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Downhill Zagreb Topological Indices and M_{dn}-Polynomial of Some Chemical Structures Applied for the Treatment of COVID-19 Patients

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Abstract

A graphical index is a numeric value corresponding to a graph which is structurally invariant and in molecular graph theory these invariants are known as topological indices. In the field of Chemical and Medical Sciences, the topological indices are used to study the chemical, biological, medical and pharmaceutical features of drugs. With reference to the previous deadly diseases, the COVID-19 pandemic has considered to be the biggest life threatening issue that modern medicines have ever tackled. COVID-19 is immedicable and even the existing treatments are only helping the certain group of sufferers. Scientists have tested available antiviral agents and got a favorable impact on recovering from pandemic. Some of these antiviral agents are remdesivir, chloroquine, hydroxychloroquine, theaflavin and dexamethasone. Keeping in view of the importance of topological indices in the study of pharmaceutical and chemical drugs, in this paper, we calculate the M_{dn}-Polynomial, some downhill Zagreb topological indices and some downhill Zagreb polynomials of some of the anti viral agents remdesivir, chloroquine, hydroxychloroquine, theaflavin and dexamethasone. The results thus obtained may be useful for the finding new medicine and vaccine for the treatment of COVID-19.

Keywords

COVID-19, Remdesivir, Chloroquine, Hydroxychloroquine, Theaflavin, Dexamethasone, M_{dn}-Polynomial, Downhill Zagreb Polynomial

1. Introduction

In the period of dynamic technical development, the large number of drugs and pharmaceutical techniques has been emerging every year which requires the massive amount of work to examine the biological and chemical properties of these drugs. Also, lots of experiments have to be done on these new drugs to find out the side effects and benefits on human body. These heavy works loaded experiments in laboratories may affect the impoverished countries especially Africa and Southeast Asia. During the initial stages of chemical experiments, the scientists have compared the structure of the compounds and its experimental values and pointed that they are closely related [1] [2]. Calculating the properties of the molecular structure of the compounds in terms of topological indices, the pharmaceutical and medical scholars may find them useful in studying the medicinal properties of the drugs.

In the modeling of medical mathematics, the structure of medicine is considered as an undirected graph, where the vertices and edges are considered to be atoms and the chemical bonds respectively. The information pertaining physiochemical properties and the biological activities of molecular graph of compounds are important in pharmaceutical drug design. These properties can be anticipated without any use of laboratories but by a conventional aid of chemical graph theory known as the topological index. A graphical index is a numeric value corresponding to a graph which is structurally invariant and in molecular graph theory these invariants are known as topological indices. The first and second Zagreb indices are extensively studied among the various classes of topological indices and have many applications in the molecular graph theory. The Zagreb indices play a vital role in the theory of total π-electron energy of alternant hydrocarbons. Gutman and Trinajstic introduced the first and second Zagreb indices in 1972 [3].

With reference to the previous deadly diseases, the COVID-19 pandemic has considered to be the biggest life threatening issue that modern medicines have ever tackled. The scientists and doctors have been working tirelessly in finding the drugs which may save the sufferers and may even protect them from getting affected. As of 26th August 2020, there were more than 24 million reported resulting in 819,000 deaths and 16,620,943 have been recovered across 188 countries and territories (from world meters information). COVID-19 is immedicable and even the existing treatments are only helping the certain group of sufferers. No treatment has been fully licensed by the food and the drug administration agency for COVID-19.

Scientists have tested some of the available antiviral agents and got a favorable impact on recovering from pandemic by using remdesivir, chloroquine, hydroxychloroquine, theaflavin and dexamethasone. The first drug to get the emergency approval from food and drug administration for the use of COVID-19 is remdesivir. It ceases the reproduction of the virus. This drug was initially used as an antiviral agent for Hepatitis C and Ebola. From the preliminary trials, it has been observed that the drug can reduce the recovery time of the COVID-19 sufferers from 15 days to 11 days. In 1930s the German scientists incorporated chloroquine as a drug against malaria. In 1946, the scientists invented the less toxic version of chloroquine called hydroxychloroquine and later the drug was approved for other diseases also. During the initial stages of the deadly pandemic, the scientists have found that both chloroquine and hydroxychloroquine can control the virus from reproducing the cells [4]. Initial reports from France and China have proposed that by giving chloroquine or hydroxychloroquine, the COVID-19 sufferers are recovered quickly. Theaflavin is a polyphenol chemical found in black tea which acts as an antiviral agent in the treatment of influenza A, B and hepatitis C virus. Lung *et al.* [5] have suggested that this drug can be used as a primary factor in producing a drug against COVID-19. British researchers on 17th July, 2020 published that dexamethasone improves the immune response of the Covid-19 positives. The recovery collaborative group of researchers has found that this drug reduces the death rate of patients on ventilators by one-third and for the patients on oxygen by one-fifth. But it may be less effective and even may be harmful for the patients who are at an earlier stage of COVID-19 infections [6]. However, in the COVID-19 treatment guidelines, the National Institutes of Health recommends only using dexamethasone in patients with COVID-19 who are on a ventilator or are receiving supplemental oxygen. For more application of topological indices, see [7]-[16].

2. M_{dn}-Polynomial and Downhill Zagreb Polynomials

Let $G=(V,E)$ be a graph of order $n=|V|$. The open neighborhood of a vertex $v\in V$ is the set $N(v)=\{u|uv\in E\}$, while the closed neighborhood is the set $N[v]=N(v)\cup\{v\}$. Each vertex in $u\in N(v)$ is called a neighbor of *v*, and $|N(v)|$ is called the degree of *v*, and denoted $deg(v)$. Any terminology in graph theory not defined here, we refer the reader to [17].

Definition 2.1. [18] Let $G=(V,E)$ be a graph. A $u-v$ path P in G is a sequence of vertices in *G*, starting with u and ending at *v*, such that consecutive vertices in P are adjacent, and no vertex is repeated. A path $\pi=v_1,v_2,\cdots,v_{k+1}$ in G is a downhill path if for every *i*, $1\le i\le k$, $deg(v_i)\ge deg(v_{i+1})$.

Definition 2.2. A vertex v is downhill dominates a vertex u if there exists a downhill path originated from v to u. The downhill neighborhood of a vertex v is denotes by $N_{dn}(v)$ and define as

$$N_{dn}(v)=\{u: v \text{ down hill dominates } u\}.$$

The downhill degree of the vertex *v*, denotes by $d_{dn}(v)$, is the number of downhill neighbors of *v*, that means $d_{dn}(v)=|N_{dn}(v)|$.

Definition 2.3. [19] Let $G=(V,E)$ be a graph. Then the first, second and forgotten downhill Zagreb indices are defined by

$$DWM_1(G)=\sum_{v\in V(G)}\left(d_{dn}(v)\right)^2,$$

$$DWM_2(G)=\sum_{vu\in E(G)}d_{dn}(v)d_{dn}(u)$$

and

$$DWF(G)=\sum_{v\in V(G)}\left(d_{dn}(v)\right)^3.$$

Definition 2.4. [20] Let $G=(V,E)$ be a graph. Then the first, second and forgotten downhill Zagreb polynomials are defined by

$$DWM_1(G,x)=\sum_{v\in V(G)} x^{(d_{dn}(v))^2},$$

$$DWM_2(G,x)=\sum_{vu\in E(G)} x^{d_{dn}(v)d_{dn}(u)}$$

and

$$DWF(G,x)=\sum_{v\in V(G)} x^{(d_{dn}(v))^3}.$$

Definition 2.5. The M_{dn}-polynomial of G is defined as

$$M_{dn}(G,x,y)=\sum_{\delta_{dn}\le i\le j\le \Delta_{dn}} m_{i,j}x^i y^j,$$

where $\delta_{dn}=\mathrm{Min}\{d_{dn}(v)|v\in V(G)\}, \Delta_{dn}=\mathrm{Max}\{d_{dn}(v)|v\in V(G)\}$ and $m_{i,j}$ is the number of edges $vu\in E(G)$ such that $\{d_{dn}(v),d_{dn}(u)\}=\{i,j\}$ and $i\le j$.

