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New Irregularity Sombor Indices and New Adriatic (*a*, *b*)-*KA* Indices of Certain Chemical Drugs

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Abstract: *In Chemical Graph Theory, several degree based topological indices were introduced and studied. In this paper, we introduce some new irregularity Sombor indices: the first, second, third, fourth and fifth irregularity Sombor indices of a graph and compute the exact formulas for some important chemical drugs which appeared in Medical Science.. Also we introduce some Adriatic (a, b)-KA indices and compute the exact formulas for chloroquine and hydroxychloroquine.*

Keywords: *irregularity Sombor index, Adriatic (a, b)-KA index, chloroquine, hydroxychloroquine.*

Mathematics Subject Classification: 05*C*05, 05*C*12, 05*C*35.

I. Introduction

In Chemical Graph Theory, concerning the definition of the topological index on the molecular graph and concerning chemical properties of drugs can be studied by the topological index calculation, see [1]. Several degree based topological indices of a graph have been appeared in the literature, see [2, 3, 4, 5] and have found some applications, especially in QSPR/QSAR study, see [6, 7].

Let G be a finite, simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. The degree $d(u)$ of a vertex u is the number of vertices adjacent to u. Let $s(u)$ be the sum of the degrees of all vertices adjacent to vertex u. For undefined term and notation, we refer the book [8]

Minus F-index or nonzero Zagreb index was introduced and studied by Kulli in [9] and Jahabani et al. in [10], defined it as

$$MF(G)=\sum_{uv\in E(G)}\left|d(u)^2-d(v)^2\right|.$$

In [11], Gutman et al. introduced σ-index of a graph G, which is defined as σ(G)

$$\sigma(G)=\sum_{uv\in E(G)}\left[d(u)-d(v)\right]^2.$$

In [12], the Sombor index of a graph G was introduced and it is defined as

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

Recently, some Sombor indices were studied, for example, in [13, 14, 15, 16, 17, 18, 19, 20, 21].

We introduce the first irregularity Sombor index of a graph G and it is defined as

$$ISO_1(G)=\sum_{uv\in E(G)}\left[\left|d(u)^2-d(v)^2\right|\right]^{\frac{1}{2}}.$$

In [22], the Adriatic (a, b)-*KA* index of a graph G was introduced and it is defined as

$$AKA^1_{a,b}(G)=\sum_{uv\in E(G)}\left[\left|d(u)^a-d(v)^a\right|\right]^b$$

where a and b are a real numbers.
We call this index as the first Adriatic (a, b)-*KA* index of a graph.

We define the second irregularity minus F-index of a graph G as

$$IMF_2(G) = \sum_{uv \in E(G)} \left| n(u)^2 - n(v)^2 \right|$$

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.

We define the second irregularity σ-index of a graph G as

$$I\sigma_2(G) = \sum_{uv \in E(G)} \left[n(u) - n(v) \right]^2.$$

We introduce the second irregularity Sombor index of a graph G and it is defined as

$$ISO_2(G) = \sum_{uv \in E(G)} \left[\left| n(u)^2 - n(v)^2 \right| \right]^{\frac{1}{2}}.$$

We propose the second Adriatic (a, b)-*KA* index of a graph G and it is defined as

$$AKA_{a,b}^2(G) = \sum_{uv \in E(G)} \left[\left| n(u)^a - n(v)^a \right| \right]^b.$$

We define the third irregularity minus F-index of a graph G as

$$IMF_3(G) = \sum_{uv \in E(G)} \left| m(u)^2 - m(v)^2 \right|$$

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.

