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REVAN INDICES OF CHLOROQUINE, HYDROXYCHLOROQUINE, REMDESIVIR: RESEARCH ADVANCES FOR THE TREATMENT OF COVID-19

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ABSTRACT

In Medical Science, the topological index calculation is used to study medical, chemical, biological, pharmaceutical properties of drugs. In this study, we establish some topological properties of chloroquine, hydroxychloroquine and remdesivir structures. We compute some Revan indices for these three chemical antiviral agents. The results obtained may be useful in finding new medicine and vaccine for the prevention and treatment of a novel coronavirus disease-19 (COVID-19).

KEYWORDS: *molecular structure, antiviral agent, Revan indices, chloroquine, hydroxychloroquine, remdesivir.*

Mathematics Subject Classification: *05C05, 05C07, 05C12.*

1. INTRODUCTION

A novel coronavirus disease (COVID-19) started in Wuhan, China in December 2019[1]. This new disease has spread very quickly to several countries in the world. As of 26 April 2020, there were more than 26 lakhs confirmed cases and more than 2 lakhs deaths worldwide (as per Wikipedia) within very short period. Now, there is no drug or no vaccine available for the treatment and prevention of COVID-19. Therefore there is urgent need to identify very effective and safe medicine and vaccine to treat this new disease. There are some antiviral agents and these were studied, for example, in [2, 3, 4, 5, 6, 7, 8, 9, 10]. In this study, we consider antiviral agents namely chloroquine, hydroxychloroquine and remdesivir. 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 erythamatosus and rheumatoid arthritis [11]. Due to COVID-19, the FDA has issued an emergency use authorization for hydroxychloroquine and chloroquine [12]. Remdesivir and chloroquine effectively inhibit the recently emerged novel coronavirus (2019-nCoV) in vitro [5]. In Medical Science, concerning the definition of the topological index on the molecular structure and corresponding chemical, biological, medical, pharmaceutical properties of drugs can be studied for the topological index calculation [13]. A molecular structure [14] 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 finding some new drugs for diseases. A topological index is a numeric quantity from the structure of a molecule. Let G be a finite, simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d_G(u)$ of a vertex u is the number of vertices adjacent 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 $d_G(u) = \Delta(G) + \delta(G) - d_G(u)$. The Revan edge connecting the Revan vertices u and v will be denoted by uv. In 1972[15], two degree based topological indices were introduced and studied.

The first and second Revan indices of a graph G were introduced by Kulli in [16], and they are defined as

$$R_1(G) = \sum_{uv \in E(G)} \left[r_G(u) + r_G(v) \right], \qquad R_2(G) = \sum_{uv \in E(G)} r_G(u) r_G(v).$$

In [17], Kulli introduced the first and second hyper Revan indices of a graph G, defined as

$$HR_1(G) = \sum_{uv \in E(G)} \left[r_G(u) + r_G(v) \right]^2, \qquad HR_2(G) = \sum_{uv \in E(G)} \left[r_G(u) r_G(v) \right]^2.$$

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The modified first and second Revan indices of a graph G were introduced by Kulli in [18], defined as

$$ {}^{m}R_1(G)=\sum_{uv\in E(G)}\frac{1}{r_G(u)+r_G(v)}, \qquad {}^{m}R_2(G)=\sum_{uv\in E(G)}\frac{1}{r_G(u)r_G(v)}. $$

The sum connectivity Revan index [19] of a graph G is defined as

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

The product connectivity Revan index [20] of a graph G is defined as

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

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

$$ R_1^a(G)=\sum_{uv\in E(G)}\left[r_G(u)+r_G(v)\right]^a, \qquad R_2^a(G)=\sum_{uv\in E(G)}\left[r_G(u)r_G(v)\right]^a. $$

The F-Revan index of a graph G is defined as [21]

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

The atom bond connectivity Revan index of a graph G is defined as

$$ ABCR(G)=\sum_{uv\in E(G)}\sqrt{\frac{r_G(u)+r_G(v)-2}{r_G(u)r_G(v)}}. $$

The geometric-arithmetic Revan index of a graph G is defined as

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

The harmonic Revan index of a graph G is defined as

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

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

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

In this paper, some Revan indices of chloroquine, hydroxychloroquine, remdesivir are determined.

