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NEW IRREGULARITY NIRMALA INDICES OF SOME CHEMICAL STRUCTURES

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ABSTRACT

Recently, a novel degree based topological index was introduced, the so called Nirmala index. In this paper, we introduce the first, second, third, fourth and fifth irregularity Nirmala indices of a graph and compute exact formulas for some important chemical structures of drugs such as chloroquine, hydroxychloroquine and remdesivir.

KEYWORDS: irregularity Nirmala indices, chemical structure.

Mathematics Subject Classification: 05C05, 05C07, 05C90.

1. INTRODUCTION

Let G be a finite, simple connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d(v)$ of a vertex v is the number of vertices adjacent to v. For additional definitions and notations, the reader may refer to [1].

A molecular graph is a graph whose vertices correspond to the atoms and the edges to the bonds. Chemical graph theory has an important effect on the development of chemical sciences. A single number that can be used to characterize some property of the graph of molecular is called a topological index. Several topological indices have been considered in Theoretical Chemistry, see [2].

In [3] Albertson introduced the irregularity index as

$$Alb(G) = \sum_{uv \in V(G)} |d(u) - d(v)|.$$

In [4], the Nirmala index of a molecular graph G was introduced and it is defined as

$$N(G) = \sum_{uv \in E(G)} [d(u) + d(v)]^{\frac{1}{2}}.$$

Recently, some Nirmala indices were studied, for example, in [5, 6, 7, 8, 9, 10, 11, 12].

The reciprocal minus connectivity index of a graph G is defined by Kulli in [13] as

$$RMic(G) = \sum_{uv \in V(G)} |d(u) - d(v)|^{\frac{1}{2}}.$$

We now call the reciprocal minus connectivity index as the first irregularity Nirmala index and it is denoted by $IN_1(G)$.

Motivated by the above research work, we introduce the second, third, fourth and fifth irregularity Nirmala indices of a graph as follows:

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The second irregularity Nirmala index of a molecular graph G is defined as

$$IN_2(G) = \sum_{uv \in V(G)} \left[|n(u) - n(v)|\right]^{\frac{1}{2}}$$

where the number $n(u)$ of vertices of G lying closer to the vertex u than to the vertex v for the edge uv of a graph G.

The third irregularity Nirmala index of a molecular graph G is defined as

$$IN_3(G) = \sum_{uv \in V(G)} \left[|m(u) - m(v)|\right]^{\frac{1}{2}}$$

where the number $m(u)$ of edges of G lying closer to the vertex u than to the vertex v for the edge uv of a graph G.

The fourth irregularity Nirmala index of a molecular graph G is defined as

$$IN_4(G) = \sum_{uv \in V(G)} \left[|\varepsilon(u) - \varepsilon(v)|\right]^{\frac{1}{2}}$$

where the number $\varepsilon(u)$ is the eccentricity of vertex u.

The fifth irregularity Nirmala index of a molecular graph G is defined as

$$IN_5(G) = \sum_{uv \in V(G)} \left[|s(u) - s(v)|\right]^{\frac{1}{2}}$$

where $s(u)$ denote the sum of the degrees of all vertices adjacent to vertex u.

The general minus index of a graph G is defined by Kulli in [13] as

$$M_i^a(G) = \sum_{uv \in V(G)} \left[|d(u) - d(v)|\right]^a.$$

Recently, some new topological indices were studied, for example, in [14, 15, 16, 17, 18,19,20, 21, 22, 23, 24, 25, 26, 27] and also some new versions of graph indices were studied, for example, in [28, 29, 30, 31, 32, 33, 34].

In this study, we compute the different types of the Nirmala indices of some significant molecular structures of drugs such as chloroquine, hydroxychloroquine, remdesivir. For molecular structures, see [35, 36].

2. RESULTS FOR CHLOROQUINE

Chloroquine is an antiviral compound (drug) which was discovered in 1934 by H.Andersag. This drug is medication primarily used to prevent and treat malaria.

Let G_1 be the chemical structure of chloroquine. This structure has 21 atoms and 23 bonds, see Figure 1.