We define the third irregularity σ-index of a graph G as

$$I\sigma_3(G) = \sum_{uv \in E(G)} \left[m(u) - m(v) \right]^2.$$

We introduce the third irregularity Sombor index of a graph G and it is defined as

$$ISO_3(G) = \sum_{uv \in E(G)} \left[\left| m(u)^2 - m(v)^2 \right| \right]^{\frac{1}{2}}.$$

We propose the third Adriatic (a, b)-*KA* index of a graph G and it is defined as

$$AKA_{a,b}^3(G) = \sum_{uv \in E(G)} \left[\left| m(u)^a - m(v)^a \right| \right]^b.$$

We define the fourth irregularity minus F-index of G as

$$IMF_4(G) = \sum_{uv \in E(G)} \left| \varepsilon(u)^2 - \varepsilon(v)^2 \right|$$

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

We define the fourth irregularity σ-index of G as

$$I\sigma_4(G) = \sum_{uv \in E(G)} \left[\varepsilon(u) - \varepsilon(v) \right]^2.$$

We introduce the fourth irregularity Sombor index of a graph G and it is defined as

$$ISO_4(G) = \sum_{uv \in E(G)} \left[\left| \varepsilon(u)^2 - \varepsilon(v)^2 \right| \right]^{\frac{1}{2}}.$$

We propose the fourth Adriatic (a, b)-*KA* index of a graph G and it is defined as

$$AKA_{a,b}^4(G) = \sum_{uv \in E(G)} \left[\left| \varepsilon(u)^a - \varepsilon(v)^a \right| \right]^b.$$

We define the fifth irregularity minus F-index of a graph G as

$$IMF_5(G) = \sum_{uv \in E(G)} \left| s(u)^2 - s(v)^2 \right|$$

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

We define the fifth irregularity σ-index of a graph G as

$$I\sigma_5(G)=\sum_{uv\in E(G)}\left[s(u)-s(v)\right]^2.$$

We introduce the fifth irregularity Sombor index of a graph G and it is defined as

$$ISO_5(G)=\sum_{uv\in E(G)}\left[\left|s(u)^2-s(v)^2\right|\right]^{\frac{1}{2}}.$$

We propose the fifth Adriatic (a, b)-*KA* index and it is defined as

$$AKA_{a,b}^{5}(G)=\sum_{uv\in E(G)}\left[\left|s(u)^a-s(v)^a\right|\right]^{b}.$$

Recently, some new topological indices were studied, for example, in [23, 24, 25, 26, 27, 28, 29, 30, 31, 32]. Also some different versions of topological indices were studied in [33, 34, 35, 36, 37. 38,].

In this paper, we determine the first, second, third, fourth and fifth irregularity Sombor indices of some important chemical drugs such as chloroquine, hydrochloroquine, which appeared in Medical Science. Also we compute the first, second, third, fourth and fifth Adriatic (a, b)-*KA* indices of chloroquine and hydroxychloroquine. For chemical drugs, see [39, 40, 41].

II. RESULTS FOR CHLOROQUINE

Chloroquine is medication primarily used to prevent and treat malaria. Let G_1 be the graph of chloroquine. This graph has 21 vertices and 23 edges, see Figure 1, see [39].

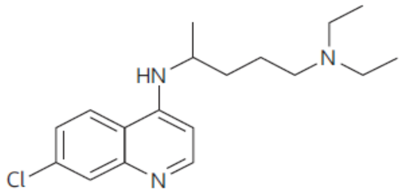

Figure 1. Molecular structure of chloroquine

From Figure 1, we obtain that (i) $\{(d(u), d(v)) \setminus uv \in E(G_1)\}$ has 5 edge set partitions,(ii)$\{(n(u), n(v)) \setminus uv \in E(G_1)\}$ has 10 edge set partitions,(iii)$\{(m(u), m(v)) \setminus uv \in E(G_1)\}$ has 12 edge set partitions,(iv) $\{(\varepsilon(u), \varepsilon(v)) \setminus uv \in E(G_1)\}$ has 7 edge set partitions,(v) $\{(s(u), s(v)) \setminus uv \in E(G_1)\}$ has 10 edge set partitions, see [39].

Table 1. Edge 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 edges	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 edges	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 edges	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 edges	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 edges	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 Adriatic (*a*, *b*)-*KA* index of chloroquine.

