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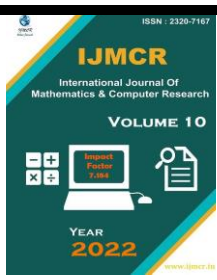

HDR-Nirmala Index

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ARTICLE INFO	ABSTRACT
Published Online: 06 July 2022 Corresponding Author: **V.R.Kulli**	In this paper, we introduce the HDR-Nirmala index and the HDR-Nirmala exponential of a graph. We compute the HDR-Nirmala index and its corresponding exponential of chloroquine, hydroxychloroquine and remdesivir. Also we establish some properties of newly defined the HDR-Nirmala index.

KEYWORDS: HDR-Nirmala index, chemical drug, graph.

I. INTRODUCTION

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*. We refer [1], for other undefined notations and terminologies.

In 1972 [2], two degree based topological indices were introduced and studied. We consider three antiviral compounds (agents) such as chloroquine, hydroxychloroquine and remdesivir. In the field of Medical Science, concerning the definition of the graphical index on the molecular structure and corresponding medical, chemical, biological, pharmaceutical properties of drugs can be studied for the graphical index calculation. A molecular structure 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 structure of a molecule.

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 as the first HDR Zagreb index. In [4], Kulli introduced the second HDR Zagreb index of a graph *G* and it is defined as

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

Recently, some HDR indices were studied, for example, in [5].

The Nirmala index was introduced by Kulli in [6] and defined it as

$$N(G) = \sum_{uv\in E(G)} \sqrt{d_G(u) + d_G(v)}.$$

Recently, some Nirmala indices were studied, for example, in [7, 8, 9, 10, 11, 12, 13, 14, 15, and 16].

Motivated by the definitions of the HDR index and Nirmala index, we introduce the HDR-Nirmala index of a graph and defined it as,

$$HDRN(G) = \sum_{uv\in E(G)} \sqrt{d_{hr}(u) + d_{hr}(v)}.$$

Considering the HDR Nirmala index, we introduce the HDR Nirmala exponential of a graph *G* and it is defined as

$$HDRN(G,x) = \sum_{uv\in E(G)} x^{\left[\left(d_{hr}(u)+d_{hr}(v)\right)\right]^{\frac{1}{2}}}.$$

In this paper, the HDR-Nirmala index and its corresponding exponential of chloroquine, hydroxychloroquine and rendesivir are computed. Also we obtain some properties of the HDR Nirmala index.

2. RESULTS AND DISCUSSION: CHLOROQUINE

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

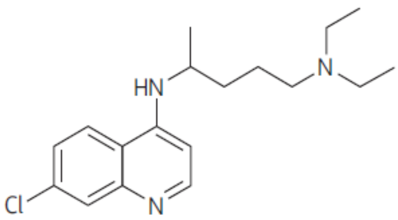

Figure 1. Graph of chloroquine

The edge set $E(G)$ can be divided into seven partitions using HDR vertex degree of end vertices of each edge as given in Table 1.

Table 1. 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

We compute the HDR Nirmala index of the molecular graph of chloroquine.

Theorem 1. Let G be the molecular graph of chloroquine. Then

$$HDRN(G) = 2\sqrt{5} + 7\sqrt{7} + 16\sqrt{2} + 2\sqrt{6} + 3\sqrt{3}.$$

Proof: Using definition and Table 1, we have

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

$$= 2\sqrt{2+3} + 7\sqrt{3+4} + 5\sqrt{3+5} + 2\sqrt{3+3}$$

$$+2\sqrt{4+4} + 3\sqrt{1+2} + 2\sqrt{1+1}.$$

After simplification, we obtain the desired result.

In Theorem 2, we determine the HDR Nirmala exponential of the molecular graph of chloroquine.

Theorem 2. Let G be the molecular graph of chloroquine. Then

$$HDRN(G,x) = 2x^{\sqrt{5}} + 7x^{\sqrt{7}} + 7x^{2\sqrt{2}}$$

$$+2x^{\sqrt{6}} + 3x^{\sqrt{3}} + 2x^{\sqrt{2}}.$$

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

$$HDRN(G,x) = \sum_{uv\in E(G)} x^{\left[\left(d_{hr}(u)+d_{hr}(v)\right)\right]^{\frac{1}{2}}}$$

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

$$+2x^{\sqrt{4+4}} + 3x^{\sqrt{1+2}} + 2x^{\sqrt{1+1}}.$$

Gives the desired result after simplification.

3. RESULTS AND DISCUSSION: HYDROXYCHLOROQUINE

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

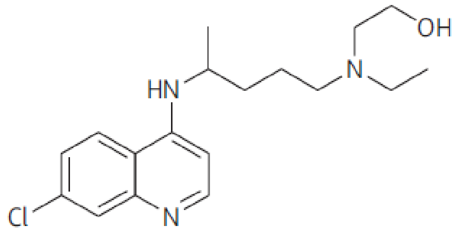

Figure 2. Graph of hydroxychloroquine

The edge set of H can be divided into nine partitions using HDR vertex degree of end vertices of each edge as given in Table 2.

Table 2. Edge partition of *H*

$d_{hr}(u), d_{hr}(v) \setminus uv \in E(H)$	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

In the following theorem, we determine the HDR Nirmala index of the molecular graph of hydroxychloroquine.

