K Banhatti Polynomials of Remdesivir, Chloroquine, Hydroxychloroquine: Research Advances for the Prevention and Treatment of COVID-19

V.R.Kulli

Department of Mathematics, Gulbarga University, Kalaburgi (Gulbarga)-585106, India

Abstract: *In this study, we obtain some topological properties of remdesivir, chloroquine, hydroxychloroquine used to inhibit the outbreak of COVID-19. We determine some K Banhatti polynomials for these three chemical structures. 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 drug and vaccine for the treatment of COVID-19.*

Keywords: *molecular structures, K Banhatti polynomials, remdesivir, chloroquine, hydroxychloroquine.*

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

I. INTRODUCTION

Coronavirus disease started in Wuhan China [1] in December 2019. At present, there is no drug and no vaccine available for the treatment and prevention of COVID-19. Thus there is urgent need to identify effective and safe drug and vaccine to treat coronavirus disease. There are of some antiviral agents, and these were studied in [2, 3, 4, 5, 6, 7, 8]. In this study, we consider three antiviral agents such as remdesivir, chloroquine and hydroxy-chloroquine.

Remdesivir and chloroquine effectively inhibit the recently emerged novel coronavirus (2019-nCOV) in vitro [5]. Chloroquine is a medication primarily used to treat malaria. Chloroquine and its derivative hydroxychloroquine have since then 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].

A molecular structure [11] 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 finding some new drugs for diseases. A topological index is a numeric quantity from the structure of a molecular. In Chemical Science, concerning 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 [12].

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. Let $d_G(e)$ denote the degree of an edge $e = uv$ in G, which is defined as $d_G(e) = d_G(u) + d_G(v) – 2$. If $e = uv$ is an edge of G, then the vertex u and edge e are incident and it is denoted by ue.

The first and second K Banhatti indices were introduced by Kulli in [13], and they are defined as

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

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

Considering the K Banhatti indices, the first and second K Banhatti polynomials of a graph are defined as:

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

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

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

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

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

Considering the hyper K hyper Banhatti indices, the first and second K hyper Banhatti polynomials of a graph G are defined as

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

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

The modified first and second Banhatti indices were introduced by Kulli in [15], defined as

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

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

Considering the modified first and second Banhatti indices, we define the modified first and second *K* Banhatti polynomials as

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

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

The sum connectivity Banhatti index and product connectivity Banhatti index [16] are defined as

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

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

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

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

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

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

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

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

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

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

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

where *a* is a real number.

We introduce the *F-K* Banhatti index of a graph *G* and it is defined as

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

Considering the *F-K* Banhatti index, we define the *F-K* Banhatti polynomial of a graph *G*, as

$$FB(G,x)=\sum_{ue}x^{d_G(u)^2+d_G(e)^2}.$$

The harmonic *K* Banhatti index [15] of a graph *G* is defined as

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

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

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

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

$$SDB(G)=\sum_{ue}\left(\frac{d_G(u)}{d_G(e)}+\frac{d_G(e)}{d_G(u)}\right)$$

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

$$SDB(G,x)=\sum_{ue}x^{\left(\frac{d_G(u)}{d_G(e)}+\frac{d_G(e)}{r_G(u)}\right)}$$

The inverse sum indeg *K* Banhatti index [18] of a graph *G* is defined as

$$ISB(G)=\sum_{ue}\frac{d_G(u)d_G(e)}{d_G(u)+r_G(e)}.$$

Considering the inverse sum *K* Banhatti index, we define the inverse sum indeg *K* Banhatti polynomial of a graph *G* is defined as

$$ISB(G,x)=\sum_{ue}x^{\frac{d_G(u)d_G(e)}{d_G(u)+d_G(e)}}.$$

Recently, some antiviral agents were studied in [18, 19, 20].

In this study, some *K* Banhatti 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 Figure 1.

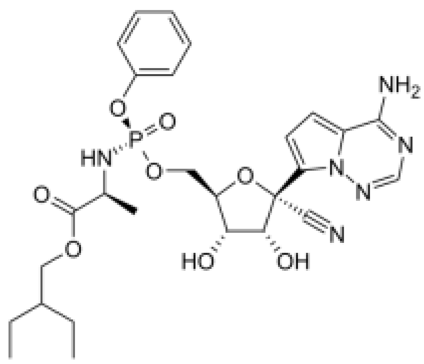

Figure 1

In R, the edge set of R can be divided into eight partitions based on the degree of end vertices of each edge as given in Table 1.

$d_R(u), d_R(v)$\ uv□$E(R)$	(1, 2)	(1, 3)	(1, 4)	(2, 2)	(2, 3)	(2, 4)	(3, 3)	(3, 4)
No. of edges	2	5	2	9	14	4	6	2

Table 1. Edge partition of *R*.

Therefore the edge degree partition of remdesivir R is given in Table 2.