Theorem 1. Let G_1 be the graph of chloroquine. Then

$$AKA^{1}_{a,b}(G_1) = \left(\left|1^a - 2^a\right|\right)^b 2 + \left(\left|1^a - 3^a\right|\right)^b 2 + \left(\left|2^a - 3^a\right|\right)^b 12.$$

Proof: From definition and by using Table 1, we deduce

$$AKA^{1}_{a,b}(G_1) = \sum_{uv\in E(G_1)} \left[\left|d(u)^a - d(v)^a\right|\right]^b$$

$$= \left(\left|1^a - 2^a\right|\right)^b 2 + \left(\left|1^a - 3^a\right|\right)^b 2 + \left(\left|2^a - 2^a\right|\right)^b 5 + \left(\left|2^a - 3^a\right|\right)^b 12 + \left(\left|3^a - 3^a\right|\right)^b 2.$$

After simplification, we get the desired result.

From Theorem 1, we obtain the following results.

Corollary 1.1. Let G_1 be the graph of chloroquine. Then

(1) $MF(G_1) = AKA^{1}_{2,1}(G_1) = 82.$

(2) $\sigma(G_1) = AKA^{1}_{1,2}(G_1) = 22.$

(3) $ISO_1(G_1) = AKA^{1}_{2,\frac{1}{2}}(G_1) = 35.9537715946$

In the following theorem, we compute the second Adriatic (*a*, *b*)-*KA* index of chloroquine.

Theorem 2. Let G_1 be the graph of chloroquine. Then

$$AKA^{2}_{a,b}(G_1) = \left(\left|1^a - 19^a\right|\right)^b 2 + \left(\left|1^a - 20^a\right|\right)^b 4 + \left(\left|2^a - 18^a\right|\right)^b 2 + \left(\left|3^a - 17^a\right|\right)^b 4 + \left(\left|4^a - 16^a\right|\right)^b 1$$
$$+ \left(\left|5^a - 15^a\right|\right)^b 4 + \left(\left|6^a - 14^a\right|\right)^b 1 + \left(\left|7^a - 13^a\right|\right)^b 3 + \left(\left|9^a - 11^a\right|\right)^b 1.$$

Proof: From definition and by using Table 1, we deduce

$$AKA^{2}_{a,b}(G_1) = \sum_{uv\in E(G_1)} \left[\left|n(u)^a - n(v)^a\right|\right]^b$$

$$= \left(\left|1^a - 19^a\right|\right)^b 2 + \left(\left|1^a - 20^a\right|\right)^b 4 + \left(\left|2^a - 18^a\right|\right)^b 2 + \left(\left|3^a - 17^a\right|\right)^b 4 + \left(\left|4^a - 16^a\right|\right)^b 1$$
$$+ \left(\left|5^a - 15^a\right|\right)^b 4 + \left(\left|6^a - 14^a\right|\right)^b 1 + \left(\left|7^a - 13^a\right|\right)^b 3 + \left(\left|9^a - 11^a\right|\right)^b 1 + \left(\left|10^a - 10^a\right|\right)^b 1.$$

After simplification, we get the desired result.

From Theorem 2, we obtain the following results.

Corollary 2.1. Let G_1 be the graph of chloroquine. Then

(1) $IMF_2(G_1) = AKA^{2}_{2,1}(G_1) = 5676.$

(2) $I\sigma_2(G_1) = AKA^{2}_{1,2}(G_1) = 4108.$

(3) $ISO_2(G_1) = AKA^{2}_{2,\frac{1}{2}}(G_1) = 344.454654398$

In the following theorem, we compute the third Adriatic (*a*, *b*)-*KA* index of chloroquine.

