Revan Polynomials of Chloroquine, Hydroxychloroquine, Remdesivir: Research for the Treatment of COVID-19

V.R.Kulli

Department of Mathematics, Gulbarga University, Kalaburgi (Gulbarga)-585106, India

Abstract: *In Chemical Science, chemical, biological, pharmaceutical properties of molecular structure are essential for drug design. These properties can be studied by topological index calculation. In this study, we obtain some topological properties of molecular structures of chloroquine, hydroxychloroquine and remdesivir. We determine some Revan polynomials for these three chemical antiviral agents. The results obtained can be helpful in finding new drug and vaccine for the treatment of COVID-19.*

Keywords: *molecular structure, Revan polynomials, antiviral agent, chloroquine, hydroxychloroquine, remdesivir.*

I. INTRODUCTION

A novel coronavirus disease started in Wuhan China in December 2019 [1]. As of 16 May 2020, there were more than 45 lakhs confirmed cases and more than 3 lakhs deaths worldwide (as per Wikipedia). So that there is urgent need to identify very effective and safe medicine and vaccine to treat this novel coronavirus disease. There are some antiviral agents and these antiviral agents were studied, for example, in [2, 3, 4, 5, 6, 7]. In this study, we consider three antiviral agents. Chloroquine is a medication primarily used to treat malaria. Chloroquine and its derivative hydroxychloroquine have since been repurposed for the treatment of a number of other conditions including HIV, systemic lupus erythmatosus and rheumatoid arthritis [8]. Due to COVID-19, the FDA has issued an emergency use authorization for hydroxychloroquine and chloroquine [9]. Remdesivir and chloroquine effectively inhibit the recently emerged novel coronavirus (2019-nCoV) in vitro [3]. In Chemical Science, concerning the definition of the topological index on the molecular structure and corresponding chemical, biological, pharmaceutical properties of drugs can be studied for the topological index calculation. A molecular structure [10] is a graph whose vertices correspond to the atoms and edges to the bonds. Studying molecular structures is a constant focus in Chemical Graph Theory: an effort to better understand molecular structures and obtaining some new drugs for diseases. A topological index is a numerical parameter mathematically derived from the graph structure. Throughout this study, we consider simple graphs which are finite connected undirected graphs without loops and multiple edges. Let G be such a graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertex u is the number of edges incident to u. Let $\Delta(G)(\delta(G))$ denote the maximum (minimum) degree among the vertices of G. The Revan vertex degree of a vertex u in G is defined as $r_G(u) = \Delta(G) + \delta(G) - d_G(u)$. The Revan edge connecting Revan vertices u and v will be denoted by uv. Two degree based topological indices were introduced and studied by Gutman et al. in [11].

The first and second Revan indices of a graph G were introduced by Kulli in [12], defined as

$$R_1(G) = \sum_{uv\in E(G)} \left[r_G(u)+r_G(v)\right],$$

$$R_2(G) = \sum_{uv\in E(G)} r_G(u)r_G(v).$$

Considering the Revan indices, the first and second Revan polynomials [12] of a graph were defined as follows:

$$R_1(G,x) = \sum_{uv\in E(G)} x^{r_G(u)+r_G(v)},$$

$$R_2(G,x) = \sum_{uv\in E(G)} x^{r_G(u)r_G(v)}.$$

The first and second hyper Revan indices of a graph were introduced in [13] and they are defined as

$$HR_1(G) = \sum_{uv\in E(G)} \left[r_G(u)+r_G(v)\right]^2,$$

$$HR_2(G) = \sum_{uv\in E(G)} \left[r_G(u)r_G(v)\right]^2.$$

Considering the hyper Revan indices, the first and second hyper Revan polynomials [13] of a graph were defined as

$$HR_1(G,x) = \sum_{uv\in E(G)} x^{\left[r_G(u)+r_G(v)\right]^2},$$

$$HR_2(G) = \sum_{uv\in E(G)} x^{\left[r_G(u)r_G(v)\right]^2}.$$

The modified first and second Revan indices of a graph were introduced by Kulli in [14], defined as

$${}^{m}R_1(G) = \sum_{uv\in E(G)} \frac{1}{r_G(u)+r_G(v)},$$

$$^{m}R_2(G) = \sum_{uv \in E(G)} \frac{1}{r_G(u) r_G(v)}.$$

Considering the modified first and second Revan indices of a graph, the modified first and second Revan polynomials are defined as

$$^{m}R_1(G,x) = \sum_{uv \in E(G)} x^{\frac{1}{r_G(u)+r_G(v)}},$$

$$^{m}R_2(G,x) = \sum_{uv \in E(G)} x^{\frac{1}{r_G(u) r_G(v)}}.$$

The sum and product connectivity Revan indices [15, 16] of a graph G are defined as

