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Computation of Modified Banhatti Sombor and Modified Diminished Sombor Indices of Certain Chemical Drugs

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Abstract: ***In this paper, we introduce the modified Banhatti Sombor and modified diminished Sombor indices of a graph. We compute these newly defined Sombor indices of certain chemical drugs. Furthermore, we compute the Banhatti Sombor and diminished Sombor indices of certain chemical drugs.***

Keywords: modified Banhatti Sombor index, modified diminished Sombor index, drug

1. Introduction

The simple graphs which are finite, undirected, connected graphs without loops and multiple edges are considered. Let G be such a 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.

In [1], Kulli introduced the Banhatti Sombor index and this index is defined as

$$BSO(G)=\sum_{uv\in E(G)}\frac{\sqrt{d_G(u)^2+d_G(v)^2}}{d_G(u)d_G(v)}.$$

Recently, some Sombor indices were studied in [2-7].

We define the modified Banhatti Sombor index of a graph G as

$$^{m}BSO(G)=\sum_{uv\in E(G)}\frac{d_G(u)d_G(v)}{\sqrt{d_G(u)^2+d_G(v)^2}}.$$

In [8], Rajathagiri introduced the diminished Sombor index and this index is defined as

$$DSO(G)=\sum_{uv\in E(G)}\frac{\sqrt{d_G(u)^2+d_G(v)^2}}{d_G(u)+d_G(v)}.$$

We define the modified diminished Sombor index of a graph G as

$$^{m}DSO(G)=\sum_{uv\in E(G)}\frac{d_G(u)+d_G(v)}{\sqrt{d_G(u)^2+d_G(v)^2}}.$$

In this research, we compute the modified Banhatti Sombor and modified diminished Sombor indices of certain chemical drugs.

2. Results and Discussion: Chloroquine

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

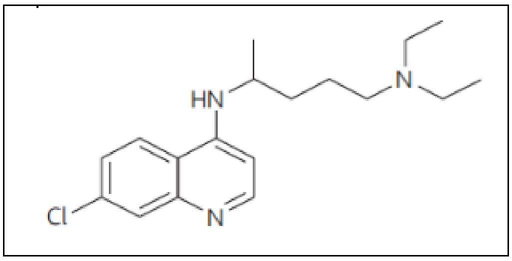

Figure 1

The edge set of G can be divided into five partitions based on the degree of end vertices of each edge as given in Table 1:

Table 1: Edge partition of G

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

We calculate the Banhatti Sombor and modified Banhatti Sombor indices of chloroquine as follows.

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

$$BSO(G)=\sqrt{5}+\frac{2\sqrt{10}}{3}+\frac{5\sqrt{2}}{2}+2\sqrt{13}+\frac{2\sqrt{2}}{3}.$$

Proof: By using the definitions and edge partition of G, we deduce

$$BSO(G)=\sum_{uv\in E(G)}\frac{\sqrt{d_G(u)^2+d_G(v)^2}}{d_G(u)d_G(v)}$$
$$=\frac{2\sqrt{1^2+2^2}}{1\times 2}+\frac{2\sqrt{1^2+3^2}}{1\times 3}+\frac{5\sqrt{2^2+2^2}}{2\times 2}$$
$$+\frac{12\sqrt{2^2+3^2}}{2\times 3}+\frac{2\sqrt{3^2+3^2}}{3\times 3}$$
$$=\sqrt{5}+\frac{2\sqrt{10}}{3}+\frac{5\sqrt{2}}{2}+2\sqrt{13}+\frac{2\sqrt{2}}{3}.$$

Theorem 2. Let G be the chemical structure of chloroquine. Then

$$^{m}BSO(G)=\frac{4}{\sqrt{5}}+\frac{6}{\sqrt{10}}+\frac{10}{\sqrt{2}}+\frac{72}{\sqrt{13}}+\frac{6}{\sqrt{2}}.$$

