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Original Article

HDR Zagreb Indices of Remdesivir, Chloroquine, Hydroxychloroquine: Research for the Treatment of COVID-19

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Abstract - *In this paper, we obtain some topological properties of remdesivir, chloroquine, hydroxychloroquine used to inhibit the outbreak of COVID-19. We determine some HDR* Zagreb indices and their *polynomials for these three chemical drugs. In Chemical Science, chemical, biological, pharmaceutical properties of molecular structure are useful for drug design. These properties can be studied by topological index calculation. Considering this, our findings may be useful in obtaining new drugs and vaccines for the treatment of COVID-19.*

Keywords - *HDR Zagreb indices, Remdesivir, chloroquine, Hydroxychloroquine.*

Mathematics Subject Classification: 05*C*05, 05*C*07, 05*C*09.

I. INTRODUCTION

A molecular structure [1] 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 find some new drugs for diseases. A topological index is a numeric quantity from the structure of a molecular. In Chemical Science, the definition of the topological index on the molecular structure and corresponding chemical, pharmaceutical, biological properties of drugs can be studied for the topological index calculation [2].

Let G be a finite, simple, connected graph with the vertex set $V(G)$ and the edge set $E(G)$. The degree $d_G(u)$ of a vertex u is the number of vertices adjacent to u. The HDR vertex degree of a vertex u in G is $d_{hr}(u) = |\{u,v \in V(G)/\ d(u, v)= \lceil R/2 \rceil$, where $d(u, v)$ is the distance between the vertices u and v in $V(G)$ and R is the radius of G [3].

The HDR Zagreb index was introduced by Alsinai et al. in [3], and it is defined as

$$HDRM_1(G) = \sum_{uv\in E(G)} \left[d_{hr}(u) + d_{hr}(v)\right]$$

Now we call this index the first HDR Zagreb index.

We now introduce the second HDR Zagreb index of a graph G, and it is defined as

$$HDRM_2(G) = \sum_{uv\in E(G)} d_{hr}(u) d_{hr}(v)$$

Considering the HDR Zagreb indices, we define the first and second HDR Zagreb polynomials of a graph as:

$$HDRM_1(G,x) = \sum_{uv\in E(G)} x^{d_{hr}(u)+d_{hr}(v)},$$

$$HDRM_2(G,x) = \sum_{uv\in E(G)} x^{d_{hr}(u)d_{hr}(v)}.$$

Recently, some Zagreb polynomials were studied, for example, in [4, 5, 6, 7].

The hyper HDR Zagreb index was introduced by Alsinai et al. in [3], and it is defined as

$$HDRHM_1(G) = \sum_{uv\in E(G)} \left[d_{hr}(u) + d_{hr}(v)\right]^2$$

Now we call this index the first hyper HDR Zagreb index.

We now introduce the second hyper HDR Zagreb index of a graph G, and it is defined as

$$HDRHM_2(G) = \sum_{uv\in E(G)} [d_{hr}(u) d_{hr}(v)]^2$$

Recently, some hyper Zagreb indices were studied, for example, in [8, 9, 10, 11].

Considering the hyper HDR Zagreb indices, we introduce the first and second hyper HDR Zagreb polynomials of a graph G, and they are defined as

$$HDRHM_1(G,x) = \sum_{uv\in E(G)} x^{\left[d_{hr}(u)+d_{hr}(v)\right]^2},$$

$$HDRHM_2(G,x) = \sum_{ue} x^{\left[d_{hr}(u)d_{hr}(v)\right]^2}.$$

We define the modified first and second HDR Zagreb indices as

$$^{m}HDRM_1(G) = \sum_{uv\in E(G)} \frac{1}{d_{hr}(u) + d_{hr}(v)},$$

$$^{m}HDRM_2(G) = \sum_{uv\in E(G)} \frac{1}{d_{hr}(u) d_{hr}(v)}.$$

Considering the modified first and second HDR Zagreb indices, we define the modified first and second HDR Zagreb polynomials as

$$^{m}HDRM_1(G,x)=\sum_{uv\in E(G)} x^{\frac{1}{d_{hr}(u)+d_{hr}(v)}},$$

$$^{m}HDRM_2(G,x)=\sum_{uv\in E(G)} x^{\frac{1}{d_{hr}(u)d_{hr}(v)}}.$$

We propose the sum connectivity HDR index and product connectivity HDR index, and they are defined as

$$SHDR(G)=\sum_{uv\in E(G)} \frac{1}{\sqrt{d_{hr}(u)+d_{hr}(v)}}$$

$$PHDR(G)=\sum_{uv\in E(G)} \frac{1}{\sqrt{d_{hr}(u)d_{hr}(v)}}$$

Recently, some connectivity indices were studied, for example, in [12, 13, 14, 15,16, 17].

Considering the sum connectivity HDR and product connectivity HDR indices, we define the sum connectivity HDR and product connectivity HDR polynomials of a graph as

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

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

We put forward the general first and second *HDR* indices of a graph *G*, and they are defined as

$$HDRM_1^a(G)=\sum_{uv\in E(G)} \left[d_{hr}(u)+d_{hr}(v)\right]^a,$$

$$HDRM_2^a(G)=\sum_{uv\in E(G)} \left[d_{hr}(u)d_{hr}(v)\right]^a.$$

Considering general first and second *HDR* indices, we define the general first and second HDR polynomials of a graph as

$$HDRM_1^a(G,x)=\sum_{uv\in E(G)} x^{\left[d_{hr}(u)+d_{hr}(v)\right]^a},$$

$$HDRM_2^a(G,x)=\sum_{uv\in E(G)} x^{\left[d_{hr}(u)d_{hr}(v)\right]^a},$$

Where *a* is a real number.

