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Original Article

ABC, GA, AG HDR Indices of Certain Chemical Drugs

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Abstract *- In this study, we introduce* the *ABC, GA, AG and inverse sum indeg HDR indices and compute these newly defined indices for some important chemical drugs such as chloroquine, hydroxychloroquine and remdesivir.*

Keywords - *Molecular structure, HDR indices, Chloroquine, Hydroxychloroquine, Remdesivir.*

I. INTRODUCTION

We consider three antiviral compounds (agents) such as chloroquine, hydroxychloroquine and remdesivir. In 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.

Let G be a 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 edges incident to u. Any undefined terms and notations can be found in the book [1].

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 [2].

The HDR Zagreb index was introduced by Alsinai et al. in [2], and it is defined as

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

In [3], Kulli introduced the second HDR Zagreb index of a graph G and it is defined as

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

We now propose the following HDR indices:

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

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

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

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

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

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

The inverse sum indeg HDR index of a graph G is defined as

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

Recently, some graphical indices were studied, for example, in [4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25]. In this paper, some HDR indices of chloroquine, hydroxychloroquine and remdesivir are computed. For graph indices see [26].

II. RESULTS AND DISCUSSION: CHLOROQUINE

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

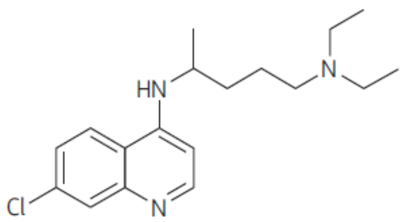

Fig. 1

In G, the edge set $E(G)$ can be divided into five 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

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

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

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

Proof: Using definition and using Table 1, we deduce

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

$$=2\sqrt{\frac{2+3-2}{2\times 3}}+7\sqrt{\frac{3+4-2}{3\times 4}}+5\sqrt{\frac{3+5-2}{3\times 5}}+2\sqrt{\frac{3+3-2}{3\times 3}}+2\sqrt{\frac{4+4-2}{4\times 4}}+3\sqrt{\frac{1+2-2}{1\times 2}}+2\sqrt{\frac{1+1-2}{1\times 1}}.$$

After simplification, we get the desired result.

In the next theorem, we determine the geometric-arithmetic HDR index of the molecular graph of chloroquine.

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

$$GAHDR(G)=6+\frac{4\sqrt{6}}{5}+4\sqrt{3}+\frac{5\sqrt{15}}{4}+2\sqrt{2}.$$

Proof: Using definition and using Table 1, we derive

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

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

gives the desired result.

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

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

$$AGHDR(G)=6+\frac{5}{\sqrt{6}}+\frac{49}{4\sqrt{3}}+\frac{20}{\sqrt{15}}+\frac{9}{2\sqrt{2}}\ .$$

Proof: From definition and using Table 1, we obtain

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

$$=2\left(\frac{2+3}{2\sqrt{2\times 3}}\right)+7\left(\frac{3+4}{2\sqrt{3\times 4}}\right)+5\left(\frac{3+5}{2\sqrt{3\times 5}}\right)+2\left(\frac{3+3}{2\sqrt{3\times 3}}\right)+2\left(\frac{4+4}{2\sqrt{4\times 4}}\right)+3\left(\frac{1+2}{2\sqrt{1\times 2}}\right)+2\left(\frac{1+1}{2\sqrt{1\times 1}}\right)$$ giving the desired result after simplification.

In the next theorem, we determine the inverse sum HDR index of the graph of chloroquine.

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

$$IHDR(G)=\frac{1351}{40}.$$

Proof: Using definition and using Table 1, we have

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

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

After simplification, we get the desired result.

III. RESULTS AND DISCUSSION: HYDROXYCHLOROQUINE

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

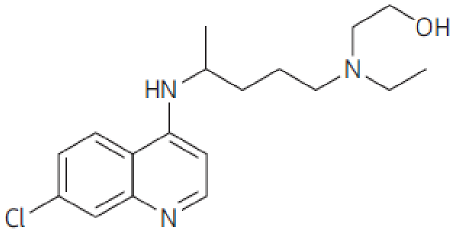

Fig. 2 Structure of hydroxychloroquine

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*

$d_{hr}(u), d_{hr}(v) \backslash uv \in E(H)$	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 atom bond connectivity HDR index of the molecular graph of hydroxychloroquine.