$d_R(u), d_R(v)$\ uv□$E(R)$	(1, 2)	(1, 3)	(1, 4)	(2, 2)	(2, 3)	(2, 4)	(3, 3)	(3, 4)
$d_R(e)$	1	2	3	2	3	4	4	5
No. of edges	2	5	2	9	14	4	6	2

Table 2. Edge degree partition of *R*

In the following theorem, we compute the general first K Banhatti polynomial of the molecular structure of remdesivir.

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

$$B_1^a(R,x) = 2x^{2^a+3^a} + 5x^{3^a+5^a} + 2x^{4^a+7^a} + 9x^{4^a+4^a} + 14x^{5^a+6^a} + 4x^{6^a+8^a} + 6x^{7^a+7^a} + 2x^{8^a+9^a}. \quad (1)$$

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

$$B_1^a(R,x) = \sum_{ue} x^{\left[d_R(u)+d_R(e)\right]^a}$$
$$= 2x^{(1+1)^a+(2+1)^a} + 5x^{(1+2)^a+(3+2)^a} + 2x^{(1+3)^a+(4+3)^a} + 9x^{(2+2)^a+(2+2)^a} + 14x^{(2+3)^a+(3+3)^a} + 4x^{(2+4)^a+(4+4)^a} + 6x^{(3+4)^a+(3+4)^a} + 2x^{(3+5)^a+(4+5)^a}$$
$$= 2x^{2^a+3^a} + 5x^{3^a+5^a} + 2x^{4^a+7^a} + 9x^{4^a+4^a} + 14x^{5^a+6^a} + 4x^{6^a+8^a} + 6x^{7^a+7^a} + 2x^{8^a+9^a}.$$

We obtain the following results from Theorem 1.

Corollary 1.1. The first K Banhatti polynomial of the molecular structure of remdesivir is

$$B_1(R,x) = 2x^5 + 14x^8 + 16x^{11} + 10x^{14} + 2x^{17}.$$

Corollary 1.2. The first hyper K Banhatti polynomial of the molecular structure of remdesivir is

$$HB_1(R,x) = 2x^{13} + 9x^{32} + 5x^{34} + 14x^{61} + 2x^{65} + 6x^{98} + 4x^{100} + 2x^{145}.$$

Corollary 1.3. The modified first K Banhatti polynomial of the molecular structure of remdesivir is

$${}^{m}B_1(R,x) = 2x^{\frac{5}{6}} + 5x^{\frac{8}{15}} + 2x^{\frac{11}{28}} + 9x^{\frac{1}{2}} + 14x^{\frac{11}{30}} + 4x^{\frac{7}{24}} + 6x^{\frac{2}{7}} + 2x^{\frac{17}{72}}.$$

Corollary 1.4. The sum connectivity K Banhatti polynomial of the molecular structure of remdesivir is

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

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

In the following theorem, we determine the general second K Banhatti polynomial of the molecular structure of remdesivir.

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

$$B_2^a(R,x) = 2x^{1^a+2^a} + 5x^{2^a+6^a} + 2x^{3^a+12^a} + 9x^{4^a+4^a} + 14x^{6^a+9^a} + 4x^{8^a+16^a} + 6x^{12^a+12^a} + 2x^{15^a+20^a}. \quad (2)$$

Proof: Using definition and Table 2, we derive

$$B_2^a(R,x) = \sum_{ue} x^{\left[d_R(u)d_R(e)\right]^a}$$
$$= 2x^{(1\times1)^a+(2\times1)^a} + 5x^{(1\times2)^a+(3\times2)^a} + 2x^{(1\times3)^a+(4\times3)^a} + 9x^{(2\times2)^a+(2\times2)^a} + 14x^{(2\times3)^a+(3\times3)^a} + 4x^{(2\times4)^a+(4\times4)^a} + 6x^{(3\times4)^a+(3\times4)^a} + 2x^{(3\times5)^a+(4\times5)^a}$$
$$= 2x^{1^a+2^a} + 5x^{2^a+6^a} + 2x^{3^a+12^a} + 9x^{4^a+4^a} + 14x^{6^a+9^a} + 4x^{8^a+16^a} + 6x^{12^a+12^a} + 2x^{15^a+20^a}.$$

From Theorem 2, we establish the following results.

Corollary 2.1. The second K Banhatti polynomial of the molecular structure of remdesivir is

$$B_2(R,x) = 2x^3 + 14x^8 + 16x^{15} + 10x^{24} + 2x^{25}.$$

Corollary 2.2. The second hyper K Banhatti polynomial of the molecular structure of remdesivir is

$$HB_2(R,x) = 2x^5 + 9x^{32} + 5x^{40} + 14x^{117} + 2x^{153} + 6x^{288} + 4x^{320} + 2x^{625}.$$

Corollary 2.3. The modified second K Banhatti polynomial of the molecular structure of remdesivir is

$${}^{m}B_2(R,x) = 2x^{\frac{3}{2}} + 5x^{\frac{2}{3}} + 2x^{\frac{5}{12}} + 9x^{\frac{1}{2}} + 14x^{\frac{5}{18}} + 4x^{\frac{3}{16}} + 6x^{\frac{1}{6}} + 2x^{\frac{7}{60}}.$$

Corollary 2.4. The product connectivity K Banhatti polynomial of the molecular structure of remdesivir is

$$PB(R,x) = 2x^{1+\frac{1}{\sqrt{2}}} + 5x^{\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{6}}} + 2x^{\frac{1}{\sqrt{3}}+\frac{1}{\sqrt{12}}} + 9x + 14x^{\frac{1}{\sqrt{6}}+\frac{1}{3}}.$$

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

In the following theorem, we compute the *F*-*K* Banhatti polynomial of the molecular structure of remdesivir.

