x (ID(G; x))|_{x=1} = \int_0^x (3t^2 + 5t + 3) dt = \left(x^3 + \frac{5}{2} x^2 + 3x \right) \Big|_{x=1} = 1 + \frac{5}{2} + 3 = 6.5.$$

The following theorem shows the M-Polynomial of some TIs.

Theorem 3.3. Let G be a chemical graph of acetaminophen ($C_8H_9NO_2$) drug. Then,

$$M(G; x, y) = 3xy^3 + 2x^2y^2 + 6x^2y^3.$$

Proof: From equation (1), The M – Polynomial of G arrives as follows.

$$\begin{aligned} M(G; x, y) &= \sum_{l \leq m} k_{l,m} x^l y^m, \text{ where } l, m \in \{1, 2, 3\}. \\ &= k_{1,3} x^1 y^3 + k_{2,2} x^2 y^2 + k_{2,3} x^2 y^3. \end{aligned}$$

Substituting the values of $k_{1,3}$, $k_{2,2}$, and $k_{2,3}$, we get,

$$M(G; x, y) = 3xy^3 + 2x^2y^2 + 6x^2y^3.$$

Now, we evaluate some indices for the molecular graph of acetaminophen using M-Polynomials derived in the previous theorem.

Theorem 3.4. Let G be a chemical graph of acetaminophen ($C_8H_9NO_2$) drug. Then, we have,

- (i) $M_1(G) = 50.$
- (ii) $M_2(G) = 53.$
- (iii) ${}^m M_2(G) = 2.5.$
- (iv) $R_\alpha(G) = 3^{\alpha+1} + 2^{2\alpha+1} + 6^{\alpha+1}.$
- (v) $RR_\alpha(G) = \frac{1}{3^{\alpha-1}} + \frac{1}{2^{2\alpha-1}} + \frac{1}{6^{\alpha-1}}.$
- (vi) $SDD(G) = 27.$
- (vii) $H(G) = 4.9.$
- (viii) $ISI(G) = 11.45.$
- (ix) $AZI(G) = 74.125.$
- (x) $F(G) = 124.$
- (xi) $Re M_3(G) = 248.$
- (xii) $ABC(G) = 8.10634.$