Theorem 5. Let H be the molecular graph of hydroxychloroquine. Then

$$ABCHDR(H) = 2 + \frac{3}{\sqrt{2}} + \frac{7\sqrt{5}}{2\sqrt{3}} + \frac{5\sqrt{2}}{\sqrt{5}} + \frac{\sqrt{3}}{\sqrt{2}} + \frac{\sqrt{2}}{\sqrt{3}} + \sqrt{2}.$$

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

$$ABCHDR(H) = \sum_{uv \in E(H)} \sqrt{\frac{d_{hr}(u) + d_{hr}(v) - 2}{d_{hr}(u) d_{hr}(v)}}$$

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

$$+1\sqrt{\frac{1+3-2}{1\times 3}} + 2\sqrt{\frac{1+2-2}{1\times 2}} + 2\sqrt{\frac{2+2-2}{2\times 2}} + 1\sqrt{\frac{1+1-2}{1\times 1}}$$

giving the desired result after simplification

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

Theorem 6. Let H be the molecular graph of hydroxychloroquine. Then

$$GAHDR(H)=8+\frac{2\sqrt{6}}{5}+4\sqrt{3}+\frac{5\sqrt{15}}{4}+\frac{\sqrt{3}}{2}+\frac{4\sqrt{2}}{3}.$$

Proof: Using definition and using Table 2, we have

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

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

$$+1\left(\frac{2\sqrt{1\times 3}}{1+3}\right)+2\left(\frac{2\sqrt{1\times 2}}{1+2}\right)+2\left(\frac{2\sqrt{2\times 2}}{2+2}\right)+1\left(\frac{2\sqrt{1\times 1}}{1+1}\right).$$

After simplification, we get the desired result

In the following theorem, we determine the arithmetic-geometric HDR index of the molecular graph of hydroxychloroquine.

Theorem 7. Let H be the molecular graph of hydroxychloroquine. Then

$$AGHDR(H)=8+\frac{5}{2\sqrt{6}}+\frac{49}{4\sqrt{3}}+\frac{20}{\sqrt{15}}+\frac{2}{\sqrt{3}}+\frac{3}{\sqrt{2}}.$$

Proof: By using definition and Table 2, we deduce

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

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

$$+1\left(\frac{1+3}{2\sqrt{1\times 3}}\right)+2\left(\frac{1+2}{2\sqrt{1\times 2}}\right)+2\left(\frac{2+2}{2\sqrt{2\times 2}}\right)+1\left(\frac{1+1}{2\sqrt{1\times 1}}\right)$$

giving the desired result after simplification

In the next theorem, we compute the inverse sum HDR index of the molecular graph of hydroxychloroquine.

Theorem 8. Let H be the molecular graph of hydroxychloroquine. Then

$$IHDR(H)=\frac{4289}{120}.$$

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

$$IHDR(H) = \sum_{uv \in E(H)} \frac{d_{hr}(u)\, d_{hr}(v)}{d_{hr}(v) + d_{hr}(u)}$$

$$= 1\left(\frac{2\times3}{2+3}\right) + 3\left(\frac{3\times3}{3+3}\right) + 7\left(\frac{3\times4}{3+4}\right) + 5\left(\frac{3\times5}{3+5}\right) + 2\left(\frac{4\times4}{4+4}\right)$$

$$+1\left(\frac{1\times3}{1+3}\right) + 2\left(\frac{1\times2}{1+2}\right) + 2\left(\frac{2\times2}{2+2}\right) + 1\left(\frac{1\times1}{1+1}\right).$$

After simplification, we get the desired result

IV. RESULTS AND DISCUSSION: REMDESIVIR

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

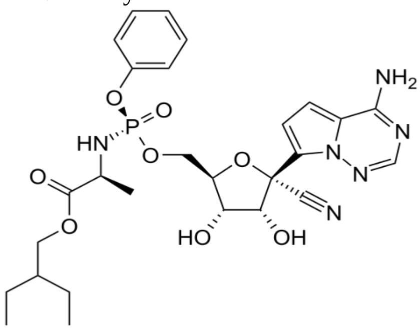

Fig. 3

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*

$d_{hr}(u), d_{hr}(v) \backslash uv \in E(R)$	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 the following theorem, we determine the atom bond connectivity HDR index of the molecular graph of remdesivir.

Theorem 9. Let R be the molecular graph of remdesivir. Then

$$ABCHDR(R)=\frac{17}{\sqrt{2}}+5\sqrt{\frac{2}{3}}+2\sqrt{\frac{5}{3}}+\frac{8}{3}+3\sqrt{\frac{2}{5}}+2\sqrt{\frac{7}{5}}+\frac{6\sqrt{2}}{5}+2\sqrt{\frac{3}{10}}+\sqrt{\frac{2}{7}}+\sqrt{\frac{11}{42}}.$$

