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# The HDR-Sombor Index

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***Abstract*** *- In this paper, we introduce the HDR-Sombor index and F-HDR index of a graph. We compute the HDR Sombor index and F-HDR index of chloroquine, hydroxychloroquine and remdesivir. Also we establish some properties of newly defined indices.*

***Keywords -*** *HDR-Somber index, F-HDR 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 Sombor index was introduced by Gutman in [6] and defined it as

$$SO(G) = \sum_{uv \in E(G)} \sqrt{d_G(u)^2 + d_G(v)^2}.$$

Recently, some Sombor indices were studied, for example, in [ 7].

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

$$HDRSO(G) = \sum_{uv \in E(G)} \sqrt{d_{hr}(u)^2 + d_{hr}(v)^2}.$$

The forgotten topological index of a graph is defined as [8]

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

The F-HDR index of a graph is defined as

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

We establish some properties of the HDR Sombor index. For more information about topological indices and polynomials see [10,11,12,13,14,15,16,17,18,19, 20].

In this paper, the HDR-Sombor and F-HDR indices of chloroquine, hydroxychloroquine and rendesivir are computed. We establish some properties of the HDR Sombor index.

## II. RESULTS AND DISCUSSION: CHLOROQUINE

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

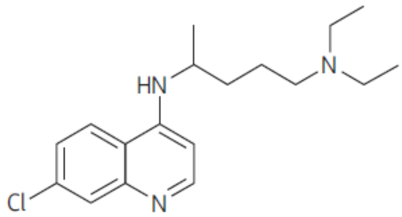


**Fig. 1. Structure of chloroquine**

In $G$, 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***

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

In the following theorem, we determine the HDR Sombor index of the molecular graph of chloroquine.

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

$$HDRSO(G) = 101.$$

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

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

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

$$= 2\sqrt{13} + 7\sqrt{25} + 5\sqrt{34} + 2\sqrt{18} + 2\sqrt{32} + 3\sqrt{5} + 2\sqrt{2} = 101.$$

In the following theorem, we compute the F-HDR index of the molecular graph of chloroquine.

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

$$FHDR(G) = 343.$$

**Proof:** Using definition and using Table 1, we have

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

$$= 2(2^2+3^2) + 7(3^2+4^2) + 5(3^2+5^2) + 2(3^2+3^2) + 2(4^2+4^2) + 3(1^2+2^2) + 2(1^2+1^2) = 343.$$

## III. RESULTS AND DISCUSSION: HYDROXYCHLOROQUINE

Let *H* be the graph of hydroxychloroquine and it has 22 vertices and 24 edges, see Fig. 2.

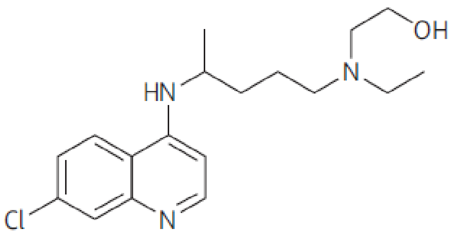


**Fig. 2. Structure of hydroxychloroquine**

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***

| $d_{hr}(u), d_{hr}(v) \setminus uv$ □ $E(H)$ | 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 Sombor index of the molecular graph of hydroxychloroquine .

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

$$HDRSO(H) = 106.5$$

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

$$HDRSO(H) = \sum_{uv \in E(H)} \sqrt{d_{hr}(u)^2 + d_{hr}(v)^2}$$

$$= 1\sqrt{2^2+3^2} + 3\sqrt{3^2+3^2} + 7\sqrt{3^2+4^2} + 5\sqrt{3^2+5^2} + 2\sqrt{4^2+4^2} + 1\sqrt{1^2+3^2} + 2\sqrt{1^2+2^2} + 2\sqrt{2^2+2^2} + 1\sqrt{1^2+1^2}$$
$$= 106.5$$

In the following theorem, we compute the F-HDR index of the molecular graph of hydroxychloroquine.

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

$$FHDR(H) = 572.$$

**Proof:** Using definition and using Table 2, we have

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

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

$$+ 2(2^2 + 2^2) + 1(1^2 + 1^2) = 572.$$

## IV. RESULTS AND DISCUSSION: REMDESIVIR

Let $R$ be the molecular structure of remdesivir. Clearly $R$ has 41 vertices and 44 edges, see Fig. 3.

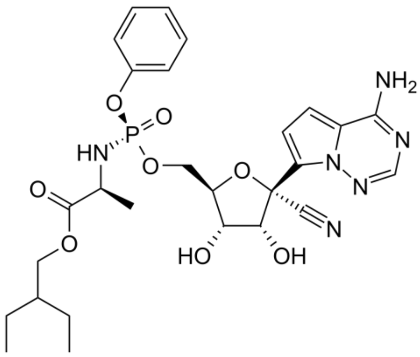


**Fig. 3 Structure of remdesivir**

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 3.

**Table 3. Edge partition of *R***

| $d_{hr}(u), d_{hr}(v) \setminus uv$ □ $E(R)$ | 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 the following theorem, we determine the HDR Sombor index of the molecular graph of remdesivir.

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

$$HDRSO(R) = 160.$$

**Proof:** From definition and by using Table 3, we obtain

$$HDRSO(R) = \sum_{uv \in E(R)} \sqrt{d_{hr}(u)^2 + d_{hr}(v)^2}$$

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

$$+4\sqrt{4^2+5^2} + 3\sqrt{5^2+5^2} + 2\sqrt{5^2+6^2} + 1\sqrt{5^2+7^2} + 1\sqrt{6^2+7^2} = 160$$

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

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

$$FHDR(R) = 1074.$$

**Proof:** Using definition and using Table 3, we have

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

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

$$+4(4^2+5^2) + 3(5^2+5^2) + 2(5^2+6^2) + 1(5^2+7^2) + 1(6^2+7^2) = 1074$$

## V. PROPERTIES OF THE HDR SOMBOR INDEX

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

$$HDRSO(G) \le \sqrt{mFHDR(G)}.$$

**Proof:** Using the Cauchy-Schwarz inequality, we obtain

$$\left( \sum_{uv \in E(G)} \sqrt{d_{hr}(u)^2 + d_{hr}(v)^2} \right)^2 \le \sum_{uv \in E(G)} 1 \sum_{uv \in E(G)} \left( d_{hr}(u)^2 + d_{hr}(v)^2 \right).$$

$$= mFHDR(G).$$

Thus $$HDRSO(G) \le \sqrt{mFHDR(G)}.$$

**Theorem 8.** Let *G* be a connected graph. Then

$$HDRSO(G) \ge \frac{1}{\sqrt{2}} HDRM_1(G)$$

Equality holds if and only if *G* is regular.

**Theorem 9.** Let *G* be a connected graph. Then

$$HDRSO(G) \le \sqrt{2}\left( HDRM_1(G) - HDRM_2(G) \right).$$

We can prove Theorem 8 and Theorem 9.

## VI. CONCLUSION

We obtain some results involving the HDR Sombor index and F-HDR index of a graph. We compute the HDR Sombor index and F-HDR index of chloroquine, hydroxychloroquine and remdesivir.

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