$$SR(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{r_G(u)+r_G(v)}}$$

$$PR(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{r_G(u) r_G(v)}}$$

Considering the sum and product connectivity Revan indices, the sum and product connectivity Revan polynomials are defined as

$$SR(G,x) = \sum_{uv \in E(G)} x^{\frac{1}{\sqrt{r_G(u)+r_G(v)}}},$$

$$PR(G,x) = \sum_{uv \in E(G)} x^{\frac{1}{\sqrt{r_G(u) r_G(v)}}}.$$

The general first and second Revan indices [7] of a graph G are defined as

$$R_1^a(G) = \sum_{uv \in E(G)} \left[r_G(u)+r_G(v)\right]^a,$$

$$R_2^a(G) = \sum_{uv \in E(G)} \left[r_G(u) r_G(v)\right]^a.$$

Considering general first and second Revan indices, we propose the first and second Revan polynomials of a graph G, defined as

$$R_1^a(G,x) = \sum_{uv \in E(G)} x^{\left[r_G(u)+r_G(v)\right]^a},$$

$$R_2^a(G,x) = \sum_{uv \in E(G)} x^{\left[r_G(u) r_G(v)\right]^a}.$$

where a is a real number.

The F-Revan index [17] of a graph G is defined as

$$FR(G) = \sum_{uv \in E(G)} \left[r_G(u)^2 + r_G(v)^2\right].$$

Considering the F-Revan index, we define the F-Revan polynomial of a graph G, as

$$FR(G,x) = \sum_{uv \in E(G)} x^{\left[r_G(u)^2 + r_G(v)^2\right]}.$$

The harmonic Revan index [7] of a graph G is defined as

$$HR(G) = \sum_{uv \in E(G)} \frac{2}{r_G(u)+r_G(v)}$$

Considering the harmonic Revan index, we define the harmonic Revan polynomial of a graph G as

$$HR(G,x) = \sum_{uv \in E(G)} x^{\frac{2}{r_G(u)+r_G(v)}}.$$

The symmetric division Revan index [7] of a graph G is defined as

$$SDR(G) = \sum_{uv \in E(G)} \left(\frac{r_G(u)}{r_G(v)} + \frac{r_G(v)}{r_G(u)}\right)$$

Considering the symmetric division Revan index, we define the symmetric devision Revan polynomial of a graph G as

$$SDR(G,x) = \sum_{uv \in E(G)} x^{\left(\frac{r_G(u)}{r_G(v)} + \frac{r_G(v)}{r_G(u)}\right)}$$

The inverse sum indeg Revan index [7] of a graph G is defined as

$$IR(G) = \sum_{uv \in E(G)} \frac{r_G(u) r_G(v)}{r_G(u)+r_G(v)}.$$

Considering the inverse sum indeg Revan index, we define the inverse sum indeg Revan polynomial of a graph G as

$$IR(G,x) = \sum_{uv \in E(G)} x^{\frac{r_G(u) r_G(v)}{r_G(u)+r_G(v)}}.$$

The minimum degree of the molecular graph of chloroquine (hydroxychloroquine or remdesivir) is 1. Therefore every Revan index of the molecular graph of chloroquine (hydroxychloroquine or remdesivir) is the reverse index of the molecular graph of chloroquine (hydroxychloroquine or remdesivir).

In this study, some Revan polynomials of chloroquine, hydroxychloroquine, remdesivir are computed.

II. RESULTS AND DISCUSSION : CHLOROQUINE

Let G be the molecular structure of chloroquine. Clearly G has 21 vertices and 23 edges, see Figure 1.

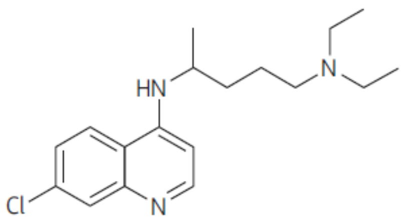

Figure 1

The edge set of G can be divided into five partitions based on the degree of end vertices of each edge as given in Table 1:

$d_G(u), d_G(v)\backslash uv\in E(G)$	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
No. of edges	2	2	5	12	2

Table 1. Edge partition of G

Clearly the vertices of G are of either of degree 1, 2 or 3. Hence $\Delta(G) = 3$ and $\delta(G) = 1$. Therefore $r_G(u) = 4 - d_G(u)$. In G, we obtain that there are five types of Revan edges based on the Revan degree of end Revan vertices of each Revan edge as given in Table 2:

$r_G(u), r_G(v)\backslash uv\in E(G)$	(3,2)	(3,1)	(2,2)	(2,1)	(1,1)
No. of edges	2	2	5	12	2

Table 2. Revan edge partition of G

In the following theorem, we determine the general first Revan polynomial of the molecular structure of chloroquine.