Theorem 3. Let H be the molecular graph of hydroxychloroquine. Then

$$HDRN(H) = 1\sqrt{5} + 3\sqrt{6} + 7\sqrt{7} + 15\sqrt{2} + 2\sqrt{3} + 6.$$

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

$$HDRN(H) = \sum_{uv\in E(H)} \sqrt{d_{hr}(u) + d_{hr}(v)}$$

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

$$+2\sqrt{4+4} + 1\sqrt{1+3} + 2\sqrt{1+2} + 2\sqrt{2+2} + 1\sqrt{1+1}$$

$$= 1\sqrt{5} + 3\sqrt{6} + 7\sqrt{7} + 5\sqrt{8} + 2\sqrt{8}$$

$$+1\sqrt{4} + 2\sqrt{3} + 2\sqrt{4} + 1\sqrt{2}.$$

After simplification, we get the desired result.

In the next theorem, we compute the HDR Nirmala exponential of the molecular graph of hydroxychloroquine.

Theorem 4. Let H be the molecular graph of hydroxychloroquine. Then

$$HDRN(H,x) = 1x^{\sqrt{5}} + 3x^{\sqrt{6}} + 7x^{\sqrt{7}}$$

$$+7x^{2\sqrt{2}}+3x^{2}+2x^{\sqrt{3}}+1x^{\sqrt{2}}$$

Proof: Using definition and using Table 2, we have

$$HDRN(H,x)=\sum_{uv\in E(H)} x^{\left[\left(d_{hr}(u)+d_{hr}(v)\right)\right]^{\frac{1}{2}}}$$

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

$$+1x^{\sqrt{1+3}}+2x^{\sqrt{1+2}}+2x^{\sqrt{2+2}}+1x^{\sqrt{1+1}}$$

After simplification, we obtain the desired result.

4. RESULTS AND DISCUSSION: REMDESIVIR

Let R be the molecular graph of remdesivir. Clearly R has 41 vertices and 44 edges, see Figure 3.

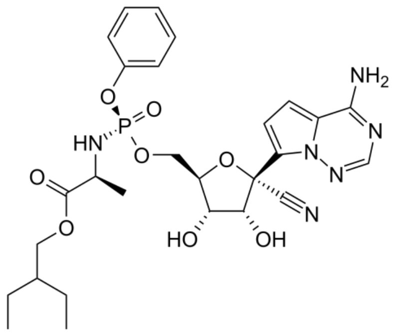

Figure 3. Graph of remdesivir

The edge set $E(R)$ can be divided into 12 partitions using HDR vertex degree of end vertices of each edge as given in Table 3.

Table 3. 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

In Theorem 5, we determine the HDR Nirmala index of the molecular graph of remdesivir.

Theorem 5. Let R be the molecular graph of remdesivir. Then

$$HDRN(R)=9\sqrt{3}+8\sqrt{5}+4\sqrt{6}+6\sqrt{2}+4\sqrt{7}$$

$$+3\sqrt{10}+2\sqrt{11}+1\sqrt{13}+26$$

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

$$HDRN(R)=\sum_{uv\in E(R)}\sqrt{d_{hr}(u)+d_{hr}(v)}$$

$$=7\sqrt{1+2}+5\sqrt{1+3}+2\sqrt{2+2}+8\sqrt{2+3}$$

$$+4\sqrt{3+3}+3\sqrt{3+5}+4\sqrt{3+4}+4\sqrt{4+5}$$

$$+3\sqrt{5+5}+2\sqrt{5+6}+1\sqrt{5+7}+1\sqrt{6+7}$$

$$=7\sqrt{3}+5\sqrt{4}+2\sqrt{4}+8\sqrt{5}+4\sqrt{6}+3\sqrt{8}+4\sqrt{7}$$

$$+4\sqrt{9}+3\sqrt{10}+2\sqrt{11}+1\sqrt{12}+1\sqrt{13}$$

Gives the desired result.

In the next theorem, we compute the HDR Nirmala exponential of the molecular graph of remdesivir.

Theorem 6. Let R be the molecular graph of remdesivir. Then

$$HDRN(R,x)=7x^{\sqrt{3}}+7x^{2}+8x^{\sqrt{5}}+4x^{\sqrt{6}}+3x^{2\sqrt{2}}$$

$$+4x^{\sqrt{7}}+4x^{3}+3x^{\sqrt{10}}+2x^{\sqrt{11}}+1x^{2\sqrt{3}}+x^{\sqrt{13}}$$

Proof: Using definition and Table 3, we have

$$HDRN(\mathrm{R},x)=\sum_{uv\in E(R)} x^{\left[\left(d_{hr}(u)+d_{hr}(v)\right)\right]^{\frac{1}{2}}}$$

$$=7x^{\sqrt{1+2}}+5x^{\sqrt{1+3}}+2x^{\sqrt{2+2}}+8x^{\sqrt{2+3}}+4x^{\sqrt{3+3}}$$

$$+3x^{\sqrt{3+5}}+4x^{\sqrt{3+4}}+4x^{\sqrt{4+5}}+3x^{\sqrt{5+5}}+2x^{\sqrt{5+6}}$$

$$+1x^{\sqrt{5+7}}+1x^{\sqrt{6+7}}$$

After simplification, we obtain the desired result.

5. PROPERTY OF THE HDR SOMBOR INDEX

Theorem 7. Let G be a connected graph with m edges. Then

$$HDRN(G)\leq\sqrt{mHDRM_1(G)}.$$

Proof: Using the Cauchy-Schwarz inequality, we obtain

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

$$\leq\sum_{uv\in E(G)}1\sum_{uv\in E(G)}\left(d_{hr}(u)+d_{hr}(v)\right).$$

$$=mHDRM_1(G).$$

Thus $\quad HDRN(G)\leq\sqrt{mHDRM_1(G)}.$

CONCLUSION

In this paper, a novel invariant is considered which is the HDR-Nirmala index. Also we have defined the HDR-Nirmala exponential of a molecular graph. Furthermore, the HDR-Nirmala index and its corresponding exponential for chloroquine, hydroxychloroquine, remdesivir are determined.

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