Theorem 3. Let *R* be the molecular structure of remdesivir. Then

$$FB(R,x) = 2x^{7} + 9x^{16} + 5x^{18} + 14x^{31}$$
$$+2x^{35} + 6x^{50} + 4x^{52} + 2x^{75}.$$

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

$$FB(R,x) = \sum_{ue} x^{d_R(u)^2 + d_R(e)^2}$$
$$= 2x^{(1^2+1^2)+(2^2+1^2)} + 5x^{(1^2+2^2)+(3^2+2^2)} + 2x^{(1^2+3^2)+(4^2+3^2)}$$
$$+9x^{(2^2+2^2)+(2^2+2^2)} + 14x^{(2^2+3^2)+(3^2+3^2)} + 4x^{(2^2+4^2)+(4^2+4^2)}$$
$$+6x^{(3^2+4^2)+(3^2+4^2)} + 2x^{(3^2+5^2)+(4^2+5^2)}$$
$$= 2x^{7} + 9x^{16} + 5x^{18} + 14x^{31}$$
$$+2x^{35} + 6x^{50} + 4x^{52} + 2x^{75}.$$

In the following theorem, the harmonic *K* Banhatti polynomial of the molecular structure of remdesivir.

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

$$H_b(R,x) = 2x^{\frac{5}{3}} + 5x^{\frac{16}{15}} + 2x^{\frac{11}{14}} + 9x$$
$$+14x^{\frac{11}{15}} + 4x^{\frac{7}{12}} + 6x^{\frac{4}{7}} + 2x^{\frac{17}{36}}.$$

Proof: Using definition and Table 2, we derive

$$H_b(R,x) = \sum_{ue} x^{\frac{2}{d_R(u)+d_R(e)}}$$
$$= 2x^{\frac{2}{1+1}+\frac{2}{2+1}} + 5x^{\frac{2}{1+2}+\frac{2}{3+2}} + 2x^{\frac{2}{1+3}+\frac{2}{4+3}}$$
$$+9x^{\frac{2}{2+2}+\frac{2}{2+2}} + 14x^{\frac{2}{2+3}+\frac{2}{3+3}} + 4x^{\frac{2}{2+4}+\frac{2}{4+4}}$$
$$+6x^{\frac{2}{3+4}+\frac{2}{3+4}} + 2x^{\frac{2}{3+5}+\frac{2}{4+5}}$$
$$= 2x^{\frac{5}{3}} + 5x^{\frac{16}{15}} + 2x^{\frac{11}{14}} + 9x$$
$$+14x^{\frac{11}{15}} + 4x^{\frac{7}{12}} + 6x^{\frac{4}{7}} + 2x^{\frac{17}{36}}.$$

In the following theorem, we determine the symmetric division *K* Banhatti polynomial of the molecular structure of remdesivir.

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

$$SDB(R,x) = 6x^{\frac{9}{2}} + 5x^{\frac{14}{3}} + 2x^{\frac{65}{12}} + 9x^{4} + 20x^{\frac{25}{6}} + 2x^{\frac{259}{60}}.$$

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

$$SDB(R,x) = \sum_{ue} x^{\frac{d_G(u)}{d_G(e)} + \frac{d_G(e)}{d_G(u)}}$$
$$= 2x^{\left(\frac{1}{1}+\frac{1}{1}\right)+\left(\frac{2}{1}+\frac{1}{2}\right)} + 5x^{\left(\frac{1}{2}+\frac{2}{1}\right)+\left(\frac{3}{2}+\frac{2}{3}\right)} + 2x^{\left(\frac{1}{2}+\frac{3}{1}\right)+\left(\frac{4}{3}+\frac{3}{4}\right)}$$
$$+9x^{\left(\frac{2}{2}+\frac{2}{2}\right)+\left(\frac{2}{2}+\frac{2}{2}\right)} + 14x^{\left(\frac{2}{3}+\frac{3}{2}\right)+\left(\frac{3}{3}+\frac{3}{3}\right)} + 4x^{\left(\frac{2}{4}+\frac{4}{2}\right)+\left(\frac{4}{4}+\frac{4}{4}\right)}$$
$$+6x^{\left(\frac{3}{4}+\frac{4}{3}\right)+\left(\frac{3}{4}+\frac{4}{3}\right)} + 2x^{\left(\frac{3}{5}+\frac{5}{3}\right)+\left(\frac{4}{5}+\frac{5}{4}\right)}$$
$$= 6x^{\frac{9}{2}} + 5x^{\frac{14}{3}} + 2x^{\frac{65}{12}} + 9x^{4} + 20x^{\frac{25}{6}} + 2x^{\frac{259}{60}}.$$

In the following theorem, we compute the inverse sum indeg *K* Banhatti polynomial of the molecular structure of remdesivir.