Proof: Let $M(G; x, y) = 3xy^3 + 2x^2y^2 + 6x^2y^3.$

$$J(f(x, y)) = 3x^4 + 2x^4 + 6x^5 = 5x^4 + 6x^5.$$

$$S_x J(f(x, y)) = \frac{5}{4} x^4 + \frac{6}{5} x^5.$$

$$(D_x D_y)(f(x, y)) = 9xy^3 + 8x^2y^2 + 36x^2y^3.$$

$$J(D_x D_y)(f(x, y)) = 9x^4 + 8x^4 + 36x^5 = 17x^4 + 36x^5.$$

$$S_x J(D_x D_y)(f(x, y)) = \frac{17}{4} x^4 + \frac{36}{5} x^5.$$

$$\begin{aligned} (D_x + D_y)(f(x, y)) &= 12xy^3 + 8x^2y^2 + 30x^2y^3. \\ (D_x^3 D_y^3)(f(x, y)) &= 81xy^3 + 128x^2y^2 + 1296x^2y^3. \\ J(D_x^3 D_y^3)(f(x, y)) &= 81x^4 + 128x^4 + 1296x^5 = 209x^4 + 1296x^5. \\ Q_{-2}J(D_x^3 D_y^3)(f(x, y)) &= 209x^2 + 1296x^3. \\ S_x^3 Q_{-2}J(D_x^3 D_y^3)(f(x, y)) &= \frac{209}{8}x^2 + \frac{1296}{27}x^3. \\ (S_x S_y)(f(x, y)) &= xy^3 + \frac{1}{2}x^2y^2 + x^2y^3. \\ (D_x^2 + D_y^2)(f(x, y)) &= 30xy^3 + 16x^2y^2 + 78x^2y^3. \\ (D_x^\alpha D_y^\alpha)(f(x, y)) &= 3^{\alpha+1}xy^3 + 2^{2\alpha+1}x^2y^2 + 6^{\alpha+1}x^2y^3. \\ (S_x^\alpha S_y^\alpha)(f(x, y)) &= \frac{1}{3^{\alpha-1}}xy^3 + \frac{1}{2^{2\alpha-1}}x^2y^2 + \frac{1}{6^{\alpha-1}}x^2y^3. \\ (D_x D_y)(D_x + D_y)(f(x, y)) &= 36xy^3 + 32x^2y^2 + 180x^2y^3. \\ (D_x S_y + D_y S_x)(f(x, y)) &= 10xy^3 + 4x^2y^2 + 13x^2y^3. \\ \left(S_x^{-\frac{1}{2}} Q_{-2} J D_x^{-\frac{1}{2}} D_y^{-\frac{1}{2}} \right) (f(x, y)) &= \sqrt{6}x^2 + \sqrt{2}x^2 + \sqrt{18}x^3. \end{aligned}$$

Using Table 4 and the above expressions, one can get,

$$\begin{aligned} M_1(G) &= 12xy^3 + 8x^2y^2 + 30x^2y^3 \Big|_{x=y=1} = 50. \\ M_2(G) &= 9xy^3 + 8x^2y^2 + 36x^2y^3 \Big|_{x=y=1} = 53. \\ {}^m M_2(G) &= xy^3 + \frac{1}{2}x^2y^2 + x^2y^3 \Big|_{x=y=1} = 2.5. \\ R_\alpha(G) &= 3^{\alpha+1}xy^3 + 2^{2\alpha+1}x^2y^2 + 6^{\alpha+1}x^2y^3 \Big|_{x=y=1} = 3^{\alpha+1} + 2^{2\alpha+1} + 6^{\alpha+1}. \\ RR_\alpha(G) &= \frac{1}{3^{\alpha-1}}xy^3 + \frac{1}{2^{2\alpha-1}}x^2y^2 + \frac{1}{6^{\alpha-1}}x^2y^3 \Big|_{x=y=1} = \frac{1}{3^{\alpha-1}} + \frac{1}{2^{2\alpha-1}} + \frac{1}{6^{\alpha-1}}. \\ SDD(G) &= 10xy^3 + 4x^2y^2 + 13x^2y^3 \Big|_{x=y=1} = 27. \\ H(G) &= 2 \left(\frac{5}{4}x^4 + \frac{6}{5}x^5 \right) \Big|_{x=1} = 4.9. \\ ISI(G) &= \frac{17}{4}x^4 + \frac{36}{5}x^5 \Big|_{x=1} = 11.45 \\ AZI(G) &= \frac{209}{8}x^2 + \frac{1296}{27}x^3 \Big|_{x=1} = 74.125. \\ F(G) &= 30xy^3 + 16x^2y^2 + 78x^2y^3 \Big|_{x=y=1} = 124. \\ Re M_3(G) &= 36xy^3 + 32x^2y^2 + 180x^2y^3 \Big|_{x=y=1} = 248. \\ ABC(G) &= \sqrt{6}x^2 + \sqrt{2}x^2 + \sqrt{18}x^3 \Big|_{x=1} = 8.10634. \end{aligned}$$

Theorem 3.5. Let G be a chemical graph of acetaminophen ($C_8H_9NO_2$) drug. Then, we get,

