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Zagreb Polynomials and Redefined Zagreb Indices for Chemical Structures Helpful in the Treatment of COVID-19

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Abstract

A topological index (TI) is a number that is helpful in predicting the properties of chemical compounds. We canestimate the physical and chemical properties of several chemical compounds. In this study, we compute Zagreb polynomials and the redefined Zagreb indices for chemical compounds used in the treatment of COVID-19 namely remdesivir, chloroquine, hydroxychloroquine and theaflavin.

Keywords: COVID-19, chloroquine, hydroxychloroquine, redefined Zagreb indices, remdesivir, theaflavin, Zagreb polynomials

Introduction

Currently, the COVID-19 pandemic is jeopardizing human health as well as the economy all over the world. Wuhan, China is its place of origin [1]. By December 2020, there were 80410714 confirmed cases of COVID including 1732088 deaths worldwide (as per world meter information). Scientists have used some existing antiviral agents to treat the disease [2, 3, 4, 5, 6]. These include chloroquine, hydroxychloroquine, remdesivir (GS5734), and theaflavin [7].

Topological Indices (TIs) are very important tools in predicting the various properties of chemical compounds. A special number in graph theoretical term which represents a molecular structure is known as a TI. The first and second Zagreb indices are the oldest molecular descriptors introduced by Gutman in 1975 [8] and their various properties are investigated in this research.

They are defined as follows:

$$M_1(G) = \sum_{uv \in E(G)} (d_u + d_v)$$

$$M_2(G) = \sum_{uv \in E(G)} (d_u \times d_v)$$

Considering the Zagreb indices in [9], Fath-Tabar introduced the first and second Zagreb polynomials which are stated as follows:

$$M_1(G,z) = \sum_{uv \in E(G)} z^{[d_u + d_v]}$$

$$M_2(G,z) = \sum_{uv \in E(G)} z^{[d_u \times d_v]}$$

$M_1(G,x)$ and $M_2(G,x)$ give us important information about molecular graphs [10]. Afterwards, the author in [11] defined the third Zagreb polynomial as follows:

$$M_3(G,z) = \sum_{uv \in E(G)} z^{[d_u - d_v]}$$

Other versions of the Zagreb polynomials are given in [12].

$$M_4(G,z) = \sum_{uv \in E(G)} z^{d_u[d_u + d_v]}$$

$$M_5(G,z) = \sum_{uv \in E(G)} z^{d_v[d_u + d_v]}$$

$$M_{a,b}(G,z) = \sum_{uv \in E(G)} z^{[a d_u + b d_v]}$$

$$M'_{a,b}(G,z) = \sum_{uv \in E(G)} z^{(d_u + a)(b + d_v)}$$

Ranjini et al. [13] introduced the redefined Zagreb indices as follows:

$$ReZG_1 = \sum_{uv \in E(G)} \frac{d_u + d_v}{d_u \times d_v}$$

$$ReZG_2 = \sum_{uv \in E(G)} \frac{d_u \times d_v}{d_u + d_v}$$

$$ReZG_3 = \sum_{uv \in E(G)} (d_u + d_v)(d_u \times d_v)$$

Many studies have investigated the topological invariants [14, 15, 16, 17, 18, 19].

2. Main Results

In this section, we will discuss Zagreb polynomials and the redefined Zagreb indices for chemical structures used in the treatment of COVID-19 namely remdesivir, chloroquine, hydroxychloroquine and theaflavin.

2.1. Zagreb Polynomials and Redefined Zagreb Indices for Remdesivir

The graph of remdesivir is given in Figure 1. There are eight types of edges present in the graph. The degree-based edge partition is given in Table 1.

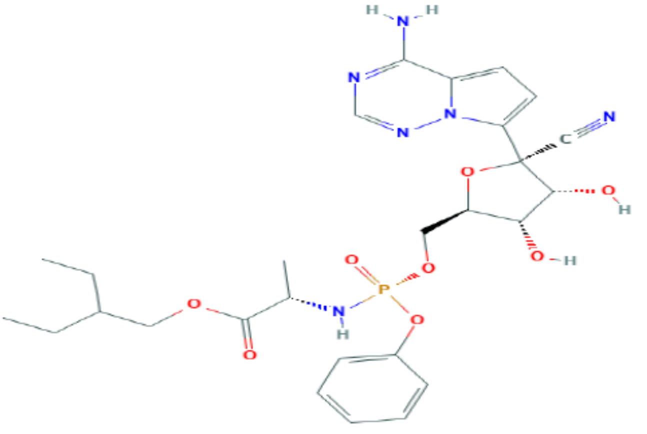

Figure 1. Chemical structure of Remdesivir (National centre for biotechnology information (PubChem))

Table 1. Partition of E (Remdesivir)

(d_u, d_v)	Frequency
(1,2)	2
(1,3)	5
(1,4)	2
(2,2)	9
(2,3)	14
(2,4)	4
(3,3)	6
(3,4)	2

Theorem 2.2.