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

$$ISB(R,x) = 2x^{\frac{7}{6}} + 5x^{\frac{28}{15}} + 2x^{\frac{68}{28}} + 9x^{2}$$
$$+14x^{\frac{27}{10}} + 4x^{\frac{10}{3}} + 6x^{\frac{24}{7}} + 2x^{\frac{295}{72}}$$

Proof: Using definition and Table 2, we derive

$$ISB(R,x) = \sum_{ue} x^{\frac{d_R(u)d_R(e)}{d_R(u)+d_R(e)}}$$
$$= 2x^{\frac{1\times1}{1+1}+\frac{2\times1}{2+1}} + 5x^{\frac{1\times2}{1+2}+\frac{3\times2}{3+2}} + 2x^{\frac{1\times3}{1+3}+\frac{4\times3}{4+3}} + 9x^{\frac{2\times2}{2+2}+\frac{2\times2}{2+2}}$$
$$+14x^{\frac{2\times3}{2+3}+\frac{3\times3}{3+3}} + 4x^{\frac{2\times4}{2+4}+\frac{4\times4}{4+4}} + 6x^{\frac{3\times4}{3+4}+\frac{3\times4}{3+4}} + 2x^{\frac{3\times5}{3+5}+\frac{4\times5}{4+5}}$$
$$= 2x^{\frac{7}{6}} + 5x^{\frac{28}{15}} + 2x^{\frac{69}{28}} + 9x^{2}$$
$$+14x^{\frac{27}{10}} + 4x^{\frac{10}{3}} + 6x^{\frac{24}{7}} + 2x^{\frac{295}{72}}$$

III. RESULTS AND DISCUSSION : CHLOROQUINE

Let *G* be the molecular structure of chloroquine. Clearly *G* has 21 vertices and 23 edges, see Figure 2.

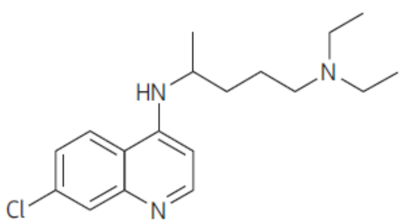

Figure 2

In *G*, the edge set *E*(*G*) can be divided into five partitions based on the degree of end vertices of each edge as given in Table 3.

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

Table 3. Edge partition of G

Thus the edge degree partition of chloroquine G is given in Table 4.

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

Table 4. Edge degree partition of G

In the following theorem, we determine the general first K Banhatti polynomial of the molecular structure of chloroquine.

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

$$B_1^a(G,x) = 2x^{2^a+3^a} + 2x^{3^a+5^a} + 5x^{4^a+4^a} + 12x^{5^a+6^a} + 2x^{7^a+7^a}. \quad (3)$$

Proof: Using definition and using Table 4, we deduce

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

$$= 2x^{(1+1)^a+(2+1)^a} + 2x^{(1+2)^a+(3+2)^a} + 5x^{(2+2)^a+(2+2)^a} + 12x^{(2+3)^a+(3+3)^a} + 2x^{(3+4)^a+(3+4)^a}$$

$$= 2x^{2^a+3^a} + 2x^{3^a+5^a} + 5x^{4^a+4^a} + 12x^{5^a+6^a} + 2x^{7^a+7^a}.$$

From Theorem 7, we establish the following results.

Corollary 7.1. The first K Banhatti polynomial of the molecular structure of chloroquine is

$$B_1(G,x) = 2x^5 + 7x^8 + 12x^{11} + 2x^{14}.$$

Corollary 7.2. The first hyper K Banhatti polynomial of the molecular structure of chloroquine is

$$HB_1(G,x) = 2x^{13} + 5x^{32} + 2x^{34} + 12x^{61} + 2x^{98}.$$

Corollary 7.3. The modified first K Banhatti polynomial of the molecular structure of chloroquine is

$${}^mB_1(G,x) = 2x^{\frac{5}{6}} + 2x^{\frac{8}{15}} + 5x^{\frac{1}{2}} + 12x^{\frac{11}{30}} + 2x^{\frac{2}{7}}.$$

Corollary 7.4. The sum connectivity K Banhatti polynomial of the molecular structure of chloroquine is

$$SB(G,x) = 2x^{\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}} + 2x^{\frac{1}{\sqrt{3}}+\frac{1}{\sqrt{5}}} + 5x + 12x^{\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{6}}} + 2x^{\frac{2}{\sqrt{7}}}.$$

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

In the following theorem, we compute the general second K Banhatti polynomial of the molecular structure of chloroquine.