2. RESULTS AND DISCUSSION: CHLOROQUINE

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

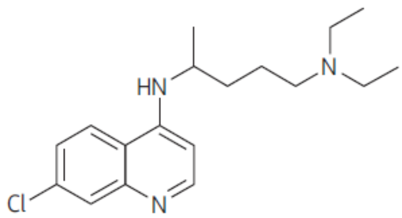

Figure 1

In G, the edge set $E(G)$ can be divided into five partitions based on the degree of end vertices of each edge as follows:

$E_1=\{uv \in E(G) \mid d_G(u)=1, d_G(v)=2\}$, $|E_1|=2$,
$E_2=\{uv \in E(G) \mid d_G(u)=1, d_G(v)=3\}$, $|E_2|=2$,

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$E_3=\{uv \in E(G) \mid d_G(u)=d_G(v)=2\}$, $|E_3|=5$,
$E_4=\{uv\in E(G) \mid d_G(u)=2, d_G(v)=3\}$, $|E_4|=12$,
$E_5=\{uv \in E(G) \mid d_G(u) = d_G(v)=3\}$, $|E_5|=2$.

Clearly the vertices of G are either of degree 1 or 2 or 3. Thus $\Delta(G) = 3$ and $\delta(G) = 1$. Thus $d_G(u) = \Delta(G) + \delta(G) – d_G(u) = 3 + 1 – d_G(u)$. Now 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 1.

Table 1. Revan edge partition of G

$r_G(u), r_G(v)\backslash uv\in E(G)$	(3,2)	(3,1)	(2,2)	(2,1)	(1,1)
Number of edges	2	2	5	12	2

In the following theorem, we compute the general first Revan index of the molecular graph of chloroquine.

Theorem 1. The general first Revan index of the molecular graph of chloroquine G is given by
$R^a_1(G)=2 \times 5^a + 7 \times 4^a + 12 \times 3^a + 2 \times 2^a$
Proof: From definition and by using Table 1, we obtain

$$R_1^a(G) = \sum_{ue\in E(G)} \left[r_G(u)+r_G(v)\right]^a$$
$$= 2(3+2)^a+2(3+1)^a+5(2+2)^a+12(2+1)^a+2(1+1)^a$$
$$= 2\times5^a + 7\times4^a + 12 \times 3^a + 2\times2^a.$$

We obtain the following results, by using Theorem 1.
Corollary 1.1. The first Revan index of the molecular graph of chloroquine is given is by
$R_1(G) = 78$.
Corollary 1.2. The first hyper Revan index of the graph of the molecular graph of chloroquine is
$HR_1(G) = 278$.
Corollary 1.3. The sum connectivity Revan index of the graph of the molecular graph of chloroquine is given by

$$SR(G) = \frac{2}{\sqrt{5}} + \frac{7}{2} + \frac{12}{\sqrt{3}} + \frac{2}{\sqrt{2}}.$$

Corollary 1.4. The modified first Revan index of the molecular graph of chloroquine is

$$^m R_1(G) = \frac{143}{20}.$$

In the following theorem, we determine the general second Revan index of the molecular graph of chloroquine.

Theorem 2. The general second Revan index of the molecular graph of chloroquine G is given by
$R^a_2(G)= 2 \times 6^a + 2 \times 3^a + 5 \times 4^a + 12 \times 2^a + 2$.
Proof: Using definition and Table 1, we derive

$$R_2^a(G) = \sum_{uv\in E(G)} \left[r_G(u) r_G(v)\right]^a$$
$$= 2(3 \times 2)^a + 2(3 \times 1)^a + 5(2 \times 2)^a +12(2\times1)^a + 2(1 \times 1)^a$$
$$= 2 \times 6^a + 2 \times 3^a + 5 \times 4^a + 12 \times 2^a + 2.$$

We establish the following results from Theorem 2,
Corollary 2.1. The second Revan index of the molecular graph of chloroquine is
$R_2(G) = 64$.
Corollary 2.2. The second hyper Revan index of the molecular graph of chloroquine is
$HR_2(G)=220$.
Corollary 2.3. The product connectivity Revan index of the molecular graph of chloroquine is

$$PR(G) = \frac{2}{\sqrt{6}} + \frac{2}{\sqrt{3}} + \frac{12}{\sqrt{2}} + \frac{9}{2}.$$

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Corollary 2.4. The modified second Revan index of the molecular graph of chloroquine is

$$^{m}R_2(G)=\frac{41}{4}.$$

In the following theorem, we compute the atom bond connectivity Revan index of the molecular graph of chloroquine.

Theorem 3. Let *G* be the molecular graph of chloroquine. Then

$FR(G) = 150.$

Proof: From definition and by using Table 1, we obtain

$$FR(G)=\sum_{ue\in E(G)}\left[r_G(u)^2+r_G(v)^2\right]$$
$$=2(3^2+2^2)+2(3^2+1^2)+5(2^2+2^2)+12(2^2+1^2)+2(1^2+1^2)$$
$$= 150$$

In the following theorem, we determine the atom bond connectivity Revan index of the molecular graph of chloroquine.