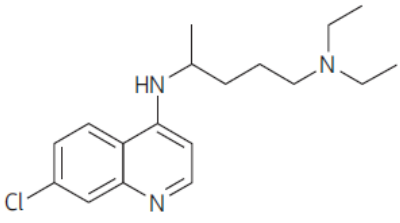

Figure 1. Chemical structure of chloroquine

From Figure 1, we obtain that

(i) $\{(d(u), d(v)) \setminus uv \in E(G_1)\}$ has 5 bond set partitions,

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(ii)$\{(n(u), n(v)) \setminus uv \in E(G_1)\}$ has 10 bond set partitions,
(iii)$\{(m(u), m(v)) \setminus uv \in E(G_1)\}$ has 12 bond set partitions,
(iv) $\{(\varepsilon(u), \varepsilon(v)) \setminus uv \in E(G_1)\}$ has 7 bond set partitions,
(iv) $\{(s(u), s(v)) \setminus uv \in E(G_1)\}$ has 10 bond set partitions.

Table 1. Bond set partitions of chloroquine

$d(u), d(v) \setminus uv \in E(G_1)$	(1, 2)	(1,3)	(2, 2)	(2, 3)	(3, 3)	
Number of bonds	2	2	5	12	2	
$n(u), n(v) \setminus uv \in E(G_1)$	(1,19)	(1,20)	(2,18)	(3,17)	(4,16)	
Number of bonds	2	4	2	4	1	
	(5,15)	(6,14)	(7,13)	(9,11)	(10,10)	
	4	1	3	1	1	
$m(u), m(v) \setminus uv \in E(G_1)$	(1,21)	(1,22)	(2,19)	(3,18)	(4,17)	(5,15)
Number of bonds	2	4	2	4	1	3
	(5,16)	(6,15)	(7,14)	(8,13)	(9,13)	(10,12)
	1	1	2	1	1	1
$\varepsilon(u), \varepsilon(v) \setminus uv \in E(G_1)$	(7,7)	(8,7)	(8,9)	(9,10)	(10,11)	
Number of bonds	1	3	3	4	5	
	(11,12)	(12,13)				
	4	3				
$s(u), s(v) \setminus uv \in E(G_1)$	(2,4)	(3,5)	(4,5)	(4,6)	(5,5)	
Number of bonds	2	2	4	2	3	
	(5,6)	(5,7)	(5,8)	(6,7)	(7,8)	
	3	2	1	2	2	

In the following theorem, we compute the different versions of Nirmala indices of chloroquine.

Theorem 1. Let G_1 be the chemical structure of chloroquine. Then

(i) $IN_1(G_1) = 16.8284271247.$

(ii) $IN_2(G_1) = 76.5918288668.$

(iii) $IN_3(G_1) = 81.3635125342.$

(iv) $IN_4(G_1) = 22.$

(v) $N_5(G_1) = 24.0457593066.$

Proof: By using the definitions and cardinalities of the bond partition of G_1, we deduce

(i) $$IN_1(G_1) = \sum_{uv \in V(G_1)} \left[|d(u) - d(v)|\right]^{\frac{1}{2}}$$

$$= (|1-2|)^{\frac{1}{2}} 2 + (|1-3|)^{\frac{1}{2}} 2 + (|2-2|)^{\frac{1}{2}} 5 + (|2-3|)^{\frac{1}{2}} 12 + (|3-3|)^{\frac{1}{2}} 2.$$

After simplification, we get the desired result.

(ii) $$IN_2(G_1) = \sum_{uv \in V(G_1)} \left[|n(u) - n(v)|\right]^{\frac{1}{2}}$$

$$= (|1-19|)^{\frac{1}{2}} 2 + (|1-20|)^{\frac{1}{2}} 4 + (|2-18|)^{\frac{1}{2}} 2 + (|3-17|)^{\frac{1}{2}} 4 + (|4-16|)^{\frac{1}{2}} 1$$

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$$+(|5-15|)^{\frac{1}{2}}4+(|6-14|)^{\frac{1}{2}}1+(|7-13|)^{\frac{1}{2}}3+(|9-11|)^{\frac{1}{2}}1+(|10-10|)^{\frac{1}{2}}1.$$

After simplification, we get the desired result.

