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Degree Ratio Euler Sombor Index of Certain Chemical Drugs

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Abstract: ***In this paper, we introduce the degree ratio Euler Sombor and the reciprocal degree ratio Euler Sombor indices of a graph. We compute these newly defined degree ratio Euler Sombor indices for certain chemical drugs.***

Keywords: degree ratio Euler Sombor index, reciprocal degree ratio Euler 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], the degree ratio Nirmala index of a graph is defined as

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

The Euler Sombor index [2] or Nirmala alpha Gourava index [3] of a graph is defined as

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

Recently, some Sombor indices were studied in [4-10].

We define the degree ratio Euler Sombor index of a graph G as

$$DREU(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G(u)^2}{d_G(v)^2} + \frac{d_G(v)^2}{d_G(u)^2} + 1}.$$

We define the reciprocal degree ratio Euler Sombor index of a graph G as

$$RDREU(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G(u)^2 d_G(v)^2}{d_G(u)^4 + d_G(v)^4 + d_G(u)^2 d_G(v)^2}}.$$

In this research, we compute the degree ratio Euler Sombor and reciprocal degree ratio Euler Sombor indices for 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.

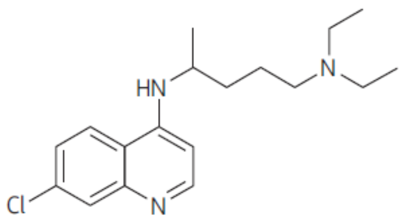

Figure 1

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

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

We calculate the degree ratio Euler Sombor and reciprocal degree ratio Euler Sombor indices of chloroquine as follows.

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

$$DREU(G) = \sqrt{21} + \frac{2}{3}\sqrt{91} + 2\sqrt{133} + 7\sqrt{3}.$$

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

$$DREU(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_G(u)^2}{d_G(v)^2} + \frac{d_G(v)^2}{d_G(u)^2} + 1}$$

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

$$+12\sqrt{\frac{2^2}{3^2} + \frac{3^2}{2^2} + 1} + 2\sqrt{\frac{3^2}{3^2} + \frac{3^2}{3^2} + 1}$$

$$= \sqrt{21} + \frac{2}{3}\sqrt{91} + 2\sqrt{133} + 7\sqrt{3}.$$

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

$$RDREU(G) = 4\sqrt{\frac{1}{21}} + 6\sqrt{\frac{1}{91}} + 7\sqrt{\frac{1}{3}} + 72\sqrt{\frac{1}{133}}.$$

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

$$RDREU(G)=\sum_{uv\in E(G)}\sqrt{\frac{d_G(u)^2\,d_G(v)^2}{d_G(u)^4+d_G(v)^4+d_G(u)^2\,d_G(v)^2}}$$

$$=2\sqrt{\frac{1^2\times2^2}{1^4+2^4+1^2\times2^2}}+2\sqrt{\frac{1^2\times3^2}{1^4+3^4+1^2\times3^2}}+5\sqrt{\frac{2^2\times2^2}{2^4+2^4+2^2\times2^2}}$$

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

$$=4\sqrt{\frac{1}{21}}+6\sqrt{\frac{1}{91}}+7\sqrt{\frac{1}{3}}+72\sqrt{\frac{1}{133}}.$$

3. Results and Discussion: Hydroxychloroquine

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

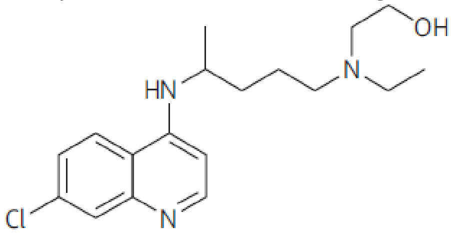

Figure 2

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 degree ratio Euler Sombor and reciprocal degree ratio Euler Sombor indices of hydroxychloroquine as follows.

Theorem 3. Let H be the chemical structure of hydroxychloroquine. Then

$$DREU(H)=2\sqrt{7}+2\sqrt{\frac{13}{2}}+6\sqrt{6}+12\sqrt{\frac{19}{3}}+\sqrt{\frac{27}{4}}.$$

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

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

$$=2\sqrt{\frac{1^2+2^2+1\times2}{1+2-2}}+2\sqrt{\frac{1^2+3^2+1\times3}{1+3-2}}+6\sqrt{\frac{2^2+2^2+2\times2}{2+2-2}}$$

$$+12\sqrt{\frac{2^2+3^2+2\times3}{2+3-2}}+2\sqrt{\frac{3^2+3^2+3\times3}{3+3-2}}$$

$$=2\sqrt{7}+2\sqrt{\frac{13}{2}}+6\sqrt{6}+12\sqrt{\frac{19}{3}}+\sqrt{\frac{27}{4}}.$$