Theorem 4. Let *G* be the molecular graph of chloroquine. Then

$$ABCR(G)=\frac{19}{\sqrt{2}}+\frac{2\sqrt{2}}{\sqrt{3}}.$$

Proof: Using definition and using Table 1, we deduce

$$ABCR(G)=\sum_{uv\in E(G)}\sqrt{\frac{r_G(u)+r_G(v)-2}{r_G(u)r_G(v)}}$$
$$=2\sqrt{\frac{3+2-2}{3\times 2}}+2\sqrt{\frac{3+1-2}{3\times 1}}+2\sqrt{\frac{2+2-2}{2\times 2}}+12\sqrt{\frac{2+1-2}{2\times 1}}+2\sqrt{\frac{1+1-2}{1\times 1}}$$
$$=\frac{19}{\sqrt{2}}+\frac{2\sqrt{2}}{\sqrt{3}}.$$

In the following theorem, we compute the geometric-arithmetic Revan index of the molecular graph of chloroquine.

Theorem 5. Let *G* be the molecular graph of chloroquine. Then

$$GAR(G)=\frac{4\sqrt{6}}{5}+\sqrt{3}+8\sqrt{2}+7.$$

Proof: From definition and by using Table 1, we derive

$$GAR(G)=\sum_{uv\in E(G)}\frac{2\sqrt{r_G(u)r_G(v)}}{r_G(u)+r_G(v)}$$
$$=2\left(\frac{2\sqrt{3\times 2}}{3+2}\right)+2\left(\frac{2\sqrt{3\times 1}}{3+1}\right)+5\left(\frac{2\sqrt{2\times 2}}{2+2}\right)+2\left(\frac{2\sqrt{2\times 1}}{2+1}\right)+2\left(\frac{2\sqrt{1\times 1}}{1+1}\right)$$
$$=\frac{4\sqrt{6}}{5}+\sqrt{3}+8\sqrt{2}+7.$$

In the following theorem, we determine the harmonic Revan index of the molecular graph of chloroquine.

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

$$HR(G)=\frac{143}{10}.$$

Proof: From definition and using Table 1, we derive

$$HR(G)=\sum_{uv\in E(G)}\frac{2}{r_G(u)+r_G(v)}$$
$$=2\left(\frac{2}{3+2}\right)+2\left(\frac{2}{3+1}\right)+5\left(\frac{2}{2+2}\right)+12\left(\frac{2}{2+1}\right)+2\left(\frac{2}{1+1}\right)$$
$$=\frac{143}{10}.$$

In the next theorem, we compute the symmetric division Revan index of the molecular graph of chloroquine.

Theorem 7. Let G be the molecular graph of chloroquine. Then

$$SDR(G)=\frac{165}{3}.$$

Proof: Using definition and using Table 1, we deduce

$$SDR(G)=\sum_{uv\in E(G)}\left(\frac{r_G(u)}{r_G(v)}+\frac{r_G(v)}{r_G(u)}\right)$$
$$=2\left(\frac{3}{2}+\frac{2}{3}\right)+2\left(\frac{3}{1}+\frac{1}{3}\right)+5\left(\frac{2}{2}+\frac{2}{2}\right)+12\left(\frac{2}{1}+\frac{1}{2}\right)+2\left(\frac{1}{1}+\frac{1}{1}\right)$$
$$=\frac{165}{3}.$$

3. RESULTS AND DISCUSSION: HYDROXYCHLOROQUINE

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

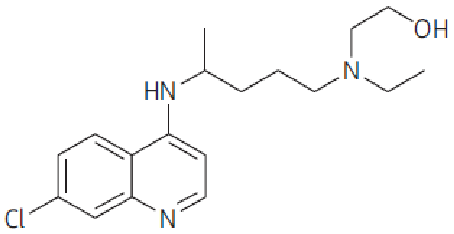

Figure 2

In H, the edge set of H can be divided into five partitions based on the degree of end vertices of each edge as follows:

$E_1=\{uv \in E(H) \mid d_H(u)=1, d_H(v)=2\}$, $|E_1|=2$,
$E_2=\{uv \in E(H) \mid d_H(u)=1, d_H(v)=3\}$, $|E_2|=2$,
$E_3=\{uv \in E(H) \mid d_H(u)=2, d_H(v)=2\}$, $|E_3|=6$,
$E_4=\{uv \in E(H) \mid d_H(u)=2, d_H(v)=3\}$, $|E_4|=12$,
$E_5=\{uv \in E(H) \mid d_H(u) = d_H(v)=3\}$, $|E_5|=2$.