Theorem 1. The general first Revan polynomial of the molecular structure of chloroquine G is

$$R_1^a(G,x) = 2x^{5^a} + 7x^{4^a} + 12x^{3^a} + 2x^{2^a}.$$

Proof: Using definition and Table 2, we deduce

$$R_1^a(G,x) = \sum_{uv\in E(G)} x^{\left[r_G(u)+r_G(v)\right]^a}$$

$$= 2x^{(3+2)^a} + 2x^{(3+1)^a} + 5x^{(2,2)^a} + 12x^{(2+1)^a} + 2x^{(1+1)^a}$$

$$= 2x^{5^a} + 7x^{4^a} + 12x^{3^a} + 2x^{2^a}.$$

From Theorem 1, we obtain the following results.

Corollary 1.1. The first Revan polynomial of the molecular structure of chloroquine is

$$R_1(G,x) = 2x^5 + 7x^4 + 12x^3 + 2x^2.$$

Corollary 1.2. The first hyper Revan polynomial of the molecular structure of chloroquine is

$$HR_1(G,x) = 2x^{25} + 7x^{16} + 12x^9 + 2x^4.$$

Corollary 1.3. The modified first Revan polynomial of the molecular structure of chloroquine is

$${}^mR_1(G,x) = 2x^{\frac{1}{5}} + 7x^{\frac{1}{4}} + 12x^{\frac{1}{3}} + 2x^{\frac{1}{2}}.$$

Corollary 1.4. The sum connectivity Revan polynomial of the molecular structure of chloroquine is

$$SR_1(G,x) = 2x^{\frac{1}{\sqrt{5}}} + 7x^{\frac{1}{2}} + 12x^{\frac{1}{\sqrt{3}}} + 2x^{\frac{1}{\sqrt{2}}}.$$

In the following theorem, we compute the general second Revan polynomial of the molecular structure of chloroquine.

Theorem 2. The general second Revan polynomial of the molecular structure of chloroquine G is

$$R_2^a(G,x) = 2x^{6^a} + 5x^{4^a} + 2x^{3^a} + 12x^{2^a} + 2x.$$

Proof: From definition and using Table 2, we derive

$$R_2^a(G,x) = \sum_{uv\in E(G)} x^{\left[r_G(u)r_G(v)\right]^a}$$

$$= 2x^{(3\times2)^a} + 2x^{(3\times1)^a} + 5x^{(2\times2)^a} + 12x^{(2\times1)^a} + 2x^{(1\times1)^a}.$$

$$= 2x^{6^a} + 5x^{4^a} + 2x^{3^a} + 12x^{2^a} + 2x.$$

We establish the following results from Theorem 2.

Corollary 2.1. The second Revan polynomial of the molecular structure of chloroquine is

$$R_2(G,x) = 2x^6 + 5x^4 + 2x^3 + 12x^2 + 2x.$$

Corollary 2.2. The second hyper Revan polynomial of the molecular structure of chloroquine is

$$HR_2(G,x) = 2x^{36} + 5x^{16} + 2x^9 + 12x^4 + 2x.$$

Corollary 2.3. The modified second Revan polynomial of the molecular structure of chloroquine is

$${}^mR_2(G,x) = 2x^{\frac{1}{6}} + 5x^{\frac{1}{4}} + 2x^{\frac{1}{3}} + 12x^{\frac{1}{2}} + 2x.$$

Corollary 2.4. The product connectivity Revan polynomial of the molecular structure of chloroquine is

$$PR(G,x) = 2x^{\frac{1}{\sqrt{6}}} + 5x^{\frac{1}{2}} + 2x^{\frac{1}{\sqrt{3}}} + 12x^{\frac{1}{\sqrt{2}}} + 2x.$$

In the following theorem, we determine the *F*-Revan polynomial of the molecular structure of chloroquine.

Theorem 3. Let G be the molecular structure of chloroquine. Then

$$FR(G,x) = 2x^{13} + 2x^{10} + 5x^8 + 12x^5 + 2x^2.$$

Proof: Using definition and Table 2, we obtain

$$FR(G,x) = \sum_{uv\in E(G)} x^{\left[r_G(u)^2+r_G(v)^2\right]}$$

$$= 2x^{3^2+2^2} + 2x^{3^2+1^2} + 5x^{2^2+2^2} + 12x^{2^2+1^2} + 2x^{1^2+1^2}$$

$$= 2x^{13} + 2x^{10} + 5x^8 + 12x^5 + 2x^2.$$

In the following theorem, we compute the harmonic Revan polynomial of the molecular structure of chloroquine.