(iii) $$IN_3(G_1)=\sum_{uv\in V(G_1)}\left[|m(u)-m(v)|\right]^{\frac{1}{2}}$$

$$=(|1-21|)^{\frac{1}{2}}2+(|1-22|)^{\frac{1}{2}}4+(|2-19|)^{\frac{1}{2}}2+(|3-18|)^{\frac{1}{2}}4+(|4-17|)^{\frac{1}{2}}1+(|5-15|)^{\frac{1}{2}}3$$
$$+(|5-16|)^{\frac{1}{2}}1+(|6-15|)^{\frac{1}{2}}1+(|7-14|)^{\frac{1}{2}}2+(|8-13|)^{\frac{1}{2}}1+(|9-13|)^{\frac{1}{2}}1+(|10-12|)^{\frac{1}{2}}1.$$

After simplification, we get the desired result.

(iv) $$IN_4(G_1)=\sum_{uv\in V(G_1)}\left[|\varepsilon(u)-\varepsilon(v)|\right]^{\frac{1}{2}}$$

$$=(|7-7|)^{\frac{1}{2}}1+(|8-7|)^{\frac{1}{2}}3+(|8-9|)^{\frac{1}{2}}3+(|9-10|)^{\frac{1}{2}}4+(|10-11|)^{\frac{1}{2}}5$$
$$+(|11-12|)^{\frac{1}{2}}4+(|12-13|)^{\frac{1}{2}}3.$$

After simplification, we get the desired result.

(v) $$IN_5(G_1)=\sum_{uv\in V(G_1)}\left[|s(u)-s(v)|\right]^{\frac{1}{2}}$$

$$=(|2-4|)^{\frac{1}{2}}2+(|3-5|)^{\frac{1}{2}}2+(|4-5|)^{\frac{1}{2}}4+(|4-6|)^{\frac{1}{2}}2+(|5-5|)^{\frac{1}{2}}3$$
$$+(|5-6|)^{\frac{1}{2}}3+(|5-7|)^{\frac{1}{2}}2+(|5-8|)^{\frac{1}{2}}1+(|6-7|)^{\frac{1}{2}}2+(|7-8|)^{\frac{1}{2}}2.$$

After simplification, we get the desired result.

3. RESULTS AND DISCUSSION: HYDROXYCHLOROQUINE

Hydroxychloroquine is another antiviral compound (drug) which has antiviral activity very similar to that of chloroquine. These compounds have been repurposed for the treatment of a number of other conditions including HIV, systemic lupus erythmatosus and rheumatoid arthritis .

Let G_2 be the chemical structure of hydroxychloroquine. This structure has 22 atoms and 24 bonds, see Figure 2.

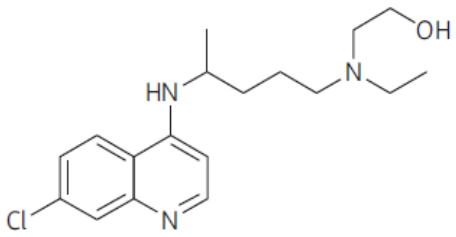

Figure 2. Chemical structure of hydroxychloroquine

From Figure 2, we obtain that
(i) $\{(d(u), d(v)) \setminus uv \in E(G_2)\}$ has 5 bond set partitions,
(ii)$\{(n(u), n(v)) \setminus uv \in E(G_2)\}$ has 9 bond set partitions,
(iii)$\{(m(u), m(v)) \setminus uv \in E(G_2)\}$ has 12 bond set partitions,
(iv) $\{(\varepsilon(u), \varepsilon(v)) \setminus uv \in E(G_2)\}$ has 7 bond set partitions,
(iv) $\{(s(u), s(v)) \setminus uv \in E(G_2)\}$ has 11 bond set partitions.

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Table 2. Bond set partitions of hydroxychloroquine

$d(u), d(v) \setminus uv \in E(G_2)$	(1, 2)	(1,3)	(2, 2)	(2, 3)	(3, 3)	
Number of bonds	2	2	6	12	2	
$n(u), n(v) \setminus uv \in E(G_2)$	(1,20)	(1,21)	(2,19)	(3,18)	(5,16)	
Number of bonds	2	4	3	4	4	
	(6,15)	(7,14)	(10,11)	(8,13)		
	3	2	1	1		
$m(u), m(v) \setminus uv \in E(G_2)$	(1,22)	(1,23)	(2,20)	(2,21)	(3,19)	(5,16)
Number of bonds	2	4	2	1	4	3
	(5,17)	(6,16)	(7,15)	(8,14)	(10,13)	(11,12)
	1	1	1	3	1	1
$\varepsilon(u), \varepsilon(v) \setminus uv \in E(G_2)$	(7,8)	(8,9)	(9,10)	(10,11)	(11,12)	
Number of bonds	3	2	3	4	6	
	(12,13)	(13,14)				
	4	2				
$s(u), s(v) \setminus uv \in E(G_2)$						
Number of bonds	(2,3)	(2,4)	(3,5)	(4,5)	(4,6)	(5,5)
	1	1	3	4	1	3
	(5,6)	(5,7)	(5,8)	(6,7)	(7,8)	
	4	2	1	2	2	

In the following theorem, we compute the different versions of Nirmala indices of hydroxychloroquine.

