K Banhatti Indices of Chloroquine and Hydroxychloroquine :Research Applied for the Treatment and Prevention of COVID-19

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Abstract: *In the present study, we establish some topological properties of chloroquine and hydroxychloroquine used to inhibit the outbreak of coronaivirus disease-19. We compute some K Banhatti indices for these two chemical structures. In the field of Medical Science, concerning the definition of the topological index on the molecular structure and corresponding medical, biological, chemical, pharmaceutical properties of drugs can be studied by the topological index calculation. In the view of this, our results may be useful in finding new drug and vaccine for the treatment and prevention of COVID-19.*

Keywords: *molecular structures, K Banhatti indices, chloroquine, hydroxychloroquine.*

I. INTRODUCTION

Coronavirus disease (COVID-19) first started in Wohan, China [1] in December 2019. It is spreading quickly several countries worldwide. As the 15 April 2020, there were more than 19 lakhs 75 thousand confirmed cases and more than 1 lakh 25 thousand deaths worldwide (as per Wikipedia). The number of COVID-19 cases and deaths are still on the rise. At present, there is no drug and no vaccine available for the treatment and prevention of COVID-19. Therefore there is urgent need to identify effective and safe drug and vaccine to treat this disease. We find use of some antiviral agents, for example, in [2, 3, 4, 5, 6, 6, 7, 8]. We consider two antiviral compounds (agents) such as chloroquine and hydroxychloroquine. Chloroquine was discovered in 1934 by H. Andersag. This compound 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 erythmatosus and rheumatoid arthritis [9]. Due to COVID-19, the FDA has issued an emergency use authorization for hydroxychloroquine and chloroquine [10]. In the field of Medical Science, concerning the definition of the topological index on the molecular structure and corresponding medical, chemical, biological, pharmaceutical properties of drugs can be studied for the topological index calculation [11]. A molecular structure (graph) [12] 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. In 1972 [13], two degree based topological indices were introduced and studied. 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. If $e= uv$ is an edge of G, then the vertex u and edge e are incident and it is denoted by ue. Let $d_G(e)$ denote the degree of an edge e in G, which is defined as $d_G(e) = d_G(u) + d_G(v) – 2$ with $e = uv$.

The first and second K Banhatti indices [14] of a graph G are defined as

$$B_1(G) = \sum_{ue} \left[d_G(u) + d_G(e) \right],$$

$$B_2(G) = \sum_{ue} d_G(u) d_G(e).$$

The first and second K hyper Banhatti indices [15] of a graph G are defined as

$$HB_1(G) = \sum_{ue} \left[d_G(u) + d_G(e) \right]^2,$$

$$HB_2(G) = \sum_{ue} \left[d_G(u) d_G(e) \right]^2.$$

The sum connectivity Banhatti index of a graph G is defined as

$$SB(G) = \sum_{ue} \frac{1}{\sqrt{d_G(u) + d_G(e)}}$$

The product connectivity Banhatti index [16] of a graph G is defined as

$$PB(G) = \sum_{ue} \frac{1}{\sqrt{d_G(u) d_G(e)}}$$

The modified first and second Banhatti indices [17] of a graph G are defined as

$${}^m B_1(G) = \sum_{ue} \frac{1}{d_G(u) + d_G(e)},$$

$${}^m B_2(G) = \sum_{ue} \frac{1}{d_G(u) d_G(e)}.$$

The general first and second Banhatti indices [18] of a graph G are defined as

$$B_1^a(G) = \sum_{ue} \left[d_G(u) + d_G(e) \right]^a,$$

$$B_2^a(G) = \sum_{ue} \left[d_G(u) d_G(e) \right]^a,$$

where a is a real number.