Theorem 4. Let G be the molecular structure of chloroquine. Then

$$HR(G,x) = 2x^{\frac{2}{5}} + 7x^{\frac{1}{2}} + 12x^{\frac{2}{3}} + 2x.$$

Proof: From definition and Table 2, we deduce

$$HR(G,x) = \sum_{uv\in E(G)} x^{\frac{2}{r_G(u)+r_G(v)}}$$

$$= 2x^{\frac{2}{3+2}} + 2x^{\frac{2}{3+1}} + 5x^{\frac{2}{2+2}} + 12x^{\frac{2}{2+1}} + 2x^{\frac{2}{1+1}}$$

$$= 2x^{\frac{2}{5}} + 7x^{\frac{1}{2}} + 12x^{\frac{2}{3}} + 2x.$$

In the following theorem, we determine the symmetric division Revan polynomial of the molecular structure of chloroquine.

Theorem 5. Let G be the molecular structure of chloroquine. Then

$$SDR(G,x)=2x^{\frac{13}{6}}+2x^{\frac{10}{3}}+12x^{\frac{5}{2}}+7x^{2}.$$

Proof: Using definition and Table 2, we derive

$$SDR(G,x)=\sum_{uv\in E(G)} x^{\left(\frac{r_G(u)}{r_G(v)}+\frac{r_G(v)}{r_G(u)}\right)}$$

$$=2x^{\left(\frac{3}{2}+\frac{2}{3}\right)}+2x^{\left(\frac{3}{1}+\frac{1}{3}\right)}+5x^{\left(\frac{2}{2}+\frac{2}{2}\right)}+12x^{\left(\frac{2}{1}+\frac{1}{2}\right)}+2x^{\left(\frac{1}{1}+\frac{1}{1}\right)}$$

$$=2x^{\frac{13}{6}}+2x^{\frac{10}{3}}+12x^{\frac{5}{2}}+7x^{2}.$$

In the following theorem, we compute the inverse sum indeg Revan polynomial of the molecular structure of chloroquine.

Theorem 6. Let G be the molecular structure of chloroquine. Then

$$IR(G,x)=2x^{\frac{6}{5}}+2x^{\frac{3}{4}}+5x+12x^{\frac{2}{3}}+2x^{\frac{1}{2}}.$$

Proof: From definition and by using Table 2, we deduce

$$IR(G,x)=\sum_{uv\in E(G)} x^{\frac{r_G(u)r_G(v)}{r_G(u)+r_G(v)}}$$

$$=2x^{\frac{3\times 2}{3+2}}+2x^{\frac{3\times 1}{3+1}}+5x^{\frac{2\times 2}{2+2}}+12x^{\frac{2\times 1}{2+1}}+2x^{\frac{1\times 1}{1+1}}$$

$$=2x^{\frac{6}{5}}+2x^{\frac{3}{4}}+5x+12x^{\frac{2}{3}}+2x^{\frac{1}{2}}.$$

III. RESULTS AND DISCUSSION: HYDROXYCHLOROQUINE

Let H be the molecular structure of hydroxychloroquine. Clearly H has 22 vertices and 24 edges, see Figure 2.

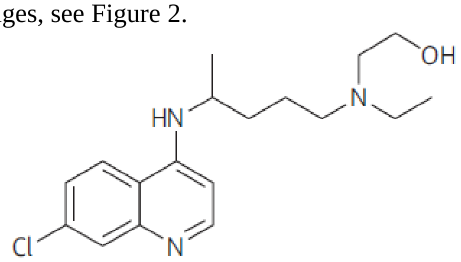

Figure 2

In H, the edge set of $E(H)$ can be divided into five partitions based on the degree of end vertices of each edge as given in Table 3:

$d_H(u), d_H(v)\backslash uv\in E(H)$	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
No. of edges	2	2	6	12	2

Table 3. Edge partition of H

The vertices of H are of either of degree 1, 2 or 3. Thus $\Delta(H)$ = 3, $\delta(H)$ = 1. Therefore $r_H(u)$ = 4 – $d_H(u)$. In H, there are five types of Revan edges based on the Revan degree of end Revan vertices of each Revan edge as given in Table 4:

$r_H(u), r_H(v)\backslash uv\in E(H)$	(3,2)	(3,1)	(2,2)	(2,1)	(1,1)
No. of edges	2	2	5	12	2

Table 4. Revan edge partition of H

In the following theorem, we compute the general first Revan polynomial of the molecular structure of hydroxychloroquine.

Theorem 7. The general first Revan polynomial of the molecular structure of hydroxychloroquine is

$$R_1^a(H,x)=2x^{5^a}+8x^{4^a}+12x^{3^a}+2x^{2^a}.$$

Proof: From definition and by using Table 4, we deduce

$$R_1^a(H,x)=\sum_{uv\in E(H)} x^{\left[r_H(u)+r_H(v)\right]^a}$$

$$=2x^{(3+2)^a}+2x^{(3+1)^a}+6x^{(2+2)^a}+12x^{(2+1)^a}+2x^{(1+1)^a}.$$

$$=2x^{5^a}+8x^{4^a}+12x^{3^a}+2x^{2^a}.$$

From Theorem 7, we obtain the following results.