Definition 2.6. Let $G=(V,E)$ be a graph. Then the first, second and forgotten downhill modified Zagreb indices are defined by

$$DWM_1^*(G)=\sum_{vu\in E(G)} d_{dn}(v)+d_{dn}(u)$$

and

$$DWF^*(G)=\sum_{vu\in E(G)} (d_{dn}(v))^2+(d_{dn}(u))^2.$$

Table 1 presented relates some of these downhill degree—based topological indices with the downhill Zagreb polynomials and M_{dn}-polynomial with the following reserved notations

$$D_x=x\frac{\partial(f(x))}{\partial x}, D_y=y\frac{\partial(f(y))}{\partial y}.$$

3. Methodology

We associated the graphs with the chemical structures of remdesivir, chloroquine, hydroxychloroquine, theaflavin and dexamethasone where atoms are represented by vertices and chemical bonds are represented by edges. Then by using the symmetry of the molecular structures of remdesivir, chloroquine, hydroxychloroquine,

Table 1. Derivation of some topological indices from the downhill Zagreb polynomials (DZP) and M_{dn}-polynomial.

Topological Index	Derivation from DZP	Topological Index	Derivation from $M_{dn}(G,x,y)$
$DWM_1(G)$	$D_x(DWM_1(G,x))\|_{x=1}$	$DWM_1^*(G)$	$(D_x+D_y)(M_{dn}(G,x,y))\|_{x=y=1}$
$DWM_2(G)$	$D_x(DWM_2(G,x))\|_{x=1}$	$DWF^*(G)$	$(D_x^2+D_y^2)(M_{dn}(G,x,y))\|_{x=y=1}$
$DWF(G)$	$D_x(DWF(G,x))\|_{x=1}$		

theaflavin and dexamethasone we counted the edges and vertices by a simple counting method. By applying the formula of the polynomial, we derived the downhill Zagreb polynomials and M_{dn}-polynomial of remdesivir, chloroquine, hydroxychloroquine, theaflavin and dexamethasone. From these downhill Zagreb polynomials and M_{dn}-polynomial we recovered 5 downhill degree-based topological indices by using Derivation. We used Matlab 2017 to plot our results.

4. Main Results

In this section, we give our main computational results. We compute downhill Zagreb polynomials and M_{dn}-polynomial of molecular graph of remdesivir.

Theorem 4.1. *Let G be the molecular graph of remdesivir. Then,*

$$DWM_1(G,x) = x^{361} + 4x^{81} + 3x^{49} + 4x^{36} + x^{25} + 5x^{16} + 3x^4 + 8x + 12,$$

$$DWM_2(G,x) = x^{171} + x^{133} + 3x^{81} + 2x^{49} + x^{36} + 2x^{24} + 2x^{18} + 4x^{16} + 2x^9 + x^7 + 4x^6 + x^5 + 2x^4 + 3x + 15,$$

$$DWF(G,x) = x^{6859} + 4x^{729} + 3x^{343} + 4x^{216} + x^{125} + 5x^{64} + 3x^8 + 8x + 12.$$

Proof. Let G be the molecular graph of remdesivir (**Figure 1**). It has 41 vertices in which one vertex of downhill degree 19, 4 vertices of downhill degree 9, 3 vertices of downhill degree 7, 4 vertices of downhill degree 6, one vertex of downhill degree 5, 5 vertices of downhill degree 4, 3 vertices of downhill degree 2, 8 vertices of downhill degree 1 and 12 vertices of downhill degree 0.

Then, $DWM_1(G,x)$ is obtained as follows.

$$\begin{aligned} DWM_1(G,x) &= \sum_{v \in V(G)} x^{(d_{dn}(v))^2} \\ &= x^{19^2} + 4x^{9^2} + 3x^{7^2} + 4x^{6^2} + x^{5^2} + 5x^{4^2} + 3x^{2^2} + 8x^{1^2} + 12x^{0^2} \\ &= x^{361} + 4x^{81} + 3x^{49} + 4x^{36} + x^{25} + 5x^{16} + 3x^4 + 8x + 12. \end{aligned}$$

The graph G has 44 edges. Suppose that $E_{a,b} = \{uv \in E(G) : d_{dn}(u) = a \text{ and } d_{dn}(v) = b\}$ and $|E_{a,b}| = m_{i,j}$. In a graph G there are 20 types of edges based on the downhill degree of the vertices of each edge. From **Figure 1**, we have $|E_{9,19}| = 1$, $|E_{7,19}| = 1$, $|E_{9,9}| = 3$, $|E_{2,9}| = 2$, $|E_{1,9}| = 2$, $|E_{7,7}| = 2$, $|E_{1,7}| = 1$, $|E_{6,6}| = 1$, $|E_{4,6}| = 2$, $|E_{1,6}| = 4$, $|E_{1,5}| = 1$, $|E_{4,4}| = 4$, $|E_{2,2}| = 2$, $|E_{1,1}| = 3$, $|E_{0,19}| = 2$, $|E_{0,9}| = 1$, $|E_{0,7}| = 3$, $|E_{0,6}| = 4$, $|E_{0,5}| = 3$ and $|E_{0,1}| = 2$.

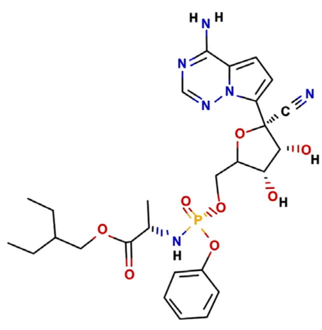

Figure 1. Chemical structure of remdesivir.

Then, $DWM_2(G,x)$ is obtained as follows.

$$
\begin{aligned}
DWM_2(G,x) &= \sum_{vu\in E(G)} x^{d_{dn}(v)d_{dn}(u)} \\
&= |E_{9,19}|x^{9\times19} + |E_{7,19}|x^{7\times19} + |E_{9,9}|x^{9\times9} + |E_{2,9}|x^{2\times9} + |E_{1,9}|x^{1\times9} \\
&\quad + |E_{7,7}|x^{7\times7} + |E_{1,7}|x^{1\times7} + |E_{6,6}|x^{6\times6} + |E_{4,6}|x^{4\times6} + |E_{1,6}|x^{1\times6} \\
&\quad + |E_{1,5}|x^{1\times5} + |E_{4,4}|x^{4\times4} + |E_{2,2}|x^{2\times2} + |E_{1,1}|x^{1\times1} + |E_{0,19}|x^{0\times19} \\
&\quad + |E_{0,9}|x^{0\times9} + |E_{0,7}|x^{0\times7} + |E_{0,6}|x^{0\times6} + |E_{0,5}|x^{0\times5} + |E_{0,1}|x^{0\times1} \\
&= x^{171} + x^{133} + 3x^{81} + 2x^{49} + x^{36} + 2x^{24} + 2x^{18} + 4x^{16} + 2x^{9} \\
&\quad + x^{7} + 4x^{6} + x^{5} + 2x^{4} + 3x + 15.
\end{aligned}
$$

Now, we calculate $DWF(G,x)$ similar to $DWM_1(G,x)$, then

$$
\begin{aligned}
DWF(G,x) &= \sum_{v\in V(G)} x^{(d_{dn}(v))^3} \\
&= x^{19^3} + 4x^{9^3} + 3x^{7^3} + 4x^{6^3} + x^{5^3} + 5x^{4^3} + 3x^{2^3} + 8x^{1^3} + 12x^{0^3} \\
&= x^{6859} + 4x^{729} + 3x^{343} + 4x^{216} + x^{125} + 5x^{64} + 3x^{8} + 8x + 12.
\end{aligned}
$$

Figure 2 is a 3D plot of remdesivir downhill Zagreb polynomials.