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

$$B_2^a(G,x) = 2x^{1^a+2^a} + 2x^{2^a+6^a} + 5x^{4^a+4^a} + 12x^{6^a+9^a} + 2x^{12^a+12^a}. \quad (4)$$

Proof: From definition and by using Table 4, we derive

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

$$= 2x^{(1\times1)^a+(2\times1)^a} + 2x^{(1\times2)^a+(3\times2)^a} + 5x^{(2\times2)^a+(2\times2)^a} + 12x^{(2\times3)^a+(3\times3)^a} + 2x^{(3\times4)^a+(3\times4)^a}$$

$$= 2x^{1^a+2^a} + 2x^{2^a+6^a} + 5x^{4^a+4^a} + 12x^{6^a+9^a} + 2x^{12^a+12^a}.$$

We establish the following results from Theorem 8.

Corollary 8.1. The second K Banhatti polynomial of the molecular structure of chloroquine is

$$B_2(G,x) = 2x^3 + 7x^8 + 12x^{15} + 2x^{24}.$$

Corollary 8.2. The second hyper K Banhatti polynomial of the molecular structure of chloroquine is

$$HB_2(G,x) = 2x^5 + 5x^{32} + 2x^{40} + 12x^{117} + 2x^{288}.$$

Corollary 8.3. The modified second K Banhatti polynomial of the molecular structure of chloroquine is

$${}^mB_2(G,x) = 2x^{\frac{3}{2}} + 2x^{\frac{2}{3}} + 5x^{\frac{1}{2}} + 12x^{\frac{5}{18}} + 2x^{\frac{1}{6}}.$$

Corollary 8.4. The product connectivity K Banhatti polynomial of the molecular structure of chloroquine is

$$PB(G,x) = 2x^{1+\frac{1}{\sqrt{2}}} + 2x^{\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{6}}} + 5x + 12x^{\frac{1}{\sqrt{6}}+\frac{1}{3}} + 2x^{\frac{1}{\sqrt{3}}}.$$

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

In the following theorem, we determine the F-K Banhatti polynomial of the molecular structure of chloroquine.

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

$$FB(G,x) = 2x^7 + 5x^{16} + 2x^{18} + 12x^{31} + 2x^{50}.$$

Proof: Using definition and Table 4, we

$$FB(G,x) = \sum_{ue} x^{d_G(u)^2+d_G(e)^2}$$

$$= 2x^{(1^2+1^2)+(2^2+1^2)} + 2x^{(1^2+2^2)+(3^2+2^2)} + 5x^{(2^2+2^2)+(2^2+2^2)} + 12x^{(2^2+3^2)+(3^2+3^2)} + 2x^{(3^2+4^2)+(3^2+4^2)}.$$

$$= 2x^{7} + 5x^{16} + 2x^{18} + 12x^{31} + 2x^{50}.$$

In the following theorem, the harmonic *K* Banhatti polynomial of the molecular structure of chloroquine.

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

$$H_b(G,x) = 2x^{\frac{5}{3}} + 2x^{\frac{16}{15}} + 5x + 12x^{\frac{11}{15}} + 2x^{\frac{4}{7}}.$$

Proof: From definition and Table 4, we obtain

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

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

$$+12x^{\frac{2}{2+3}+\frac{2}{3+3}} + 2x^{\frac{2}{3+4}+\frac{2}{3+4}}$$

$$= 2x^{\frac{5}{3}} + 2x^{\frac{16}{15}} + 5x + 12x^{\frac{11}{15}} + 2x^{\frac{4}{7}}.$$

In the following theorem, we compute the symmetric division *K* Banhatti polynomial of the molecular structure of chloroquine.

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

$$SDB(G,x) = 2x^{\frac{9}{2}} + 2x^{\frac{14}{3}} + 5x^{4} + 14x^{\frac{25}{6}}.$$

Proof: From definition and by using Table 4, we deduce

$$SDB(G,x) = \sum_{ue} x^{\left(\frac{d_G(u)}{d_G(e)}+\frac{d_G(e)}{d_G(u)}\right)}$$

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

$$+12x^{\left(\frac{2}{3}+\frac{3}{2}\right)+\left(\frac{3}{3}+\frac{3}{3}\right)} + 2x^{\left(\frac{3}{4}+\frac{4}{3}\right)+\left(\frac{3}{4}+\frac{4}{3}\right)}$$

$$= 2x^{\frac{9}{2}} + 2x^{\frac{14}{3}} + 5x^{4} + 14x^{\frac{25}{6}}.$$

In the following theorem, we determine the inverse sum indeg *K* Banhatti polynomial of the molecular structure of chloroquine.

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

$$ISB(G,x) = 2x^{\frac{7}{6}} + 2x^{\frac{28}{15}} + 5x^{2} + 12x^{\frac{27}{10}} + 2x^{\frac{24}{7}}.$$

Proof: From definition and by using Table 4, we derive

$$ISB(G,x) = \sum_{ue} x^{\frac{d_G(u)d_G(e)}{d_G(u)+d_G(e)}}$$

$$= 2x^{\frac{1\times1}{1+1}+\frac{2\times1}{2+1}} + 2x^{\frac{1\times2}{1+2}+\frac{3\times2}{3+2}} + 5x^{\frac{2\times2}{2+2}+\frac{2\times2}{2+2}}$$

$$+12x^{\frac{2\times3}{2+3}+\frac{3\times3}{3+3}} + 2x^{\frac{3\times4}{3+4}+\frac{3\times4}{3+4}}$$

$$= 2x^{\frac{7}{6}} + 2x^{\frac{28}{15}} + 5x^{2} + 12x^{\frac{27}{10}} + 2x^{\frac{24}{7}}.$$

IV. RESULTS AND DISCUSSION: HYDROXYCHLOROQUINE

Let *H* be the molecular structure of hydroxychloroquine. By calculation, *H* has 22 vertices and 24 edges, see Figure 3.