The atom bond connectivity Banhatti index [19] of a graph G is defined as

$$ABCB(G)=\sum_{ue}\sqrt{\frac{d_G(u)+d_G(e)-2}{d_G(u)d_G(e)}}$$

The geometric-arithmetic Banhatti index [20] of a graph G is defined as

$$GAB(G)=\sum_{ue}\frac{2\sqrt{d_G(u)d_G(e)}}{d_G(u)+d_G(e)}$$

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

$$AGB(G)=\sum_{ue}\frac{d_G(u)+d_G(e)}{2\sqrt{d_G(u)d_G(e)}}$$

The harmonic K Banhatti index [17] of a graph G is defined as

$$H_b(G)=\sum_{ue}\frac{2}{d_G(u)+d_G(e)}$$

The inverse sum K Banhatti of a graph G is defined as

$$IB(G)=\sum_{ue}\frac{d_G(u)d_G(e)}{d_G(e)+d_G(u)}$$

In this study, some K Banhatti indices of chloroquine and hydroxychloroquine are computed.

II. CHLOROQUINE: RESULTS AND DISCUSSION

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

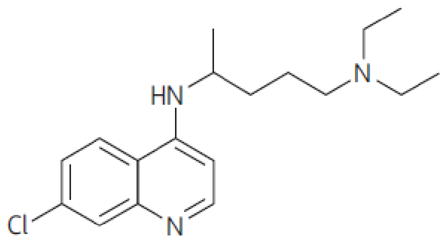

Figure 1. Structure of chloroquine

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

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

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

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

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

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

Then the edge degree partition of G is given in Table 1:

$d_G(u), d_G(v)\backslash uv \in E(G)$	(1,2)	(1,2)	(2,2)	(2,3)	(3,3)
$d_G(e)$	1	2	2	3	4
No. of edges	2	2	5	12	2

Table 1. Edge degree partition of G

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

Theorem 1. Let G be the molecular graph of chloroquine. Then
$B^a_1(G)=2\times2^a+4\times3^a+10\times4^a+14\times5^a+12\times6^a+4\times7^a$.

Proof: From definition and using Table 1, we deduce

$$B_1^a(G)=\sum_{ue}\left[d_G(u)+d_G(e)\right]^a$$

$=2[(1+1)^a+(2+1)^a]+2[(1+2)^a+(3+2)^a]$
$+5[(2+2)^a+(2+2)^a]+12[(2+3)^a+(3+3)^a]$
$+2[(3+4)^a+(3+4)^a]$
$=2\times2^a+4\times3^a+10\times4^a+14\times5^a+12\times6^a+4\times7^a$.

Using Theorem 1, we obtain the following results.

Corollary 1.1. The first K Banhatti index of the graph of chloroquine is given by

$B_1(G)=226$.

Corollary 1.2. The first K-hyper Banhatti index of the graph of chloroquine is given by

$HB_1(G)=1182$.

Corollary 1.3. The sum connectivity Banhatti index of the graph of chloroquine is given by

$$SB(G)=\frac{2}{\sqrt{2}}+\frac{4}{\sqrt{3}}+\frac{14}{\sqrt{5}}+\frac{12}{\sqrt{6}}+\frac{4}{\sqrt{7}}+5.$$

Corollary 1.4. The modified first K Banhatti index of the graph of chloroquine is

$${}^mB_1(G)=\frac{2143}{210}.$$

In the following theorem, we compute the general second K Banhatti index of the molecular graph of chloroquine.

Theorem 2. Let G be the molecular graph of chloroquine. Then
$B^a_2(G)=2+4\times2^a+10\times4^a+14\times6^a+12\times9^a+4\times12^a$.

Proof: Using definition and Table 1, we derive

$$B_2^a(G)=\sum_{ue}\left[d_G(u)d_G(e)\right]^a$$

$=2[(1\times1)^a+(2\times1)^a]+2[(1\times2)^a+(3\times2)^a]$
$+5[(2\times2)^a+(2\times2)^a]+12[(2\times3)^a+(3\times3)^a]$
$+2[(3\times4)^a+(3\times4)^a]$
$=2+4\times2^a+10\times4^a+14\times6^a+12\times9^a+4\times12^a$.

Using Theorem 2, we get the following results.

Corollary 2.1. The second K Banhatti index of the graph of chloroquine is given by

$B_2(G)=290$.

Corollary 2.2. The second K-hyper Banhatti index of the graph of chloroquine is

$HB_2(G)=2230$.