Let G be the graph of Remdesivir. The Zagreb polynomials are stated as follows:

(1) $M_1(G,z) = 2z^3+14z^4+16z^5+10z^6+2z^7$

(2) $M_2(G,z) = 2z^2+5z^3+11z^4+14z^6+4z^8+6z^9+2z^{12}$

(3) $M_3(G,z) = 2z^3+9z^2+18z+15$

(4) $M_4(G,z) = 2z^3+5z^4+2z^5+9z^8+14z^{10}+4z^{12}+6z^{18}+2z^{36}$

(5) $M_5(G,z) = 2z^6+5z^{12}+2z^{20}+9z^8+14z^{15}+4z^{24}+6z^{18}+2z^{48}$

(6) $M_{a,b}(G,z) = 2z^{a+2b}+5z^{a+3b}+2z^{a+3b}+9z^{2a+2b}+14z^{2a+3b}+4z^{2a+4b}+6z^{3a+3b}+2z^{3a+4b}$

(7) $M'_{a,b}(G,z) = 2z^{(1+a)(2+b)}+5z^{(1+a)(3+b)}+2z^{(1+a)(4+b)}+9z^{(2+a)(2+b)}+14z^{(2+a)(3+b)}+4z^{(2+a)(4+b)}+6z^{(3+a)(3+b)}+2z^{(3+a)(4+b)}$

Proofs:

1. $M_1(G,z) = \sum_{uv\in E(G)} z^{[d_u+d_v]}$

$= |E_{\{1,2\}}(G)|\, z^3 + |E_{\{1,3\}}(G)|\, z^4 + |E_{\{1,4\}}(G)|\, z^5 + |E_{\{2,2\}}(G)|\, z^4 + |E_{\{2,3\}}(G)| z^5 +$

$|E_{\{2,4\}}(G)| z^6 + |E_{\{3,3\}}(G)| z^6 + |E_{\{3,4\}}(G)| z^7$

$= 2z^3+14z^4+16z^5+10z^6+2z^7$

2. $M_2(G,z) = \sum_{uv\in E(G)} z^{[d_u\times d_v]}$

$= |E_{\{1,2\}}(G)|\, z^2 + |E_{\{1,3\}}(G)|\, z^3 + |E_{\{1,4\}}(G)|\, z^4 + |E_{\{2,2\}}(G)|\, z^4 + |E_{\{2,3\}}(G)| z^6 +$

$|E_{\{2,4\}}(G)| z^8 + |E_{\{3,3\}}(G)| z^9 + |E_{\{3,4\}}(G)| z^{12}$

$= 2z^2+5z^3+11z^4+14z^6+4z^8+6z^9+2z^{12}$

3. $M_3(G,z) = \sum_{uv\in E(G)} z^{[d_u-d_v]}$

$= |E_{\{1,2\}}(G)|\, z^1 + |E_{\{1,3\}}(G)|\, z^2 + |E_{\{1,4\}}(G)|\, z^3 + |E_{\{2,2\}}(G)|\, z^0 + |E_{\{2,3\}}(G)| z^1 +$

$|E_{\{2,4\}}(G)| z^2 + |E_{\{3,3\}}(G)| z^0 + |E_{\{3,4\}}(G)| z^1$

$= 2z^3+9z^2+18z+15$

4. $M_4(G,z) = \sum_{uv\in E(G)} z^{d_u[d_u+d_v]}$

$=|E_{\{1,2\}}(G)| z^3+|E_{\{1,3\}}(G)| z^4+|E_{\{1,4\}}(G)| z^5+|E_{\{2,2\}}(G)| z^8+|E_{\{2,3\}}(G)|z^{10}+$