Theorem 3. Let G_1 be the graph of chloroquine. Then

$$AKA^{3}_{a,b}(G_1) = \left(\left|1^a - 21^a\right|\right)^b 2 + \left(\left|1^a - 22^a\right|\right)^b 4 + \left(\left|2^a - 19^a\right|\right)^b 2 + \left(\left|3^a - 18^a\right|\right)^b 4 + \left(\left|4^a - 17^a\right|\right)^b 1$$
$$+ \left(\left|5^a - 15^a\right|\right)^b 3 + \left(\left|5^a - 16^a\right|\right)^b 1 + \left(\left|6^a - 15^a\right|\right)^b 1 + \left(\left|7^a - 14^a\right|\right)^b 2 + \left(\left|8^a - 13^a\right|\right)^b 1$$
$$+ \left(\left|9^a - 13^a\right|\right)^b 1 + \left(\left|10^a - 12^a\right|\right)^b 1.$$

Proof: From definition and by using Table 1, we deduce

$$AKA^{3}_{a,b}(G_1) = \sum_{uv\in E(G_1)} \left[\left|m(u)^a - m(v)^a\right|\right]^b$$

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

From Theorem 3, we obtain the following results.

Corollary 3.1. Let G_1 be the graph of chloroquine. Then

(1) $IMF_3(G_1)=AKA^3_{2,1}(G_1)=6610.$

(2) $I\sigma_3(G_1)=AKA^3_{1,2}(G_1)=4856.$

(3) $ISO_3(G_1)=AKA^3_{2,\frac{1}{2}}(G_1)=377.048515406$

In the following theorem, we compute the fourth Adriatic (*a*, *b*)-*KA* index of chloroquine.

Theorem 4. Let G_1 be the graph of chloroquine. Then

$$AKA^4_{a,b}(G_1)=\left(\left|8^a-7^a\right|\right)^b 3+\left(\left|8^a-9^a\right|\right)^b 3+\left(\left|9^a-10^a\right|\right)^b 4+\left(\left|10^a-11^a\right|\right)^b 5$$
$$+\left(\left|11^a-12^a\right|\right)^b 4+\left(\left|12^a-13^a\right|\right)^b 3.$$

Proof: From definition and by using Table 1, we deduce

$$AKA^4_{a,b}(G_1)=\sum_{uv\in E(G_1)}\left[\left|\varepsilon(u)^a-\varepsilon(v)^a\right|\right]^b$$
$$=\left(\left|7^a-7^a\right|\right)^b 1+\left(\left|8^a-7^a\right|\right)^b 3+\left(\left|8^a-9^a\right|\right)^b 3+\left(\left|9^a-10^a\right|\right)^b 4+\left(\left|10^a-11^a\right|\right)^b 5$$
$$+\left(\left|11^a-12^a\right|\right)^b 4+\left(\left|12^a-13^a\right|\right)^b 3.$$

From Theorem 4, we obtain the following results.

Corollary 4.1. Let G_1 be the graph of chloroquine. Then

(1) $IMF_4(G_1)=AKA^4_{2,1}(G_1)=444.$

(2) $I\sigma_4(G_1)=AKA^4_{1,2}(G_1)=22.$

(3) $ISO_4(G_1)=AKA^4_{2,\frac{1}{2}}(G_1)=98.5200672577$

In the following theorem, we compute the fifth Adriatic (*a*, *b*)-*KA* index of chloroquine.

Theorem 5. Let G_1 be the graph of chloroquine. Then

$$AKA^5_{a,b}(G_1)=\left(\left|2^a-4^a\right|\right)^b 2+\left(\left|3^a-5^a\right|\right)^b 2+\left(\left|4^a-5^a\right|\right)^b 4+\left(\left|4^a-6^a\right|\right)^b 2$$
$$+\left(\left|5^a-6^a\right|\right)^b 3+\left(\left|5^a-7^a\right|\right)^b 2+\left(\left|5^a-8^a\right|\right)^b 1+\left(\left|6^a-7^a\right|\right)^b 2+\left(\left|7^a-8^a\right|\right)^b 2.$$

Proof: From definition and by using Table 1, we deduce

$$AKA^5_{a,b}(G_1)=\sum_{uv\in E(G_1)}\left[\left|s(u)^a-s(v)^a\right|\right]^b$$
$$=\left(\left|2^a-4^a\right|\right)^b 2+\left(\left|3^a-5^a\right|\right)^b 2+\left(\left|4^a-5^a\right|\right)^b 4+\left(\left|4^a-6^a\right|\right)^b 2+\left(\left|5^a-5^a\right|\right)^b 3$$
$$+\left(\left|5^a-6^a\right|\right)^b 3+\left(\left|5^a-7^a\right|\right)^b 2+\left(\left|5^a-8^a\right|\right)^b 1+\left(\left|6^a-7^a\right|\right)^b 2+\left(\left|7^a-8^a\right|\right)^b 2.$$

From Theorem 5, we obtain the following results.