Theorem 2. Let G_2 be the chemical structure of hydroxychloroquine. Then

(i) $IN_1(G_2) = 16.8284271247.$

(ii) $IN_2(G_2) = 85.2616617298.$

(iii) $IN_3(G_2) = 86.256195554.$

(iv) $IN_4(G_2) = 24.$

(v) $IN_5(G_2) = 24.6315457442.$

Proof: By using the definitions and cardinalities of the bond partition of G_2, we deduce

(i) $$IN(G_2) = \sum_{uv \in V(G_2)} \left[|d(u) - d(v)|\right]^{\frac{1}{2}}$$

$$= (|1-2|)^{\frac{1}{2}} 2 + (|1-3|)^{\frac{1}{2}} 2 + (|2-2|)^{\frac{1}{2}} 6 + (|2-3|)^{\frac{1}{2}} 12 + (|3-3|)^{\frac{1}{2}} 2$$

$$= 14 + 2\sqrt{2}.$$

After simplification, we get the desired result.

(ii) $$IN_2(G_2) = \sum_{uv \in V(G_2)} \left[|n(u) - n(v)|\right]^{\frac{1}{2}}$$

$$= (|1-20|)^{\frac{1}{2}} 2 + (|1-21|)^{\frac{1}{2}} 4 + (|2-19|)^{\frac{1}{2}} 3 + (|3-18|)^{\frac{1}{2}} 4 + (|5-16|)^{\frac{1}{2}} 4$$

$$+ (|6-15|)^{\frac{1}{2}} 3 + (|7-14|)^{\frac{1}{2}} 2 + (|10-11|)^{\frac{1}{2}} 1 + (|8-13|)^{\frac{1}{2}} 1$$

$$= 2\sqrt{19} + 3\sqrt{17} + 4\sqrt{15} + 4\sqrt{11} + 2\sqrt{7} + 9\sqrt{5} + 10.$$

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After simplification, we get the desired result.

(iii) $$IN_3(G_2)=\sum_{uv\in V(G_2)}\left[|m(u)-m(v)|\right]^{\frac{1}{2}}$$

$$=(|1-22|)^{\frac{1}{2}}2+(|1-23|)^{\frac{1}{2}}4+(|2-20|)^{\frac{1}{2}}2+(|2-21|)^{\frac{1}{2}}1+(|3-19|)^{\frac{1}{2}}4+(|5-16|)^{\frac{1}{2}}3$$
$$+(|5-17|)^{\frac{1}{2}}1+(|6-16|)^{\frac{1}{2}}1+(|7-15|)^{\frac{1}{2}}1+(|8-14|)^{\frac{1}{2}}3+(|10-13|)^{\frac{1}{2}}1+(|11-12|)^{\frac{1}{2}}1$$
$$=4\sqrt{22}+\sqrt{19}+3\sqrt{11}+\sqrt{10}+3\sqrt{6}+4\sqrt{5}+3\sqrt{3}+8\sqrt{2}+17.$$

After simplification, we get the desired result.

(iv) $$IN_4(G_2)=\sum_{uv\in V(G_2)}\left[|\varepsilon(u)-\varepsilon(v)|\right]^{\frac{1}{2}}$$

$$=(|7-8|)^{\frac{1}{2}}3+(|8-9|)^{\frac{1}{2}}2+(|9-10|)^{\frac{1}{2}}3+(|10-11|)^{\frac{1}{2}}4+(|11-12|)^{\frac{1}{2}}6$$
$$+(|12-13|)^{\frac{1}{2}}4+(|13-14|)^{\frac{1}{2}}2$$
$$=24.$$

After simplification, we get the desired result.