- (i) $M_1^\alpha(G) = 5 \times 4^\alpha + 6 \times 5^\alpha$.
- (ii) $M_2^\alpha(G) = 3^{\alpha+1} + 2 \times 4^\alpha + 6^{\alpha+1}$.
- (iii) $HM_1(G) = 230$.
- (iv) $HM_2(G) = 275$.
- (v) $RM_2(G) = 14$.
- (vi) $Re M_1(G) = 11$.
- (vii) $Re M_2(G) = 11.45$.
- (viii) $N_z(G) = 54$.
- (ix) $\chi_{\frac{1}{2}} N_z(G) = 21.9017$.
- (x) $R_{\frac{-1}{2}}^0(G) = 8.2676$.
- (xi) $R_\alpha^0(G) = 3(1)^\alpha + 5(2)^\alpha + 3(3)^\alpha$.
- (xii) $R(G) = 5.182$.
- (xiii) $RR(G) = 23.89309$.
- (xiv) $RRR(G) = 10.4853$.
- (xv) $R'(G) = 4$.
- (xvi) $SCI(G) = \chi(G) = 5.18328$.
- (xvii) $AG(G) = 11.58782$.
- (xviii) $SEI_\alpha(G) = 3\alpha + 10\alpha^2 + 3\alpha^3, \alpha \neq 1$.
- (xix) $H_k(G) = \frac{5}{2^k} + 6\left(\frac{2}{5}\right)^k$
- (xx) $OGA_k(G) = 3\left(\frac{\sqrt{3}}{2}\right)^k + 6\left(\frac{2\sqrt{6}}{5}\right)^k + 2$.
- (xxi) $OGA(G) = 10.476852$.
- (xxii) $SK(G) = 25$.
- (xxiii) $SK_1(G) = 26.5$.
- (xxiv) $SK_2(G) = 57.5$.
- (xxv) $M_1^\varepsilon(G) = 115$.
- (xxvi) $IRM(G) = 18$.
- (xxvii) $A(G) = 12$.
- (xxviii) $B(G) = 6$.
- (xxix) $SO(G) = 36.777$.

Proof: Let the chemical graph of acetaminophen be taken as G.

- (i) $M_1^\alpha(G) = k_{1,3} \times 4^\alpha + k_{2,2} \times 4^\alpha + k_{2,3} \times 5^\alpha = 5 \times 4^\alpha + 6 \times 5^\alpha$.
- (ii) $M_2^\alpha(G) = k_{1,3} \times 3^\alpha + k_{2,2} \times 4^\alpha + k_{2,3} \times 6^\alpha = 3^{\alpha+1} + 2 \times 4^\alpha + 6^{\alpha+1}$.

Put $\alpha = 2$ in (i) and (ii), we get,

$$HM_1(G) = 230 ; HM_2(G) = 275.$$

If $\alpha = \frac{1}{2}, \frac{-1}{2}$,

We obtain $RR(G) = 23.89309 ; R(G) = 5.182$ directly from (ii).

$$OGA_k(G) = k_{1,3} \times \left(\frac{2\sqrt{1 \times 3}}{1+3}\right)^k + k_{2,2} \times \left(\frac{2\sqrt{2 \times 2}}{2+2}\right)^k + k_{2,3} \times \left(\frac{2\sqrt{2 \times 3}}{2+3}\right)^k = 3\left(\frac{\sqrt{3}}{2}\right)^k + 6\left(\frac{2\sqrt{6}}{5}\right)^k + 2.$$

$OGA(G) = 10.476852$ would be got from $OGA_k(G)$ when $k = 1$.

One can arrive remaining TIs by substituting the values of $d_u, d_w, j_1 = 3, j_2 = 5, j_3 = 3, k_{1,3} = 3, k_{2,2} = 2$, and $k_{2,3} = 6$ in the rules mentioned in Table 1.

We derive the multiplicative TIs of Acetaminophen as follows,

Theorem 3.6. For a chemical graph of acetaminophen ($C_8H_9NO_2$) drug G, we obtain,