Proof: By using the definitions and edge partition of G, we deduce

$$^{m}BSO(G)=\sum_{uv\in E(G)}\frac{d_G(u)d_G(v)}{\sqrt{d_G(u)^2+d_G(v)^2}}$$
$$=\frac{2\times1\times2}{\sqrt{1^2+2^2}}+\frac{2\times1\times3}{\sqrt{1^2+3^2}}+\frac{5\times2\times2}{\sqrt{2^2+2^2}}$$
$$+\frac{12\times2\times3}{\sqrt{2^2+3^2}}+\frac{2\times3\times3}{\sqrt{3^2+3^2}}$$
$$=\frac{4}{\sqrt{5}}+\frac{6}{\sqrt{10}}+\frac{10}{\sqrt{2}}+\frac{72}{\sqrt{13}}+\frac{6}{\sqrt{2}}.$$

We calculate the diminished Sombor and modified diminished Sombor indices of chloroquine as follows.

Theorem 3. Let G be the chemical structure of chloroquine. Then

$$DSO(G)=\frac{2\sqrt{5}}{3}+\frac{\sqrt{10}}{2}+\frac{5\sqrt{2}}{2}+\frac{12\sqrt{13}}{5}+\sqrt{2}.$$

Proof: By using the definitions and edge partition of G, we deduce

$$DSO(G)=\sum_{uv\in E(G)}\frac{\sqrt{d_G(u)^2+d_G(v)^2}}{d_G(u)+d_G(v)}$$
$$=\frac{2\sqrt{1^2+2^2}}{1+2}+\frac{2\sqrt{1^2+3^2}}{1+3}+\frac{5\sqrt{2^2+2^2}}{2+2}$$
$$+\frac{12\sqrt{2^2+3^2}}{2+3}+\frac{2\sqrt{3^2+3^2}}{3+3}$$
$$=\frac{2\sqrt{5}}{3}+\frac{\sqrt{10}}{2}+\frac{5\sqrt{2}}{2}+\frac{12\sqrt{13}}{5}+\sqrt{2}.$$

Theorem 4. Let G be the chemical structure of chloroquine. Then

$$^{m}DSO(G)=\frac{6}{\sqrt{5}}+\frac{8}{\sqrt{10}}+\frac{10}{\sqrt{2}}+\frac{60}{\sqrt{13}}+\frac{4}{\sqrt{2}}.$$

Proof: By using the definitions and edge partition of G, we deduce

$$^{m}DSO(G)=\sum_{uv\in E(G)}\frac{d_G(u)+d_G(v)}{\sqrt{d_G(u)^2+d_G(v)^2}}$$
$$=\frac{2\times(1+2)}{\sqrt{1^2+2^2}}+\frac{2\times(1+3)}{\sqrt{1^2+3^2}}+\frac{5\times(2+2)}{\sqrt{2^2+2^2}}$$
$$+\frac{12\times(2+3)}{\sqrt{2^2+3^2}}+\frac{2\times(3+3)}{\sqrt{3^2+3^2}}$$
$$=\frac{6}{\sqrt{5}}+\frac{8}{\sqrt{10}}+\frac{10}{\sqrt{2}}+\frac{60}{\sqrt{13}}+\frac{4}{\sqrt{2}}.$$

3. Results and Discussion: Hydroxychloroquine

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

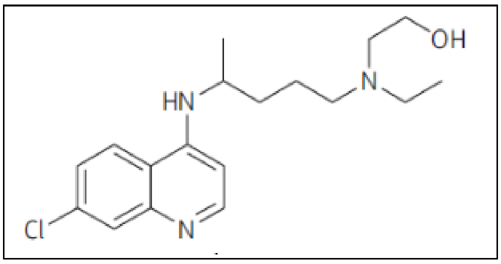

Figure 2

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 given in Table 2:

Table 2: Edge partition of H

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

We calculate the Banhatti Sombor and modified Banhatti Sombor indices of hydroxychloroquine as follows.