$|E_{\{2,4\}}(G)|z^{12}+ |E_{\{3,3\}}(G)|z^{18} +|E_{\{3,4\}}(G)|z^{36}$

$= 2z^3+5z^4+2z^5+9z^8+14z^{10}+4x^{12}+6z^{18}+2z^{36}$

5. $M_5(G,z) = \sum_{uv\in E(G)} z^{d_v[d_u+d_v]}$

$=|E_{\{1,2\}}(G)| z^6+|E_{\{1,3\}}(G)| z^{12}+|E_{\{1,4\}}(G)| z^{20}+|E_{\{2,2\}}(G)| z^8+|E_{\{2,3\}}(G)|z^{15}+$

$|E_{\{2,4\}}(G)|z^{24}+ |E_{\{3,3\}}(G)|z^{18} +|E_{\{3,4\}}(G)|z^{48}$

$=2z^6+5z^{12}+2z^{20}+9z^8+14z^{15}+4z^{24}+6z^{18}+2z^{48}$

6. $M_{a,b}(G,z) = \sum_{uv\in E(G)} z^{[ad_u+bd_v]}$

$=|E_{\{1,2\}}(G)| z^{a+2b}+|E_{\{1,3\}}(G)| z^{a+3b}+|E_{\{1,4\}}(G)| z^{a+4b}+|E_{\{2,2\}}(G)|z^{2a+2b}+ |E_{\{2,3\}}(G)|z^{2a+3b} + |E_{\{2,4\}}(G)|z^{2a+4b}+ |E_{\{3,3\}}(G)|z^{3a+3b} +|E_{\{3,4\}}(G)|z^{3a+4b}$

$= 2z^{a+2b}+5z^{a+3b}+2z^{a+3b}+9z^{2a+2b}+14z^{2a+3b}+4z^{2a+4b}+6z^{3a+3b}+2z^{3a+4b}$

7. $M'_{a,b}(G,z) = \sum_{uv\in E(G)} z^{(d_u+a)(b+d_v)}$

$=|E_{\{1,2\}}(G)| z^{(1+a)(2+b)} + |E_{\{1,3\}}(G)| z^{(1+a)(3+b)}+|E_{\{1,4\}}(G)| z^{(1+a)(4+b)}+ |E_{\{2,2\}}(G)|z^{(2+a)(2+b)}+ |E_{\{2,3\}}(G)|z^{(2+a)(3+b)} + |E_{\{2,4\}}(G)|z^{(2+a)(4+b)}+ |E_{\{3,3\}}(G)|z^{(3+a)(3+b)} +|E_{\{3,4\}}(G)|z^{(3+a)(4+b)}$

$=2z^{(1+a)(2+b)}+5z^{(1+a)(3+b)}+2z^{(1+a)(4+b)}+9z^{(2+a)(2+b)}+14z^{(2+a)(3+b)}+4z^{(2+a)(4+b)}+6z^{(3+a)(3+b)}+2z^{(3+a)(4+b)}$

Theorem 2.3.

Let G be the graph of Remdesivir. The redefined Zagreb indices are given below.

(1) $ReZG_1$=41
(2) $ReZG_2$=52.64
(3) $ReZG_3$=1948

Proofs:

1. $ReZG_1 = \sum_{uv \in E(G)} \frac{d_u + d_v}{d_u \times d_v}$

$= (2)\left(\frac{3}{2}\right) + (5)\left(\frac{4}{3}\right) + (2)\left(\frac{5}{4}\right) + (9)\left(\frac{4}{4}\right) + (14)\left(\frac{5}{6}\right) + (4)\left(\frac{6}{8}\right) + (6)\left(\frac{6}{9}\right) + (2)\left(\frac{7}{12}\right)$

$= 41$

2. $ReZG_2 = \sum_{uv \in E(G)} \frac{d_u \times d_v}{d_u + d_v}$

$= (2)\left(\frac{2}{3}\right) + (5)\left(\frac{3}{4}\right) + (2)\left(\frac{4}{5}\right) + (9)\left(\frac{4}{4}\right) + (14)\left(\frac{6}{5}\right) + (4)\left(\frac{8}{6}\right) + (6)\left(\frac{9}{6}\right) + (2)\left(\frac{12}{7}\right)$

$= 52.64$

3. $ReZG_3 = \sum_{uv \in E(G)} (d_u + d_v)(d_u \times d_v)$

$= (2)(2\text{x}3) + (5)(3\text{x}4) + (2)(4 \text{ x } 5) + (9)(4 \text{ x } 4) + (14)(6 \text{ x } 5) + (4)(8 \text{ x } 6) + (6)(9 \text{ x } 6) + (9)(12\text{x}7)$

$= 1948$

2.4. Zagreb Polynomials and Redefined Zagreb Indices for Chloroquine

The graph of chloroquine is given in Figure 2. There are five types of edges present in the graph. The degree-based edge partition is given in Table 2.