Corollary 7.1. The first Revan polynomial of the molecular structure of hydroxychloroquine is

$$R_1(H,x)=2x^5+8x^4+12x^3+2x^2.$$

Corollary 7.2. The first hyper Revan polynomial of the molecular structure of hydroxychloroquine is

$$HR_1(H,x)=2x^{25}+8x^{16}+12x^9+2x^4.$$

Corollary 7.3. The modified first Revan polynomial of the molecular structure of hydroxychloroquine is

$${}^mR_1(H,x)=2x^{\frac{1}{5}}+8x^{\frac{1}{4}}+12x^{\frac{1}{3}}+2x^{\frac{1}{2}}.$$

Corollary 7.4. The sum connectivity Revan polynomial of the molecular structure of hydroxychloroquine is

$$SR_1(H,x)=2x^{\frac{1}{\sqrt{5}}}+8x^{\frac{1}{2}}+12x^{\frac{1}{\sqrt{3}}}+2x^{\frac{1}{\sqrt{2}}}.$$

In the following theorem, we determine the general second Revan polynomial of the molecular structure of hydroxychloroquine.

Theorem 8. The general second Revan polynomial of the molecular structure of hydroxychloroquine is

$$R_2^a(H,x)=2x^{6^a}+6x^{4^a}+2x^{3^a}+12x^{2^a}+2x.$$

Proof: Using definition and Table 2, we obtain

$$R_2^a(H,x)=\sum_{uv\in E(H)} x^{\left[r_H(u)r_H(v)\right]^a}$$

$$=2x^{(3\times 2)^a}+2x^{(3\times 1)^a}+6x^{(2\times 2)^a}+12x^{(2\times 1)^a}+2x^{(1\times 1)^a}.$$

$$=2x^{6^a}+6x^{4^a}+2x^{3^a}+12x^{2^a}+2x.$$

From Theorem 8, we establish the following results.

Corollary 8.1. The second Revan polynomial of the molecular structure of hydroxychloroquine is

$$R_2(H,x) = 2x^6 + 6x^4 + 2x^3 + 12x^2 + 2x.$$

Corollary 8.2. The second hyper Revan polynomial of the molecular structure of hydroxychloroquine is

$$HR_2(H,x) = 2x^{36} + 6x^{16} + 2x^9 + 12x^4 + 2x.$$

Corollary 8.3. The modified second Revan polynomial of the molecular structure of hydroxychloroquine is

$${}^mR_2(H,x) = 2x^{\frac{1}{6}} + 6x^{\frac{1}{4}} + 2x^{\frac{1}{3}} + 12x^{\frac{1}{2}} + 2x.$$

Corollary 8.4. The product connectivity Revan polynomial of the molecular structure of hydroxychloroquine is

$$PR(H,x) = 2x^{\frac{1}{\sqrt{6}}} + 6x^{\frac{1}{2}} + 2x^{\frac{1}{\sqrt{3}}} + 12x^{\frac{1}{\sqrt{2}}} + 2x.$$

In the following theorem, we compute the *F*-Revan polynomial of the molecular structure of hydroxychloroquine.

Theorem 9. Let *H* be the molecular structure of hydroxychloroquine. Then

$$FR(H,x) = 2x^{13} + 2x^{10} + 6x^8 + 12x^5 + 2x^2.$$

Proof: Using definition and Table 4, we derive

$$FR(H,x) = \sum_{uv\in E(H)} x^{\left[r_H(u)^2 + r_H(v)^2\right]}$$

$$= 2x^{3^2+2^2} + 2x^{3^2+1^2} + 6x^{2^2+2^2} + 12x^{2^2+1^2} + 2x^{1^2+1^2}.$$

$$= 2x^{13} + 2x^{10} + 6x^8 + 12x^5 + 2x^2.$$

In the following theorem, we compute the harmonic Revan polynomial of the molecular structure of hydroxychloroquine.

Theorem 10. Let *H* be the molecular structure of hydroxychloroquine. Then

$$HR(H,x) = 2x^{\frac{2}{5}} + 8x^{\frac{1}{2}} + 12x^{\frac{2}{3}} + 2x.$$

Proof: Using definition and Table 4, we obtain

$$HR(H,x) = \sum_{uv\in E(H)} x^{\frac{2}{r_H(u)+r_H(v)}}$$

$$= 2x^{\frac{2}{3+2}} + 2x^{\frac{2}{3+1}} + 6x^{\frac{2}{2+2}} + 12x^{\frac{2}{2+1}} + 2x^{\frac{2}{1+1}}$$

$$= 2x^{\frac{2}{5}} + 8x^{\frac{1}{2}} + 12x^{\frac{2}{3}} + 2x.$$

In the following theorem, we determine the symmetric division Revan polynomial of the molecular structure of hydroxychloroquine.