(v) $$IN_5(G_2)=\sum_{uv\in V(G_2)}\left[|s(u)-s(v)|\right]^{\frac{1}{2}}$$

$$=(|2-3|)^{\frac{1}{2}}1+(|2-4|)^{\frac{1}{2}}1+(|3-5|)^{\frac{1}{2}}3+(|4-5|)^{\frac{1}{2}}4+(|4-6|)^{\frac{1}{2}}1+(|5-5|)^{\frac{1}{2}}3$$
$$+(|5-6|)^{\frac{1}{2}}4+(|5-7|)^{\frac{1}{2}}2+(|5-8|)^{\frac{1}{2}}1+(|6-7|)^{\frac{1}{2}}2+(|7-8|)^{\frac{1}{2}}2$$
$$=7\sqrt{2}+\sqrt{3}+13.$$

After simplification, we get the desired result.

4. RESULTS AND DISCUSSION: REMDESIVIR

Let G_3 be the molecular graph of remdesivir. This graph has 41 atoms and 44 bonds.

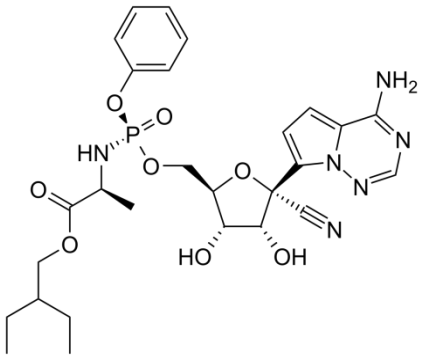

Figure 3. Chemical structure of remdesivir

From Figure 2, we obtain that
(i) $\{(d(u), d(v)) \setminus uv \in E(G_3)\}$ has 8 bond set partitions,
(ii)$\{(n(u), n(v)) \setminus uv \in E(G_3)\}$ has 25 bond set partitions,
(iii)$\{(m(u), m(v)) \setminus uv \in E(G_3)\}$ has 23 bond set partitions,
(iv) $\{(\varepsilon(u), \varepsilon(v)) \setminus uv \in E(G_3)\}$ has 11 bond set partitions,
(iv) $\{(s(u), s(v)) \setminus uv \in E(G_3)\}$ has 23 bond set partitions.

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Table 3. Bond set partitions of remdesivir

$d(u)$, $d(v)\setminus uv\in E(G_3)$	(1,2)	(1, 3)	(1, 4)	(2, 2)	(2, 3)	(2, 4)	(3, 3)	(3, 4)
Number of bonds	2	5	2	9	14	4	6	2
$n(u)$, $n(v)\setminus uv\in E(G_3)$	(1,6)	(1,34)	(1,38)	(1,39)	(2,37)	(3,12)	(3,23)	(3,36)
Number of bonds	1	1	2	9	8	1	1	2
	(4,32)	(4,33)	(4,34)	(4,35)	(5,34)	(6,32)	(6,33)	(8,31)
	1	1	1	1	2	1	2	1
	(9,30)	(10,29)	(11,28)	(12,24)	(13,24)	(13,25)	(17,22)	(18,21)
	1	1	1	1	1	1	1	1
	(19,20)							
	1							
$m(u)$,$m(v)\setminus uv\in E(G_3)$	(1,42)	(1,43)	(2,8)	(2,32)	(2,40)	(2,41)	(3,39)	(4,15)
Number of bonds	2	9	1	1	2	6	2	1
	(4,39)	(4,26)	(5,37)	(5,38)	(6,35)	(6,37)	(7,36)	(8,35)
	1	1	2	1	1	2	1	2
	(10,33)	(11,32)	(15,27)	(16,26)	(16,27)	(20,23)	(21,22)	
	1	2	1	1	1	1	2	
$\varepsilon(u)$,$\varepsilon(v)\setminus uv\in E(G_3)$	(9,10)	(10,11)	(11,12)	(12,13)	(13,13)	(13,14)	(14,15)	(15,16)
Number of bonds	2	4	4	7	1	7	5	4
	(16,16)	(16,17)	(17,18)					
	1	4	5					
$s(u)$,$s(v)\setminus uv\in E(G_3)$	(2,4)	(3,6)	(3,7)	(3,8)	(4,4)	(4,5)	(4,6)	(4,7)
Number of bonds	2	3	1	1	2	4	2	1
	(4,9)	(5,5)	(5,6)	(5,7)	(5,8)	(5,9)	(6,6)	(6,7)
	1	2	6	1	2	1	1	3
	(6,8)	(7,7)	(7,8)	(7,9)	(8,8)	(8,9)	(9,9)	
	1	4	1	1	1	2	1	

In the following theorem, we compute the different versions of Nirmala indices of remdesivir.