We have, the vertices of H are either of degree 1 or 2 or 3. Hence $\Delta(H) = 3$ and $\delta(H) = 1$. Therefore $r_H(u) = \Delta(H) + \delta(H) - d_H(u) = 4 - d_H(u)$. 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 2.

Table 2. Revan edge partition of H

$r_H(u), r_H(v) \backslash uv \in E(H)$	(3, 2)	(3, 1)	(2, 2)	(2, 1)	(1, 1)
Number of edges	2	2	6	12	2

In the following theorem, we determine the general first Revan index of the molecular graph of hydroxychloroquine.

Theorem 8. The general first Revan index of the molecular graph of hydroxychloroquine H is

$$R^a_1(H) = 2 \times 5^a + 8 \times 4^a + 12 \times 3^a + 2 \times 2^a.$$

Proof: Using definition and Table 2, we deduce

$$R_1^a(H) = \sum_{uv \in E(H)} \left[r_H(u) + r_H(v)\right]^a$$
$$= 2(3+2)^a + 2(3+1)^a + 6(2+2)^a + 12(2+1)^a + 2(1+1)^a$$
$$= 2 \times 5^a + 8 \times 4^a + 12 \times 3^a + 2 \times 2^a.$$

We establish the following results from Theorem 8.

Corollary 8.1. The first Revan index of the molecular graph of hydroxychloroquine is

$$R_1(H) = 82.$$

Corollary 8.2. The first hyper Revan index of the molecular graph of hydroxychloroquine is

$$HR_1(H) = 294.$$

Corollary 8.3. The sum connectivity Revan index of the molecular graph of hydroxychloroquine is

$$SR(H) = 4 + \frac{2}{\sqrt{5}} + \frac{12}{\sqrt{3}} + \frac{2}{\sqrt{2}}.$$

Corollary 8.4. The modified first Revan index of the molecular graph of hydroxychloroquine is

$${}^m R_1(H) = \frac{37}{5}.$$

In the following theorem, we compute the general second Revan index of the molecular graph of hydroxychloroquine.

Theorem 9. The general second Revan index of the molecular graph of hydroxychloroquine is

$$R^a_2(H) = 2 \times 6^a + 2 \times 3^a + 6 \times 4^a + 12 \times 2^a + 2.$$

Proof: From definition and using Table 2, we derive

$$R_2^a(H) = \sum_{uv \in E(H)} \left[r_H(u) r_H(v)\right]^a$$
$$= 2(3 \times 2)^a + 2(3 \times 1)^a + 6(2 \times 2)^a + 12(2 \times 1)^a + 2(1 \times 1)^a$$
$$= 2 \times 6^a + 2 \times 3^a + 6 \times 4^a + 12 \times 2^a + 2.$$

We obtain the following results by using Theorem 9.

Corollary 9.1. The second Revan index of the molecular graph of hydroxychloroquine is

$$R_2(H) = 68.$$

Corollary 9.2. The second hyper Revan index of the molecular graph of hydroxychloroquine is

$$HR_2(H) = 236.$$

Corollary 9.3. The product connectivity Revan index of the molecular graph of hydroxychloroquine is

$$PR(H) = 5 + \frac{2}{\sqrt{6}} + \frac{2}{\sqrt{3}} + \frac{12}{\sqrt{2}}.$$

Corollary 9.4. The modified second Revan index of the molecular graph of hydroxychloroquine is

$${}^m R_2(H) = \frac{21}{2}.$$

In the following theorem, we determine the F-Revan index of the molecular graph of hydroxychloroquine.

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

$FR(H) = 158.$

Proof: Using definition and using Table 2, we deduce

$$FR(H) = \sum_{uv \in E(H)} \left[r_H(u)^2 + r_H(v)^2 \right]$$
$$= 2(3^2 + 2^2) + 2(3^2 + 1^2) + 6(2^2 + 2^2) + 12(2^2 + 1^2) + 2(1^2 + 1^2)$$
$$= 158.$$

In the next theorem, we compute the atom bond connectivity Revan index of the molecular graph of hydroxychloroquine.