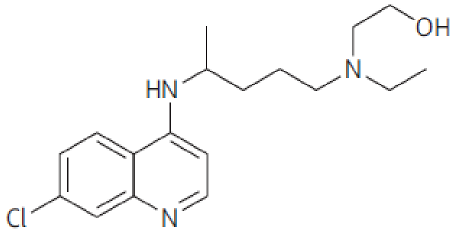

Figure 3

The edge set of *H* can be divided into five partitions based on degrees of end vertices of each edge as given in Table 5.

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

Table 5. Edge partition of *H*

Hence the edge degree partition of hydroxychloroquine is given in Table 6.

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

Table 6. Edge degree partition of *H*

In the following theorem, we determine the general first *K* Banhatti polynomial of the molecular structure of hydroxychloroquine.

Theorem 13. Let *H* be the molecular structure of hydroxychloroquine. Then

$$B_1^a(H,x) = 2x^{2^a+3^a} + 2x^{3^a+5^a} + 6x^{4^a+4^a}$$
$$+12x^{5^a+6^a} + 2x^{7^a+7^a}. \qquad (5)$$

Proof: From definition and by using Table 6, we obtain

$$B_1^a(H,x) = \sum_{ue} x^{[d_H(u)+d_H(e)]^a}$$

$$= 2x^{(1+1)^a+(2+1)^a} + 2x^{(1+2)^a+(3+2)^a} + 6x^{(2+2)^a+(2+2)^a}$$

$$+12x^{(2+3)^a+(3+3)^a} + 2x^{(3+4)^a+(3+4)^a}.$$

$$= 2x^{2^a+3^a} + 2x^{3^a+5^a} + 6x^{4^a+4^a}$$

$$+12x^{5^a+6^a} + 2x^{7^a+7^a}.$$

We obtain the following results by using Theorem 13.

Corollary 13.1. The first *K* Banhatti polynomial of the molecular structure of hydroxychloroquine *H* is

$$B_1(H,x) = 2x^{5} + 8x^{8} + 12x^{11} + 2x^{14}.$$

Corollary 13.2. The first hyper *K* Banhatti polynomial of the molecular structure of hydroxychloroquine *H* is

$$HB_1(H,x) = 2x^{13} + 6x^{32} + 2x^{34} + 12x^{61} + 2x^{98}.$$

Corollary 13.3. The modified first *K* Banhatti polynomial of the molecular structure of hydroxychloroquine *H* is

$$^{m}B_1(H,x) = 2x^{\frac{5}{6}} + 2x^{\frac{8}{15}} + 6x^{\frac{1}{2}} + 12x^{\frac{11}{30}} + 2x^{\frac{2}{7}}.$$

Corollary 13.4. The sum connectivity *K* Banhatti polynomial of the molecular structure of hydroxychloroquine is

$$SB(H,x) = 2x^{\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{3}}} + 2x^{\frac{1}{\sqrt{3}}+\frac{1}{\sqrt{5}}} + 6x + 12x^{\frac{1}{\sqrt{5}}+\frac{1}{\sqrt{6}}} + 2x^{\frac{2}{\sqrt{7}}}.$$

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

In the following theorem, we determine the general second *K* Banhatti polynomial of the molecular structure of hydroxychloroquine.

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

$$B_2^a(H,x) = 2x^{1^a+2^a} + 2x^{2^a+6^a} + 6x^{4^a+4^a} + 12x^{6^a+9^a} + 2x^{12^a+12^a}. \quad (6)$$

Proof: Using definition and Table 6, we deduce

$$B_2^a(H,x) = \sum_{ue} x^{[d_H(u)d_H(e)]^a}$$

$$= 2x^{(1\times1)^a+(2\times1)^a} + 2x^{(1\times2)^a+(3\times2)^a} + 6x^{(2\times2)^a+(2\times2)^a} + 12x^{(2\times3)^a+(3\times3)^a} + 2x^{(3\times4)^a+(3\times4)^a}.$$

$$= 2x^{1^a+2^a} + 2x^{2^a+6^a} + 6x^{4^a+4^a} + 12x^{6^a+9^a} + 2x^{12^a+12^a}.$$

We establish the following results from Theorem 14.