Theorem 4.2. *Let G be the molecular graph of remdesivir. Then,*

$$
\begin{aligned}
M_{dn}(G,x,y) = {} & x^9y^{19} + x^7y^{19} + 3x^9y^9 + 2x^2y^9 + 2xy^9 + 2x^7y^7 + xy^7 + x^6y^6 \\
& + 2x^4y^6 + 4xy^6 + xy^5 + 4x^4y^4 + 2x^2y^2 + 3xy + 2y^{19} + y^9 \\
& + 3y^7 + 4y^6 + 3y^5 + 2y.
\end{aligned}
$$

Proof. From Theorem 4.1 and using the definition $M_{dn}(G,x,y)$, we have

$$
\begin{aligned}
M_{dn}(G,x,y) &= \sum_{\delta_{dn}\le i\le j\le \Delta_{dn}} m_{i,j}x^iy^j \\
&= |E_{9,19}|x^9y^{19} + |E_{7,19}|x^7y^{19} + |E_{9,9}|x^9y^9 + |E_{2,9}|x^2y^9 + |E_{1,9}|xy^9 \\
&\quad + |E_{7,7}|x^7y^7 + |E_{1,7}|xy^7 + |E_{6,6}|x^6y^6 + |E_{4,6}|x^4y^6 + |E_{1,6}|xy^6 \\
&\quad + |E_{1,5}|xy^5 + |E_{4,4}|x^4y^4 + |E_{2,2}|x^2y^2 + |E_{1,1}|xy + |E_{0,19}|x^0y^{19} \\
&\quad + |E_{0,9}|x^0y^9 + |E_{0,7}|x^0y^7 + |E_{0,6}|x^0y^6 + |E_{0,5}|x^0y^5 + |E_{0,1}|x^0y \\
&= x^9y^{19} + x^7y^{19} + 3x^9y^9 + 2x^2y^9 + 2xy^9 + 2x^7y^7 + xy^7 + x^6y^6 \\
&\quad + 2x^4y^6 + 4xy^6 + xy^5 + 4x^4y^4 + 2x^2y^2 + 3xy + 2y^{19} + y^9 + 3y^7 \\
&\quad + 4y^6 + 3y^5 + 2y.
\end{aligned}
$$

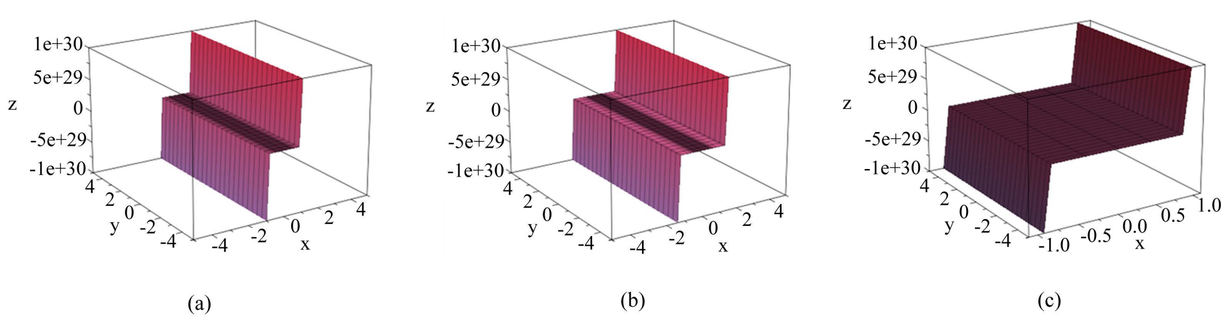

Figure 2. Plotting of remdesivir downhill Zagreb polynomials. (a) $DWM_1(G, x)$; (b) $DWM_2(G, x)$; (c) $DWF(G, x)$.

Figure 3 is a 3D plot of M_{dn}-polynomial of remdesivir.

Now using the Theorem 4.1, we calculate the first, second and forgotten downhill Zagreb indices of the molecular graph of remdesivir in the following theorem.

Theorem 4.3. *Let G be the molecular graph of remdesivir. Then,*

$$DWM_1(G) = 1101,$$

$$DWM_2(G) = 894,$$

$$DWF(G) = 12145.$$

Proof. Let

$$DWM_1(G,x) = f(x) = x^{361} + 4x^{81} + 3x^{49} + 4x^{36} + x^{25} + 5x^{16} + 3x^4 + 8x + 12.$$

Then

$$D_x f(x) = 361x^{361} + 324x^{81} + 147x^{49} + 144x^{36} + 25x^{25} + 80x^{16} + 12x^4 + 8x.$$

From Table 1,

$$DWM_1(G) = D_x f(x)\big|_{x=1} = 1101.$$

For $DWM_2(G)$, let

$$DWM_2(G,x) = h(x) = x^{171} + x^{133} + 3x^{81} + 2x^{49} + x^{36} + 2x^{24} + 2x^{18} + 4x^{16} + 2x^9 + x^7 + 4x^6 + x^5 + 2x^4 + 3x + 15.$$

Then

$$D_x h(x) = 171x^{171} + 133x^{133} + 243x^{81} + +98x^{49} + 36x^{36} + 48x^{24} + 36x^{18} + 64x^{16} + 18x^9 + 7x^7 + 24x^6 + 5x^5 + +8x^4 + 3x.$$

From Table 1,

$$DWM_2(G) = D_x h(x)\big|_{x=1} = 894.$$

Now, for $DWF(G)$. Let

$$DWF(G,x) = g(x) = x^{6859} + 4x^{729} + 3x^{343} + 4x^{216} + x^{125} + 5x^{64} + 3x^8 + 8x + 12.$$

Then

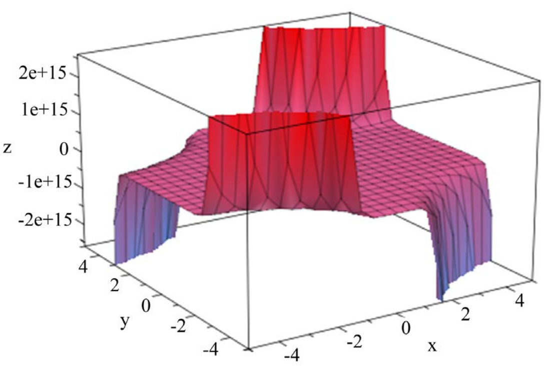

Figure 3. Plotting of M_{dn}-polynomial of remdesivir.

$$D_x g(x) = 6859x^{6859} + 2916x^{729} + 1029x^{343} + 864x^{216} + 125x^{125} + 320x^{64} + 24x^{8} + 8x.$$

From Table 1,

$$DWF(G) = D_x g(x)\big|_{x=1} = 12145.$$

Now using the Theorem 4.2, we calculate the first, second and forgotten downhill modified Zagreb indices of the molecular graph of remdesivir in the following theorem.