Theorem 3. Let G_3 be the chemical structure of remdesivir. Then

(i) $IN_1(G_3) = 34.1920236765.$

(ii) $IN_2(G_3) = 222.972451158.$

(iii) $IN_3(G_3) = 231.774038525.$

(iv) $IN_4(G_3) = 42.$

(v) $IN_5(G_3) = 44.763935737.$

Proof: By using the definitions and cardinalities of the bond partition of G_2, we deduce

(i) $$IN_1(G_3) = \sum_{uv\in V(G_3)} \left[|d(u)-d(v)|\right]^{\frac{1}{2}}$$

$$= (|1-2|)^{\frac{1}{2}}2 + (|1-3|)^{\frac{1}{2}}5 + (|1-4|)^{\frac{1}{2}}2 + (|2-2|)^{\frac{1}{2}}9 + (|2-3|)^{\frac{1}{2}}14$$

$$+ (|3-3|)^{\frac{1}{2}}6 + (|3-4|)^{\frac{1}{2}}2.$$

After simplification, we get the desired result.

(ii) $$IN_2(G_3) = \sum_{uv\in V(G_3)} \left[|n(u)-n(v)|\right]^{\frac{1}{2}}$$

$$= (|1-6|)^{\frac{1}{2}}1 + (|1-34|)^{\frac{1}{2}}1 + (|1-38|)^{\frac{1}{2}}2 + (|1-39|)^{\frac{1}{2}}9 + (|2-37|)^{\frac{1}{2}}8 + (|3-12|)^{\frac{1}{2}}1$$

$$+(|3-23|)^{\frac{1}{2}}1+(|3-36|)^{\frac{1}{2}}2+(|4-32|)^{\frac{1}{2}}1+(|4-33|)^{\frac{1}{2}}1+(|4-34|)^{\frac{1}{2}}1+(|4-35|)^{\frac{1}{2}}1$$
$$+(|5-34|)^{\frac{1}{2}}2+(|6-32|)^{\frac{1}{2}}1+(|6-33|)^{\frac{1}{2}}2+(|8-31|)^{\frac{1}{2}}1+(|9-30|)^{\frac{1}{2}}1+(|10-29|)^{\frac{1}{2}}1$$
$$+(|11-28|)^{\frac{1}{2}}1+(|12-24|)^{\frac{1}{2}}1+(|13-24|)^{\frac{1}{2}}1+(|13-25|)^{\frac{1}{2}}1+(|17-22|)^{\frac{1}{2}}1$$
$$+(|18-21|)^{\frac{1}{2}}1+(|19-20|)^{\frac{1}{2}}1.$$

After simplification, we get the desired result.

(iii) $$IN_3(G_3)=\sum_{uv\in V(G_3)}\left[|m(u)-m(v)|\right]^{\frac{1}{2}}$$

$$=(|1-42|)^{\frac{1}{2}}2+(|1-43|)^{\frac{1}{2}}9+(|2-8|)^{\frac{1}{2}}1+(|2-32|)^{\frac{1}{2}}1+(|2-40|)^{\frac{1}{2}}2+(|2-41|)^{\frac{1}{2}}6$$
$$+(|3-39|)^{\frac{1}{2}}2+(|4-15|)^{\frac{1}{2}}1+(|4-39|)^{\frac{1}{2}}1+(|4-26|)^{\frac{1}{2}}1+(|5-37|)^{\frac{1}{2}}2+(|5-38|)^{\frac{1}{2}}1$$
$$+(|6-35|)^{\frac{1}{2}}1+(|6-37|)^{\frac{1}{2}}2+(|7-36|)^{\frac{1}{2}}1+(|8-35|)^{\frac{1}{2}}2+(|10-33|)^{\frac{1}{2}}1+(|11-32|)^{\frac{1}{2}}2$$
$$+(|15-27|)^{\frac{1}{2}}1+(|6-26|)^{\frac{1}{2}}1+(|6-27|)^{\frac{1}{2}}1+(|20-23|)^{\frac{1}{2}}1+(|21-22|)^{\frac{1}{2}}2.$$

After simplification, we get the desired result.