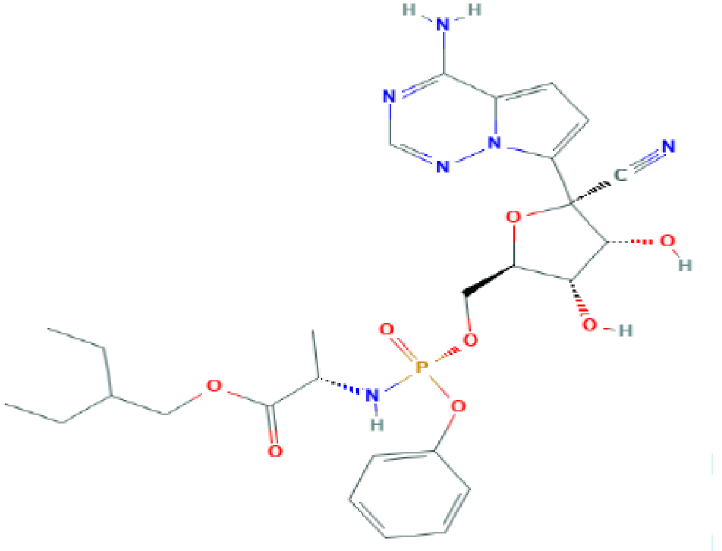

Figure 2. Chemical structure of of Chloroquine (National centre for biotechnology information (PubChem))

Table 2. Partition of E (Chloroquine)

(du, dv)	Frequency
(1, 2)	2
(1,3)	2
(2,2)	5
(2,3)	12
(3,3)	2

Theorem 2.5.

Let G be the graph of Chloroquine. The Zagreb polynomials are stated as follows:

(1) $M_1(G,z) = 2z^3+7z^4+12z^5+2z^6$

(2) $M_2(G,z) = 2z^2+2z^3+5z^4+12z^6+2z^9$

(3) $M_3(G,z) = 2z^2+14z+7$

(4) $M_4(G,z) = 2z^3+2z^4+5z^8+12z^{10}+2z^{18}$

(5) $M_5(G,z) = 2z^6+2z^{12}+5z^8+12z^{15}+2z^{18}$

(6) $M_{a,b}(G,z) = 2z^{a+2b}+2z^{a+3b}+5z^{2a+2b}+12z^{2a+3b}+2z^{3a+3b}$

(7) $M'_{a,b}(G,z) = 2z^{(1+a)(2+b)}+2z^{(1+a)(3+b)}+5z^{(2+a)(2+b)}+12z^{(2+a)(3+b)}$ $+2z^{(3+a)(3+b)}$

Proofs:

$$M_1(G,z) = \sum_{uv\in E(G)} z^{[d_u+d_v]}$$

$$= |E_{\{1,2\}}(G)|\, z^3 + |E_{\{1,3\}}(G)|\, z^4 + |E_{\{2,2\}}(G)|\, z^4 + |E_{\{2,3\}}(G)|\, z^5 + |E_{\{3,3\}}(G)|\, z^6$$

$$= 2z^3+7z^4+12z^5+2z^6$$

1. $M_2(G,z) = \sum_{uv\in E(G)} z^{[d_u\times d_v]}$

$$= |E_{\{1,2\}}(G)|\, z^2 + |E_{\{1,3\}}(G)|\, z^3 + |E_{\{2,2\}}(G)|\, z^4 + |E_{\{2,3\}}(G)|\, z^6 + |E_{\{3,3\}}(G)|\, z^9$$

$$= 2z^2+2z^3+5z^4+12z^6+2z^9$$

2. $M_3(G,z) = \sum_{uv\in E(G)} z^{[d_u-d_v]}$

$=|E_{\{1,2\}}(G)|\, z^1+|E_{\{1,3\}}(G)|\, z^2+|E_{\{2,2\}}(G)|\, z^0+|E_{\{2,3\}}(G)|z^1+|E_{\{3,3\}}(G)|z^0$

