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Some New Topological Invariants for Chemical Structures Used in the Treatment of COVID-19 Patients

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Abstract. A topological index plays an important rule in predicting physicochemical properties of a molecular structure. There are more than 150 topological indices present in literature but not a single index predict perfect result. In this paper, we will introduce some new topological invariants namely Maxmin indices and Maxmin polynomials and calculate results for Chloroquine and Hydroxychloroquine. These structures are helpful in the treatment of COVID-19 patients.

2010 AMS Classification: 05C09

Keywords: Maxmin indices, COVID-19, Chloroquine, Hydroxychloroquine.

1. Introduction

Currently, the COVID-19 pandemic is disarray human and world economy. It is started in a Wuhan [9] but has rapidly spread in and in all over the world. As of 3 April 2020, there were 1116643 cases, including 59158 deaths worldwide (as per world meter information). The novel corona virus (2019-nCoV) is a betacoronavirus. No vaccination is available right now for disease. It is therefore urgent need to identify appropriate antiviral agents to combat the pathogen. An compelling analysis to drug discovery is to test whether existing drugs are efficient in the treatment of this viral diseases. Scientist tested some existing antiviral drugs [10, 11, 19, 22, 24] and got conclusive results to inhibit the infection. Some of these antiviral compounds are chloroquine and hydroxychloroquine. Chloroquine is a nucleotide analog drug having broad spectrum activity developed to prevent Ebola virus infection [20]. It is also efficient for treatment of 2019-nCoV [19]. Chloroquine is a broadspectrum antiviral drug [15, 23] effective for treating malaria and autoimmune disease. Hydroxychloroquine has antiviral activity very similar to that of chloroquine. Hydroxychloroquine reduce the acute evolution of COVID-19. These properties can be predicted without using any lab by means of graph theory tools known as topological index.

A graph having no loop or multiple edge in known as simple graph. A molecular graph is a simple graph in which atoms and bounds are represented by vertex and edge set respectively. The degree of vertex is the number of edges attached with that vertex. The maximum and minimum degrees of graph is represented by $\Delta(G)$ and $\delta(G)$. The concept of maxmin vertex degree a_v, is define as $a_v = \Delta(G) + \delta(G) - d_g(v)$.

The first and second Maxmin indices are

$$MX_1(G) = \sum_{uv \epsilon E(G)} (a_u + a_v)$$

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$$MX_2(G) = \sum_{uv\epsilon E(G)} (a_u \times a_v)$$

Now, the first and second hyper Maxmin indices are

$$HMX_1(G) = \sum_{uv\epsilon E(G)} (a_u + a_v)^2$$

$$HMX_2(G) = \sum_{uv\epsilon E(G)} (a_u \times a_v)^2$$

With the help of Maxmin and hyper Maxmin indices, we now able to write the Maxmin and hyper Maxmin polynomials.

$$MX_1(G, y) = \sum_{uv\epsilon E(G)} y^{(a_u+a_v)}$$

$$MX_2(G, y) = \sum_{uv\epsilon E(G)} y^{(a_u\times a_v)}$$

and

$$HMX_1(G, y) = \sum_{uv\epsilon E(G)} y^{(a_u+a_v)^2}$$

$$HMX_2(G, y) = \sum_{uv\epsilon E(G)} y^{(a_u\times a_v)^2}$$

Many topological indices are studied in [1–8, 12–14, 16–18, 21].

2. Maxmin Indices and Polynomials

In this section, we will compute Maxmin indices, hyper Maxmin indices, Maxmin polynomials and hyper Maxmin polynomials for Chloroquine and Hydroxychloroquine. We will discuss these results in two subsections. The first subsection contain results for Chloroquine and the second subsection is about the computational results of Hydroxychloroquine.

2.1. **Maxmin indices and polynomials for Chloroquine.** Here, we will discuss Maxmin and hyper Maxmin indices of Chloroquine and also their Maxmin polynomials. The Figure 1 shows the graph of Chloroquine, there are five type of edges present in Chloroquine graph. The degree based edge and maxmin edge partition of Chloroquine is given in Table 1.