The harmonic HDR index of a graph *G* is defined as

$$HDRH_b(G)=\sum_{uv\in E(G)} \frac{2}{d_{hr}(u)+d_{hr}(v)}.$$

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

$$HDRH_b(G,x)=\sum_{uv\in E(G)} x^{\frac{2}{d_{hr}(u)+d_{he}(v)}}.$$

The symmetric division HDR index of a graph *G* is defined as

$$SDHDR(G)=\sum_{uv\in E(G)} \left(\frac{d_{hr}(u)}{d_{hr}(v)}+\frac{d_{hr}(v)}{d_{hr}(u)}\right)$$

Considering the symmetric division HDR index, we define the symmetric division HDR polynomial of a graph *G* as

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

Coronavirus disease started in Wuhan, China [18] in December 2019. There are some antiviral agents, and these were studied in [19, 20, 21, 22, 23, 24]. In this study, we consider three antiviral agents such as remdesivir, chloroquine and hydroxychloroquine. Remdesivir and chloroquine effectively inhibit the recently emerged novel coronavirus (2019-nCOV) in vitro [19]. Chloroquine is a medication primarily used to treat malaria. Chloroquine and its derivative hydroxychloroquine have since then been repurposed for the treatment of a number of other conditions, including HIV, systemic lupus erythmatosus and rheumatoid arthritis [24]. Due to COVID-19, the FDA has issued an emergency use authorization for hydroxychloroquine and chloroquine [25].

In this paper, some HDR Zagreb indices and their polynomials of remdesivir, chloroquine, hydroxychloroquine are determined.

II. RESULTS AND DISCUSSION: REMDESIVIR

Let *R* be the molecular structure of remdesivir. Clearly, *R* has 41 vertices and 44 edges. See Fig. 1.

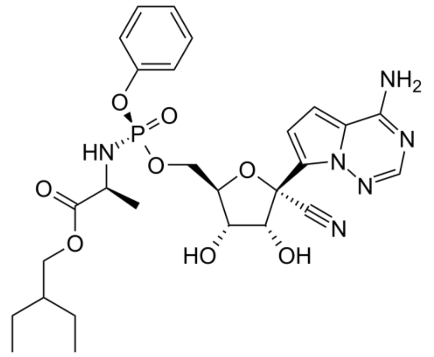

Fig. 1

In *R*, the edge set of *R* can be divided into 12 partitions using HDR vertex degree of end vertices of each edge, as given in Table 1.

Table 1. Edge partition of *R*

$d_{hr}(u), d_{hr}(v) \setminus uv \in E(R)$	Number of edges
(1, 2)	7
(1, 3)	5
(2, 2)	2
(2, 3)	8
(3, 3)	4
(3, 5)	3
(3, 4)	4
(4, 5)	4
(5, 5)	3
(5, 6)	2
(5, 7)	1
(6, 7)	1

Theorem 1. Let R be the molecular graph of remdesivir. Then

$$HDRM_1^a(R) = 7\times3^a+7\times4^a+10\times4^a+8\times5^a+4\times6^a+3\times8^a +4\times7^a+4\times9^a+3\times10^a+2\times11^a+12^a+13^a \qquad (1)$$

Proof: From the definition and using Table 1, we deduce

$$HDRM_1^a(R) = \sum_{uv\in E(R)} \left[d_{hr}(u)+d_{hr}(v)\right]^a$$

$$=7(1+2)^a+5(1+3)^a+2(2+2)^a+8(2+3)^a +4(3+3)^a+3(3+5)^a+4(3+4)^a+4(4+5)^a +3(5+5)^a+2(5+6)^a+1(5+7)^a+1(6+7)^a$$

gives the desired result.

From Theorem 1, we establish the following results.

Corollary 1.1. The first *HDR* Zagreb index of the molecular structure of remdesivir is

$$HDRM_1(R) = 278.$$

Corollary 1.2. The first hyper *HDR* Zagreb index of the molecular structure of remdesivir is

$$HDRHM_1(R) = 2086.$$

Corollary 1.3. The first modified HDR Zagreb index of the molecular structure of remdesivir is

$${}^mHDRM_1(R) = 8.38294760795.$$

Corollary 1.4. The sum connectivity *HDR* index of the molecular structure of remdesivir is

$$SHDR(R) = 18.7757364272.$$

Proof: Put a = 1, 2, – 1, – ½ in equation (1), we get the desired results.

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

Theorem 2. Let R be the molecular structure of remdesivir. Then

$$HDRM_1^a(\mathrm{R},x) = 7x^{3^a}+7x^{4^a}+8x^{5^a}+4x^{6^a}+3x^{8^a} +4x^{7^a}+4x^{9^a}+3x^{10^a}+2x^{11^a}+x^{12^a}+x^{13^a}. \qquad (2)$$

Proof: From the definition and by using Table 1, we deduce

$$HDRM_1^a(R,x) = \sum_{uv\in E(R)} x^{\left[d_{hr}(u)+d_{hr}(v)\right]^a}$$

$$=7x^{(1+2)^a}+5x^{(1+3)^a}+2x^{(2+2)^a}+8x^{(2+3)^a} +4x^{(3+3)^a}+3x^{(3+5)^a}+4x^{(3+4)^a}+4x^{(4+5)^a} +3x^{(5+5)^a}+2x^{(5+6)^a}+x^{(5+7)^a}+x^{(6+7)^a}$$

After simplification, we get the desired result.

We get the following results from Theorem 2.

Corollary 2.1. The first HDR Zagreb polynomial of the molecular structure of remdesivir is

$$HDRM_1(R,x) = 7x^3+7x^4+8x^5+4x^6+3x^8 +4x^7+4x^9+3x^{10}+2x^{11}+x^{12}+x^{13}$$

Corollary 2.2. The first hyper HDR Zagreb polynomial of the molecular structure of remdesivir is

$$HDRHM_1(R,x) = 7x^9+7x^{16}+8x^{25}+4x^{36}+3x^{64} +4x^{49}+4x^{81}+3x^{10}+2x^{121}+x^{144}+x^{169}$$

Corollary 2.3. The modified first HDR Zagreb polynomial of the molecular structure of remdesivir is

$${}^mHDRM_1(R,x) = 7x^{\frac{1}{3}}+7x^{\frac{1}{4}}+8x^{\frac{1}{5}}+4x^{\frac{1}{6}}+3x^{\frac{1}{8}} +4x^{\frac{1}{7}}+4x^{\frac{1}{9}}+3x^{\frac{1}{10}}+2x^{\frac{1}{11}}+x^{\frac{1}{12}}+x^{\frac{1}{13}}$$