$= 2z^2+14z+7$

3. $M_4(G,z)=\sum_{uv\in E(G)} z^{d_u[d_u+d_v]}$

$=|E_{\{1,2\}}(G)|\, z^3+|E_{\{1,3\}}(G)|\, z^4+|E_{\{2,2\}}(G)|\, z^8+|E_{\{2,3\}}(G)|z^{10}+|E_{\{3,3\}}(G)|z^{18}$

$= 2z^3+2z^4+5z^8+12z^{10}+2z^{18}$

4. $M_5(G,z)=\sum_{uv\in E(G)} z^{d_v[d_u+d_v]}$

$=|E_{\{1,2\}}(G)|\, z^6+|E_{\{1,3\}}(G)|\, z^{12}+|E_{\{2,2\}}(G)|\, z^8+|E_{\{2,3\}}(G)|z^{15}+|E_{\{3,3\}}(G)|z^{18}$

$=2z^6+5z^8+2z^{12}+12z^{15}+2z^{18}$

5. $M_{a,b}(G,z)=\sum_{uv\in E(G)} z^{[ad_u+bd_v]}$

$=|E_{\{1,2\}}(G)|\, z^{a+2b}+|E_{\{1,3\}}(G)|\, z^{a+3b}+|E_{\{2,2\}}(G)|z^{2a+2b}+|E_{\{2,3\}}(G)|z^{2a+3b}+|E_{\{3,3\}}(G)|z^{3a+3b}$

$= 2z^{a+2b}+2z^{a+3b}+5z^{2a+2b}+12z^{2a+3b}+2z^{3a+3b}$

6. $M'_{a,b}(G,z) = \sum_{uv\in E(G)} z^{(d_u+a)(b+d_v)}$

$=|E_{\{1,2\}}(G)|\, z^{(1+a)(2+b)}+|E_{\{1,3\}}(G)|\, z^{(1+a)(3+b)}+|E_{\{2,2\}}(G)|z^{(2+a)(2+b)}+|E_{\{2,3\}}(G)|z^{(2+a)(3+b)}+|E_{\{3,3\}}(G)|z^{(3+a)(3+b)}$

$=2z^{(1+a)(2+b)}+2z^{(1+a)(3+b)}+5z^{(2+a)(2+b)}+12z^{(2+a)(3+b)}+2z^{(3+a)(3+b)}$

Theorem 2.6.

Let G be the graph of chloroquine. The redefined Zagreb indices are given below.

(1) $ReZG_1$=22

(2) $ReZG_2$=25.23

(3) $ReZG_3$=584

Proofs:

1. $ReZG_1 = \sum_{uv\in E(G)} \frac{d_u+d_v}{d_u\times d_v}$

$= (2)\left(\frac{3}{2}\right)+(2)\left(\frac{4}{3}\right)+(5)\left(\frac{4}{4}\right)+(12)\left(\frac{5}{6}\right)+(2)\left(\frac{6}{9}\right)=22$

2. $ReZG_2 = \sum_{uv\in E(G)} \frac{d_u\times d_v}{d_u+d_v}$

$= (2)\left(\frac{2}{3}\right)+(2)\left(\frac{3}{4}\right)+(5)\left(\frac{4}{4}\right)+(12)\left(\frac{6}{5}\right)+(2)\left(\frac{9}{6}\right) =25.23$

3. $ReZG_3 = \sum_{uv\in E(G)}(d_u + d_v)\,(d_u \times d_v)$

= (2) (2x3) +(5) (3x4) + (9) (4 x 4) + (14) (6 x 5) + (6) (9 x 6) = 584

2.7. Zagreb Polynomials and Redefined Zagreb Indices for Hydroxychloroquine.

The graph of hydroxychloroquine is given in Figure 3. There are five types of edges present in the graph. The degree-based edge partition is given in Table 3.