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

$$ABCR(H) = \frac{20}{\sqrt{2}} + \frac{2\sqrt{2}}{\sqrt{3}}.$$

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

$$ABCR(H) = \sum_{uv \in E(H)} \sqrt{\frac{d_H(u) + d_H(v) - 2}{d_H(u)d_H(v)}}$$
$$= 2\sqrt{\frac{3+2-2}{3\times 2}} + 2\sqrt{\frac{3+1-2}{3\times 1}} + 6\sqrt{\frac{2+2-2}{2\times 2}} + 12\sqrt{\frac{2+1-2}{2\times 1}} + 2\sqrt{\frac{1+1-2}{1\times 1}}$$
$$= \frac{20}{\sqrt{2}} + \frac{2\sqrt{2}}{\sqrt{3}}.$$

In the following theorem, we compute geometric-arithmetic Revan index of the molecular graph of hydroxychloroquine.

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

$$GAR(H) = \frac{4\sqrt{6}}{5} + \sqrt{3} + 8\sqrt{2} + 8.$$

Proof: Using definition and using Table 2, we derive

$$GAR(H) = \sum_{uv \in E(H)} \frac{2\sqrt{r_H(u)r_H(v)}}{r_H(u) + r_H(v)}$$
$$= 2\left(\frac{2\sqrt{3\times 2}}{3+2}\right) + 2\left(\frac{2\sqrt{3\times 1}}{3+1}\right) + 6\left(\frac{2\sqrt{2\times 2}}{2+2}\right) + 12\left(\frac{2\sqrt{2\times 1}}{2+1}\right) + 2\left(\frac{2\sqrt{1\times 1}}{1+1}\right)$$
$$= \frac{4\sqrt{6}}{5} + \sqrt{3} + 8\sqrt{2} + 8.$$

In the following theorem, we compute the harmonic Revan index of the molecular graph of hydroxychloroquine.

Theorem 13. Let *H* be the molecular graph of hydroxychloroquine. Then

$$HR(H) = \frac{148}{10}.$$

Proof: Using definition and by using Table 2, we derive

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

$$= 2\left(\frac{2}{3+2}\right) + 2\left(\frac{2}{3+1}\right) + 6\left(\frac{2}{2+2}\right) + 12\left(\frac{2}{2+1}\right) + 2\left(\frac{2}{1+1}\right)$$
$$= \frac{148}{10}.$$

In the next theorem, we determine the symmetric division Revan index of the molecular graph of hydroxychloroquine.

Theorem 14. Let H be the molecular graph of hydroxychloroquine. Then

$$SDR(H) = \frac{171}{3}.$$

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

$$SDR(H) = \sum_{uv \in E(H)} \left(\frac{r_H(u)}{r_H(v)} + \frac{r_H(v)}{r_H(u)}\right)$$
$$= 2\left(\frac{3}{2} + \frac{2}{3}\right) + 2\left(\frac{3}{1} + \frac{1}{3}\right) + 6\left(\frac{2}{2} + \frac{2}{2}\right) + 12\left(\frac{2}{1} + \frac{1}{2}\right) + 2\left(\frac{1}{1} + \frac{1}{1}\right)$$
$$= \frac{171}{3}.$$

4. RESULTS AND DISCUSSION: REMDESIVIR

Let G be the molecular graph of remdesivir. This graph has 41 vertices and 44 edges.

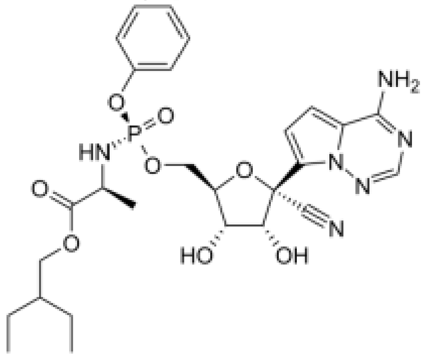

Figure 3

In G, the edge set of G can be divided into 8 partitions based on the degree of end vertices of each edge as follows:

$E_1 = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 2\}$, $|E_1| = 2$,
$E_2 = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 3\}$, $|E_2| = 5$,
$E_3 = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 4\}$, $|E_3| = 2$,
$E_4 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_4| = 9$,
$E_5 = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_5| = 14$.
$E_6 = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 4\}$, $|E_6| = 4$.
$E_7 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}$, $|E_7| = 6$.
$E_8 = \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 4\}$, $|E_8| = 2$.

The vertices of G are either of degree 1, 2, 3 or 4. Therefore $\Delta(G) = 4$, $\delta(G) = 1$. Thus $r_G(u) = \Delta(G) + \delta(G) - d_G(u) = 5 - d_G(u)$. In G, there are 8 types of Revan edges based on the Revan degree of end Revan vertices of each Revan edge as given in Table 3.