Theorem 4.4. *Let G be the molecular graph of remdesivir. Then,*

$$DWM_1^*(G) = 407,$$

$$DWF^*(G) = 3589.$$

Proof. Let

$$\begin{aligned} M_{dn}(G,x,y) &= f(x,y) \\ &= x^9y^{19} + x^7y^{19} + 3x^9y^9 + 2x^2y^9 + 2xy^9 + 2x^7y^7 + xy^7 \\ &\quad + x^6y^6 + 2x^4y^6 + 4xy^6 + xy^5 + 4x^4y^4 + 2x^2y^2 + 3xy \\ &\quad + 2y^{19} + y^9 + 3y^7 + 4y^6 + 3y^5 + 2y. \end{aligned}$$

Then

$$\begin{aligned} &(D_x + D_x) f(x,y) \\ &= 28x^9y^{19} + 26x^7y^{19} + 54x^9y^9 + 22x^2y^9 + 20xy^9 + 28x^7y^7 \\ &\quad + 8xy^7 + 12x^6y^6 + 20x^4y^6 + 28xy^6 + 6xy^5 + 32x^4y^4 \\ &\quad + 8x^2y^2 + 6xy + 38y^{19} + 9y^9 + 21y^7 + 24y^6 + 15y^5 + 2y, \end{aligned}$$

$$\begin{aligned} &(D_x^2 + D_y^2) f(x,y) \\ &= 442x^9y^{19} + 410x^7y^{19} + 486x^9y^9 + 170x^2y^9 + 164xy^9 + 196x^7y^7 \\ &\quad + 50xy^7 + 72x^6y^6 + 140x^4y^6 + 148xy^6 + 26xy^5 + 128x^4y^4 \\ &\quad + 16x^2y^2 + 6xy + 722y^{19} + 81y^9 + 147y^7 + 144y^6 + 75y^5 + 2y. \end{aligned}$$

Using Table 1, we have

$$DWM_1^*(G) = (D_x + D_x) f(x,y)\big|_{x=y=1} = 407,$$

$$DWF^*(G) = (D_x^2 + D_y^2) f(x,y)\big|_{x=y=1} = 3589.$$

We evaluate the downhill Zagreb polynomials and M_{dn}-polynomial of the molecular graph of chloroquine in the following two theorems.

Theorem 4.5. *Let G be the molecular graph of chloroquine. Then,*

$$DWM_1(G,x) = 3x^{81} + x^{49} + x^{25} + x^{16} + 6x^4 + 4x + 6,$$

$$DWM_2(G,x) = 2x^{81} + 2x^{18} + x^{14} + x^{10} + x^9 + 2x^7 + 5x^4 + x + 8,$$

$$DWF(G,x) = 3x^{729} + x^{343} + x^{125} + x^{64} + 6x^8 + 4x + 6.$$

Proof. Let G be the molecular graph of chloroquine (Figure 4). It has 22 vertices in which 3 vertices of downhill degree 9, one vertex of downhill degree 7,

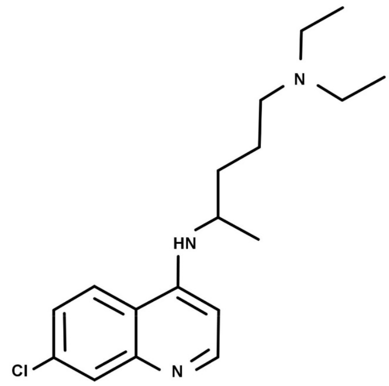

Figure 4. Chemical structure of chloroquine.

one vertex of downhill degree 5, one vertex of downhill degree 4, 6 vertices of downhill degree 2, 4 vertices of downhill degree 1 and 6 vertices of downhill degree 0.

Then, $DWM_1(G,x)$ is obtained as follows.

$$DWM_1(G,x) = \sum_{v\in V(G)} x^{(d_{dn}(v))^2}$$
$$= 3x^{9^2} + x^{7^2} + x^{5^2} + x^{4^2} + 6x^{2^2} + 4x^{1^2} + 6x^{0^2}$$
$$= 3x^{81} + x^{49} + x^{25} + x^{16} + 6x^4 + 4x + 6.$$

The graph G has 23 edges. In a graph G there are 13 types of edges based on the downhill degree of the vertices of each edge. From **Figure 4**, we have $|E_{9,9}| = 2$, $|E_{2,9}| = 2$, $|E_{1,9}| = 1$, $|E_{2,7}| = 1$, $|E_{1,7}| = 2$, $|E_{2,5}| = 1$, $|E_{1,4}| = 1$, $|E_{2,2}| = 4$, $|E_{1,1}| = 1$, $|E_{0,9}| = 2$, $|E_{0,5}| = 2$, $|E_{0,4}| = 2$ and $|E_{0,1}| = 2$.

Then, $DWM_2(G,x)$ is obtained as follows.

$$DWM_2(G,x) = \sum_{vu\in E(G)} x^{d_{dn}(v)d_{dn}(u)}$$
$$= |E_{9,9}|x^{9\times9} + |E_{2,9}|x^{2\times9} + |E_{1,9}|x^{1\times9} + |E_{2,7}|x^{2\times7} + |E_{1,7}|x^{1\times7}$$
$$+ |E_{2,5}|x^{2\times5} + |E_{1,4}|x^{1\times4} + |E_{2,2}|x^{2\times2} + |E_{1,1}|x^{1\times1} + |E_{0,9}|x^{0\times9}$$
$$+ |E_{0,5}|x^{0\times5} + |E_{0,4}|x^{0\times4} + |E_{0,1}|x^{0\times1}$$
$$= 2x^{81} + 2x^{18} + x^{14} + x^{10} + x^9 + 2x^7 + 5x^4 + x + 8.$$

Now, we calculate $DWF(G,x)$ similar to $DWM_1(G,x)$, then

$$DWF(G,x) = \sum_{v\in V(G)} x^{(d_{dn}(v))^3}$$
$$= 3x^{9^3} + x^{7^3} + x^{5^3} + x^{4^3} + 6x^{2^3} + 4x^{1^3} + 6x^{0^3}$$
$$= 3x^{729} + x^{343} + x^{125} + x^{64} + 6x^8 + 4x + 6.$$

Figure 5 is a 3D plot of downhill Zagreb polynomials of chloroquine.