(iv) $$IN_4(G_3)=\sum_{uv\in V(G_3)}\left[|\varepsilon(u)-\varepsilon(v)|\right]^{\frac{1}{2}}$$

$$=(|9-10|)^{\frac{1}{2}}2+(|10-11|)^{\frac{1}{2}}4+(|11-12|)^{\frac{1}{2}}4+(|12-13|)^{\frac{1}{2}}7+(|13-13|)^{\frac{1}{2}}1+(|13-14|)^{\frac{1}{2}}7$$
$$+(|14-15|)^{\frac{1}{2}}5+(|15-16|)^{\frac{1}{2}}4+(|16-16|)^{\frac{1}{2}}1+(|16-17|)^{\frac{1}{2}}4+(|17-18|)^{\frac{1}{2}}5.$$

After simplification, we get the desired result.

(v) $$IN_5(G_3)=\sum_{uv\in V(G_3)}\left[|s(u)-s(v)|\right]^{\frac{1}{2}}$$

$$=(|2-4|)^{\frac{1}{2}}2+(|3-6|)^{\frac{1}{2}}3+(|3-7|)^{\frac{1}{2}}1+(|3-8|)^{\frac{1}{2}}1+(|4-4|)^{\frac{1}{2}}2+(|4-5|)^{\frac{1}{2}}4$$
$$+(|4-6|)^{\frac{1}{2}}2+(|4-7|)^{\frac{1}{2}}1+(|4-9|)^{\frac{1}{2}}1+(|5-5|)^{\frac{1}{2}}2+(|5-6|)^{\frac{1}{2}}6+(|5-7|)^{\frac{1}{2}}1$$
$$+(|5-8|)^{\frac{1}{2}}2+(|5-9|)^{\frac{1}{2}}1+(|6-6|)^{\frac{1}{2}}1+(|6-7|)^{\frac{1}{2}}3+(|6-8|)^{\frac{1}{2}}1+(|7-7|)^{\frac{1}{2}}4$$
$$+(|7-8|)^{\frac{1}{2}}1+(|7-9|)^{\frac{1}{2}}1+(|8-8|)^{\frac{1}{2}}1+(|8-9|)^{\frac{1}{2}}2+(|9-9|)^{\frac{1}{2}}1.$$

After simplification, we get the desired result.

5. CONCLUSION

In this study, we have found computational values of molecular structures such as chloroquine, hydroxychloroquine and remdesivir. These values can be useful in planning the effective use of these drugs in Medical Science.

REFERENCES

[1] V.R.Kulli, *College Graph Theory*, Vishwa International Publications, Gulbarga, India (2012).
[2] V.R.Kulli, Graph indices, in *Hand Book of Research on Advanced Applications of Application Graph Theory in Modern Society*, M. Pal. S. Samanta and A. Pal, (eds.) IGI Global, USA (2019) 66-91.
[3] M.O.Albertson, The irregularity of a graph, *Ars Combnatoria*, 46 (1997) 219-225.
[4] V.R.Kulli, Nirmala index, *International Journal of Mathematics Trends and Technology*, 67(3) (2021) 8.12.