Corollary 5.1. Let G_1 be the graph of chloroquine. Then

(1) $IMF_5(G_1)=AKA^5_{2,1}(G_1)=308.$

(2) $I\sigma_5(G_1)=AKA^4_{1,2}(G_1)=52.$

(3) $ISO_5(G_1)=AKA^5_{2,\frac{1}{2}}(G_1)=76.8223757242$

III. RESULTS FOR HYDROXYCHLOROQUINE

Let G_2 be the graph of hydroxychloroquine. This graph has 22 vertices and 24 edges, see Figure 2, see [39].

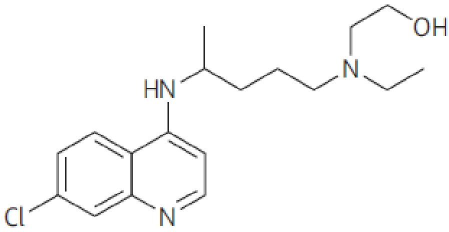

Figure 2. Molecular structure of hydroxychloroquine

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

Table 2. Edge 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 edges	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 edges	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 edges	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 edges	3	2	3	4	6	
	(12,13)	(13,14)				
	4	2				
$s(u), s(v) \setminus uv \in E(G_2)$	(2,3)	(2,4)	(3,5)	(4,5)	(4,6)	(5,5)
Number of edges	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 Adriatic (a, b)-KA index of hydroxychloroquine.

Theorem 6. Let G_2 be the graph of hydroxychloroquine. Then

$$AKA_{a,b}^{1}(G_2) = \left(\left|1^a - 2^a\right|\right)^b 2 + \left(\left|1^a - 3^a\right|\right)^b 2 + \left(\left|2^a - 3^a\right|\right)^b 12.$$

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

$$AKA_{a,b}^{1}(G_2) = \sum_{uv \in E(G_2)} \left[\left|d(u)^a - d(v)^a\right|\right]^b$$

$$= \left(\left|1^a - 2^a\right|\right)^b 2 + \left(\left|1^a - 3^a\right|\right)^b 2 + \left(\left|2^a - 2^a\right|\right)^b 5 + \left(\left|2^a - 3^a\right|\right)^b 12 + \left(\left|3^a - 3^a\right|\right)^b 2.$$

After simplification, we get the desired result.

From Theorem 6, we obtain the following results.

Corollary 6.1. Let G_2 be the graph of hydroxychloroquine. Then

(1) $MF\left(G_2\right) = AKA_{2,1}^{1}\left(G_2\right) = 82.$

(2) $\sigma(G_2) = AKA^1_{1,2}(G_2) = 22.$

(3) $ISO_1(G_2) = AKA^1_{2,\frac{1}{2}}(G_2) = 35.9537715946$

In the following theorem, we compute the second Adriatic (*a*, *b*)-*KA* index of hydroxychloroquine.