Theorem 4.6. *Let G be the molecular graph of chloroquine. Then,*

$$M_{dn}(G,x,y) = 2x^9y^9 + 2x^2y^9 + xy^9 + x^2y^7 + 2xy^7 + x^2y^5 + xy^4$$
$$+ 4x^2y^2 + xy + 2y^9 + 2y^5 + 2y^4 + 2y.$$

Proof. From Theorem 4.5 and using the definition $M_{dn}(G,x,y)$, we have

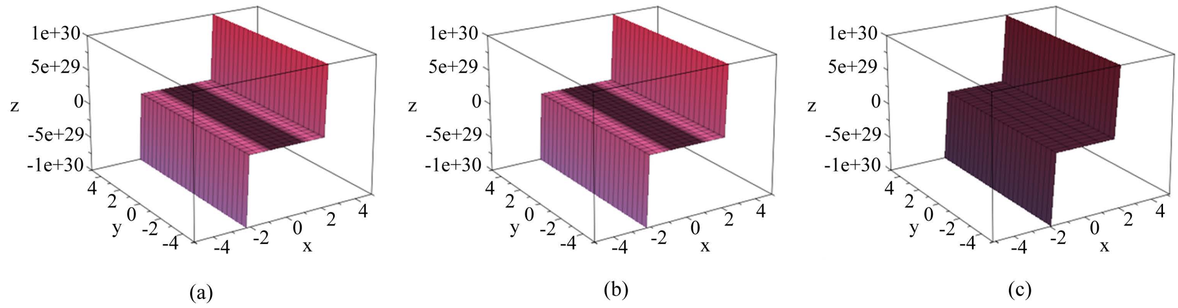

Figure 5. Plotting of downhill Zagreb polynomials of chloroquine. (a) $DWM_1(G, x)$; (b) $DWM_2(G, x)$; (c) $DWF(G, x)$.

$$\begin{aligned}
M_{dn}(G,x,y) &= \sum_{\delta_{dn}\le i\le j\le \Delta_{dn}} m_{i,j} x^i y^j \\
&= |E_{9,9}| x^9 y^9 + |E_{2,9}| x^2 y^9 + |E_{1,9}| xy^9 + |E_{2,7}| x^2 y^7 + |E_{1,7}| xy^7 \\
&\quad + |E_{2,5}| x^2 y^5 + |E_{1,4}| x^1 y^4 + |E_{2,2}| x^2 y^2 + |E_{1,1}| xy + |E_{0,9}| x^0 y^9 \\
&\quad + |E_{0,5}| x^0 y^5 + |E_{0,4}| x^0 y^4 + |E_{0,1}| x^0 y \\
&= 2x^9 y^9 + 2x^2 y^9 + xy^9 + x^2 y^7 + 2xy^7 + x^2 y^5 + xy^4 + 4x^2 y^2 \\
&\quad + xy + 2y^9 + 2y^5 + 2y^4 + 2y.
\end{aligned}$$

Figure 6 is a 3D plot of M_{dn}-polynomial of chloroquine.

Now using the Theorem 4.5, we calculate the first, second and forgotten downhill Zagreb indices of the molecular graph of chloroquine in the following theorem.

Theorem 4.7. *Let G be the molecular graph of chloroquine. Then,*

$$DWM_1(G) = 361,$$

$$DWM_2(G) = 266,$$

$$DWF(G) = 2771.$$

Proof. The proof similarly to the proof of Theorem 4.3.

Now using the Theorem 4.6, we calculate the first, second and forgotten downhill modified Zagreb indices of the molecular graph of chloroquine in the following theorem.

Theorem 4.8. *Let G be the molecular graph of chloroquine. Then,*

$$DWM_1^*(G) = 161,$$

$$DWF^*(G) = 1055.$$

Proof. The proof similarly to the proof of Theorem 4.4.

We evaluate the downhill Zagreb polynomials and M_{dn}-polynomial of the molecular graph of hydroxychloroquine in the following two theorems.

Theorem 4.9. *Let G be the molecular graph of hydroxychloroquine. Then,*

$$DWM_1(G,x) = 3x^{81} + x^{64} + x^{25} + x^{16} + 8x^4 + 3x + 6,$$

$$DWM_2(G,x) = 2x^{81} + 2x^{18} + 2x^{16} + x^{10} + x^9 + x^8 + 6x^4 + x + 8,$$

$$DWF(G,x) = 3x^{729} + x^{512} + x^{125} + x^{64} + 8x^8 + 3x + 6.$$

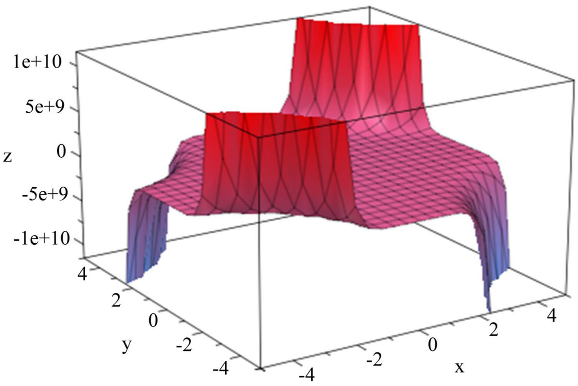

Figure 6. Plotting of M_{dn}-polynomial of chloroquine.

Proof. Let G be the molecular graph of hydroxychloroquine (**Figure 7**). It has 23 vertices in which 3 vertices of downhill degree 9, one vertex of downhill degree 8, one vertex of downhill degree 5, one vertex of downhill degree 4, 8 vertices of downhill degree 2, 3 vertices of downhill degree 1 and 6 vertices of downhill degree 0.

Then, $DWM_1(G,x)$ is obtained as follows.

$$DWM_1(G,x)=\sum_{v\in V(G)} x^{(d_{dn}(v))^2}$$
$$=3x^{9^2}+x^{8^2}+x^{5^2}+x^{4^2}+8x^{2^2}+3x^{1^2}+6x^{0^2}$$
$$=3x^{81}+x^{64}+x^{25}+x^{16}+8x^{4}+3x+6.$$

The graph G has 24 edges. In a graph G there are 14 types of edges based on the downhill degree of the vertices of each edge. From **Figure 7**, we have $|E_{9,9}|=2$, $|E_{2,9}|=2$, $|E_{1,9}|=1$, $|E_{2,8}|=2$, $|E_{1,8}|=1$, $|E_{2,5}|=1$, $|E_{1,4}|=1$, $|E_{2,2}|=5$,, $|E_{1,1}|=1$, $|E_{0,9}|=2$, $|E_{0,5}|=2$, $|E_{0,4}|=2$, $|E_{0,2}|=1$ and $|E_{0,1}|=2$.

Then, $DWM_2(G,x)$ is obtained as follows.

$$DWM_2(G,x)=\sum_{vu\in E(G)} x^{d_{dn}(v)d_{dn}(u)}$$
$$=|E_{9,9}|x^{9\times 9}+|E_{2,9}|x^{2\times 9}+|E_{1,9}|x^{1\times 9}+|E_{2,8}|x^{2\times 8}+|E_{1,8}|x^{1\times 8}$$
$$+|E_{2,5}|x^{2\times 5}+|E_{1,4}|x^{1\times 4}+|E_{2,2}|x^{2\times 2}+|E_{1,1}|x^{1\times 1}+|E_{0,9}|x^{0\times 9}$$
$$+|E_{0,5}|x^{0\times 5}+|E_{0,4}|x^{0\times 4}+|E_{0,2}|x^{0\times 2}+|E_{0,1}|x^{0\times 1}$$
$$=2x^{81}+2x^{18}+2x^{16}+x^{10}+x^{9}+x^{8}+6x^{4}+x+8.$$