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[5] V.R.Kulli, V.Lokesha and Nirupadi K, Computation of inverse Nirmala indices of certain nanostructures, *International Journal of Mathematical Combinatorics*, 2 (2021) 32-39.
[6] V.R.Kulli, Neighborhood Nirmala index and its exponential of nanocones and dendrimers,*International Journal of Engineering Sciences and Research Technology*, 10(5) (2021) 47-56.
[7] V.R.Kulli, On multiplicative inverse Nirmala indices, *Annals of Pure and Applied Mathematics*, 23(2) (2021) 57-61.
[8] V.R.Kulli, Different versions of Nirmala index of certain chemical structures, *International Journal of Mathematics Trends and Technology*, 67(7) (2021) 56-63.
[9] V.R.Kulli, B.Chaluvaraju and T.V.Asha, Computation of Nirmala indices of some chemical networks, *Journal of Ultra Scientist of Physical Sciences-A*, 33(4) (2021) 30-41.
[10] V.R.Kulli and I.Gutman, On some mathematical properties of Nirmala index, *Annals of Pure and Applied Mathematics*, 23(2) (2021) 93-99.
[11] I.Gutman and V.R.Kulli, Nirmala energy, *Open Journal of Discrete Applied Mathematics*, 4(2) (2021) 11-16.
[12] I.Gutman, V.R.Kulli and I.Redzepovic, Nirmala index of Kragujevac trees, *International Journal of Mathematics Trends and Technology*, 67(6) (2021) 44-49.
[13] V.R.Kulli, Computation of some minus indices of titania nanotubes, *International Journal of Current Research in Science and Technology*, 4(12) (2018) 9-13.
[14] V.R.Kulli, Neighborhood Sombor index of some nanostructures, *International Journal of Mathematics Trends and Technology*, 67(5) (2021) 101-108.
[15] S.Alikhani and N.Ghanbari, Sombor index of polymers, *MATCH Commun. Math. Comput. Chem.* 86 (2021).
[16] R.Cruz, I.Gutman and J.Rada, Sombor index of chemical graphs, *Appl. Math. Comput.* 399 (2021) 126018.
[17] H.Deng, Z.Tang and R.Wu, Molecular trees with extremal values of Sombor indices, *Int. J. Quantum Chem.*DOI: 10.1002/qua.26622.
[18] B.Horoldagva and C.Xu, On Sombor index of graphs, *MATCH Commun. Math. Comput. Chem.* 86 (2021).
[19] V.R.Kulli, Sombor indices of certain graph operators, *International Journal of Engineering Sciences and Research Technology*, 10(1) (2021) 127-134.
[20] V.R.Kulli, Multiplicative Sombor indices of certain nanotubes, *International Journal of Mathematical Archive*, 12(3) (2021) 1-5.
[21] V.R.Kulli, δ-Sombor index and its exponential for certain nanotubes, *Annals of Pure and Applied Mathematics*, 23(1) (2021) 37-42.
[22] V.R.Kulli and I.Gutman, Computation of Sombor indices of certain networks, *SSRG International Journal of Applied Chemistry*, 8(1) (2021) 1-5.
[23] I.Redzepović, Chemical applicability of Sombor indices, *J. Serb. Chem. Soc.*(2021) https://doi.org/10.2298/JSC20:1215006R.
[24] T.Reti, T. Došlić and A. Ali, On the Sombor index of graphs, *Contributions of Mathematics*, 3 (2021) 11-18.
[25] V.R.Kulli, Computation of multiplicative Banhatti-Sombor indices of certain benzenoid systems, *International Journal of Mathematical Archive*, 12(4) (2021) 24-30.
[26] V.R.Kulli, On Banhatti-Sombor indices, *SSRG International Journal of Applied Chemistry*, 8(1) (2021) 21-25.
[27] V.R.Kulli, On second Banhatti-Sombor indices, *International Journal of Mathematical Archive*, 12(5) (2021) 11-16.
[28] M.Ghorbaniand and M.A.Hosseinzadeh, A new version of Zagreb indices, *Filomat*, 26(1) (2012) 93-100.
[29] A.Graovac and M.Ghorbani, A new version of atom bond connectivity index, *Acta Cimica Slovenica*, 57(2) (2010) 609-612
[30] V.R.Kulli, Two new multiplicative atom bond connectivity indices, *Annals of Pure and Applied Mathematics*, 13(1) (2017) 1-7.
[31] V.R.Kulli, Some new multiplicative geometric-arithmetic indices, *Journal of Ultra Scientist of Physical Sciences*, A, 29(2) (2017) 52-57.

[32] V.R.Kulli, New arithmetic-geometric indices, *Annals of Pure and Applied Mathematics*, 13(2) (2017) 165-172.
[33] V.R.Kulli, Different versions of multiplicative arithmetic-geometric indices of some chemical structures, *International Journal of Engineering Sciences and Research Technology*, 10(6) (2021) 34-44.
[34] V.R.Kulli, Some new versions of multiplicative geometric-arithmetic indices of certain chemical drugs, *International Journal of Mathematical Archive*, 12(7) (2021) 35-44.
[35] B.Chaluvaraju and A.B.Shaikh, Different versions of atom bond connectivity indices of some molecular structures: Applied for the treatment and prevention of COVID-19, *Polycyclic Aromatic Compounds*, DOI: 10.1080/10406638.2021.1872655.
[36] V.R.Kulli, Revan indices of chloroquine, hydroxychloroquine, remdesivir: Research Advances for the treatment of COVOD-19, *International Journal of Engineering Sciences and research technology*, 9(5) (2020) 73-84.