Theorem 5. Let H be the chemical structure of hydroxychloroquine. Then

$$BSO(H)=\sqrt{5}+\frac{2\sqrt{10}}{3}+3\sqrt{2}+2\sqrt{13}+\frac{2\sqrt{2}}{3}.$$

Proof: By using the definitions and edge partition of H, we deduce

$$BSO(H)=\sum_{uv\in E(H)}\frac{\sqrt{d_H(u)^2+d_H(v)^2}}{d_H(u)d_H(v)}$$
$$=\frac{2\sqrt{1^2+2^2}}{1\times2}+\frac{2\sqrt{1^2+3^2}}{1\times3}+\frac{6\sqrt{2^2+2^2}}{2\times2}$$
$$+\frac{12\sqrt{2^2+3^2}}{2\times3}+\frac{2\sqrt{3^2+3^2}}{3\times3}$$
$$=\sqrt{5}+\frac{2\sqrt{10}}{3}+3\sqrt{2}+2\sqrt{13}+\frac{2\sqrt{2}}{3}.$$

Theorem 6. Let H be the chemical structure of hydroxychloroquine. Then

$$^{m}BSO(H)=\frac{4}{\sqrt{5}}+\frac{6}{\sqrt{10}}+\frac{12}{\sqrt{2}}+\frac{72}{\sqrt{13}}+\frac{6}{\sqrt{2}}.$$

Proof: By using the definitions and edge partition of H, we deduce

$$^{m}BSO(H)=\sum_{uv\in E(H)}\frac{d_H(u)d_H(v)}{\sqrt{d_H(u)^2+d_H(v)^2}}$$
$$=\frac{2\times1\times2}{\sqrt{1^2+2^2}}+\frac{2\times1\times3}{\sqrt{1^2+3^2}}+\frac{6\times2\times2}{\sqrt{2^2+2^2}}$$
$$+\frac{12\times2\times3}{\sqrt{2^2+3^2}}+\frac{2\times3\times3}{\sqrt{3^2+3^2}}$$
$$=\frac{4}{\sqrt{5}}+\frac{6}{\sqrt{10}}+\frac{12}{\sqrt{2}}+\frac{72}{\sqrt{13}}+\frac{6}{\sqrt{2}}.$$

We calculate the diminished Sombor and modified diminished Sombor indices of hydroxychloroquine as follows.

Theorem 7. Let H be the chemical structure of hydroxychloroquine. Then

$$DSO(H)=\frac{2\sqrt{5}}{3}+\frac{\sqrt{10}}{2}+3\sqrt{2}+\frac{12\sqrt{13}}{5}+\sqrt{2}.$$

Proof: By using the definitions and edge partition of H, we deduce

$$DSO(H)=\sum_{uv\in E(H)}\frac{\sqrt{d_H(u)^2+d_H(v)^2}}{d_H(u)+d_H(v)}$$

$$=\frac{2\sqrt{1^2+2^2}}{1+2}+\frac{2\sqrt{1^2+3^2}}{1+3}+\frac{6\sqrt{2^2+2^2}}{2+2}$$

$$+\frac{12\sqrt{2^2+3^2}}{2+3}+\frac{2\sqrt{3^2+3^2}}{3+3}$$

$$=\frac{2\sqrt{5}}{3}+\frac{\sqrt{10}}{2}+3\sqrt{2}+\frac{12\sqrt{13}}{5}+\sqrt{2}.$$

Theorem 8. Let H be the chemical structure of hydroxychloroquine. Then

$$^{m}DSO(H)=\frac{6}{\sqrt{5}}+\frac{8}{\sqrt{10}}+\frac{12}{\sqrt{2}}+\frac{60}{\sqrt{13}}+\frac{4}{\sqrt{2}}.$$

