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Revan-Nirmala Index

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Abstract. In this paper, we propose the Revan-Nirmala index of a graph. Considering the Revan- Nirmala index, we propose the Revan-Nirmala exponential of a graph. We compute the Revan- Nirmala index and Revan Nirmala exponential of chloroquine, hydroxychloroquine and remdesivir.

Keywords: Revan Nirmala index, Revan Nirmala exponential, chemical drug

AMS Mathematics Subject Classification (2010): 05*C*05, 05*C*07, 05*C*09, 05*C*92

1. Introduction

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 $\Delta(G)$ ($\delta(G)$) denote the maximum(minimum) degree among the vertices of G. The Revan vertex degree of a vertex u in G is defined as $d_G(u) = \Delta(G) + \delta(G) - d_G(u)$. The Revan edge connecting the Revan vertices u and v will be denoted by uv. We refer [1], for other undefined notations and terminologies.

The first and second Revan indices of a graph G were introduced by Kulli in [2], and they are defined as

$$R_1(G) = \sum_{uv\in E(G)} \left[r_G(u) + r_G(v)\right], \qquad R_2(G) = \sum_{uv\in E(G)} r_G(u) r_G(v).$$

Recently, some Revan indices were studied, for example, in [3, 4, 5, 6, 7, 8].

The Nirmala index was introduced by Kulli in [9] and defined it as

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

Recently, some Nirmala indices were studied, for example, in [10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22].

Motivated by the definitions of the Revan and Nirmala indices, we introduce the Revan-Nirmala index of a graph and defined it as,

$$RN(G) = \sum_{uv \in E(G)} \sqrt{r_G(u) + r_G(v)}.$$

Considering the Revan-Nirmala index, we propose the Revan-Nirmala exponential of a graph G and it is defined as

$$RN(G,x) = \sum_{uv \in E(G)} x^{\sqrt{r_G(u)+r_G(v)}}.$$

In this paper, the Revan-Nirmala index and its corresponding exponential of chloroquine, hydroxychloroquine and rendesivir are determined.

2. Results for chloroquine

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

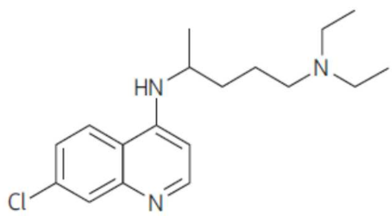

Figure 1: Structure of chloroquine

In G, the edge set $E(G)$ can be divided into five partitions based on the degree of end vertices of each edge as follows:

$E_1=\{uv \in E(G) \mid d_G(u)=1, d_G(v)=2\}$, $|E_1|=2$,
$E_2=\{uv \in E(G) \mid d_G(u)=1, d_G(v)=3\}$, $|E_2|=2$,
$E_3=\{uv \in E(G) \mid d_G(u)=d_G(v)=2\}$, $|E_3|=5$,
$E_4=\{uv \in E(G) \mid d_G(u)=2, d_G(v)=3\}$, $|E_4|=12$,
$E_5=\{uv \in E(G) \mid d_G(u) = d_G(v)=3\}$, $|E_5|=2$.

Clearly the vertices of G are either of degree 1 or 2 or 3. Thus $\Delta(G) = 3$ and $\delta(G) = 1$. Thus $d_G(u) = \Delta(G) + \delta(G) - d_G(u) = 3 + 1 - d_G(u)$. Now we obtain that there are five types of Revan edges based on the Revan degree of end Revan vertices of each Revan edge as given in Table 1.

$r_G(u), r_G(v) \backslash uv \in E(G)$	(3,2)	(3,1)	(2,2)	(2,1)	(1,1)
Number of edges	2	2	5	12	2

Table 1: Revan edge partition of G

We determine the Revan-Nirmala index of the molecular structure of chloroquine.

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

$$RN(G) == 2\sqrt{5} + 14 + 12\sqrt{3} + 2\sqrt{2}.$$

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

$$RN(G)=\sum_{uv\in E(G)}\sqrt{r_G(u)+r_G(v)}=2\sqrt{3+2}+2\sqrt{3+1}+5\sqrt{2+2}+12\sqrt{2+1}+2\sqrt{1+1}$$
$$=2\sqrt{5}+14+12\sqrt{3}+2\sqrt{2}.$$

In next theorem, we determine the Revan-Nirmala exponential of chloroquine.