Theorem 11. Let *H* be the molecular structure of hydroxychloroquine. Then

$$SDR(H,x) = 2x^{\frac{13}{6}} + 2x^{\frac{10}{3}} + 12x^{\frac{5}{2}} + 8x^2.$$

Proof: From definition and using Table 4, we have

$$SDR(H,x) = \sum_{uv\in E(H)} x^{\left(\frac{r_H(u)}{r_H(v)} + \frac{r_H(v)}{r_H(u)}\right)}$$

$$= 2x^{\left(\frac{3}{2}+\frac{2}{3}\right)} + 2x^{\left(\frac{3}{1}+\frac{1}{3}\right)} + 6x^{\left(\frac{2}{2}+\frac{2}{2}\right)} + 12x^{\left(\frac{2}{1}+\frac{1}{2}\right)} + 2x^{\left(\frac{1}{1}+\frac{1}{1}\right)}$$

$$= 2x^{\frac{13}{6}} + 2x^{\frac{10}{3}} + 12x^{\frac{5}{2}} + 8x^2.$$

In the following theorem, we compute the inverse sum indeg Revan polynomial of the molecular structure of hydroxychloroquine.

Theorem 12. Let *H* be the molecular structure of hydroxychloroquine. Then

$$IR(H,x) = 2x^{\frac{6}{5}} + 2x^{\frac{3}{4}} + 6x + 12x^{\frac{2}{3}} + 2x^{\frac{1}{2}}.$$

Proof: Using definition and Table 4, we deduce

$$IR(H,x) = \sum_{uv\in E(H)} x^{\frac{r_H(u)r_H(v)}{r_H(u)+r_H(v)}}$$

$$= 2x^{\frac{3\times2}{3+2}} + 2x^{\frac{3\times1}{3+1}} + 6x^{\frac{2\times2}{2+2}} + 12x^{\frac{2\times1}{2+1}} + 2x^{\frac{1\times1}{1+1}}$$

$$= 2x^{\frac{6}{5}} + 2x^{\frac{3}{4}} + 6x + 12x^{\frac{2}{3}} + 2x^{\frac{1}{2}}.$$

IV. RESULTS AND DISCUSSION : REMDESVIR

Let *G* be the molecular structure of remdesivir. Clearly *G* has 41 vertices and 44 edges, see Figure 3.

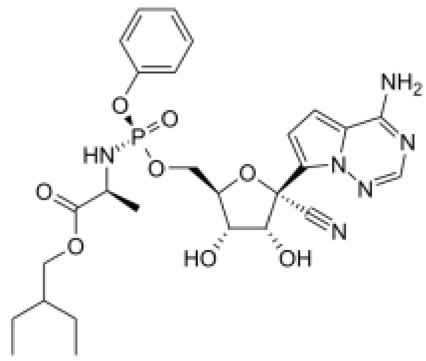

Figure 3

In *G*, the edge set $E(G)$ can be divided into eight partitions based on the degree of end vertices of each edge as given in Table 5:

$d_G(u), d_G(v)\backslash uv\in E(G)$	(1, 2)	(1, 3)	(1, 4)	(2, 2)	(2, 3)	(2, 4)	(3, 3)	(3, 4)
No. of edges	2	5	2	9	14	4	6	2

Table 5. Edge partition of *G*

Clearly the vertices of *G* are of either of degree 1, 2, 3 or 4. Hence $\Delta(G) = 4$ and $\delta(G) = 1$. Hence $r_G(u) = \Delta(G) + \delta(G) - d_G(u) = 5 - d_G(u)$. In *G*, there are eight types of Revan edges based on the Revan degree of end Revan vertices of each Revan edge as given in Table 6:

$r_G(u), r_G(v)\backslash uv \in E(G)$	(4, 3)	(4, 2)	(4, 1)	(3, 3)	(3, 2)	(3, 1)	(2, 2)	(2, 1)
No. of edges	2	5	2	9	14	4	6	2

Table 6. Revan edge partition of G

In the following theorem, we compute the general first Revan polynomial of the molecular structure of remdesivir.