Now, we calculate $DWF(G,x)$ similar to $DWM_1(G,x)$, then

$$DWF(G,x)=\sum_{v\in V(G)} x^{(d_{dn}(v))^3}$$
$$=3x^{9^3}+x^{8^3}+x^{5^3}+x^{4^3}+8x^{2^3}+3x^{1^3}+6x^{0^3}$$
$$=3x^{729}+x^{512}+x^{125}+x^{64}+8x^{8}+3x+6.$$

Theorem 4.10. *Let G be the molecular graph of hydroxychloroquine. Then,*

$$M_{dn}(G,x,y)=2x^9y^9+2x^2y^9+xy^9+2x^2y^8+xy^8+x^2y^5+xy^4$$
$$+5x^2y^2+xy+2y^9+2y^5+2y^4+y^2+y.$$

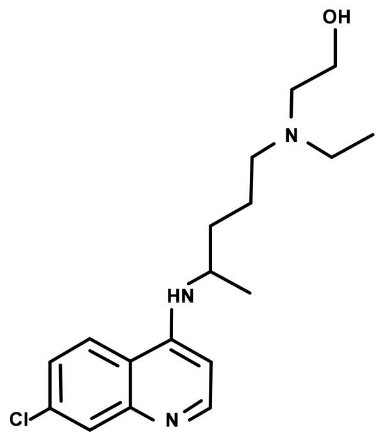

Figure 7. Chemical structure of hydroxychloroquine.

Proof. From Theorem 4.9 and using the definition $M_{dn}(G,x,y)$, we have

$$M_{dn}(G,x,y)=\sum_{\delta_{dn}\le i\le j\le\Delta_{dn}} m_{i,j}x^i y^j$$
$$=|E_{9,9}|x^9y^9+|E_{2,9}|x^2y^9+|E_{1,9}|xy^9+|E_{2,8}|x^2y^8+|E_{1,8}|xy^8$$
$$+|E_{2,5}|x^2y^5+|E_{1,4}|x^1y^4+|E_{2,2}|x^2y^2+|E_{1,1}|xy+|E_{0,9}|x^0y^9$$
$$+|E_{0,5}|x^0y^5+|E_{0,4}|x^0y^4+|E_{0,2}|x^0y^2+|E_{0,1}|x^0y$$
$$=2x^9y^9+2x^2y^9+xy^9+2x^2y^8+xy^8+x^2y^5+xy^4+5x^2y^2$$
$$+xy+2y^9+2y^5+2y^4+y^2+y.$$

Figure 8 is a 3D plot of downhill Zagreb polynomials of hydroxychloroquine.

Figure 9 is a 3D plot of M_{dn}-polynomial of hydroxychloroquine.

Now by using the Theorem 4.9, we calculate the first, second and forgotten downhill Zagreb indices of the molecular graph of hydroxychloroquine in the following theorem.

Theorem 4.11. *Let G be the molecular graph of hydroxychloroquine. Then,*

$$DWM_1(G)=383,$$
$$DWM_2(G)=282,$$
$$DWF(G)=2955.$$

Proof. The proof similarly to the proof of Theorem 4.3.

Now, by using the Theorem 4.10, we can calculate the first, second and forgotten downhill modified Zagreb indices of the molecular graph of hydroxychloroquine in the following theorem.

Theorem 4.12. *Let G be the molecular graph of hydroxychloroquine. Then,*

$$DWM_1^*(G)=170,$$
$$DWF^*(G)=1114.$$

Proof. The proof is similar to the proof of Theorem 4.4.

We evaluate the downhill Zagreb polynomials and M_{dn}-polynomial of the molecular graph of theaflavin in the following two results.

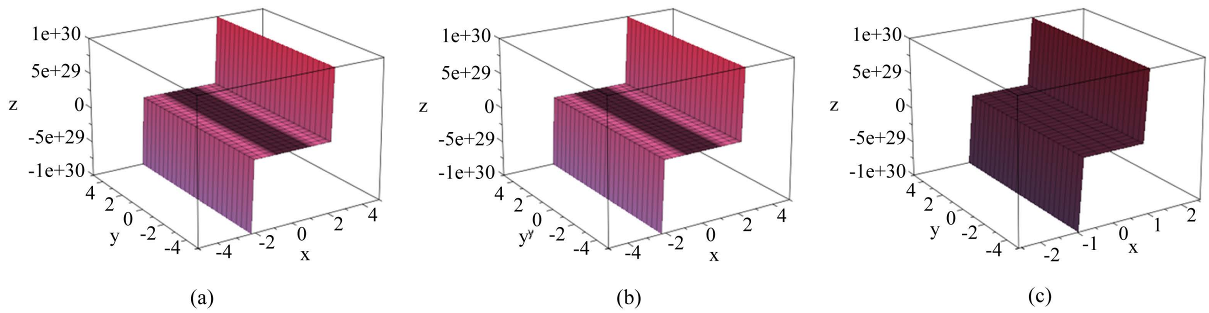

Figure 8. Plotting of downhill Zagreb polynomials of hydroxychloroquine. (a) $DWM_1(G, x)$; (b) $DWM_2(G, x)$; (c) $DWF(G, x)$.

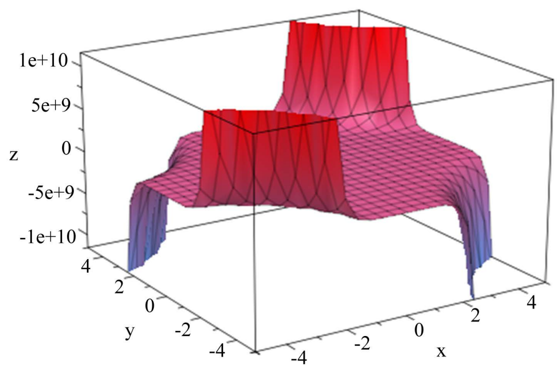

Figure 9. Plotting of M_{dn}-polynomial of hydroxychloroquine.

Theorem 4.13. *Let G be the molecular graph of theaflavin. Then,*

$$DWM_1(G,x) = 9x^{324} + 9x^{49} + 2x^9 + 12,$$

$$DWM_2(G,x) = 8x^{324} + 6x^{49} + 32,$$

$$DWF(G,x) = 9x^{5832} + 9x^{343} + 2x^{27} + 12.$$

Proof. Let G be the molecular graph of theaflavin (Figure 10). It has 41 vertices in which 9 vertices of downhill degree 18, 9 vertices of downhill degree 7, 2 vertices of downhill degree 3 and 21 vertices of downhill degree 0.

Then, $DWM_1(G,x)$ is obtained as follows.

$$\begin{aligned} DWM_1(G,x) &= \sum_{v\in V(G)} x^{(d_{dn}(v))^2} \\ &= 9x^{18^2} + 9x^{7^2} + 2x^{3^2} + 12x^{0^2} \\ &= 9x^{324} + 9x^{49} + 2x^9 + 12. \end{aligned}$$

The graph G has 46 edges. In a graph G there are 5 types of edges based on the downhill degree of the vertices of each edge. From Figure 10, we have $|E_{18,18}| = 8$, $|E_{7,7}| = 6$, $|E_{0,18}| = 11$, $|E_{0,7}| = 15$ and $|E_{0,3}| = 6$.