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

$$ABCHDR(R)=\sum_{uv\in E(R)}\sqrt{\frac{d_{hr}(u)+d_{hr}(v)-2}{d_{hr}(u)d_{hr}(v)}}$$

$$=7\sqrt{\frac{1+2-2}{1\times 2}}+5\sqrt{\frac{1+3-2}{1\times 3}}+2\sqrt{\frac{2+2-2}{2\times 2}}+8\sqrt{\frac{2+3-2}{2\times 3}}+4\sqrt{\frac{3+3-2}{3\times 3}}+3\sqrt{\frac{3+5-2}{3\times 5}}$$

$$+4\sqrt{\frac{3+4-2}{3\times 4}}+4\sqrt{\frac{4+5-2}{4\times 5}}+3\sqrt{\frac{5+5-2}{5\times 5}}+2\sqrt{\frac{5+6-2}{5\times 6}}+1\sqrt{\frac{5+7-2}{5\times 7}}+1\sqrt{\frac{6+7-2}{6\times 7}}$$

After simplification, we get the desired result

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

Theorem 10. Let R be the molecular graph of remdesivir. Then

$$GAHDR(R)=\frac{14\sqrt{2}}{3}+\frac{5\sqrt{3}}{2}+\frac{16\sqrt{6}}{5}+\frac{3\sqrt{15}}{4}+\frac{16\sqrt{3}}{7}+\frac{16\sqrt{5}}{9}+\frac{4\sqrt{30}}{11}+\frac{\sqrt{35}}{6}+\frac{2\sqrt{42}}{13}+9.$$

Proof: Using definition and using Table 3, we have

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

$$=7\left(\frac{2\sqrt{1\times 2}}{1+2}\right)+5\left(\frac{2\sqrt{1\times 3}}{1+3}\right)+2\left(\frac{2\sqrt{2\times 2}}{2+2}\right)+8\left(\frac{2\sqrt{2\times 3}}{2+3}\right)+4\left(\frac{2\sqrt{3\times 3}}{3+3}\right)+3\left(\frac{2\sqrt{3\times 5}}{3+5}\right)$$

$$+4\left(\frac{2\sqrt{3\times 4}}{3+4}\right)+4\left(\frac{2\sqrt{4\times 5}}{4+5}\right)+3\left(\frac{2\sqrt{5\times 5}}{5+5}\right)+2\left(\frac{2\sqrt{5\times 6}}{5+6}\right)+1\left(\frac{2\sqrt{5\times 7}}{5+7}\right)+1\left(\frac{2\sqrt{6\times 7}}{6+7}\right)$$

giving the desired result after simplification

In the following theorem, we determine the arithmetic-geometric HDR index of the molecular graph of hydroxychloroquine.

Theorem 11. Let R be the molecular graph of hydroxychloroquine. Then

$$AGHDR(R)=\frac{21}{2\sqrt{2}}+\frac{10}{\sqrt{3}}+\frac{20}{\sqrt{6}}+\frac{10}{\sqrt{15}}+\frac{7}{\sqrt{3}}+\frac{9}{\sqrt{5}}+\frac{11}{\sqrt{30}}+\frac{6}{\sqrt{35}}+\frac{13}{2\sqrt{42}}+9.$$

Proof: By using definition and Table 3, we deduce

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

$$=7\left(\frac{1+2}{2\sqrt{1\times 2}}\right)+5\left(\frac{1+3}{2\sqrt{1\times 3}}\right)+2\left(\frac{2+2}{2\sqrt{2\times 2}}\right)+8\left(\frac{2+3}{2\sqrt{2\times 3}}\right)+4\left(\frac{3+3}{2\sqrt{3\times 3}}\right)+3\left(\frac{3+5}{2\sqrt{3\times 5}}\right)$$

$$+4\left(\frac{3+4}{2\sqrt{3\times 4}}\right)+4\left(\frac{4+5}{2\sqrt{4\times 5}}\right)+3\left(\frac{5+5}{2\sqrt{5\times 5}}\right)+2\left(\frac{5+6}{2\sqrt{5\times 6}}\right)+1\left(\frac{5+7}{2\sqrt{5\times 7}}\right)+1\left(\frac{6+7}{2\sqrt{6\times 7}}\right)$$

After simplification, we obtain the desired result

In the next theorem, we compute the inverse sum HDR index of the molecular graph of hydroxychloroquine.

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

$$IHDR(R)=66.4896797647.$$

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

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

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

$$+4\left(\frac{3\times 4}{3+4}\right)+4\left(\frac{4\times 5}{4+5}\right)+3\left(\frac{5\times 5}{5+5}\right)+2\left(\frac{5\times 6}{5+6}\right)+1\left(\frac{5\times 7}{5+7}\right)+1\left(\frac{6\times 7}{6+7}\right)$$

gives the desired result.

V. CONCLUSION

In this paper, we have computed the ABC HDR index, GA HDR index, AG HDR index and inverse sum indeg HDR index of chloroquine, hydroxychloroquine and remdesivir. In Medical Science, chemical, medical, biological, pharmaceutical properties of molecular structure are essential for drug design. These properties can be studied by the graphical index calculation. In the view of this, our results may be useful in Medical Science.

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