Theorem 13. The general first Revan polynomial of the molecular structure of remdesivir is

$$R_1^a(G,x) = 2x^{7^a} + 14x^{6^a} + 16x^{5^a} + 10x^{4^a} + 2x^{3^a}.$$

Proof: From definition and by using Table 6, we deduce

$$R_1^a(G,x) = \sum_{uv\in E(G)} x^{\left[r_G(u)+r_G(v)\right]^a}$$

$$= 2x^{(4+3)^a} + 5x^{(4+2)^a} + 2x^{(4+1)^a} + 9x^{(3+3)^a}$$
$$+14x^{(3+2)^a} + 4x^{(3+1)^a} + 6x^{(2+2)^a} + 2x^{(2+1)^a}$$
$$= 2x^{7^a} + 14x^{6^a} + 16x^{5^a} + 10x^{4^a} + 2x^{3^a}.$$

We establish the following results from Theorem 13.

Corollary 13.1. The first Revan polynomial of the molecular structure of remdesivir is

$$R_1(G,x) = 2x^7 + 14x^6 + 16x^5 + 10x^4 + 2x^3.$$

Corollary 13.2. The first hyper Revan polynomial of the molecular structure of remdesivir is

$$HR_1(G,x) = 2x^{49} + 14x^{36} + 16x^{25} + 10x^{16} + 2x^9.$$

Corollary 13.3. The modified first Revan polynomial of the molecular structure of remdesivir is

$${}^{m}R_1(G,x) = 2x^{\frac{1}{7}} + 14x^{\frac{1}{6}} + 16x^{\frac{1}{5}} + 10x^{\frac{1}{4}} + 2x^{\frac{1}{3}}.$$

Corollary 13.4. The sum connectivity Revan polynomial of the molecular structure of remdesivir is

$$SR_1(G,x) = 2x^{\frac{1}{\sqrt{7}}} + 14x^{\frac{1}{\sqrt{6}}} + 16x^{\frac{1}{\sqrt{5}}} + 10x^{\frac{1}{2}} + 2x^{\frac{1}{\sqrt{3}}}.$$

In the following theorem, we determine the general second Revan polynomial of the molecular structure of remdesivir.

Theorem 14. The general second Revan polynomial of the molecular structure of remdesivir is

$$R_2^a(G,x) = 2x^{12^a} + 9x^{9^a} + 5x^{8^a} + 14x^{6^a}$$
$$+8x^{4^a} + 4x^{3^a} + 2x^{2^a}.$$

Proof: From definition and using Table 6, we derive

$$R_2^a(G,x) = \sum_{uv\in E(G)} x^{\left[r_G(u)r_G(v)\right]^a}$$

$$= 2x^{(4\times3)^a} + 5x^{(4\times2)^a} + 2x^{(4\times1)^a} + 9x^{(3\times3)^a} + 14x^{(3\times2)^a}$$
$$+4x^{(3\times1)^a} + 6x^{(2\times2)^a} + 2x^{(2\times1)^a}.$$
$$= 2x^{12^a} + 9x^{9^a} + 5x^{8^a} + 14x^{6^a} + 8x^{4^a} + 4x^{3^a} + 2x^{2^a}.$$

From Theorem 14, we obtain the following results.

Corollary 14.1. The second Revan polynomial of the molecular structure of remdesivir is

$$R_2(G,x) = 2x^{12} + 9x^9 + 5x^8 + 14x^6 + 8x^4 + 4x^3 + 2x^2.$$

Corollary 14.2. The second hyper Revan polynomial of the molecular structure of remdesivir is

$$HR_2(G,x) = 2x^{144} + 9x^{81} + 5x^{64} + 14x^{36} + 8x^{16} + 4x^9 + 2x^4.$$

Corollary 14.3. The modified second Revan polynomial of the molecular structure of remdesivir is

$${}^{m}R_2(G,x) =$$
$$2x^{\frac{1}{12}} + 9x^{\frac{1}{9}} + 5x^{\frac{1}{8}} + 14x^{\frac{1}{6}} + 8x^{1/4} + 4x^{\frac{1}{3}} + 2x^{\frac{1}{2}}$$

Corollary 14.4. The product connectivity Revan polynomial of the molecular structure of remdesivir is

$$PR(G,x) = 2x^{\frac{1}{\sqrt{12}}} + 9x^{\frac{1}{3}} + 5x^{\frac{1}{\sqrt{8}}} + 14x^{\frac{1}{\sqrt{6}}} + 8x^{2} + 4x^{\frac{1}{\sqrt{3}}} + 2x^{\frac{1}{\sqrt{2}}}.$$

In the following theorem, we compute the F-Revan polynomial of the molecular structure of remdesivir.

Theorem 15. Let G be the molecular structure of remdesivir. Then

$$FR(G,x) = 2x^{25} + 5x^{20} + 9x^{18} + 2x^{17}$$
$$+14x^{13} + 4x^{10} + 6x^8 + 2x^5.$$

Proof: From definition and by using Table 6, we deduce

$$FR(G,x) = \sum_{uv\in E(G)} x^{\left[r_G(u)^2+r_G(v)^2\right]}$$

$$= 2x^{4^2+3^2} + 5x^{4^2+2^2} + 2x^{4^2+1^2} + 9x^{3^2+3^2} + 14x^{3^2+2^2}$$
$$+4x^{3^2+1^2} + 6x^{2^2+2^2} + 2x^{2^2+1^2}$$
$$= 2x^{25} + 5x^{20} + 9x^{18} + 2x^{17} + 14x^{13} + 4x^{10} + 6x^8 + 2x^5.$$

In the following theorem, we determine the harmonic Revan polynomial of the molecular structure of remdesivir.