Corollary 2.4. The sum connectivity HDR polynomial of the molecular structure of remdesivir is

$$SHDR(R,x) = 7x^{\frac{1}{\sqrt{3}}}+7x^{\frac{1}{2}}+8x^{\frac{1}{\sqrt{5}}}+4x^{\frac{1}{\sqrt{6}}}+3x^{\frac{1}{\sqrt{8}}} +4x^{\frac{1}{\sqrt{7}}}+4x^{\frac{1}{3}}+3x^{\frac{1}{\sqrt{10}}}+2x^{\frac{1}{\sqrt{11}}}+x^{\frac{1}{\sqrt{12}}}+x^{\frac{1}{\sqrt{13}}}$$

Proof: Put a = 1, 2, – 1, – ½ in equation (2), we establish the desired results.

Theorem 3. Let R be the molecular graph of remdesivir. Then

$$HDRM_2^a(R) = 7\times2^a+5\times3^a+2\times4^a+8\times6^a+4\times9^a+3\times15^a +4\times12^a+4\times20^a+3\times25^a+2\times30^a+35^a+42^a \qquad (3)$$

Proof: From the definition and using Table 1, we deduce

$$HDRM_2^a(R) = \sum_{uv\in E(R)} \left[d_{hr}(u)d_{hr}(v)\right]^a$$

$$=7(1\times2)^a+5(1\times3)^a+2(2\times2)^a+8(2\times3)^a +4(3\times3)^a+3(3\times5)^a+4(3\times4)^a+4(4\times5)^a +3(5\times5)^a+2(5\times6)^a+1(5\times7)^a+1(6\times7)^a$$

gives the desired result.

From Theorem 3, we establish the following results.

Corollary 3.1. The second *HDR* Zagreb index of the molecular structure of remdesivir is

$$HDRM_2(R) = 506.$$

Corollary 3.2. The second hyper *HDR* Zagreb index of the molecular structure of remdesivir is

$$HDRHM_2(R) = 10182.$$

Corollary 3.3. The second modified HDR Zagreb index of the molecular structure of remdesivir is

$$ {}^{m}HDRM_2(R) = 8.4168253968. $$

Corollary 3.4. The product connectivity *HDR* index of the molecular structure of remdesivir is

$$ PHDR(R) = 17.5480254425. $$

Proof: Put *a* = 1, 2, – 1, – ½ in equation (3), we get the desired results.

In the following theorem, we compute the general second HDR Zagreb polynomial of the molecular structure of remdesivir.

Theorem 4. Let *R* be the molecular structure of remdesivir. Then

$$ HDRM_2^a(\mathrm{R}, x) = 7x^{2^a} + 5x^{3^a} + 2x^{4^a} + 8x^{6^a} $$
$$ +4x^{9^a} + 3x^{15^a} + 4x^{12^a} + 4x^{20^a} $$
$$ +3x^{25^a} + 2x^{30^a} + x^{35^a} + x^{42^a} \qquad (4) $$

Proof: From the definition and by using Table 1, we deduce

$$ HDRM_2^a(R, x) = \sum_{uv \in E(R)} x^{\left[d_{hr}(u) d_{hr}(v)\right]^a} $$
$$ = 7x^{(1\times2)^a} + 5x^{(1\times3)^a} + 2x^{(2\times2)^a} + 8x^{(2\times3)^a} $$
$$ +4x^{(3\times3)^a} + 3x^{(3\times5)^a} + 4x^{(3\times4)^a} + 4x^{(4\times5)^a} $$
$$ +3x^{(5\times5)^a} + 2x^{(5\times6)^a} + x \times^{(5\times7)^a} + x^{(6\times7)^a} $$

After simplification, we get the desired result.

We get the following results from Theorem 4.

Corollary 4.1. The second HDR Zagreb polynomial of the molecular structure of remdesivir is

$$ HDRM_2(R, x) = 7x^2 + 5x^3 + 2x^4 + 8x^6 + 4x^9 $$
$$ +3x^{15} + 4x^{12} + 4x^{20} + 3x^{25} + 2x^{30} + x^{35} + x^{42} $$

Corollary 4.2. The second hyper HDR Zagreb polynomial of the molecular structure of remdesivir is

$$ HDRHM_2(R, x) = 7x^4 + 5x^9 + 2x^{16} + 8x^{36} $$
$$ +4x^{81} + 3x^{225} + 4x^{144} + 4x^{400} + 3x^{625} $$
$$ +3x^{625} + 2x^{900} + x^{1225} + x^{1764} $$

Corollary 4.3. The modified second HDR Zagreb polynomial of the molecular structure of remdesivir is

$$ {}^{m}HDRM_2(R, x) = 7x^{\frac{1}{3}} + 7x^{\frac{1}{4}} + 8x^{\frac{1}{5}} + 4x^{\frac{1}{6}} + 3x^{\frac{1}{8}} $$
$$ +4x^{\frac{1}{7}} + 4x^{\frac{1}{9}} + 3x^{\frac{1}{10}} + 2x^{\frac{1}{11}} + x^{\frac{1}{12}} + x^{\frac{1}{13}} $$

Corollary 4.4. The product connectivity HDR polynomial of the molecular structure of remdesivir is

$$ PHDR(R, x) = 7x^{\frac{1}{\sqrt{3}}} + 7x^{\frac{1}{2}} + 8x^{\frac{1}{\sqrt{5}}} + 4x^{\frac{1}{\sqrt{6}}} + 3x^{\frac{1}{\sqrt{8}}} $$
$$ +4x^{\frac{1}{\sqrt{7}}} + 4x^{\frac{1}{3}} + 3x^{\frac{1}{\sqrt{10}}} + 2x^{\frac{1}{\sqrt{11}}} + x^{\frac{1}{\sqrt{12}}} + x^{\frac{1}{\sqrt{13}}} $$

Proof: Put *a* = 1, 2, – 1, – ½ in equation (4), we establish the desired results.