Corollary 14.1. The second *K* Banhatti polynomial of the molecular structure of hydroxychloroquine *H* is

$$B_2(H,x) = 2x^3 + 8x^8 + 12x^{15} + 2x^{24}.$$

Corollary 14.2. The second hyper *K* Banhatti polynomial of the molecular structure of hydroxychloroquine *H* is

$$HB_2(H,x) = 2x^5 + 6x^{32} + 2x^{40} + 12x^{117} + 2x^{288}.$$

Corollary 14.3. The modified second *K* Banhatti polynomial of the molecular structure of hydroxychloroquine *H* is

$$^{m}B_2(H,x) = 2x^{\frac{3}{2}} + 2x^{\frac{2}{3}} + 6x^{\frac{1}{2}} + 12x^{\frac{5}{18}} + 2x^{\frac{1}{6}}.$$

Corollary 14.4. The product connectivity *K* Banhatti polynomial of the molecular structure of hydroxychloroquine *H* is

$$PB(H,x) = 2x^{1+\frac{1}{\sqrt{2}}} + 2x^{\frac{1}{\sqrt{2}}+\frac{1}{\sqrt{6}}} + 6x + 12x^{\frac{1}{\sqrt{6}}+\frac{1}{3}} + 2x^{\frac{1}{\sqrt{3}}}.$$

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

In the following theorem, we compute the *F-K* Banhatti polynomial of the molecular structure of hydroxychloroquine.

Theorem 15. Let *H* be the molecular structure of hydroxychloroquine. Then

$$FB(H,x) = 2x^7 + 6x^{16} + 2x^{18} + 12x^{31} + 2x^{50}.$$

Proof: From definition and using Table 6, we obtain

$$FB(H,x) = \sum_{ue} x^{d_H(u)^2+d_H(e)^2}$$

$$= 2x^{(1^2+1^2)+(2^2+1^2)} + 2x^{(1^2+2^2)+(3^2+2^2)} + 6x^{(2^2+2^2)+(2^2+2^2)} + 12x^{(2^2+3^2)+(3^2+3^2)} + 2x^{(3^2+4^2)+(3^2+4^2)}$$

$$= 2x^7 + 6x^{16} + 2x^{18} + 12x^{31} + 2x^{50}.$$

In the following theorem, the harmonic *K* Banhatti polynomial of the molecular structure of hydroxychloroquine.

Theorem 16. Let *H* be the molecular structure of hydroxychloroquine. Then

$$H_b(H,x) = 2x^{\frac{5}{3}} + 2x^{\frac{16}{15}} + 6x + 12x^{\frac{11}{15}} + 2x^{\frac{4}{7}}.$$

Proof: From definition and using Table 6, we have

$$H_b(H,x) = \sum_{ue} x^{\frac{2}{d_H(u)+d_H(e)}}$$

$$= 2x^{\frac{2}{1+1}+\frac{2}{2+1}} + 2x^{\frac{2}{1+2}+\frac{2}{3+2}} + 6x^{\frac{2}{2+2}+\frac{2}{2+2}} + 12x^{\frac{2}{2+3}+\frac{2}{3+3}} + 2x^{\frac{2}{3+4}+\frac{2}{3+4}}$$

$$= 2x^{\frac{5}{3}} + 2x^{\frac{16}{15}} + 6x + 12x^{\frac{11}{15}} + 2x^{\frac{4}{7}}.$$

In the following theorem, we compute the symmetric division *K* Banhatti polynomial of the molecular structure of hydroxychloroquine.

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

$$SDB(H,x) = 2x^{\frac{9}{2}} + 2x^{\frac{14}{3}} + 6x^4 + 14x^{\frac{25}{6}}.$$

Proof: From definition and using Table 6, we deduce

$$SDR(H,x) = \sum_{ue} x^{\left(\frac{d_H(u)}{d_H(e)}+\frac{d_H(e)}{d_H(u)}\right)}$$

$$= 2x^{\left(\frac{1}{1}+\frac{1}{1}\right)+\left(\frac{2}{1}+\frac{1}{2}\right)} + 2x^{\left(\frac{1}{2}+\frac{2}{1}\right)+\left(\frac{3}{2}+\frac{2}{3}\right)} + 6x^{\left(\frac{2}{2}+\frac{2}{2}\right)+\left(\frac{2}{2}+\frac{2}{2}\right)} + 12x^{\left(\frac{2}{3}+\frac{3}{2}\right)+\left(\frac{3}{3}+\frac{3}{3}\right)} + 2x^{\left(\frac{3}{4}+\frac{4}{3}\right)+\left(\frac{3}{4}+\frac{4}{3}\right)}$$

$$= 2x^{\frac{9}{2}} + 2x^{\frac{14}{3}} + 6x^4 + 14x^{\frac{25}{6}}.$$

In the following theorem, we compute the inverse sum indeg K Banhatti polynomial of the molecular structure of hydroxychloroquine.