Corollary 2.3. The product connectivity Banhatti index of the graph of chloroquine is

$$PB(G)=11+\frac{4}{\sqrt{2}}+\frac{2}{\sqrt{3}}+\frac{14}{\sqrt{6}}.$$

Corollary 2.4. The modified second K Banhatti index of the graph of chloroquine is

$$^{m}B_2(G)=\frac{21}{2}.$$

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

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

$$ABCB(G)=8+\frac{28}{\sqrt{2}}+2\sqrt{\frac{5}{3}}.$$

Proof: Using definition and using Table 1, we deduce

$$ABCB(G)=\sum_{uv\in E(G)}\left[\sqrt{\frac{d_G(u)+d_G(e)-2}{d_G(u)d_G(e)}}+\sqrt{\frac{d_G(v)+d_G(e)-2}{d_G(v)d_G(e)}}\right]$$

$$=2\left(\sqrt{\frac{1+1-2}{1\times1}}+\sqrt{\frac{2+1-2}{2\times1}}\right)$$

$$+2\left(\sqrt{\frac{1+2-2}{1\times2}}+\sqrt{\frac{3+2-2}{3\times2}}\right)$$

$$+5\left(\sqrt{\frac{2+2-2}{2\times2}}+\sqrt{\frac{2+2-2}{2\times2}}\right)$$

$$+12\left(\sqrt{\frac{2+3-2}{2\times3}}+\sqrt{\frac{3+3-2}{3\times3}}\right)$$

$$+2\left(\sqrt{\frac{3+4-2}{3\times4}}+\sqrt{\frac{3+4-2}{3\times4}}\right)$$

$$=8+\frac{28}{\sqrt{2}}+2\sqrt{\frac{5}{3}}.$$

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

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

$$GAB(G)=24+\frac{8\sqrt{2}}{3}+\frac{28\sqrt{6}}{5}+\frac{16\sqrt{3}}{7}.$$

Proof: Using definition and using Table 1, we derive

$$GAB(G)=\sum_{uv\in E(G)}\left[\frac{2\sqrt{d_G(u)d_G(e)}}{d_G(u)+d_G(e)}+\frac{2\sqrt{d_G(v)d_G(e)}}{d_G(v)+d_G(e)}\right]$$

$$=2\left(\frac{2\sqrt{1\times1}}{1+1}+\frac{2\sqrt{2\times1}}{2+1}\right)+2\left(\frac{2\sqrt{1\times2}}{1+2}+\frac{2\sqrt{3\times2}}{3+2}\right)$$

$$+5\left(\frac{2\sqrt{2\times2}}{2+2}+\frac{2\sqrt{2\times2}}{2+2}\right)+12\left(\frac{2\sqrt{2\times3}}{2+3}+\frac{2\sqrt{3\times3}}{3+3}\right)$$

$$+2\left(\frac{2\sqrt{3\times4}}{3+4}+\frac{2\sqrt{3\times4}}{3+4}\right)$$

$$=24+\frac{8\sqrt{2}}{3}+\frac{28\sqrt{6}}{5}+\frac{16\sqrt{3}}{7}.$$

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

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

$$AGB(G)=24+\frac{6}{\sqrt{2}}+\frac{7}{\sqrt{3}}+\frac{35}{\sqrt{6}}.$$

Proof: From definition and using Table 1, we obtain

$$AGB(G)=\sum_{uv\in E(G)}\left[\frac{d_G(u)+d_G(e)}{2\sqrt{d_G(u)d_G(e)}}+\frac{d_G(v)+d_G(e)}{2\sqrt{d_G(v)d_G(e)}}\right]$$

$$=2\left(\frac{1+1}{2\sqrt{1\times1}}+\frac{2+1}{2\sqrt{2\times1}}\right)+2\left(\frac{1+2}{2\sqrt{1\times2}}+\frac{3+2}{2\sqrt{3\times2}}\right)$$

$$+5\left(\frac{2+2}{2\sqrt{2\times2}}+\frac{2+2}{2\sqrt{2\times2}}\right)+12\left(\frac{2+3}{2\sqrt{2\times3}}+\frac{3+3}{2\sqrt{3\times3}}\right)$$

$$+2\left(\frac{3+4}{2\sqrt{3\times4}}+\frac{3+4}{2\sqrt{3\times4}}\right)$$

$$=24+\frac{6}{\sqrt{2}}+\frac{7}{\sqrt{3}}+\frac{35}{\sqrt{6}}.$$

In the following theorem, we compute the harmonic K-Banhatti index of the molecular graph of chloroquine.