In the following theorem, we compute the harmonic HDR index and its polynomial of the molecular structure of remdesivir.

Theorem 5. Let *R* be the molecular structure of remdesivir. Then

$$ (i)\,\mathrm{HDR}\,H_b(R) = 16.765895216. $$

$$ \text{(ii) } HDRH_b(R, x) = 7x^{\frac{2}{3}} + 7x^{\frac{1}{2}} + 8x^{\frac{2}{5}} + 4x^{\frac{1}{3}} $$
$$ +3x^{\frac{1}{4}} + 4x^{\frac{2}{7}} + 4x^{\frac{2}{9}} + 8x^{\frac{2}{5}} $$
$$ +3x^{\frac{1}{5}} + 2x^{\frac{2}{11}} + x^{\frac{1}{6}} + x^{\frac{2}{13}} $$

Proof: (i) Using definition and Table 1, we derive

$$ HDRH_b(R) = \sum_{uv \in E(R)} \frac{2}{d_{hr}(u) + d_{hr}(v)} $$
$$ = \frac{7\times2}{1+2} + \frac{5\times2}{1+3} + \frac{2\times2}{2+2} + \frac{8\times2}{2+3} + \frac{4\times2}{3+3} + \frac{3\times2}{3+5} $$
$$ + \frac{4\times2}{3+4} + \frac{4\times2}{4+5} + \frac{3\times2}{5+5} + \frac{2\times2}{5+6} + \frac{1\times2}{5+7} + \frac{1\times2}{6+7} $$

After simplification, we get the desired result.

(ii) Using definition and Table 1, we derive

$$ HDRH_b(R, x) = \sum_{ue} x^{\frac{2}{d_{hr}(u) + d_{hr}(v)}} $$
$$ = 7x^{\frac{2}{3}} + 7x^{\frac{1}{2}} + 8x^{\frac{2}{5}} + 4x^{\frac{1}{3}} + 3x^{\frac{1}{4}} + 4x^{\frac{2}{7}} $$
$$ +4x^{\frac{2}{9}} + 8x^{\frac{2}{5}} + 3x^{\frac{1}{5}} + 2x^{\frac{2}{11}} + x^{\frac{1}{6}} + x^{\frac{2}{13}} $$

gives the desired result.

In the following theorem, we determine the symmetric division HDR index and its polynomial of the molecular structure of remdesivir.

Theorem 6. Let *R* be the molecular structure of remdesivir. Then

$$ \text{(i)} \quad SDHDR(R) = 101.03809524. $$

$$ \text{(ii)} \quad SDHDR(R, x) = 7x^{\frac{5}{2}} + 5x^{\frac{10}{3}} + 9x^2 + 8x^{\frac{13}{6}} $$
$$ +3x^{\frac{34}{15}} + 2x^{\frac{31}{60}} + x^{\frac{74}{35}} + x^{\frac{85}{42}} $$

Proof: From the definition and by using Table 1, we deduce

$$ \text{(i)} \qquad SDHDR(R) = \sum_{uv \in E(R)} \left(\frac{d_{hr}(u)}{d_{hr}(v)} + \frac{d_{hr}(v)}{d_{hr}(u)} \right) $$
$$ = 7\left(\frac{1}{2} + \frac{2}{1}\right) + 5\left(\frac{1}{3} + \frac{3}{1}\right) + 2\left(\frac{2}{2} + \frac{2}{2}\right) + 8\left(\frac{2}{3} + \frac{3}{2}\right) $$
$$ +4\left(\frac{3}{3} + \frac{3}{3}\right) + 3\left(\frac{3}{5} + \frac{5}{3}\right) + 4\left(\frac{3}{4} + \frac{4}{3}\right) + 4\left(\frac{4}{5} + \frac{5}{4}\right) $$
$$ +3\left(\frac{5}{5} + \frac{5}{5}\right) + 2\left(\frac{5}{6} + \frac{6}{5}\right) + 1\left(\frac{5}{7} + \frac{7}{5}\right) + 1\left(\frac{6}{7} + \frac{7}{6}\right) $$

After simplification, we get the desired result.

$$ (ii) SDHDR(R, x) = \sum_{uv \in E(R)} x^{\frac{d_{hr}(u)}{d_{hr}(v)} + \frac{d_{hr}(v)}{d_{hr}(u)}} $$

$$= 7x^{\left(\frac{1}{2}+\frac{2}{1}\right)} + 5x^{\left(\frac{1}{3}+\frac{3}{1}\right)} + 2x^{\left(\frac{2}{2}+\frac{2}{2}\right)} + 8x^{\left(\frac{2}{3}+\frac{3}{2}\right)}$$
$$+4x^{\left(\frac{3}{4}+\frac{4}{3}\right)} + 4x^{\left(\frac{4}{5}+\frac{5}{4}\right)} + 3x^{\left(\frac{5}{5}+\frac{5}{5}\right)} + 2x^{\left(\frac{5}{6}+\frac{6}{5}\right)}$$
$$+x^{\left(\frac{5}{7}+\frac{7}{5}\right)} + x^{\left(\frac{6}{7}+\frac{7}{6}\right)}$$

After simplification, we get the desired result.

III. RESULTS AND DISCUSSION: CHLOROQUINE

Let G be the molecular structure of chloroquine. Clearly, G has 21 vertices and 23 edges. See Fig. 2.

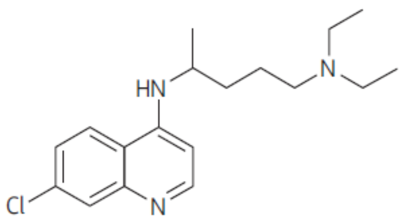

Fig. 2

In G, the edge set $E(G)$ can be divided into 7 partitions using HDR vertex degree of end vertices of each edge as given in Table 2.