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

$$ISB(H,x) = 2x^{\frac{7}{6}} + 2x^{\frac{28}{15}} + 6x^2 + 12x^{\frac{27}{10}} + 2x^{\frac{24}{7}}.$$

Proof: From definition and Table 6, we derive

$$ISB(H,x) = \sum_{ue} x^{\frac{d_H(u)d_H(e)}{d_H(u)+d_H(e)}}$$

$$= 2x^{\frac{1\times1}{1+1}+\frac{2\times1}{2+1}} + 2x^{\frac{1\times2}{1+2}+\frac{3\times2}{3+2}} + 6x^{\frac{2\times2}{2+2}+\frac{2\times2}{2+2}}$$

$$+12x^{\frac{2\times3}{2+3}+\frac{3\times3}{3+3}} + 2x^{\frac{3\times4}{3+4}+\frac{3\times4}{3+4}}$$

$$= 2x^{\frac{7}{6}} + 2x^{\frac{28}{15}} + 6x^2 + 12x^{\frac{27}{10}} + 2x^{\frac{24}{7}}.$$

V. REFERENCES

[1] C.Huang, et al., "*Clinical features of patients infected with 2019 novel coronavirus in Wuhan, China*", *The Lancet* Vol. 395, 10223, pp. 497-506 2020, doi: 10.1016/S0140-6736(20) 30183-5.

[2] J.S. Morse, T Lalonde, S. Xu and M.R. Liu, "*Learning from the past: Possible urgent prevention and treatment options for severe acute respiratory infections caused by 2019 nCoV*", *Chem. Bio.Chem* 21(5) (2020) 730-738. doi:10.10D2/cbic.202000047.

[3] J.Lung, et al. "*The potential chemical structure of anti-SARS CoV-2 RNA dependent RNA polymerase*", *J. Med. Virol*, (2020) 1-5, doi:10-1002/jmv.25761.

[4] D.Wang, B. Hu, C. Hu, "*et al Clinical characteristics of 138 hospitalized patients with 2019 novel coronavirus-infected pneumonia in Wuhan, China*", *JAMA* (2020) doi:10.1001/jama-2020.1585.

[5] M.Wang, et al., Remdesivir and chloroquine "*effectively inhabit the recently emerged novel coronavirus (2019-nCoV) in vitro*", *Cell Research*, Vol. 30, pp. 269-271, 2020. doi:10.1038/s41422-020-0282-0.

[6] E.Schrenzenmeier and T. Dorner, "*Mechanisms of action of hydroxychloroquine and chloroquine implications of rheumatology*", *Nat. Rev. Rheumatol*, Vol. 16 (2020) 155-166.

[7] D.Zhou, S.M. Dai and Q. Tongg, "*COVID-19: a recommendation to examine the effect of hydroxychloroquine in preventing infection and progression*", *J. Antimicrob. Chemother*. 2020:dkaa 114, doi:10.1093/jac.dkaa114.

[8] X.Xu, et al., "*Evolution of the novel coronavirus from the ongoing Wuhan outbreak and modeling of its spike protein for risk of human transmission*", *Sci. China Life Sci.* Vol. 63(3). pp. 457-460, 2020 doi:10.1007/s 11427-020-1637-5.

[9] D.Plantone and T. Koudriavtseva, "*Current and future use of chloroquine and hydroxychloroquine in infections, immune, Neoplastic and Neurological disease: A Mini-Review*", *Clin. Drug Investing*, Vol. 38(8), pp. 653-671, 2018 doi: 10.1007/s40261-018-4056-y (PubMed: 29737455).

[10] "*FDA: Emergency Use Authorization Information (Link)".*

[11] I.Gutman and O.E. Polansky, "*Mathematical Concepts in Organic Chemistry",* Springer, Berlin (1986).

[12] V.R.Kulli, B. Chaluvaraju and T.V. Asha, "*Multiplicative product connectivity and sum connectivity indices of chemical structures in drugs*", Research Review International Journal of Multidisciplinary, 4(2) (2019) 949-953.

[13] V.R.Kulli, "*On K Banhatti indices of graphs*", Journal of Computer and Mathematical Sciences, 7(2016) 213-218.

[14] V.R.Kulli, "*On K hyper-Banhatti indices and coindices of graphs*", International Research Journal of Pure Algebra, 6(5) (2016) 300-304.

[15] V.R.Kulli, "*New K Banhatti topological indices*", International Journal of Fuzzy Mathematical Archive, 12(1) (2017) 29-37.

[16] V.R.Kulli, B. Chaluvaraju and H.S. Boregowda, "*Connectivity Banhatti indices for certain families of benzenoid systems*", *Journal of Ultra Chemistry*, 13(4) (2017) 81-87.

[17] V.R.Kulli, "*Computing Banhatti indices of networks*", International Journal of Advances in Mathematics, 2018(1) 2018) 31-40.

[18] V.R.Kulli, "*K Banhatti indices of chloroquine and hydroxychloroquine: Research Applied for the treatment and prevention of COVID-19*", SSRG International Journal of Applied Chemistry, 7(1)(2020) 63-68.

[19] V.R.Kulli, "*Revan indices of chloroquine and hydroxychloroquine, remdesivir: Research advances for the treatment of COVID-19*", International Journal of Engineering Sciences and Research Technology, 9(5) (2020) 73-84.

[20] V.R.Kulli, "*Revan indices of chloroquine and hydroxychloroquine, remdesivir: Research advances for the treatment of COVID-19*", SSRG International Journal of Applied Chemistry, 7(2) (2020) 6-12.