Theorem 7. Let G_2 be the graph of hydroxychloroquine. Then

$$AKA^2_{a,b}(G_2) = \left(\left|1^a - 19^a\right|\right)^b 2 + \left(\left|1^a - 20^a\right|\right)^b 4 + \left(\left|2^a - 18^a\right|\right)^b 2 + \left(\left|3^a - 17^a\right|\right)^b 4 + \left(\left|4^a - 16^a\right|\right)^b 1$$
$$+ \left(\left|5^a - 15^a\right|\right)^b 4 + \left(\left|6^a - 14^a\right|\right)^b 1 + \left(\left|7^a - 13^a\right|\right)^b 3 + \left(\left|9^a - 11^a\right|\right)^b 1.$$

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

$$AKA^2_{a,b}(G_2) = \sum_{uv \in E(G_2)} \left[\left|n(u)^a - n(v)^a\right|\right]^b$$
$$= \left(\left|1^a - 19^a\right|\right)^b 2 + \left(\left|1^a - 20^a\right|\right)^b 4 + \left(\left|2^a - 18^a\right|\right)^b 2 + \left(\left|3^a - 17^a\right|\right)^b 4 + \left(\left|4^a - 16^a\right|\right)^b 1$$
$$+ \left(\left|5^a - 15^a\right|\right)^b 4 + \left(\left|6^a - 14^a\right|\right)^b 1 + \left(\left|7^a - 13^a\right|\right)^b 3 + \left(\left|9^a - 11^a\right|\right)^b 1 + \left(\left|10^a - 10^a\right|\right)^b 1.$$

After simplification, we get the desired result.

From Theorem 7, we obtain the following results.

Corollary 7.1. Let G_2 be the graph of hydroxychloroquine. Then

(1) $IMF_2(G_2) = AKA^2_{2,1}(G_2) = 6800.$

(2) $I\sigma_2(G_2) = AKA^2_{1,2}(G_2) = 4840.$

(3) $ISO_2(G_2) = AKA^2_{2,\frac{1}{2}}(G_2) = 392.647120481$

In the following theorem, we compute the third Adriatic (*a*, *b*)-*KA* index of hydroxychloroquine.

Theorem 8. Let G_2 be the graph of hydroxychloroquine. Then

$$AKA^3_{a,b}(G_2) = \left(\left|1^a - 21^a\right|\right)^b 2 + \left(\left|1^a - 22^a\right|\right)^b 4 + \left(\left|2^a - 19^a\right|\right)^b 2 + \left(\left|3^a - 18^a\right|\right)^b 4 + \left(\left|4^a - 17^a\right|\right)^b 1$$
$$+ \left(\left|5^a - 15^a\right|\right)^b 3 + \left(\left|5^a - 16^a\right|\right)^b 1 + \left(\left|6^a - 15^a\right|\right)^b 1 + \left(\left|7^a - 14^a\right|\right)^b 2 + \left(\left|8^a - 13^a\right|\right)^b 1$$
$$+ \left(\left|9^a - 13^a\right|\right)^b 1 + \left(\left|10^a - 12^a\right|\right)^b 1.$$

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

$$AKA^3_{a,b}(G_2) = \sum_{uv \in E(G_2)} \left[\left|m(u)^a - m(v)^a\right|\right]^b$$
$$= \left(\left|1^a - 21^a\right|\right)^b 2 + \left(\left|1^a - 22^a\right|\right)^b 4 + \left(\left|2^a - 19^a\right|\right)^b 2 + \left(\left|3^a - 18^a\right|\right)^b 4 + \left(\left|4^a - 17^a\right|\right)^b 1$$
$$+ \left(\left|5^a - 15^a\right|\right)^b 3 + \left(\left|5^a - 16^a\right|\right)^b 1 + \left(\left|6^a - 15^a\right|\right)^b 1 + \left(\left|7^a - 14^a\right|\right)^b 2 + \left(\left|8^a - 13^a\right|\right)^b 1$$
$$+ \left(\left|9^a - 13^a\right|\right)^b 1 + \left(\left|10^a - 12^a\right|\right)^b 1.$$

From Theorem 8, we obtain the following results.

Corollary 8.1. Let G_1 be the graph of hydroxychloroquine. Then

(1) $IMF_3(G_2) = AKA^3_{2,1}(G_2) = 7556.$

(2) $I\sigma_3(G_2) = AKA^3_{1,2}(G_2) = 5640.$

(3) $ISO_3(G_2) = AKA^3_{2,\frac{1}{2}}(G_2) = 409.131075569$

In the following theorem, we compute the fourth Adriatic (*a*, *b*)-*KA* index of hydroxychloroquine.