Table 3. Revan edge partition of G

$r_G(u), r_G(v)\backslash uv\in E(G)$	(4, 3)	(4, 2)	(4, 1)	(3, 3)	(3, 2)	(3, 1)	(2, 2)	(2, 1)
Number of edges	2	5	2	9	14	4	6	2

In the following theorem, we compute the general first Revan index of the molecular graph of remdesivir.

Theorem 15. The general first Revan index of the molecular graph of remdesivir G is

$$R^a_1(G) = 2 \times 7^a + 14 \times 6^a + 16 \times 5^a + 10 \times 4^a + 2 \times 3^a.$$

Proof: From definition and using Table 3, we deduce

$$R_1^a(G) = \sum_{uv\in E(G)} \left[r_G(u)+r_G(v)\right]^a$$
$$= 2(4 + 3)^a + 5(4 + 2)^a + 2(4 + 1)^a + 9(3 + 3)^a + 14(3 + 2)^a + 4(3 + 1)^a + 6(2 + 2)^a + 2(2 + 1)^a$$
$$= 2 \times 7^a + 14 \times 6^a + 16 \times 5^a + 10 \times 4^a + 2 \times 3^a.$$

We obtain the following results from Theorem 15.

Corollary 15.1. The first Revan index of the molecular graph of remdesivir is

$$R_1(G) = 224.$$

Corollary 15.2. The first hyper Revan index of the molecular graph of remdesivir is

$$HR_1(G) = 1180.$$

Corollary 15.3. The sum connectivity Revan index of the molecular graph of remdesivir is

$$SR(G) = \frac{2}{\sqrt{7}} + \frac{14}{\sqrt{6}} + \frac{16}{\sqrt{5}} + \frac{10}{\sqrt{4}} + \frac{2}{\sqrt{3}}.$$

Corollary 15.4. The modified first Revan index of the molecular graph of remdesivir is

$$^{m}R_1(G) = \frac{629}{70}.$$

In the following theorem, we determine the general second Revan index of the molecular graph of remdesivir.

Theorem 16. The general second Revan index of the molecular graph of remdesivir G is given by

$$R^a_2(G) = 2 \times 12^a + 5 \times 8^a + 9 \times 9^a + 14 \times 6^a + 8 \times 4^a + 4 \times 3^a + 2 \times 2^a.$$

Proof: Using definition and Table 3, we derive

$$R_2^a(G) = \sum_{uv\in E(G)} \left[r_G(u)+r_G(v)\right]^a$$
$$= 2(4 \times 3)^a + 5(4 \times 2)^a + 2(4 \times 1)^a + 9(3 \times 3)^a + 14(3 \times 2)^a + 4(3 \times 1)^a + 6(2 \times 2)^a + 2(2 \times 1)^a$$
$$= 2 \times 12^a + 5 \times 8^a + 9 \times 9^a + 14 \times 6^a + 8 \times 4^a + 4 \times 3^a + 2 \times 2^a.$$

We establish the following results from Theorem 16.

Corollary 16.1. The second Revan index of the molecular graph of remdesivir is

$$R_2(G) = 277.$$

Corollary 16.2. The second hyper Revan index of the molecular graph of remdesivir is

$$HR_2(G) = 2013.$$

Corollary 16.3. The product connectivity Revan index of the molecular graph of remdesivir is

$$PR(G) = 7 + \frac{5}{\sqrt{8}} + \frac{14}{\sqrt{6}} + \frac{5}{\sqrt{3}} + \frac{2}{\sqrt{2}}.$$

Corollary 16.4. The modified second Revan index of the molecular graph of remdesivir is

$$^{m}R_2(G) = \frac{191}{24}.$$

In the following theorem, we compute the F-Revan index of the molecular graph of remdesivir.

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

$$FR(G) = 626.$$

Proof: From definition and using Table 3, we have

$$FR(G)=\sum_{uv\in E(G)}\left[r_G(u)^2+r_G(v)^2\right]$$
$$= 2(4^2 + 3^2)+5(4^2 + 2^2)+2(4^2 + 1^2)+9(3^2 + 3^2)+14(3^2 + 2^2) + 4(3^2 + 1^2) + 6(2^2 + 2^2) + 2(2^2 + 1^2)$$
$$= 626.$$

In the next theorem, we determine the atom bond connectivity Revan index of the molecular graph of remdesivir.