- (i) $W_1^\alpha(G) = 1^{3\alpha} \times 2^{5\alpha} \times 3^{3\alpha}$.
- (ii) $NK(G) = 864$.
- (iii) $II_1(G) = 746496$.
- (iv) $MZ_1^\alpha(G) = 2^{10\alpha} \times 5^{6\alpha}$.
- (v) $MZ_2^\alpha(G) = 2^{10\alpha} \times 3^{9\alpha}$.
- (vi) $II_1^*(G) = 1.6 \times 10^7$.
- (vii) $II_2(G) = 2.0155 \times 10^7$.
- (viii) $HII_1(G) = 2.56 \times 10^{14}$.
- (ix) $HII_2(G) = 4.0624 \times 10^{14}$.
- (x) $SCII(G) = 0.00025$.
- (xi) $PCII(G) = 0.000223$.
- (xii) $SFII(G) = 1.8 \times 10^{-6}$.
- (xiii) $PFII(G) = 4.9615 \times 10^{-8}$.
- (xiv) $F_1II(G) = 5.558 \times 10^5$.
- (xv) $F_2II(G) = 20155392$.
- (xvi) $GA^\alpha II(G) = \left(\frac{\sqrt{3}}{2}\right)^{3\alpha} \times \left(\frac{2\sqrt{6}}{5}\right)^{6\alpha}$.
- (xvii) $ABCII(G) = 0.03402$.
- (xviii) $HII(G) = 0.000128$.
- (xix) $GAI(G) = 0.57465$.
- (xx) $AZII(G) = 644972544$.

Proof: Applying the values of degrees d_u, d_w of vertices u and w, and $j_1 = 3, j_2 = 5, j_3 = 3, k_{1,3} = 3, k_{2,2} = 2, k_{2,3} = 6$ in the formulae presented in Table 2, one can compute multiplicative TIs.