Theorem 16. Let G be the molecular structure of remdesivir. Then

$$HR(G,x) = 2x^{\frac{2}{7}} + 14x^{\frac{1}{3}} + 16x^{\frac{2}{5}} + 10x^{\frac{1}{2}} + 2x^{\frac{2}{3}}.$$

Proof: Using definition and Table 6, we derive

$$HR(G,x) = \sum_{uv\in E(G)} x^{\frac{2}{r_G(u)+r_G(v)}}$$

$$= 2x^{\frac{2}{4+3}} + 5x^{\frac{2}{4+2}} + 2x^{\frac{2}{4+1}} + 9x^{\frac{2}{3+3}} + 14x^{\frac{2}{3+2}}$$

$$+4x^{\frac{2}{3+1}}+6x^{\frac{2}{2+2}}+2x^{\frac{2}{2+1}}$$
$$=2x^{\frac{2}{7}}+14x^{\frac{1}{3}}+16x^{\frac{2}{5}}+10x^{\frac{1}{2}}+2x^{\frac{2}{3}}.$$

In the following theorem, we compute the symmetric division Revan polynomial of the molecular structure of remdesivir.

Theorem 17. Let G be the molecular structure of remdesivir. Then

$$SDR(G,x)=2x^{\frac{25}{12}}+7x^{\frac{5}{2}}+2x^{\frac{17}{4}}+15x^{2}+14x^{\frac{13}{6}}+4x^{\frac{10}{3}}.$$

Proof: From definition and by using Table 6, we obtain

$$SDR(G,x)=\sum_{uv\in E(G)} x^{\left(\frac{r_G(u)}{r_G(v)}+\frac{r_G(v)}{r_G(u)}\right)}$$
$$=2x^{\frac{4}{3}+\frac{3}{4}}+5x^{\frac{4}{2}+\frac{2}{4}}+2x^{\frac{4}{1}+\frac{1}{4}}+9x^{\frac{3}{3}+\frac{3}{3}}+14x^{\frac{3}{2}+\frac{2}{3}}$$
$$+4x^{\frac{3}{1}+\frac{1}{3}}+6x^{\frac{2}{2}+\frac{2}{2}}+2x^{\frac{2}{1}+\frac{1}{2}}$$
$$=2x^{\frac{25}{12}}+7x^{\frac{5}{2}}+2x^{\frac{17}{4}}+15x^{2}+14x^{\frac{13}{6}}+4x^{\frac{10}{3}}.$$

In the following theorem, we determine the inverse sum indeg Revan polynomial of the molecular structure of remdesivir.

Theorem 18. Let G be the molecular structure of remdesivir. Then

$$IR(G,x)=2x^{\frac{12}{7}}+5x^{\frac{4}{3}}+2x^{\frac{4}{5}}+9x^{\frac{3}{2}}+14x^{\frac{6}{5}}$$
$$+4x^{\frac{3}{4}}+6x+2x^{\frac{2}{3}}.$$

Proof: Using definition and Table 6, we deduce

$$IR(G,x)=\sum_{uv\in E(G)} x^{\frac{r_G(u)r_G(v)}{r_G(u)+r_G(v)}}$$
$$=2x^{\frac{4\times3}{4+3}}+5x^{\frac{4\times2}{4+2}}+2x^{\frac{4\times1}{4+1}}+9x^{\frac{3\times3}{3+3}}+14x^{\frac{3\times2}{3+2}}$$
$$+4x^{\frac{3\times1}{3+1}}+6x^{\frac{2\times2}{2+2}}+2x^{\frac{2\times1}{2+1}}$$
$$=2x^{\frac{12}{7}}+5x^{\frac{4}{3}}+2x^{\frac{4}{5}}+9x^{\frac{3}{2}}+14x^{\frac{6}{5}}+4x^{\frac{3}{4}}+6x+2x^{\frac{2}{3}}.$$

V. CONCLUSION

In this study, the expressions of some Revan polynomials of chloroquine, hydroxychloroquine and remdesiver have been determined. In Chemical Science, chemical, biological, pharmaceutical properties of molecular structure are required for drug design. In Mathematical Chemistry, these properties can be studied by the topological index calculation. Thus the results obtained in this paper may be useful in finding new drug and vaccine for the treatment of COVID-19.

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