Table 2. Edge partition of *G*

$d_{hr}(u), d_{hr}(v) \setminus uv \in E(G)$	Number of edges
(2, 3)	2
(3, 4)	7
(3, 5)	5
(3, 3)	2
(4, 4)	2
(1, 2)	3
(1, 1)	2

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

$$HDRM_1^a(G) = 2\times5^a+7\times7^a+7\times8^a+2\times6^a+3\times3^a+2\times2^a \quad (5)$$

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

$$HDRM_1^a(G) = \sum_{uv\in E(G)} \left[d_{hr}(u)+d_{hr}(v)\right]^a$$
$$=2(2+3)^a+7(3+4)^a+5(3+5)^a+2(3+3)^a$$
$$+2(4+4)^a+3(1+2)^a+2(1+1)^a$$

gives the desired result.

From Theorem 7, we establish the following results.

Corollary 7.1. The first *HDR* Zagreb index of the molecular structure of chloroquine is

$$HDRM_1(G) = 140.$$

Corollary 7.2. The first hyper *HDR* Zagreb index of the molecular structure of chloroquine is

$$HDRHM_1(G) = 820.$$

Corollary 7.3. The first modified HDR Zagreb index of the molecular structure of chloroquine is

$$^{m}HDRM_1(G) = \frac{193}{120}.$$

Corollary 7.4. The sum connectivity *HDR* index of the molecular structure of chloroquine is

$$SHDR(G) = 9.97781318709.$$

Proof: Put a = 1, 2, – 1, – ½ in equation (5), we get the desired results.

In the following theorem, we compute the general first HDR Zagreb polynomial of the molecular structure of chloroquine.

Theorem 8. Let G be the molecular structure of chloroquine. Then

$$HDRM_1^a(G,x) = 2x^{5^a} + 7x^{7^a} + 7x^{8^a}$$
$$+2x^{6^a} + 3x^{3^a} + 2x^{2^a} \quad (6)$$

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

$$HDRM_1^a(G,x) = \sum_{uv\in E(G)} x^{\left[d_{hr}(u)+d_{hr}(v)\right]^a}$$
$$= 2x^{(2+3)^a} + 7x^{(3+4)^a} + 5x^{(3+5)^a} + 2x^{(3+3)^a}$$
$$+2x^{(4+4)^a} + 3x^{(1+2)^a} + 2x^{(1+1)^a}$$

After simplification, we get the desired result.

We get the following results from Theorem 8.

Corollary 8.1. The first HDR Zagreb polynomial of the molecular structure of chloroquine is

$$HDRM_1(G,x) = 2x^5 + 7x^7 + 7x^8 + 2x^6$$
$$+3x^3 + 2x^2$$

Corollary 8.2. The first hyper HDR Zagreb polynomial of the molecular structure of chloroquine is

$$HDRM_1(G,x) = 2x^{25} + 7x^{49} + 7x^{64} + 2x^{36}$$
$$+3x^9 + 2x^4$$

Corollary 8.3. The modified first HDR Zagreb polynomial of the molecular structure of chloroquine is

$$^{m}HDRM_1(G,x) = 2x^{\frac{1}{5}} + 7x^{\frac{1}{7}} + 5x^{\frac{1}{8}} + 2x^{\frac{1}{6}}$$
$$+3x^{\frac{1}{3}} + 2x^{\frac{1}{2}}.$$

Corollary 8.4. The sum connectivity HDR polynomial of the molecular structure of remdesivir is

$$SHDRM(R,x) = 2x^{\frac{1}{\sqrt{5}}} + 7x^{\frac{1}{\sqrt{7}}} + 7x^{\frac{1}{\sqrt{8}}} + 2x^{\frac{1}{\sqrt{6}}}$$
$$+3x^{\frac{1}{\sqrt{3}}} + 2x^{\frac{1}{\sqrt{2}}}$$

Proof: Put a = 1, 2, – 1, – ½ in equation (6), we establish the desired results.

Theorem 9. Let G be the molecular graph of chloroquine. Then

$$HDRM_2^a(G) = 2\times6^a+7\times12^a+5\times15^a+2\times9^a$$

$+2\times16^a + 3\times2^a + 2\times1^a$ (7)

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

$$HDRM_2^a(G) = \sum_{uv\in E(G)} \left[d_{hr}(u)d_{hr}(v)\right]^a$$

$=2(2\times3)^a+7(3\times4)^a+5(3\times5)^a+2(3\times3)^a$
$+2(4\times4)^a+3(1\times2)^a+2(1\times1)^a$

gives the desired result.

From Theorem 9, we establish the following results.

Corollary 9.1. The second *HDR* Zagreb index of the molecular structure of chloroquine is

$$HDRM_2(G) = 229.$$

Corollary 9.2. The second hyper *HDR* Zagreb index of the molecular structure of chloroquine is

$$HDRHM_2(G) = 2893.$$

Corollary 9.3. The second modified HDR Zagreb index of the molecular structure of chloroquine is

$${}^m HDRM_2(G) = \frac{367}{72}.$$

Corollary 9.4. The product connectivity *HDR* index of the molecular structure of chloroquine is

$$PHDR(G) = 9.41620398205.$$

Proof: Put a = 1, 2, – 1, – ½ in equation (7), we get the desired results.

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

Theorem 10. Let G be the molecular structure of chloroquine. Then

$$HDRM_2^a(G,x) = 2x^{6^a} + 7x^{12^a} + 5x^{15^a} + 2x^{9^a} + 2x^{16^a} + 3x^{2^a} + 2x^{1^a} \quad (8)$$

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

$$HDRM_2^a(G,x) = \sum_{uv\in E(G)} x^{\left[d_{hr}(u)d_{hr}(v)\right]^a}$$

$$= 2x^{(2\times3)^a} + 7x^{(3\times4)^a} + 5x^{(3\times5)^a} + 2x^{(3\times3)^a} + 2x^{(4\times4)^a} + 3x^{(1\times2)^a} + 2x^{(1\times1)^a}$$

After simplification, we get the desired result.

We get the following results from Theorem 10.