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

$$H_b(G)=\frac{2143}{105}.$$

Proof: From definition and using Table 1, we have

$$H_b(G)=\sum_{uv\in E(G)}\left[\frac{2}{d_G(u)+d_G(e)}+\frac{2}{d_G(v)+d_G(e)}\right]$$

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

$$+5\left(\frac{2}{2+2}+\frac{2}{2+2}\right)+12\left(\frac{2}{2+3}+\frac{2}{3+3}\right)$$

$$+2\left(\frac{2}{3+4}+\frac{2}{3+4}\right)$$

$$=\frac{2143}{105}.$$

In the next theorem, we determine the inverse sum K-Banhatti index of the graph of chloroquine.

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

$$IB(G)=\frac{5809}{105}.$$

Proof: Using definition and using Table 1, we have

$$IB(G)=\sum_{uv\in E(G)}\left[\frac{d_G(u)d_G(e)}{d_G(u)+d_G(e)}+\frac{d_G(v)d_G(e)}{d_G(v)+d_G(e)}\right]$$

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

$$+5\left(\frac{2\times 2}{2+2}+\frac{2\times 2}{2+2}\right)+12\left(\frac{2\times 3}{2+3}+\frac{3\times 3}{3+3}\right)$$
$$+2\left(\frac{3\times 4}{3+4}+\frac{3\times 4}{3+4}\right)$$
$$=\frac{5809}{105}.$$

III. HYDROXYCHLOROQUINE: RESULTS AND DISCUSSION

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

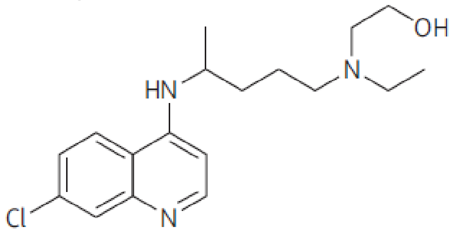

Figure 2. Structure of hydroxychloroquine

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

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

Then the edge degree partition of H is given in Table 2:

$d_H(u), d_H(v)\backslash uv\in E(H)$	(1,2)	(1,3)	(2,2)	(2,3)	(3,3)
$d_G(e)$	1	2	2	3	4
No. of edges	2	2	6	12	2

Table 2. Edge degree partition of H

In the following theorem, we compute the general first K Banhatti index of the molecular graph of hydroxychloroquine.

Theorem 8. Let H be the molecular graph of hydroxychloroquine. Then
$B^a_1(H)=2\times2^a+4\times3^a+12\times4^a+14\times5^a+12\times6^a+4\times7^a$.

Proof: Using definition and Table 2, we deduce

$$B_1^a(H)=\sum_{ue}\left[d_H(u)+d_H(e)\right]^a$$
$$=2[(1+1)^a+(2+1)^a]+2[(1+2)^a+(3+2)^a]$$
$$+6[(2+2)^a+(2+2)^a]+12[(2+3)^a+(3+3)^a]$$
$$+2[(3+4)^a+(3+4)^a]$$
$$=2\times2^a+4\times3^a+12\times4^a+14\times5^a+12\times6^a+4\times7^a.$$

We obtain the following results by using Theorem 8.

Corollary 8.1. The first K Banhatti index of the graph of hydroxychloroquine is given by
$B_1(H)=234$.

Corollary 8.2. The first K-hyper Banhatti index of the graph of hydroxychloroquine is
$HB_1(H)=1214$.