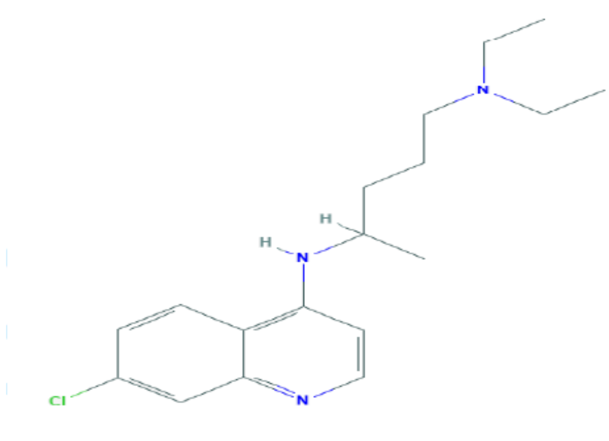

Figure 1. Graph of Chloroquine

(d_u, d_v)	(a_u, a_v)	Frequency
(1,2)	(3,2)	2
(1,3)	(3,1)	2
(2,2)	(2,2)	5
(2,3)	(2,1)	12
(3,3)	(1,1)	2

Table 1. Partition of $E(Chloroquine)$

Theorem 2.1. *Let G be the graph of Chloroquine. The first and second Maxmin indices are,*

(1) $MX_1(G) = 78$
(2) $MX_2(G) = 64$

Proof.

$$\begin{aligned} MX_1(G) &= \sum_{uv\epsilon E(G)} (a_u + a_v) \\ &= (3+2)(2) + (3+1)(2) + (2+2)(5) \\ &\quad (2+1)(12) + (1+1)(2) \\ &= 78. \end{aligned}$$

$$\begin{aligned} MX_2(G) &= \sum_{uv\epsilon E(G)} (a_u \times a_v) \\ &= (3\times 2)(2) + (3\times 1)(2) + (2\times 2)(5) \\ &\quad (2\times 1)(12) + (1\times 1)(2) \\ &= 64. \end{aligned}$$

Hence the proof is completed. □

Theorem 2.2. *Let G be the graph of Chloroquine. The first and second Maxmin polynomials are,*

(1) $MX_1(G, y) = 2y^5 + 7y^4 + 12y^3 + 2y^2$
(2) $MX_2(G, y) = 2y^6 + 5y^4 + 2y^3 + 12y^2 + 2y$

Proof.

$$\begin{aligned} MX_1(G, y) &= \sum_{uv\epsilon E(G)} y^{(a_u + a_v)} \\ &= 2y^{(3+2)} + 2y^{(3+1)} + 5y^{(2+2} \\ &\quad 12y^{(2+1)} + 2y^{(1+1)} \\ &= 2y^5 + 7y^4 + 12y^3 + 2y^2. \end{aligned}$$

$$\begin{aligned} MX_2(G, y) &= \sum_{uv\epsilon E(G)} y^{(a_u \times a_v)} \\ &= 2x^{(3\times 2)} + 2x^{(3\times 1)} + 5y^{(2\times 2} \\ &\quad 12y^{(2\times 1)} + 2y^{(1\times 1)} \\ &= 2y^6 + 5y^4 + 2y^3 + 12y^2 + 2y. \end{aligned}$$

Hence the proof is completed. □

Theorem 2.3. *Let G be the graph of Chloroquine. The first and second hyper Maxmin indices are,*

(1) $HMX_1(G) = 248$
(2) $HMX_2(G) = 220$

Proof.

$$\begin{aligned} HMX_1(G) &= \sum_{uv\epsilon E(G)} (a_u + a_v)^2 \\ &= (3+2)^2(2) + (3+1)^2(2) + (2+2)^2(5) \\ &\quad (2+1)^2(12) + (1+1)^2(2) \\ &= 248. \end{aligned}$$

$$\begin{aligned} HMX_2(G) &= \sum_{uv\epsilon E(G)} (a_u.a_v)^2 \\ &= (3\times 2)^2(2) + (3\times 1)^2(2) + (2\times 2)^2(5) \\ &\quad (2\times 1)^2(12) + (1\times 1)^2(2) \\ &= 220. \end{aligned}$$