Corollary 10.1. The second HDR Zagreb polynomial of the molecular structure of chloroquine is

$$HDRM_1(G,x) = 2x^6 + 7x^{12} + 5x^{15} + 2x^9 + 2x^{16} + 3x^2 + 2x^1$$

Corollary 10.2. The second hyper HDR Zagreb polynomial of the molecular structure of chloroquine is

$$HDRM_2(G,x) = 2x^{36} + 7x^{144} + 5x^{225} + 2x^{81} + 2x^{196} + 3x^4 + 2x^1$$

Corollary 10.3. The modified second HDR Zagreb polynomial of the molecular structure of chloroquine is

$${}^m HDRM_1(R,x) = 2x^{\frac{5}{6}} + 5x^{\frac{8}{15}} + 2x^{\frac{11}{28}} + 9x^{\frac{1}{2}} + 14x^{\frac{11}{30}} + 4x^{\frac{7}{24}} + 6x^{\frac{2}{7}} + 2x^{\frac{17}{72}}.$$

Corollary 10.4. The sum connectivity HDR polynomial of the molecular structure of chloroquine is

$$SHDR(R,x) = 2x^{\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}} + 5x^{\frac{1}{\sqrt{3}}+\frac{1}{\sqrt{5}}} + 2x^{\frac{1}{2}+\frac{1}{\sqrt{7}}} + 9x + 14x^{\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{6}}} + 4x^{\frac{1}{\sqrt{6}}+\frac{1}{\sqrt{8}}} + 6x^{\frac{2}{\sqrt{7}}} + 2x^{\frac{1}{\sqrt{8}}+\frac{1}{3}}.$$

Proof: Put a = 1, 2, – 1, – ½ in equation (8), we establish the desired results.

In the following theorem, the harmonic HDR index and its polynomial of the molecular structure of chloroquine.

Theorem 11. Let G be the molecular structure of chloroquine. Then

(i) $\text{HDR}\,H_b(G) = \frac{553}{360}$

(ii) $\text{HDR}\,H_b(G,x) = 2x^{\frac{2}{5}} + 7x^{\frac{2}{7}} + 7x^{\frac{1}{4}} + 2x^{\frac{1}{3}} + 3x^{\frac{2}{3}} + 2x^1$

Proof: (i) From the definition and Table 2, we obtain

$$HDRH_b(G) = \sum_{uv\in E(G)} \frac{2}{d_{hr}(u) + d_{hr}(v)}$$

$$= \frac{2\times2}{2+3} + \frac{7\times2}{3+4} + \frac{5\times2}{3+5} + \frac{2\times2}{3+3} + \frac{2\times2}{4+4} + \frac{3\times2}{1+2} + \frac{2\times2}{1+1}$$

After simplification, we get the desired result.

(ii) From the definition and Table 2, we obtain

$$HDRH_b(G,x) = \sum_{ue} x^{\frac{2}{d_{hr}(u)+d_{hr}(v)}}$$

$$= 2x^{\frac{2}{2+3}} + 7x^{\frac{2}{3+4}} + 5x^{\frac{2}{3+5}} + 2x^{\frac{2}{3+3}} + 2x^{\frac{2}{4+4}} + 3x^{\frac{2}{1+2}} + 2x^{\frac{2}{1+1}}$$

gives the desired result.

In the following theorem, we compute the symmetric division HDR index and its polynomial of the molecular structure of chloroquine.

Theorem 12. Let G be the molecular structure of chloroquine. Then

(i) $SDHDR(G) = \frac{525}{12}$

(ii) $SDHDR(G,x) = 2x^{\frac{13}{6}} + 7x^{\frac{25}{12}} + 5x^{\frac{34}{15}} + 3x^{\frac{5}{2}} + 6x^2$

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

(i) $$SDHDR(G)=\sum_{uv\in E(G)}\left(\frac{d_{hr}(u)}{d_{hr}(v)}+\frac{d_{hr}(v)}{d_{hr}(u)}\right)$$

$$=2\left(\frac{2}{3}+\frac{3}{2}\right)+7\left(\frac{3}{4}+\frac{4}{3}\right)+5\left(\frac{3}{5}+\frac{5}{3}\right)+2\left(\frac{3}{3}+\frac{3}{3}\right)$$
$$+2\left(\frac{4}{4}+\frac{4}{4}\right)+3\left(\frac{1}{2}+\frac{2}{1}\right)+2\left(\frac{1}{1}+\frac{1}{1}\right)$$

gives the desired result.

$$(ii)SDHDR(G,x)=\sum_{uv\in E(G)}x^{\frac{d_{hr}(u)}{d_{hr}(v)}+\frac{d_{hr}(v)}{d_{hr}(u)}}$$
$$=2x^{\left(\frac{2}{3}+\frac{3}{2}\right)}+7x^{\left(\frac{3}{4}+\frac{4}{3}\right)}+5x^{\left(\frac{3}{5}+\frac{5}{3}\right)}+2x^{\left(\frac{3}{3}+\frac{3}{3}\right)}$$
$$+2x^{\left(\frac{4}{4}+\frac{4}{4}\right)}+3x^{\left(\frac{1}{2}+\frac{2}{1}\right)}+2x^{\left(\frac{1}{1}+\frac{1}{1}\right)}$$

After simplification, we get the desired result.

IV. RESULTS AND DISCUSSION: HYDROXYCHLOROQUINE

Let H be the graph of hydroxychloroquine. By calculation, H has 22vertices and 24 edges, see Fig. 3.

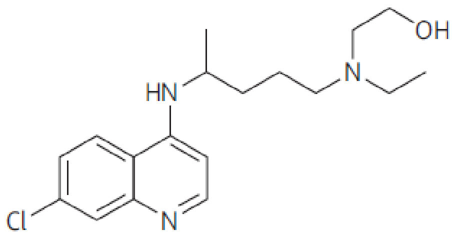

Fig. 3

The edge set of H can be divided into nine partitions using the HDR vertex degree of end vertices of each edge, as given in Table 3.