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

$$SB(H)=\frac{2}{\sqrt{2}}+\frac{4}{\sqrt{3}}+\frac{14}{\sqrt{5}}+\frac{12}{\sqrt{6}}+\frac{4}{\sqrt{7}}+6$$

Corollary 8.4. The modified first K Banhatti index of the graph of hydroxychloroquine is

$$^{m}B_1(H)=\frac{1124}{105}.$$

In the next theorem, we determine the general second K Banhatti index of the molecular graph of hydroxychloroquine.

Theorem 9. Let H be the molecular graph of hydroxychloroquine. Then
$B^a_2(H)=2+4\times2^a+12\times4^a+14\times6^a+12\times9^a+4\times12^a$.

Proof: From definition and Table 1, we derive

$$B_2^a(H)=\sum_{ue}\left[d_H(u)d_H(e)\right]^a$$
$$=\sum_{uv\in E(H)}\left(\left[d_H(u)d_H(e)\right]^a+\left[d_H(v)d_H(e)\right]^a\right)$$
$$=2[(1\times1)^a+(2\times1)^a]+2[(1\times2)^a+(3\times2)^a]$$
$$+6[(2\times2)^a+(2\times2)^a]+12[(2\times3)^a+(3\times3)^a]$$
$$+2[(3\times4)^a+(3\times4)^a]$$
$$=2+4\times2^a+12\times4^a+14\times6^a+12\times9^a+4\times12^a.$$

We establish the following results by using Theorem 9,

Corollary 9.1. The second K Banhatti index of the graph of hydroxychloroquine is given by
$B_2(H)=298$.

Corollary 9.2. The second K-hyper Banhatti index of the graph of hydroxychloroquine is
$HB_2(H)=2262$.

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

$$PB(H)=12+\frac{4}{\sqrt{2}}+\frac{2}{\sqrt{3}}+\frac{14}{\sqrt{6}}.$$

Corollary 9.4. The modified second K Banhatti index of the graph of hydroxychloroquine is

$$^{m}B_2(H)=11.$$

In the following theorem, we determine the atom bond connectivity Banhatti index of the molecular graph of hydroxychloroquine.

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

$$ABCB(H)=8+\frac{30}{\sqrt{2}}+2\sqrt{\frac{5}{3}}.$$

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

$$ABCB(H)=\sum_{uv\in E(H)}\left[\sqrt{\frac{d_H(u)+d_H(e)-2}{d_H(u)d_H(e)}}+\sqrt{\frac{d_H(v)+d_H(e)-2}{d_H(v)d_H(e)}}\right]$$
$$=2\left(\sqrt{\frac{1+1-2}{1\times1}}+\sqrt{\frac{2+1-2}{2\times1}}\right)$$
$$+2\left(\sqrt{\frac{1+2-2}{1\times2}}+\sqrt{\frac{3+2-2}{3\times2}}\right)$$
$$+6\left(\sqrt{\frac{2+2-2}{2\times2}}+\sqrt{\frac{2+2-2}{2\times2}}\right)$$
$$+12\left(\sqrt{\frac{2+3-2}{2\times3}}+\sqrt{\frac{3+3-2}{3\times3}}\right)$$
$$+2\left(\sqrt{\frac{3+4-2}{3\times4}}+\sqrt{\frac{3+4-2}{3\times4}}\right)$$
$$=8+\frac{30}{\sqrt{2}}+2\sqrt{\frac{5}{3}}.$$