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

$$ABCR(G)=6+\sqrt{\frac{5}{3}}+4\sqrt{\frac{2}{3}}+\frac{27}{\sqrt{2}}+\sqrt{3}.$$

Proof: By using definition and Table 3, we deduce

$$ABCR(G)=\sum_{uv\in E(G)}\sqrt{\frac{r_G(u)+r_G(v)-2}{r_G(u)r_G(v)}}$$
$$=2\sqrt{\frac{4+3-2}{4\times 3}}+5\sqrt{\frac{4+2-2}{4\times 2}}+2\sqrt{\frac{4+1-2}{4\times 1}}+9\sqrt{\frac{3+3-2}{3\times 3}}$$
$$+14\sqrt{\frac{3+2-2}{3\times 2}}+4\sqrt{\frac{3+1-2}{3\times 1}}+6\sqrt{\frac{2+2-2}{2\times 2}}+2\sqrt{\frac{2+1-2}{2\times 1}}$$
$$=6+\sqrt{\frac{5}{3}}+4\sqrt{\frac{2}{3}}+\frac{27}{\sqrt{2}}+\sqrt{3}.$$

In the following theorem, we compute the geometric-arithmetic Revan index of the molecular graph of remdesivir.

Theorem 19. Let G be the molecular graph of remdesivir. Then

$$GAR(G)=\frac{8\sqrt{3}}{7}+\frac{28\sqrt{6}}{5}+\frac{83}{3}+\frac{14\sqrt{2}}{3}+2\sqrt{3}.$$

Proof: Using definition and using Table 3, we derive

$$GAR(G)=\sum_{uv\in E(G)}\frac{2\sqrt{r_G(u)r_G(v)}}{r_G(u)+r_G(v)}$$
$$=2\left(\frac{2\sqrt{4\times 3}}{4+3}\right)+5\left(\frac{2\sqrt{4\times 2}}{4+2}\right)+2\left(\frac{2\sqrt{4\times 1}}{4+1}\right)+9\left(\frac{2\sqrt{3\times 3}}{3+3}\right)$$
$$+14\left(\frac{2\sqrt{3\times 2}}{3+2}\right)+4\left(\frac{2\sqrt{3\times 1}}{3+1}\right)+6\left(\frac{2\sqrt{2\times 2}}{2+2}\right)+2\left(\frac{2\sqrt{2\times 1}}{2+1}\right)$$
$$=\frac{8\sqrt{3}}{7}+\frac{28\sqrt{6}}{5}+\frac{83}{3}+\frac{14\sqrt{2}}{3}+2\sqrt{3}.$$

In the following theorem, we determine the harmonic Revan index of the molecular graph of remdesivir.

Theorem 20. Let G be the molecular graph of remdesivir. Then

$$HR(G)=\frac{629}{35}.$$

Proof: From definition and by using Table 3, we have

$$HR(G)=\sum_{uv\in E(G)}\frac{2}{r_G(u)+r_G(v)}$$
$$=2\left(\frac{2}{4+3}\right)+5\left(\frac{2}{4+2}\right)+2\left(\frac{2}{4+1}\right)+9\left(\frac{2}{3+3}\right)+14\left(\frac{2}{3+2}\right)+4\left(\frac{2}{3+1}\right)+6\left(\frac{2}{2+2}\right)+2\left(\frac{2}{2+1}\right)$$
$$=\frac{629}{35}.$$

In the next theorem, we compute the symmetric division Revan index of the molecular graph of remdesivir.

Theorem 21. Let G be the molecular graph of remdesivir. Then

$$SDR(G)=\frac{623}{6}.$$

Proof: Using definition and Table 3, we deduce

$$SDR(G)=\sum_{uv\in E(G)}\left(\frac{r_G(u)}{r_G(v)}+\frac{r_G(v)}{r_G(u)}\right)$$
$$=2\left(\frac{4}{3}+\frac{3}{4}\right)+5\left(\frac{4}{2}+\frac{2}{4}\right)+2\left(\frac{4}{1}+\frac{1}{4}\right)+9\left(\frac{3}{3}+\frac{3}{3}\right)+14\left(\frac{3}{2}+\frac{2}{3}\right)+4\left(\frac{3}{1}+\frac{1}{3}\right)+6\left(\frac{2}{2}+\frac{2}{2}\right)+2\left(\frac{2}{1}+\frac{1}{2}\right)$$
$$=\frac{623}{6}.$$

Remark : The minimum degree of the molecular structure of chloroquine (hydroxychloroquine or remdesivir) is 1. Thus every Revan index of the molecular structure of chloroquine (hydroxychloroquine or remdesivir) is the reverse index of the chloroquine (hydroxychloroquine or remdesivir).