Table 3. Edge partition of H

$d_{hr}(u), d_{hr}(v) \setminus uv$ □ $E(H)$	Number of edges
(2, 3)	1
(3, 3)	3
(3, 4)	7
(3, 5)	5
(4, 4)	2
(1, 3)	1
(1, 2)	2
(2, 2)	2
(1, 1)	1

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

$$HDRM_1^a(H) = 5^a+3\times6^a+7\times7^a+5\times8^a+2\times8^a$$
$$+4^a+2\times3^a+2\times4^a+2^a \qquad (9)$$

Proof: From the definition and using Table 3, we deduce

$$HDRM_1^a(H)=\sum_{uv\in E(R)}\left[d_{hr}(u)+d_{hr}(v)\right]^a$$
$$=1(2+3)^a+3(3+3)^a+7(3+4)^a+5(3+5)^a+2(4+4)^a$$
$$+1(1+3)^a+2(1+2)^a+2(2+2)^a+1(1+1)^a$$

gives the desired result.

From Theorem 13, we establish the following results.

Corollary 13.1. The first *HDR* Zagreb index of the molecular structure of hydroxychloroquine is

$$HDRM_1(H)=148.$$

Corollary 13.2. The first hyper *HDR* Zagreb index of the molecular structure of hydroxychloroquine is

$$HDRHM_1(H)=994.$$

Corollary 13.3. The first modified HDR Zagreb index of the molecular structure of hydroxychloroquine is

$${}^{m}HDRM_1(H)=\frac{499}{120}.$$

Corollary 13.4. The sum connectivity HDR index of the molecular structure of hydroxychloroquine is

$$SHDR(H)=10.1543908317.$$

Proof: Put a = 1, 2, – 1, – ½ in equation (9), we get the desired results.

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

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

$$HDRM_1^a(H,x)=x^{5^a}+3x^{6^a}+7x^{7^a}+7x^{8^a}$$
$$+4x^{4^a}+2x^{3^a}+x^{2^a} \qquad (10)$$

Proof: From the definition and by using Table 3, we deduce

$$HDRM_1^a(H,x)=\sum_{uv\in E(H)}x^{\left[d_{hr}(u)+d_{hr}(v)\right]^a}$$
$$=1x^{(2+3)^a}+3x^{(3+3)^a}+7x^{(3+4)^a}+5x^{(3+5)^a}$$
$$+2x^{(4+4)^a}+1x^{(1+3)^a}+2x^{(1+2)^a}+2x^{(2+2)^a}$$
$$+1x^{(1+1)^a}$$

After simplification, we get the desired result.

We get the following results from Theorem 14.

Corollary 14.1. The first HDR Zagreb polynomial of the molecular structure of hydroxychloroquine is

$$HDRM_1(H,x)=x^5+3x^6+7x^7+7x^8$$
$$+3x^4+2x^3+x^2$$

Corollary 14.2. The first hyper HDR Zagreb polynomial of the molecular structure of hydroxychloroquine is

$$HDRHM_1(H,x)=x^{25}+3x^{36}+7x^{49}+7x^{64}$$
$$+3x^{16}+2x^9+x^4$$

Corollary 14.3. The modified first HDR Zagreb polynomial of the molecular structure of hydroxychloroquine is

$$ {}^{m}HDRM_1(H,x) = x^{\frac{1}{5}} + 3x^{\frac{1}{6}} + 7x^{\frac{1}{7}} + 7x^{\frac{1}{8}} + 3x^{\frac{1}{4}} + 2x^{\frac{1}{3}} + x^{\frac{1}{2}} $$

Corollary 14.4. The sum connectivity HDR polynomial of the molecular structure of remdesivir is

$$ SHDRM(H,x) = x^{\frac{1}{\sqrt{5}}} + 3x^{\frac{1}{\sqrt{6}}} + 7x^{\frac{1}{\sqrt{7}}} + 7x^{\frac{1}{\sqrt{8}}} + 3x^{\frac{1}{2}} + 2x^{\frac{1}{\sqrt{3}}} + x^{\frac{1}{\sqrt{2}}} $$

Proof: Put a = 1, 2, – 1, – ½ in equation (10), we establish the desired results.

Theorem 15. Let H be the molecular graph of hydroxychloroquine. Then

$$ HDRM_2^a(H) = 2\times6^a+7\times12^a+5\times15^a+2\times9^a +2\times16^a +3\times2^a+2\times1^a \qquad (11) $$

Proof: From the definition and using Table 3, we deduce

$$ HDRM_2^a(H) = \sum_{uv\in E(H)} \left[d_{hr}(u)d_{hr}(v)\right]^a $$
$$ =2(2\times3)^a+7(3\times4)^a+5(3\times5)^a+2(3\times3)^a +2(4\times4)^a+3(1\times2)^a+2(1\times1)^a $$

gives the desired result.

From Theorem 15, we establish the following results.

Corollary 15.1. The second *HDR* Zagreb index of the molecular structure of hydroxychloroquine is

$$ HDRM_2(H) = 229. $$

Corollary 15.2. The second hyper *HDR* Zagreb index of the molecular structure of hydroxychloroquine is

$$ HDRHM_2(H) = 2893. $$

Corollary 15.3. The second modified HDR Zagreb index of the molecular structure of hydroxychloroquine is

$$ {}^{m}HDRM_2(H) = 5.0972222222. $$

Corollary 15.4. The sum connectivity *HDR* index of the molecular structure of hydroxychloroquine is

$$ PHDR(H) = 9.41620398205. $$

Proof: Put a = 1, 2, – 1, – ½ in equation (11), we get the desired results.

In the following theorem, we compute the general second HDR Zagreb index and its polynomial of the molecular structure of hydroxychloroquine.

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

$$ HDRM_2^a(H,x) = 2x^{6^a} + 7x^{12^a} + 5x^{15^a} + 2x^{9^a} + 2x^{16^a} + 3x^{2^a} + 2x^{1^a} \qquad (12) $$

Proof: From the definition and by using Table 3, we deduce

$$ HDRM_2^a(H,x) = \sum_{uv\in E(H)} x^{\left[d_{hr}(u)d_{hr}(v)\right]^a} $$
$$ = 2x^{(2\times3)^a} + 7x^{(3\times4)^a} + 5x^{(3\times5)^a} + 2x^{(3\times3)^a} + 2x^{(4\times4)^a} + 3x^{(1\times2)^a} + 2x^{(1\times1)^a} $$

After simplification, we get the desired result.