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

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

$$GAB(H)=26+\frac{8\sqrt{2}}{3}+\frac{28\sqrt{6}}{5}+\frac{16\sqrt{3}}{7}.$$

Proof: Using definition and using Table 2, we have

$$GAB(H)=\sum_{uv\in E(H)}\left[\frac{2\sqrt{d_H(u)d_H(e)}}{d_H(u)+d_H(e)}+\frac{2\sqrt{d_H(v)d_H(e)}}{d_H(v)+d_H(e)}\right]$$
$$=2\left(\frac{2\sqrt{1\times1}}{1+1}+\frac{2\sqrt{2\times1}}{2+1}\right)+2\left(\frac{2\sqrt{1\times2}}{1+2}+\frac{2\sqrt{3\times2}}{3+2}\right)$$
$$+6\left(\frac{2\sqrt{2\times2}}{2+2}+\frac{2\sqrt{2\times2}}{2+2}\right)+12\left(\frac{2\sqrt{2\times3}}{2+3}+\frac{2\sqrt{3\times3}}{3+3}\right)$$
$$+2\left(\frac{2\sqrt{3\times4}}{3+4}+\frac{2\sqrt{3\times4}}{3+4}\right)$$
$$=26+\frac{8\sqrt{2}}{3}+\frac{28\sqrt{6}}{5}+\frac{16\sqrt{3}}{7}.$$

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

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

$$AGB(H)=26+\frac{6}{\sqrt{2}}+\frac{7}{\sqrt{3}}+\frac{35}{\sqrt{6}}.$$

Proof: By using definition and Table 2, we deduce

$$AGB(H)=\sum_{uv\in E(H)}\left[\frac{d_H(u)+d_H(e)}{2\sqrt{d_H(u)d_H(e)}}+\frac{d_H(v)+d_H(e)}{2\sqrt{d_H(v)d_H(e)}}\right]$$
$$=2\left(\frac{1+1}{2\sqrt{1\times1}}+\frac{2+1}{2\sqrt{2\times1}}\right)+2\left(\frac{1+2}{2\sqrt{1\times2}}+\frac{3+2}{2\sqrt{3\times2}}\right)$$
$$+6\left(\frac{2+2}{2\sqrt{2\times2}}+\frac{2+2}{2\sqrt{2\times2}}\right)+12\left(\frac{2+3}{2\sqrt{2\times3}}+\frac{3+3}{2\sqrt{3\times3}}\right)$$
$$+2\left(\frac{3+4}{2\sqrt{3\times4}}+\frac{3+4}{2\sqrt{3\times4}}\right)$$
$$=26+\frac{6}{\sqrt{2}}+\frac{7}{\sqrt{3}}+\frac{35}{\sqrt{6}}.$$

In the following theorem, we compute the harmonic K-Banhatti index of the molecular graph of hydroxychloroquine.

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

$$H_b(H)=\frac{2248}{105}.$$

Proof: From definition and using Table 2, we derive

$$H_b(H)=\sum_{uv\in E(H)}\left[\frac{2}{d_H(u)+d_H(e)}+\frac{2}{d_H(v)+d_H(e)}\right]$$
$$=2\left(\frac{2}{1+1}+\frac{2}{2+1}\right)+2\left(\frac{2}{1+2}+\frac{2}{3+2}\right)$$
$$+6\left(\frac{2}{2+2}+\frac{2}{2+2}\right)+12\left(\frac{2}{2+3}+\frac{2}{3+3}\right)$$
$$+2\left(\frac{2}{3+4}+\frac{2}{3+4}\right)$$
$$=\frac{2248}{105}.$$

In the next theorem, we compute the inverse sum K-Banhatti index of the molecular graph of hydroxychloroquine.

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

$$IB(H)=\frac{6019}{105}.$$

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

$$IB(H)=\sum_{uv\in E(H)}\left[\frac{d_H(u)d_H(e)}{d_H(u)+d_H(e)}+\frac{d_H(v)d_H(e)}{d_H(v)+d_H(e)}\right]$$
$$=2\left(\frac{1\times1}{1+1}+\frac{2\times1}{2+1}\right)+2\left(\frac{1\times2}{1+2}+\frac{3\times2}{3+2}\right)$$
$$+6\left(\frac{3\times2}{2+2}+\frac{2\times2}{2+2}\right)+12\left(\frac{2\times3}{2+3}+\frac{3\times3}{3+3}\right)$$
$$+2\left(\frac{3\times4}{3+4}+\frac{3\times4}{3+4}\right)$$
$$=\frac{6019}{105}.$$

IV. CONCLUSION

In this study, the expressions of some K Banhatti indices of chloroquine and hydroxychloroquine have been determined. 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 results may be useful in finding new drug and vaccine for the treatment and prevention of coronavirus disease-19.

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