5. CONCLUSION

In this study, the expressions of some Revan indices of chloroquine, hydroxychloroquine and remdesivir have been completed. In Medical Science, chemical, medical, biological, pharmaceutical properties of molecular structure are essential for drug design. These properties can be studied by the topological index calculation. In the view of this, our can be helpful in obtaining new drug and vaccine for the treatment and prevention of coronavirus disease-19

REFERENCES

[1] C. Huang, et al., Clinical features of patients infected with 2019 novel coronavirus in Wuhan, China, *The Lancet* 395, 10223, (2020) 497-506. doi: 10.1016/S0140-6736(20) 30183-5.
[2] J.S.Morse, T. Lalonde, S. Xu and W.R. Liu, Learning from the past: Possible urgent preventation and treatment options for severe acute respiratory infections caused by 2019 nCov. *ChemBioChem*, 21(5) (2020) 730-758. doi: 10.1002/cbic.202000047.
[3] J. Lung, et.al., The potential chemical structure of anit-SARS-CoV-2 RNA-dependent RNA polymerase, *J.Med.Virol.* (2020) 1-5. doi: 10.1002/jmv.25761.
[4] D. Wang, B. Hu, C He, et al, Clinical characteristics of 138 hospitalized patient with 2019 novel coronavirus infected pneumania in Wuhan, China, *JAMA* (2020). doi: 10.1001/jama.2020.1585.
[5] M. Wang, et al., Remdesivir and chloroquine effectively inhibit the recently emerged novel coronavirus (2019-nCoV) in vitro, *Cell Research*, 30 (2020) 269-271. doi:10.1038/s41422-020-0282-0.
[6] E. Schrenzenmeier and T. Dorner, Mechanisms of action of hydroxychloroquine and chloroquine implications of rheumatology, *Nat. Rev. Rheumatol*, 16 (2020) 155-166.

[7] D. Zhou, S.M. Dai and Q. Tongg, COVID-19: a recommendation to examine the effect of hydroxychloroquine in preventing infection and progression, *J. Antimicrob. Chemother*. (2020):dkaa 114, doi:10.1093/jac.dkaa114.

[8] X. Xu, et al., Evolution of the novel coronavirus from the ongoing Wuhan outbreak and modeling of its spike protein for risk of human transmission, *Sci. China Life Sci.* 63(3) (2020) 457-460. doi:10.1007/s 11427-020-1637-5.

[9] V.R.Kulli, K Banhatti indices of chloroquine and hydroxychloroquine: Research Applied for the treatment and prevention of COVID-19, *SSRG International Journal of Applied Chemistry*, 7(1) (2020) 63-68

[10] V.R.Kulli, Research in applied applications of neighborhood Dakshayani indices of two chemical structures in COVID-19, submitted.

[11] D. Plantone and T. Koudriavtseva, Current and future use of chloroquine and hydroxychloroquine in infections, immune, Neoplastic and Neurological disease: A Mini-Review, *Clin Drug Investing*, 38(8) (2018) 653-671. doi: 10.1007/s40261-018-4056-y (PubMed: 29737455).

[12] FDA: Emergency Use Authorization Information (Link).

[13] V.R.Kulli, B. Chaluvaraju and T.V. Asha, Multiplicative product connectivity and sum connectivity indices of chemical structures in drugs, *Research Review International Journal of Multidisciplinary*, 4(2) (2019) 949-953.

[14] I. Gutman and O.E. Polansky, *Mathematical Concepts in Organic Chemistry,* Springer, Berlin (1986).

[15] I. Gutman and N. Trinajstić, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Lett.* 17 (1972) 535-538.

[16] V.R.Kulli, Revan indices of oxide and honeycomb networks, *International Journal of Mathematics and its Applications*, 5(4-E) (2017) 663-667.

[17] V.R.Kulli, Hyper Revan indices and their polynomials of silicate networks, *International Journal of Current Research in Science and Technology*, 4(3) (2018) 17-21.

[18] V.R.Kulli, Computing the F-Revan and modified Revan indices of certain nanostructures, J. Comp. and Math. Sci. 9(10) (2018) 1326-1333.

[19] V.R.Kulli, The sum connectivity Revan index of silicate and hexagonal networks, *Annals of Pure and Applied Mathematics*, 14(3) (2017) 401-406.

[20] V.R. Kulli, On the product connectivity Revan index of certain nanotubes, *Journal of Computer and Mathematical Sciences,* 8(10) (2017) 562-567.

[21] V.R.Kulli, F-Revan index and R-Revan polynomial of some families of benzenoid systems, *Journal of Global Research in mathematical Archives*, 5(11) (2018) 1-6.