We get the following results from Theorem 16.

Corollary 16.1. The second HDR Zagreb polynomial of the molecular structure of hydroxychloroquine is

$$ HDRM_1(H,x) = 2x^6 + 7x^{12} + 5x^{15} + 2x^9 + 2x^{16} + 3x^2 + 2x^1 $$

Corollary 16.2. The second hyper HDR Zagreb polynomial of the molecular structure of hydroxychloroquine is

$$ HDRM_2(H,x) = 2x^{36} + 7x^{144} + 5x^{225} + 2x^{81} + 2x^{196} + 3x^4 + 2x^1 $$

Corollary 16.3. The modified second HDR Zagreb polynomial of the molecular structure of hydroxychloroquine is

$$ {}^{m}HDRM_1(H,x) = 2x^{\frac{5}{6}} + 5x^{\frac{8}{15}} + 2x^{\frac{11}{28}} + 9x^{\frac{1}{2}} + 14x^{\frac{11}{30}} + 4x^{\frac{7}{24}} + 6x^{\frac{2}{7}} + 2x^{\frac{17}{72}}. $$

Corollary 16.4. The product connectivity HDR polynomial of the molecular structure of hydroxychloroquine is

$$ SHDR(H,x) = 2x^{\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}} + 5x^{\frac{1}{\sqrt{3}}+\frac{1}{\sqrt{5}}} + 2x^{\frac{1}{2}+\frac{1}{\sqrt{7}}} + 9x + 14x^{\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{6}}} + 4x^{\frac{1}{\sqrt{6}}+\frac{1}{\sqrt{8}}} + 6x^{\frac{2}{\sqrt{7}}} + 2x^{\frac{1}{\sqrt{8}}+\frac{1}{3}}. $$

Proof: Put a = 1, 2, – 1, – ½ in equation (12), we establish the desired results.

In the following theorem, the harmonic HDR index and its polynomial of the molecular structure of hydroxychloroquine.

Theorem 17. Let H be the molecular structure of hydroxychloroquine. Then

(i) HDR $H_b(H) = \frac{539}{360}$

(ii) HDR $H_b(H,x) = x^{\frac{2}{5}} + 3x^{\frac{1}{3}} + 7x^{\frac{2}{7}} + 7x^{\frac{1}{4}} + 3x^{\frac{1}{2}} + 2x^{\frac{2}{3}} + 2x^1$

Proof: (i) From the definition and Table 3, we obtain

$$ HDRH_b(H) = \sum_{uv\in E(H)} \frac{2}{d_{hr}(u)+d_{hr}(v)} $$
$$ = \frac{1\times2}{2+3} + \frac{3\times2}{3+3} + \frac{7\times2}{3+4} + \frac{5\times2}{3+5} + \frac{2\times2}{4+4} + \frac{1\times2}{1+3} + \frac{2\times2}{1+2} + \frac{2\times2}{2+2} + \frac{1\times2}{1+1} $$

After simplification, we get the desired result.

(ii) From the definition and Table 3, we obtain

$$HDRH_b(R,x)=\sum_{uv\in E(H)} x^{\frac{2}{d_{hr}(u)+d_{hr}(v)}}$$
$$=1x^{\frac{2}{2+3}}+3x^{\frac{2}{3+3}}+7x^{\frac{2}{3+4}}+5x^{\frac{2}{3+5}}+2x^{\frac{2}{4+4}}$$
$$+1x^{\frac{2}{1+3}}+2x^{\frac{2}{1+2}}+2x^{\frac{2}{2+2}}+2x^{\frac{2}{1+1}}$$

gives the desired result.

In the following theorem, we compute the symmetric division HDR index and its polynomial of the molecular structure of hydroxychloroquine.

Theorem 18. Let H be the molecular structure of chloroquine. Then

(i) $SDHDR(H)=\frac{653}{12}$

(ii) $SDHDR(H,x)=x^{\frac{13}{6}}+7x^{\frac{25}{12}}+5x^{\frac{34}{15}}+x^{\frac{10}{3}}$
$$+2x^{\frac{5}{2}}+8x^{2}$$

Proof: From the definition and by using Table 3, we deduce

(i) $$SDHDR(H)=\sum_{uv\in E(H)}\left(\frac{d_{hr}(u)}{d_{hr}(v)}+\frac{d_{hr}(v)}{d_{hr}(u)}\right)$$
$$=1\left(\frac{2}{3}+\frac{3}{2}\right)+3\left(\frac{3}{3}+\frac{3}{3}\right)+7\left(\frac{3}{4}+\frac{4}{3}\right)$$
$$+5\left(\frac{3}{5}+\frac{5}{3}\right)+2\left(\frac{4}{4}+\frac{4}{4}\right)+1\left(\frac{1}{3}+\frac{3}{1}\right)$$
$$+2\left(\frac{1}{2}+\frac{2}{1}\right)+2\left(\frac{2}{2}+\frac{2}{2}\right)+1\left(\frac{1}{1}+\frac{1}{1}\right)$$

gives the desired result.

$$(ii)SDHDR(H,x)=\sum_{uv\in E(H)} x^{\frac{d_{hr}(u)}{d_{hr}(v)}+\frac{d_{hr}(v)}{d_{hr}(u)}}$$
$$=1x^{\left(\frac{2}{3}+\frac{3}{2}\right)}+3x^{\left(\frac{3}{3}+\frac{3}{3}\right)}+7x^{\left(\frac{3}{4}+\frac{4}{3}\right)}+5x^{\left(\frac{3}{5}+\frac{5}{3}\right)}+2x^{\left(\frac{4}{4}+\frac{4}{4}\right)}$$
$$+1x^{\left(\frac{1}{3}+\frac{3}{1}\right)}+2x^{\left(\frac{1}{2}+\frac{2}{1}\right)}+2x^{\left(\frac{2}{2}+\frac{2}{2}\right)}+1x^{\left(\frac{1}{1}+\frac{1}{1}\right)}$$

After simplification, we get the desired result.

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