Theorem 9. Let G_2 be the graph of hydroxychloroquine. Then

$$AKA^4_{a,b}(G_2) = \left(|8^a - 7^a|\right)^b 3 + \left(|8^a - 9^a|\right)^b 3 + \left(|9^a - 10^a|\right)^b 4 + \left(|10^a - 11^a|\right)^b 5 + \left(|11^a - 12^a|\right)^b 4 + \left(|12^a - 13^a|\right)^b 3.$$

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

$$AKA^4_{a,b}(G_2) = \sum_{uv \in E(G_2)} \left[\left|\varepsilon(u)^a - \varepsilon(v)^a\right|\right]^b$$
$$= \left(|7^a - 7^a|\right)^b 1 + \left(|8^a - 7^a|\right)^b 3 + \left(|8^a - 9^a|\right)^b 3 + \left(|9^a - 10^a|\right)^b 4 + \left(|10^a - 11^a|\right)^b 5 + \left(|11^a - 12^a|\right)^b 4 + \left(|12^a - 13^a|\right)^b 3.$$

From Theorem 9, we obtain the following results.

Corollary 9.1. Let G_2 be the graph of hydroxychloroquine. Then

(1) $IMF_4(G_2) = AKA^4_{2,1}(G_2) = 512.$

(2) $I\sigma_4(G_2) = AKA^4_{1,2}(G_2) = 24.$

(3) $ISO_4(G_2) = AKA^4_{2,\frac{1}{2}}(G_2) = 110.439454886$

In the following theorem, we compute the fifth Adriatic (*a*, *b*)-*KA* index of hydroxychloroquine.

Theorem 10. Let G_2 be the graph of hydroxychloroquine. Then

$$AKA^5_{a,b}(G_2) = \left(|2^a - 4^a|\right)^b 2 + \left(|3^a - 5^a|\right)^b 2 + \left(|4^a - 5^a|\right)^b 4 + \left(|4^a - 6^a|\right)^b 2 + \left(|5^a - 6^a|\right)^b 3 + \left(|5^a - 7^a|\right)^b 2 + \left(|5^a - 8^a|\right)^b 1 + \left(|6^a - 7^a|\right)^b 2 + \left(|7^a - 8^a|\right)^b 2.$$

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

$$AKA^5_{a,b}(G_2) = \sum_{uv \in E(G_2)} \left[\left|s(u)^a - s(v)^a\right|\right]^b$$
$$= \left(|2^a - 4^a|\right)^b 2 + \left(|3^a - 5^a|\right)^b 2 + \left(|4^a - 5^a|\right)^b 4 + \left(|4^a - 6^a|\right)^b 2 + \left(|5^a - 5^a|\right)^b 3 + \left(|5^a - 6^a|\right)^b 3 + \left(|5^a - 7^a|\right)^b 2 + \left(|5^a - 8^a|\right)^b 1 + \left(|6^a - 7^a|\right)^b 2 + \left(|7^a - 8^a|\right)^b 2.$$

From Theorem 10, we obtain the following results.

Corollary 10.1. Let G_2 be the graph of hydroxychloroquine. Then

(1) $IMF_5(G_2) = AKA^5_{2,1}(G_2) = 308.$

(2) $I\sigma_5(G_2) = AKA^5_{1,2}(G_2) = 50.$

(3) $ISO_5(G_2) = AKA^5_{2,\frac{1}{2}}(G_2) = 78.4388309219$

Conclusion

In this paper, we have introduced the first, second, third, fourth and fifth irregularity Sombor indices of a graph and we have also determined these newly defined irregularity Sombor indices for some important chemical drugs such as chloroquine, hydroxychloroquine, which appeared in Chemical Science. Furthermore, we have computed the first, second, third, fourth and fifth Adriatic (*a*, *b*)-*KA* indices for chloroquine and hydroxychloroquine.

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