Hence the proof is completed. □

Theorem 2.4. *Let G be the graph of Chloroquine. The first and second hyper Maxmin polynomials are,*

(1) $HMX_1(G, y) = 2y^{25} + 7y^{16} + 12y^9 + 2y^4$
(2) $HMX_2(G, y) = 2y^{36} + 5y^{16} + 2y^9 + 12y^4 + 2y$

Proof.

$$\begin{aligned} HMX_1(G, x) &= \sum_{uv\epsilon E(G)} y^{(a_u+a_v)^2} \\ &= 2y^{(3+2)^2} + 2y^{(3+1)^2} + 5y^{(2+2)^2} \\ &\quad 12y^{(2+1)^2} + 2y^{(1+1)^2} \\ &= 2y^{25} + 7y^{16} + 12y^9 + 2y^4. \end{aligned}$$

$$\begin{aligned} HMX_2(G, x) &= \sum_{uv\epsilon E(G)} y^{(a_u.a_v)^2} \\ &= 2y^{(3\times 2)^2} + 2y^{(3\times 1)^2} + 5y^{(2\times 2)^2} \\ &\quad 12y^{(2\times 1)^2} + 2y^{(1\times 1)^2} \\ &= 2y^{36} + 5y^{16} + 2y^9 + 12y^4 + 2y. \end{aligned}$$

Hence the proof is completed. □

2.2. **Maxmin indices and polynomials for Hydroxychloroquine.** In this section, we will discuss Maxmin and hyper Maxmin indices of Hydroxychloroquine and also their Maxmin polynomials. The Figure 2 shows the graph of Hydroxychloroquine, there are five type of edges present in Chloroquine graph. The degree based edge and maxmin edge partition of Hydroxychloroquine is given in Table 2.

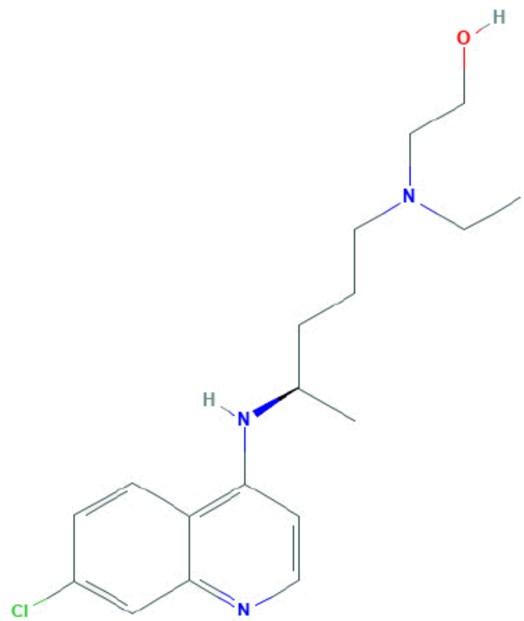

Figure 2. Graph of Hydroxychloroquine

(d_u, d_v)	(a_u, a_v)	Frequency
(1,2)	(3,2)	2
(1,3)	(3,1)	2
(2,2)	(2,2)	6
(2,3)	(2,1)	12
(3,3)	(1,1)	2

Table 2. Partition of $E(Hydroxychloroquine)$

Theorem 2.5. *Let G be the graph of Hydroxychloroquine. The first and second reverse Maxmin indices are*

(1) $MX_1(G) = 82$
(2) $MX_2(G) = 68$

Proof.

$$\begin{aligned} MX_1(G) &= \sum_{uv\epsilon E(G)} (a_u + a_v) \\ &= (3+2)(2) + (3+1)(2) + (2+2)(6) \\ &\quad (2+1)(12) + (1+1)(2) \\ &= 82. \\ MX_2(G) &= \sum_{uv\epsilon E(G)} (a_u \times a_v) \\ &= (3\times 2)(2) + (3\times 1)(2) + (2\times 2)(6) \\ &\quad (2\times 1)(12) + (1\times 1)(2) \\ &= 68. \end{aligned}$$