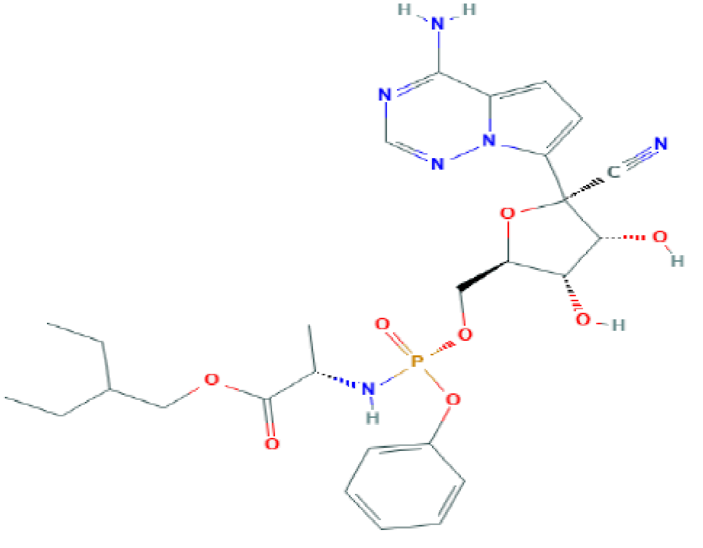

Figure 3. Chemical structure of Hydroxychloroquine (National centre for biotechnology information (PubChem))

Table 3. Partition of E (Hydroxychloroquine)

(du, dv)	Frequency
(1, 2)	2
(1,3)	2
(2,2)	6
(2,3)	12
(3,3)	2

Theorem 2.8.

Let G be the graph of hydroxychloroquine. The Zagreb polynomials are stated as follows:

(1) $M_1(G,z) = 2z^3+8z^4+12z^5+2z^6$

(2) $M_2(G,z) = 2z^2+2z^3+6z^4+12z^6+2z^9$

(3) $M_3(G,z) = 2z^2+14z+8$

(4) $M_4(G,z) = 2z^3+2z^4+6z^8+12z^{10}+2z^{18}$

(5) $M_5(G,z) = 2z^6+6z^8+2z^{12}+12z^{15}+2z^{18}$

(6) $M_{a,b}(G,z) = 2z^{a+2b}+2z^{a+3b}+6z^{2a+2b}+12z^{2a+3b}+zx^{3a+3b}$

(7) $M'_{a,b}(G,z) = 2z^{(1+a)(2+b)}+2z^{(1+a)(3+b)}+6z^{(2+a)(2+b)}+12z^{(2+a)(3+b)}$ $+2z^{(3+a)(3+b)}$

Proofs:

1. $M_1(G,z) = \sum_{uv\in E(G)} z^{[d_u+d_v]}$

$=|E_{\{1,2\}}(G)|\, z^3+|E_{\{1,3\}}(G)|\, z^4 +|E_{\{2,2\}}(G)|\, z^4+|E_{\{2,3\}}(G)| z^5+ |E_{\{3,3\}}(G)| z^6$

$= 2z^3+ 8z^4+12z^5+2z^6$

2. $M_2(G,z) = \sum_{uv\in E(G)} z^{[d_u\times d_v]}$

$=|E_{\{1,2\}}(G)|\, z^2+|E_{\{1,3\}}(G)|\, z^3 +|E_{\{2,2\}}(G)|\, z^4+|E_{\{2,3\}}(G)| z^6+ |E_{\{3,3\}}(G)| z^9$

$=2z^2+2z^3+6z^4+12z^6+2z^9$

3. $M_3(G,z) = \sum_{uv\in E(G)} z^{[d_u-d_v]}$

$=|E_{\{1,2\}}(G)|\ z^1+|E_{\{1,3\}}(G)|\ z^2+|E_{\{2,2\}}(G)|\ z^0+|E_{\{2,3\}}(G)|z^1+|E_{\{3,3\}}(G)|z^0$

$=2z^2+14z+8$

4. $M_4(G,z)=\sum_{uv\in E(G)} z^{d_u[d_u+d_v]}$

$=|E_{\{1,2\}}(G)|\ z^3+|E_{\{1,3\}}(G)|\ z^4+|E_{\{2,2\}}(G)|\ z^8+|E_{\{2,3\}}(G)|z^{10}+|E_{\{3,3\}}(G)|z^{18}$

$=2z^3+2z^4+6z^8+12z^{10}+2z^{18}$

5. $M_5(G,z)=\sum_{uv\in E(G)} z^{d_v[d_u+d_v]}$

$=|E_{\{1,2\}}(G)|\ z^6+|E_{\{1,3\}}(G)|\ z^{12}+|E_{\{2,2\}}(G)|\ z^8+|E_{\{2,3\}}(G)|z^{15}+|E_{\{3,3\}}(G)|z^{18}$