Proof: By using the definitions and edge partition of H, we deduce

$$^{m}DSO(H)=\sum_{uv\in E(H)}\frac{d_H(u)+d_H(v)}{\sqrt{d_H(u)^2+d_H(v)^2}}$$

$$=\frac{2\times(1+2)}{\sqrt{1^2+2^2}}+\frac{2\times(1+3)}{\sqrt{1^2+3^2}}+\frac{6\times(2+2)}{\sqrt{2^2+2^2}}$$

$$+\frac{12\times(2+3)}{\sqrt{2^2+3^2}}+\frac{2\times(3+3)}{\sqrt{3^2+3^2}}$$

$$=\frac{6}{\sqrt{5}}+\frac{8}{\sqrt{10}}+\frac{12}{\sqrt{2}}+\frac{60}{\sqrt{13}}+\frac{4}{\sqrt{2}}.$$

4. Results and Discussion: Remdesivir

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

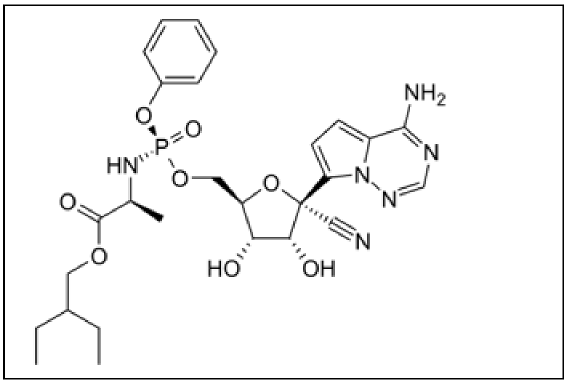

Figure 3

In R, the edge set $E(R)$ can be divided into eight partitions based on the degree of end vertices of each edge as given in Table 3:

Table 3: Edge partition of R

$d_G(u), d_G(v)\backslash uv\in E(R)$	(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

We calculate the Banhatti Sombor and modified Banhatti Sombor indices of remdesivir as follows.

Theorem 9. Let R be the chemical structure of remdesivir. Then

$$BSO(R)=2\sqrt{5}+\frac{5\sqrt{10}}{3}+\frac{\sqrt{17}}{2}$$

$$+\frac{9\sqrt{2}}{2}+\frac{7\sqrt{13}}{3}+2\sqrt{2}+\frac{5}{6}.$$

Proof: By using the definitions and edge partition of R, we deduce

$$BSO(R)=\sum_{uv\in E(R)}\frac{\sqrt{d_R(u)^2+d_R(v)^2}}{d_R(u)d_R(v)}$$

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

$$+\frac{9\sqrt{2^2+2^2}}{2\times 2}+\frac{14\sqrt{2^2+3^2}}{2\times 3}+\frac{4\sqrt{2^2+4^2}}{2\times 4}$$

$$+\frac{6\sqrt{3^2+3^2}}{3\times 3}+\frac{2\sqrt{3^2+4^2}}{3\times 4}$$

$$=2\sqrt{5}+\frac{5\sqrt{10}}{3}+\frac{\sqrt{17}}{2}+\frac{9\sqrt{2}}{2}+\frac{7\sqrt{13}}{3}+2\sqrt{2}+\frac{5}{6}.$$

Theorem 10. Let R be the chemical structure of remdesivir. Then

$$^{m}BSO(R)=\frac{20}{\sqrt{5}}+\frac{15}{\sqrt{10}}+\frac{8}{\sqrt{17}}+\frac{36}{\sqrt{2}}+\frac{84}{\sqrt{13}}+\frac{24}{5}.$$