Theorem 4. Let H be the chemical structure of hydroxychloroquine. Then

$$RDREU(H)=2\sqrt{\frac{1}{7}}+2\sqrt{\frac{2}{13}}6\sqrt{\frac{1}{6}}+12\sqrt{\frac{3}{19}}+2\sqrt{\frac{4}{27}}.$$

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

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

$$=2\sqrt{\frac{1+2-2}{1^2+2^2+1\times2}}+2\sqrt{\frac{1+3-2}{1^2+3^2+1\times3}}+6\sqrt{\frac{2+2-2}{2^2+2^2+2\times2}}$$

$$+12\sqrt{\frac{2+3-2}{2^2+3^2+2\times3}}+2\sqrt{\frac{3+3-2}{3^2+3^2+3\times3}}$$

$$=2\sqrt{\frac{1}{7}}+2\sqrt{\frac{2}{13}}+6\sqrt{\frac{1}{6}}+12\sqrt{\frac{3}{19}}+2\sqrt{\frac{4}{27}}.$$

4. Results and Discussion: REMDESVIR

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

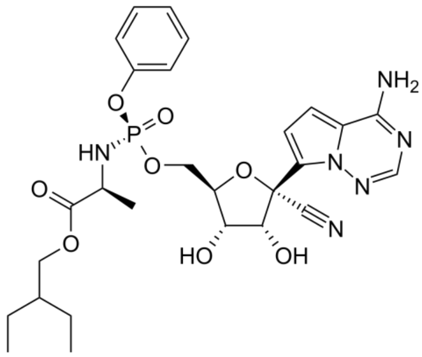

Figure 3

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 degree ratio Euler Sombor and reciprocal degree ratio Euler Sombor indices of remdesivir as follows.

Theorem 5. Let R be the chemical structure of remdesivir. Then

$$DREU(R)=8\sqrt{7}+5\sqrt{\frac{13}{2}}+9\sqrt{6}+14\sqrt{\frac{19}{3}}+6\sqrt{\frac{27}{4}}+2\sqrt{\frac{37}{5}}.$$

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

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

$$=2\sqrt{\frac{1^2+2^2+1\times2}{1+2-2}}+5\sqrt{\frac{1^2+3^2+1\times3}{1+3-2}}+2\sqrt{\frac{1^2+4^2+1\times4}{1+4-2}}$$

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$$+9\sqrt{\frac{2^2+2^2+2\times 2}{2+2-2}}+14\sqrt{\frac{2^2+3^2+2\times 3}{2+3-2}}+4\sqrt{\frac{2^2+4^2+2\times 4}{2+4-2}}$$
$$+6\sqrt{\frac{3^2+3^2+3\times 3}{3+3-2}}+2\sqrt{\frac{3^2+4^2+3\times 4}{3+4-2}}$$
$$=8\sqrt{7}+5\sqrt{\frac{13}{2}}+9\sqrt{6}+14\sqrt{\frac{19}{3}}+6\sqrt{\frac{27}{4}}+2\sqrt{\frac{37}{5}}.$$

Theorem 6. Let R be the chemical structure of remdesivir. Then

$$RDREU(R)=8\sqrt{\frac{1}{7}}+5\sqrt{\frac{2}{13}}+9\sqrt{\frac{1}{6}}+14\sqrt{\frac{3}{19}}+6\sqrt{\frac{4}{27}}+2\sqrt{\frac{5}{37}}.$$

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

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

$$=2\sqrt{\frac{1+2-2}{1^2+2^2+1\times 2}}+5\sqrt{\frac{1+3-2}{1^2+3^2+1\times 3}}+2\sqrt{\frac{1+4-2}{1^2+4^2+1\times 4}}$$
$$+9\sqrt{\frac{2+2-2}{2^2+2^2+2\times 2}}+14\sqrt{\frac{2+3-2}{2^2+3^2+2\times 3}}+4\sqrt{\frac{2+4-2}{2^2+4^2+2\times 4}}$$
$$+6\sqrt{\frac{3+3-2}{3^2+3^2+3\times 3}}+2\sqrt{\frac{3+4-2}{3^2+4^2+3\times 4}}$$
$$=8\sqrt{\frac{1}{7}}+5\sqrt{\frac{2}{13}}+9\sqrt{\frac{1}{6}}+14\sqrt{\frac{3}{19}}+6\sqrt{\frac{4}{27}}+2\sqrt{\frac{5}{37}}.$$

5. Conclusion

In this research, the degree ratio Euler Sombor and reciprocal degree ratio Euler Sombor indices for certain chemical structures are determined.

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