$=2z^6+6z^8+2z^{12}+12z^{15}+2z^{18}$

6. $M_{a,b}(G,z)=\sum_{uv\in E(G)} z^{[ad_u+bd_v]}$

$=|E_{\{1,2\}}(G)|\ z^{a+2b}+|E_{\{1,3\}}(G)|\ z^{a+3b}+|E_{\{2,2\}}(G)|z^{2a+2b}+|E_{\{2,3\}}(G)|z^{2a+3b}+|E_{\{3,3\}}(G)|z^{3a+3b}$

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

7. $M'_{a,b}(G,z)=\sum_{uv\in E(G)} z^{(d_u+a)(b+d_v)}$

$=|E_{\{1,2\}}(G)|\ z^{(1+a)(2+b)}+|E_{\{1,3\}}(G)|\ z^{(1+a)(3+b)}+|E_{\{2,2\}}(G)|\ z^{(2+a)(2+b)}+|E_{\{2,3\}}(G)|z^{(2+a)(3+b)}+|E_{\{3,3\}}(G)|z^{(3+a)(3+b)}$

$=2z^{(1+a)(2+b)}+2z^{(1+a)(3+b)}+6z^{(2+a)(2+b)}+12z^{(2+a)(3+b)}+2z^{(3+a)(3+b)}$

Theorem 2.9.

Let G be the graph of hydroxychloroquine. The redefined Zagreb indices are given below.

(1) $ReZG_1$=23

(2) $ReZG_2$=26.23

(3) $ReZG_3$=600

Proofs:

1. $ReZG_1 = \sum_{uv \in E(G)} \frac{d_u + d_v}{d_u \times d_v}$

$$= (2)\left(\frac{3}{2}\right) + (2)\left(\frac{4}{3}\right) + (6)\left(\frac{4}{4}\right) + (12)\left(\frac{5}{6}\right) + (2)\left(\frac{6}{9}\right)$$

=23

2. $ReZG_2 = \sum_{uv \in E(G)} \frac{d_u \times d_v}{d_u + d_v}$

$$= (2)\left(\frac{2}{3}\right) + (2)\left(\frac{3}{4}\right) + (6)\left(\frac{4}{4}\right) + (12)\left(\frac{6}{5}\right) + (2)\left(\frac{9}{6}\right)$$

=26.23

3. $ReZG_3 = \sum_{uv \in E(G)} (d_u + d_v)\,(d_u \times d_v)$

= (2) (2x3) +(2) (3x4) + (6) (4 x 4) + (12) (6 x 5) + (2) (9 x 6) = 600

2.10. Zagreb Polynomials and Redefined Zagreb Indices for Theaflavin

The graph of theaflavin is given in Figure 4. There are three types of edges present in the graph. The degree-based edge partition is given in Table 4.

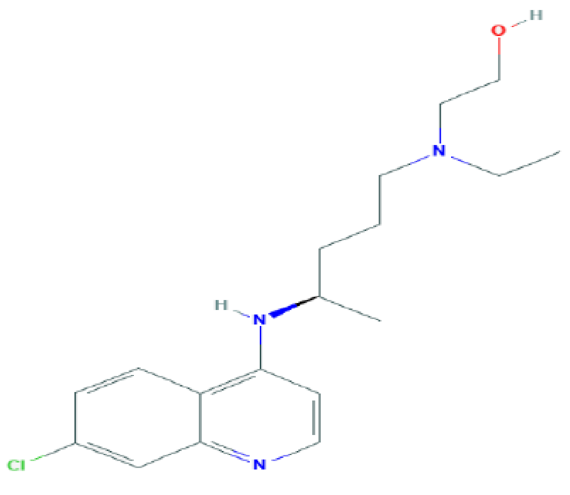

Figure 4. Chemical Structure of Theaflavin (National Centre for Biotechnology information (PubChem))

Table 4. Partition of E(Theaflavin)

(du,dv)	Frequency
(1,3)	10
(2,3)	22
(3,3)	14

Theorem 2.11.