Then, $DWM_2(G,x)$ is obtained as follows.

$$\begin{aligned} DWM_2(G,x) &= \sum_{vu\in E(G)} x^{d_{dn}(v)d_{dn}(u)} \\ &= |E_{18,18}|x^{18\times18} + |E_{7,7}|x^{7\times7} + |E_{0,18}|x^{0\times18} + |E_{0,7}|x^{0\times7} + |E_{0,3}|x^{0\times3} \\ &= 8x^{324} + 6x^{49} + 32. \end{aligned}$$

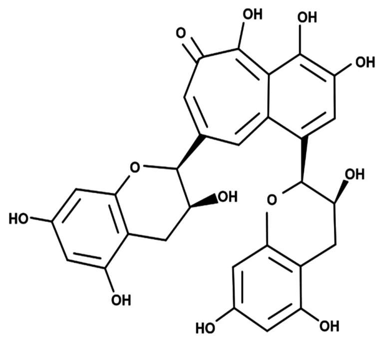

Figure 10. Chemical structure of theaflavin.

Now, we calculate $DWF(G,x)$ similar to $DWM_1(G,x)$, then

$$\begin{aligned} DWF(G,x) &= \sum_{v \in V(G)} x^{(d_{dn}(v))^3} \\ &= 9x^{18^3} + 9x^{7^3} + 2x^{3^3} + 12x^{0^3} \\ &= 9x^{5832} + 9x^{343} + 2x^{27} + 12. \end{aligned}$$

Figure 11 is a 3D plot of theaflavin downhill Zagreb polynomials.

Theorem 4.14. *Let G be the molecular graph of theaflavin. Then,*

$$M_{dn}(G,x,y) = 8x^{18}y^{18} + 6x^7y^7 + 11y^{18} + 15y^7 + 6y^3.$$

Proof. From Theorem 4.13 and using the definition $M_{dn}(G,x,y)$, we have

$$\begin{aligned} M_{dn}(G,x,y) &= \sum_{\delta_{dn} \le i \le j \le \Delta_{dn}} m_{i,j} x^i y^j \\ &= |E_{18,18}| x^{18} y^{18} + |E_{7,7}| x^7 y^7 + |E_{0,18}| x^0 y^{18} + |E_{0,7}| x^0 y^7 + |E_{0,3}| x^0 y^3 \\ &= 8x^{18}y^{18} + 6x^7y^7 + 11y^{18} + 15y^7 + 6y^3. \end{aligned}$$

Figure 12 is a 3D plot of M_{dn}-polynomial of theaflavin.

Now using the Theorem 4.13, we calculate the first, second and forgotten downhill Zagreb indices of the molecular graph of theaflavin in the following theorem.

Theorem 4.15. *Let G be the molecular graph of theaflavin. Then,*

$$DWM_1(G) = 3375,$$

$$DWM_2(G) = 2886,$$

$$DWF(G) = 55629.$$

Proof. The proof similarly to the proof of Theorem 4.3.

Now, by using the Theorem 4.14, we can calculate the first, second and forgotten downhill modified Zagreb indices of the molecular graph of theaflavin in the following result.

Theorem 4.16. *Let G be the molecular graph of theaflavin. Then,*

$$DWM_1^*(G) = 693,$$

$$DWF^*(G) = 10125.$$

Proof. The proof similarly to the proof of Theorem 4.4.

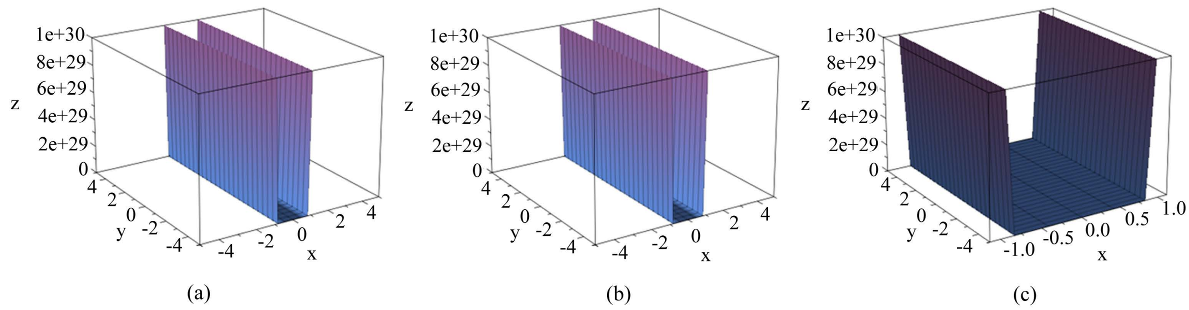

Figure 11. Plotting of theaflavin downhill Zagreb polynomials. (a) $DWM_1(G, x)$; (b) $DWM_2(G, x)$; (c) $DWF(G, x)$.

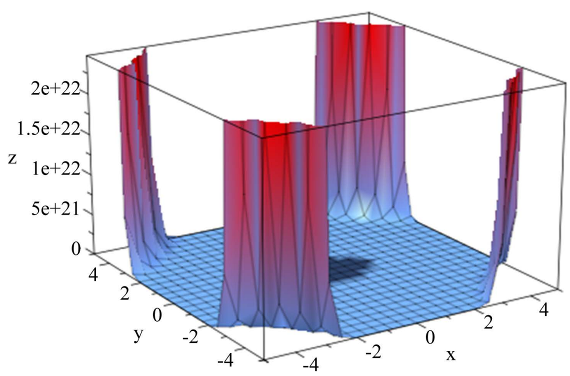

Figure 12. Plotting of M_{dn}-polynomial of theaflavin.

We evaluate the downhill Zagreb polynomials and M_{dn}-polynomial of the molecular graph of dexamethasone in the following two results.

Theorem 4.17. *Let G be the molecular graph of dexamethasone. Then,*

$$DWM_1(G,x) = 4x^{225} + 3x^{16} + 2x^9 + 2x^4 + 5x + 12,$$

$$DWM_2(G,x) = 2x^{225} + 2x^{60} + 2x^{45} + 2x^{30} + x^{16} + x^{15} + 2x^4 + 2x^3 + 2x + 15,$$

$$DWF(G,x) = 4x^{3375} + 3x^{64} + 2x^{27} + 2x^8 + 5x + 12.$$

Proof. Let G be the molecular graph of dexamethasone (**Figure 13**). It has 28 vertices in which 4 vertices of downhill degree 15, 3 vertices of downhill degree 4, 2 vertices of downhill degree 3, 2 vertices of downhill degree 2, 5 vertices of downhill degree 1 and 12 vertices of downhill degree 0.

Then, $DWM_1(G,x)$ is obtained as follows.

$$\begin{aligned} DWM_1(G,x) &= \sum_{v\in V(G)} x^{(d_{dn}(v))^2} \\ &= 4x^{15^2} + 3x^{4^2} + 2x^{3^2} + 2x^{2^2} + 5x^{1^2} + 12x^{0^2} \\ &= 4x^{225} + 3x^{16} + 2x^9 + 2x^4 + 5x + 12. \end{aligned}$$

The graph G has 31 edges. In a graph G there are 14 types of edges based on the downhill degree of the vertices of each edge. From **Figure 13**, we have $|E_{15,15}| = 2$, $|E_{4,15}| = 2$, $|E_{3,15}| = 2$, $|E_{2,15}| = 2$, $|E_{1,15}| = 1$, $|E_{4,4}| = 1$, $|E_{1,4}| = 2$, $|E_{1,3}| = 2$, $|E_{1,1}| = 2$, $|E_{0,15}| = 5$, $|E_{0,4}| = 3$, $|E_{0,3}| = 2$, $|E_{0,2}| = 4$ and $|E_{0,1}| = 1$.