Hence the proof is completed. □

Theorem 2.6. *Let G be the graph of Hydroxychloroquine. The first and second Maxmin polynomials are*

(1) $MX_1(G,y) = 2y^5 + 8y^4 + 12y^3 + 2y^2$
(2) $MX_2(G,y) = 2y^6 + 6y^4 + 2y^3 + 12y^2 + 2y$

Proof.

$$\begin{aligned} MX_1(G,y) &= \sum_{uv\epsilon E(G)} y^{(a_u+a_v)} \\ &= 2y^{(3+2)} + 2y^{(3+1)} + 6y^{(2+2} \\ &\quad 12y^{(2+1)} + 2y^{(1+1)} \\ &= 2y^5 + 8y^4 + 12y^3 + 2y^2. \end{aligned}$$

$$\begin{aligned} MX_2(G,y) &= \sum_{uv\epsilon E(G)} y^{(a_u\times a_v)} \\ &= 2y^{(3\times2)} + 2y^{(3\times1)} + 6y^{(2\times2} \\ &\quad 12y^{(2\times1)} + 2y^{(1\times1)} \\ &= 2y^6 + 6y^4 + 2y^3 + 12y^2 + 2y. \end{aligned}$$

Hence the proof is completed. □

Theorem 2.7. *Let G be the graph of Hydroxychloroquine. The first and second hyper Maxmin indices are*

(1) $HMX_1(G) = 264$
(2) $HMX_2(G) = 236$

Proof.

$$\begin{aligned} HMX_1(G) &= \sum_{uv\epsilon E(G)} (a_u + a_v)^2 \\ &= (3+2)^2(2) + (3+1)^2(2) + (2+2)^2(6) \\ &\quad (2+1)^2(12) + (1+1)^2(2) \\ &= 264. \end{aligned}$$

$$\begin{aligned} HMX_2(G) &= \sum_{uv\epsilon E(G)} (a_u.a_v)^2 \\ &= (3\times2)^2(2) + (3\times1)^2(2) + (2\times2)^2(6) \\ &\quad (2\times1)^2(12) + (1\times1)^2(2) \\ &= 236. \end{aligned}$$

Hence the proof is completed. □

Theorem 2.8. *Let G be the graph of Hydroxychloroquine. The first and second hyper Maxmin polynomials are*

(1) $HMX_1(G,y) = 2y^{25} + 8y^{16} + 12y^9 + 2y^4$
(2) $HMX_2(G,y) = 2y^{36} + 6y^{16} + 2y^9 + 12y^4 + 2y$

Proof.

$$\begin{aligned} HMX_1(G,y) &= \sum_{uv\epsilon E(G)} y^{(a_u+a_v)^2} \\ &= 2y^{(3+2)^2} + 2y^{(3+1)^2} + 6y^{(2+2)^2} \\ &\quad 12y^{(2+1)^2} + 2y^{(1+1)^2} \\ &= 2y^{25} + 8y^{16} + 12y^9 + 2y^4. \end{aligned}$$

$$\begin{aligned} HMX_2(G,y) &= \sum_{uv\epsilon E(G)} y^{(a_u.a_v)^2} \\ &= 2y^{(3\times2)^2} + 2y^{(3\times1)^2} + 6y^{(2\times2)^2} \\ & \quad 12y^{(2\times1)^2} + 2y^{(1\times1)^2} \\ &= 2y^{36} + 6y^{16} + 2y^9 + 12y^4 + 2y. \end{aligned}$$

Hence the proof is completed. □

3. Conclusion

Topological indices associate a single number with a chemical structure. In quantitative structure activity relationship, knowledge of topological indices plays an important rule. In this article, we introduce some new topological invariants and calculate results for Chloroquine and Hydroxychloroquine. These structure are helpful in the treatment of COVID-19 patients.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this article.

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