Proof: By using the definitions and edge partition of H, we deduce

$$^{m}BSO(R)=\sum_{uv\in E(R)}\frac{d_R(u)d_R(v)}{\sqrt{d_R(u)^2+d_R(v)^2}}$$

$$=\frac{2\times(1\times 2)}{\sqrt{1^2+2^2}}+\frac{5\times(1\times 3)}{\sqrt{1^2+3^2}}+\frac{2\times(1\times 4)}{\sqrt{1^2+4^2}}+\frac{9\times(2\times 2)}{\sqrt{2^2+2^2}}$$

$$+\frac{14\times(2\times 3)}{\sqrt{2^2+3^2}}+\frac{4\times(2\times 4)}{\sqrt{2^2+4^2}}+\frac{6\times(3\times 3)}{\sqrt{3^2+3^2}}+\frac{2\times(3\times 4)}{\sqrt{3^2+4^2}}$$

$$=\frac{20}{\sqrt{5}}+\frac{15}{\sqrt{10}}+\frac{8}{\sqrt{17}}+\frac{36}{\sqrt{2}}+\frac{84}{\sqrt{13}}+\frac{24}{5}.$$

We calculate the diminished Sombor and modified diminished Sombor indices of remdesivir as follows.

Theorem 11. Let R be the chemical structure of remdesivir. Then

$$DSO(R)=\frac{2\sqrt{5}}{3}+\frac{5\sqrt{10}}{4}+\frac{2\sqrt{17}}{5}+\frac{9\sqrt{2}}{2}+\frac{14\sqrt{13}}{5}+\frac{4\sqrt{5}}{3}+3\sqrt{2}+\frac{10}{7}.$$

Proof: By using the definitions and edge partition of R, we deduce

$$DSO(R)=\sum_{uv\in E(R)}\frac{\sqrt{d_R(u)^2+d_R(v)^2}}{d_R(u)+d_R(v)}$$
$$=\frac{2\sqrt{1^2+2^2}}{1+2}+\frac{5\sqrt{1^2+3^2}}{1+3}+\frac{2\sqrt{1^2+4^2}}{1+4}+\frac{9\sqrt{2^2+2^2}}{2+2}+\frac{14\sqrt{2^2+3^2}}{2+3}+\frac{4\sqrt{2^2+4^2}}{2+4}+\frac{6\sqrt{3^2+3^2}}{3+3}+\frac{2\sqrt{3^2+4^2}}{3+4}$$
$$=\frac{2\sqrt{5}}{3}+\frac{5\sqrt{10}}{4}+\frac{2\sqrt{17}}{5}+\frac{9\sqrt{2}}{2}+\frac{14\sqrt{13}}{5}+\frac{4\sqrt{5}}{3}+3\sqrt{2}+\frac{10}{7}.$$

Theorem 12. Let R be the chemical structure of remdesivir. Then

$$^{m}DSO(R)=\frac{18}{\sqrt{5}}+\frac{20}{\sqrt{10}}+\frac{10}{\sqrt{17}}+\frac{30}{\sqrt{2}}+\frac{70}{\sqrt{13}}+\frac{14}{5}.$$

Proof: By using the definitions and edge partition of R, we deduce

$$^{m}DSO(R)=\sum_{uv\in E(R)}\frac{d_R(u)+d_R(v)}{\sqrt{d_R(u)^2+d_R(v)^2}}$$
$$=\frac{2(1+2)}{\sqrt{1^2+2^2}}+\frac{5(1+3)}{\sqrt{1^2+3^2}}+\frac{2(1+4)}{\sqrt{1^2+4^2}}+\frac{9(2+2)}{\sqrt{2^2+2^2}}+\frac{14(2+3)}{\sqrt{2^2+3^2}}+\frac{4(2+4)}{\sqrt{2^2+4^2}}+\frac{6(3+3)}{\sqrt{3^2+3^2}}+\frac{2(3+4)}{\sqrt{3^2+4^2}}$$
$$=\frac{18}{\sqrt{5}}+\frac{20}{\sqrt{10}}+\frac{10}{\sqrt{17}}+\frac{30}{\sqrt{2}}+\frac{70}{\sqrt{13}}+\frac{14}{5}.$$

5. Conclusion

In this research, we have computed the modified Banhatti Sombor and modified diminished Sombor indices of certain chemical drugs. Also we have computed the Banhatti Sombor and diminished Sombor indices of certain chemical drugs.

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