Then, $DWM_2(G,x)$ is obtained as follows.

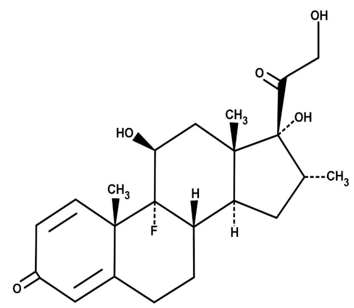

Figure 13. Chemical structure of dexamethasone.

$$\begin{aligned} DWM_2(G,x) &= \sum_{vu\in E(G)} x^{d_{dn}(v)d_{dn}(u)} \\ &= |E_{15,15}|x^{15\times15} + |E_{4,15}|x^{4\times15} + |E_{3,15}|x^{3\times15} + |E_{2,15}|x^{2\times15} \\ &\quad + |E_{1,15}|x^{1\times15} + |E_{4,4}|x^{4\times4} + |E_{1,4}|x^{1\times4} + |E_{1,3}|x^{1\times3} + |E_{1,1}|x^{1\times1} \\ &\quad + |E_{0,15}|x^{0\times15} + |E_{0,4}|x^{0\times4} + |E_{0,3}|x^{0\times3} + |E_{0,2}|x^{0\times2} + |E_{0,1}|x^{0\times1} \\ &= 2x^{225} + 2x^{60} + 2x^{45} + 2x^{30} + x^{16} + x^{15} + 2x^4 + 2x^3 + 2x + 15. \end{aligned}$$

Now, we calculate $DWF(G,x)$ similar to $DWM_1(G,x)$, then

$$\begin{aligned} DWF(G,x) &= \sum_{v\in V(G)} x^{(d_{dn}(v))^3} \\ &= 4x^{15^3} + 3x^{4^3} + 2x^{3^3} + 2x^{2^3} + 5x^{1^3} + 12x^{0^3} \\ &= 4x^{3375} + 3x^{64} + 2x^{27} + 2x^8 + 5x + 12. \end{aligned}$$

Figure 14 is a plot of dexamethasone downhill Zagreb polynomials.

Theorem 4.18. *Let G be the molecular graph of dexamethasone. Then,*

$$\begin{aligned} M_{dn}(G,x,y) &= 2x^{15}y^{15} + 2x^4y^{15} + 2x^3y^{15} + 2x^2y^{15} + xy^{15} + x^4y^4 \\ &\quad + 2xy^4 + 2xy^3 + 2xy + 5y^{15} + 3y^4 + 2y^3 + 4y^2 + y. \end{aligned}$$

Proof. From Theorem 4.17 and using the definition $M_{dn}(G,x,y)$, we have

$$\begin{aligned} M_{dn}(G,x,y) &= \sum_{\delta_{dn}\le i\le j\le\Delta_{dn}} m_{i,j}x^iy^j \\ &= |E_{15,15}|x^{15}y^{15} + |E_{4,15}|x^4y^{15} + |E_{3,15}|x^3y^{15} + |E_{2,15}|x^2y^{15} \\ &\quad + |E_{1,15}|xy^{15} + |E_{4,4}|x^4y^4 + |E_{1,4}|x^1y^4 + |E_{1,3}|xy^3 + |E_{1,1}|xy \\ &\quad + |E_{0,15}|x^0y^{15} + |E_{0,4}|x^0y^4 + |E_{0,3}|x^0y^3 + |E_{0,2}|x^0y^2 + |E_{0,1}|x^0y \\ &= 2x^{15}y^{15} + 2x^4y^{15} + 2x^3y^{15} + 2x^2y^{15} + xy^{15} + x^4y^4 + 2xy^4 \\ &\quad + 2xy^3 + 2xy + 5y^{15} + 3y^4 + 2y^3 + 4y^2 + y. \end{aligned}$$

Now using the Theorem 4.17, we calculate the first, second and forgotten downhill Zagreb indices of the molecular graph of dexamethasone in the following theorem.

Theorem 4.19. *Let G be the molecular graph of dexamethasone. Then,*

$$DWM_1(G) = 979,$$

$$DWM_2(G) = 767,$$

$$DWF(G) = 13767.$$

Proof. The proof similarly to the proof of Theorem 4.3.

Figure 15 is a 3D plot M_{dn}-polynomial of dexamethasone.

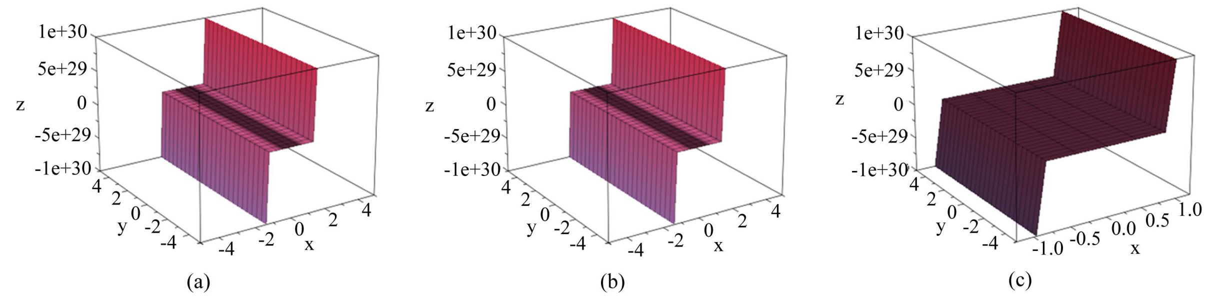

Figure 14. Plotting of dexamethasone downhill Zagreb polynomials. (a) $DWM_1(G, x)$; (b) $DWM_2(G, x)$; (c) $DWF(G, x)$.

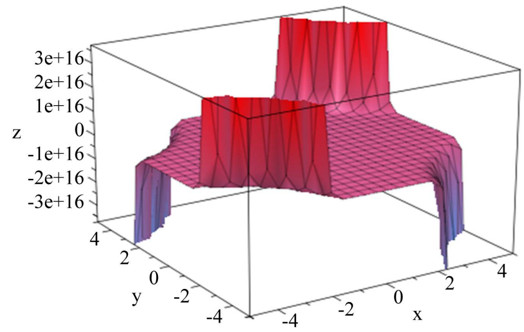

Figure 15. Plotting of M_{dn}-polynomial of dexamethasone.

Now, by using the Theorem 4.18, we can calculate the first, second and forgotten downhill modified Zagreb indices of the molecular graph of dexamethasone in the following theorem.

Theorem 4.20. *Let G be the molecular graph of dexamethasone. Then,*

$$DWM_1^*(G) = 316,$$

$$DWF^*(G) = 3832.$$

Proof. The proof similarly to the proof of Theorem 4.4.

5. Conclusion

In this research work, some properties and calculations of the chemical compounds which are used for the treatment of COVID-19 in terms of first, second and forgotten downhill Zagreb indices and polynomials are obtained. In particular, remdesivir, chloroquine, hydroxychloroquine, theaflavin and dexamethasone. We evaluate some downhill Zagreb indices, M_{dn}-polynomial and some downhill Zagreb Polynomials of these structures with 3D graphical representation. As topological indices are very important to predict different properties and activities such as acentric factor, enthalpy, boiling point, critical pressure, entropy, etc. our results and calculations will be useful to maybe developing new drug and vaccine for the treatment of COVID-19.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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