Let G be the graph of theaflavin. The Zagreb polynomials are stated as follows:

(1) $M_1(G,z) = 10z^4+22z^5+14z^6$
(2) $M_2(G,z) = 10z^3+22z^6+14z^9$
(3) $M_3(G,z) = 10z^2+22z+14$
(4) $M_4(G,z) = 10z^4+22z^{12}+14z^{18}$
(5) $M_5(G,z) = 10z^{12}+22z^{15}+14z^{18}$
(6) $M_{a,b}(G,z) = 10z^{a+3b}+22z^{2a+3b}+14z^{3a+3b}$
(7) $M'_{a,b}(G,z) = 10z^{(1+a)(3+b)}+22z^{(2+a)(3+b)}+14z^{(3+a)(3+b)}$

Proofs:

$$M_1(G,z) = \sum_{uv\in E(G)} z^{[d_u+d_v]}$$
$$=|E_{\{1,3\}}(G)|\, z^4 + |E_{\{2,3\}}(G)| z^5 + |E_{\{3,3\}}(G)| z^6$$
$$= 10z^4+22z^5+14z^6$$

1. $M_2(G,z) = \sum_{uv\in E(G)} z^{[d_u\times d_v]}$
$$=|E_{\{1,3\}}(G)|\, z^3 + |E_{\{2,3\}}(G)| z^6 + |E_{\{3,3\}}(G)| z^9$$
$$=10z^3+22z^6+14z^9$$

2. $M_3(G,z) = \sum_{uv\in E(G)} z^{[d_u-d_v]}$
$$=|E_{\{1,3\}}(G)|\, z^2 + |E_{\{2,3\}}(G)| z^1 + |E_{\{3,3\}}(G)| z^0$$
$$= 10z^2+22z+14$$

3. $M_4(G,z) = \sum_{uv\in E(G)} z^{d_u[d_u+d_v]}$
$$=|E_{\{1,3\}}(G)|\, z^4 + |E_{\{2,3\}}(G)| z^{10} + |E_{\{3,3\}}(G)| z^{18}$$
$$= 10z^4+22z^{10}+14z^{18}$$

4. $M_5(G,z) = \sum_{uv\in E(G)} z^{d_v[d_u+d_v]}$

$=|E_{\{1,3\}}(G)|\, z^{12} + |E_{\{2,3\}}(G)| z^{15} + |E_{\{3,3\}}(G)| z^{18}$

$=10z^{12}+22z^{15}+14z^{18}$

5. $M_{a,b}(G,z) = \sum_{uv\in E(G)} z^{[ad_u+bd_v]}$

$=|E_{\{1,3\}}(G)|\, z^{a+3b} + |E_{\{2,3\}}(G)| z^{2a+3b} + |E_{\{3,3\}}(G)| z^{3a+3b}$

$= 10z^{a+3b}+22z^{2a+3b}+14z^{3a+3b}$

6. $M'_{a,b}(G,z) = \sum_{uv\in E(G)} z^{(d_u+a)(b+d_v)}$

$= |E_{\{1,3\}}(G)|\, z^{(1+a)(3+b)} + |E_{\{2,3\}}(G)| z^{(2+a)(3+b)} + |E_{\{3,3\}}(G)| z^{(3+a)(3+b)}$

$=10z^{(1+a)(3+b)}+22z^{(2+a)(3+b)}+14z^{(3+a)(3+b)}$

Theorem 2.12.

Let G be the graph of theaflavin. The redefined Zagreb indices are given below.

1. $ReZG_1$=41
2. $ReZG_2$=40.9
3. $ReZG_3$=1536

Proofs:

1. $ReZG_1 = \sum_{uv\in E(G)} \frac{d_u+d_v}{d_u\times d_v}$

$= (10)\left(\frac{4}{3}\right)+(22)\left(\frac{5}{6}\right)+(14)\left(\frac{6}{9}\right)$

$=41$

2. $ReZG_2 = \sum_{uv\in E(G)} \frac{d_u\times d_v}{d_u+d_v}$

$= (10)\left(\frac{3}{4}\right)+(22)\left(\frac{6}{5}\right)+(14)\left(\frac{9}{6}\right)$

$=40.9$

3. $ReZG_3 = \sum_{uv\in E(G)}(d_u + d_v)\,(d_u \times d_v)$

= (10) (3x4) + (22) (6 x 5) + (14) (9 x 6)

= 1536

3. Conclusion

In this article, we calculated the Zagreb polynomials and the redefined Zagreb indices for the chemical compounds used in the treatment of COVID-19. It has been demonstrated with certainty that the TIs help to anticipate their numerous properties without setting off to the wet lab.

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