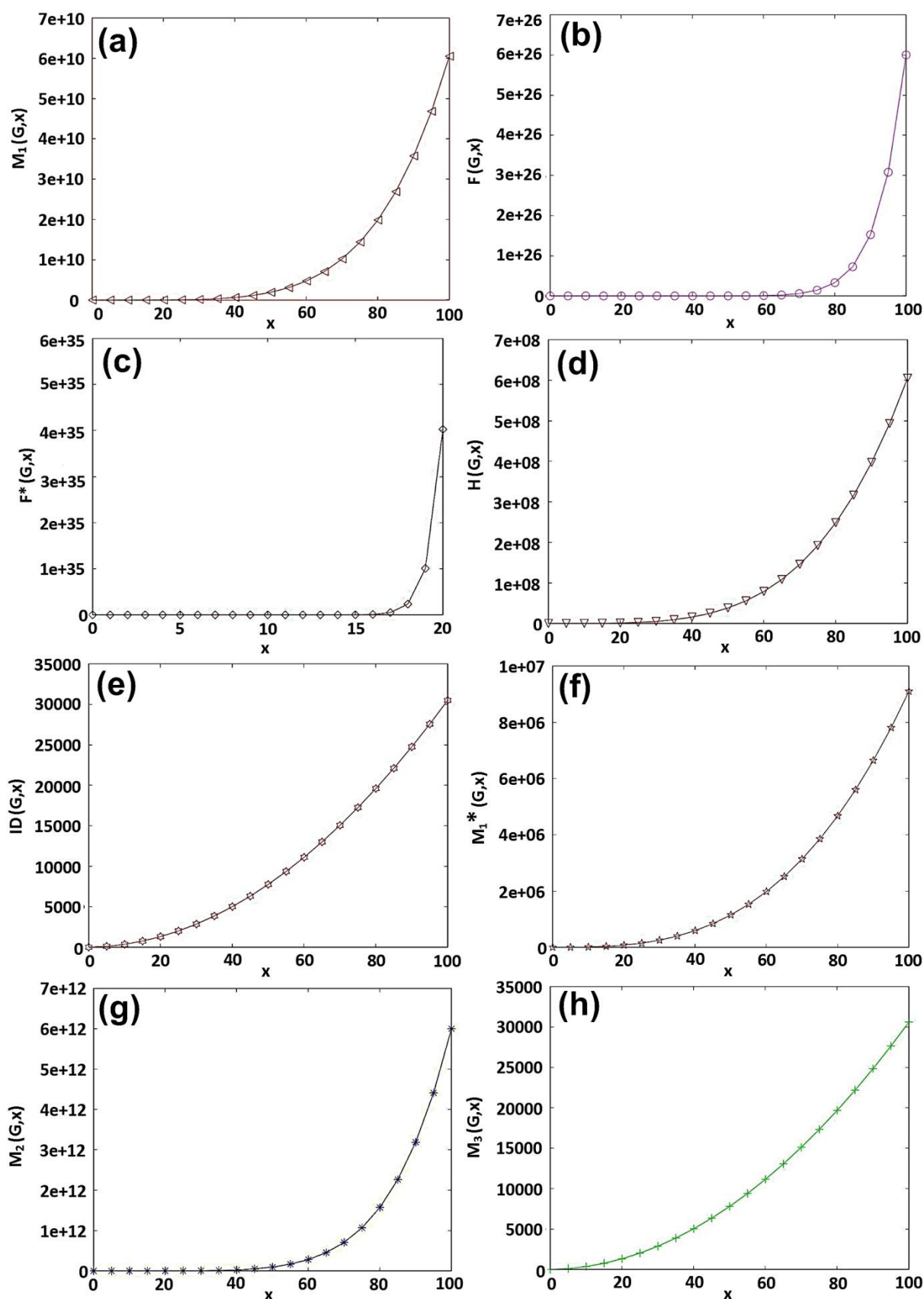


Figure 2. Plotting (a) M_1 , (b) F , (c) F^* , (d) H , (e) ID , (f) M_1^* , (g) M_2 , and (h) M_3 polynomials of Acetaminophen ($C_8H_9NO_2$) drug.

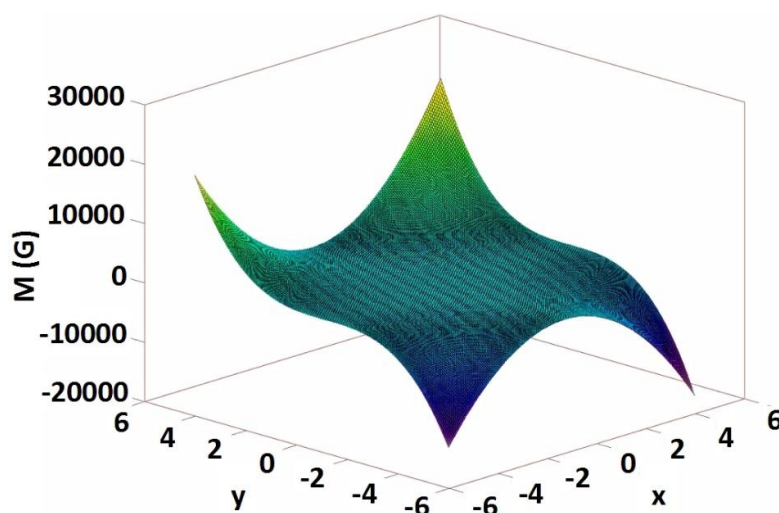


Figure 3. Plotting the M -polynomial of Acetaminophen ($C_8H_9NO_2$) drug.

The graphs plotted in Figure 2 represent the various polynomials of Acetaminophen drug, which are self-explanatory to somewhat extent. Interestingly, the Modified Forgotten index progresses rapidly than that of others. The behavior of $ID(G,x)$ and $M_3(G,x)$ polynomials is almost similar. Figure 3 illustrates the 3D surface plot for the M -polynomial of Acetaminophen.

4. Conclusions

For the first time, we have presented the numerical examination of several important sums and product connectivity TIs for the molecular graph of Acetaminophen drug, especially irregularity ($IRM(G)$, $A(G)$, $B(G)$), SK, ABC, SDD and Sombor indices. The Zagreb, Harmonic, Forgotten, and Inverse degree polynomials were also computed with graphical representations. Furthermore, the closed form of M -polynomial of Acetaminophen was successfully initiated, and their accurate expressions were obtained. The computed indices can offer potential applications in pharmaceutical sciences such as the drug designing field, data mining, and chemical documentation studies.

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Conflicts of Interest

The authors declare no conflict of interest.

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