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

$$RN(G,x)=2x^{\sqrt{5}}+7x^{2}+12x^{\sqrt{3}}+2x^{\sqrt{2}}.$$

Proof: Using definition and using Table 1, we have

$$RN(G,x)=\sum_{uv\in E(G)}x^{\sqrt{r_G(u)+r_G(v)}}=2x^{\sqrt{3+2}}+2x^{\sqrt{3+1}}+5x^{\sqrt{2+2}}+12x^{\sqrt{2+1}}+2x^{\sqrt{1+1}}$$
$$=2x^{\sqrt{5}}+7x^{2}+12x^{\sqrt{3}}+2x^{\sqrt{2}}.$$

3. Results for hydroxychloroquine

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

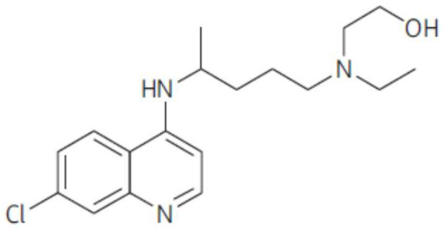

Figure 2: Structure of hydroxychloroquine

In H, the edge set of H can be divided into five partitions based on the degree of end vertices of each edge as follows:

$E_1=\{uv \in E(H) \mid d_H(u)=1, d_H(v)=2\}$, $|E_1|=2$,
$E_2=\{uv \in E(H) \mid d_H(u)=1, d_H(v)=3\}$, $|E_2|=2$,
$E_3=\{uv \in E(H) \mid d_H(u)=2, d_H(v)=2\}$, $|E_3|=6$,
$E_4=\{uv \in E(H) \mid d_H(u)=2, d_H(v)=3\}$, $|E_4|=12$,
$E_5=\{uv \in E(H) \mid d_H(u) = d_H(v)=3\}$, $|E_5|=2$.

We have, the vertices of H are either of degree 1 or 2 or 3. Hence $\Delta(H) = 3$ and $\delta(H) = 1$. Therefore $r_H(u) = \Delta(H) + \delta(H) - d_H(u) = 4 - d_H(u)$. In H, there are five types of Revan edges based on the revan degree of end revan vertices of each revan edge as given in Table 2.

$r_H(u), r_H(v)\backslash uv\in E(H)$	(3, 2)	(3, 1)	(2, 2)	(2, 1)	(1, 1)
Number of edges	2	2	6	12	2

Table 2: Revan edge partition of H

In Theorem 3, we determine the Revan-Nirmala index of hydroxychloroquine.

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

$$RN(H) == 2\sqrt{5} + 16 + 12\sqrt{3} + 2\sqrt{2}.$$

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

$$RN(H) = \sum_{uv \in E(H)} \sqrt{r_H(u) + r_H(v)}$$

$$= 2\sqrt{3+2} + 2\sqrt{3+1} + 6\sqrt{2+2} + 12\sqrt{2+1} + 2\sqrt{1+1}$$

$$= 2\sqrt{5} + 16 + 12\sqrt{3} + 2\sqrt{2}.$$

In Theorem 4, we compute the Revan-Nirmala exponential of hydroxychloroquine.

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

$$RN(H, x) == 2x^{\sqrt{5}} + 8x^2 + 12x^{\sqrt{3}} + 2x^{\sqrt{2}}.$$

Proof: Using definition and using Table 2, we have

$$RN(H, x) = \sum_{uv \in E(H)} x^{\sqrt{r_H(u) + r_H(v)}} = 2x^{\sqrt{3+2}} + 2x^{\sqrt{3+1}} + 5x^{\sqrt{2+2}} + 12x^{\sqrt{2+1}} + 2x^{\sqrt{1+1}}$$

$$= 2x^{\sqrt{5}} + 8x^2 + 12x^{\sqrt{3}} + 2x^{\sqrt{2}}.$$

4. Results for remdesivir

Let G be the molecular structure of remdesivir. This graph has 41 vertices and 44 edges.

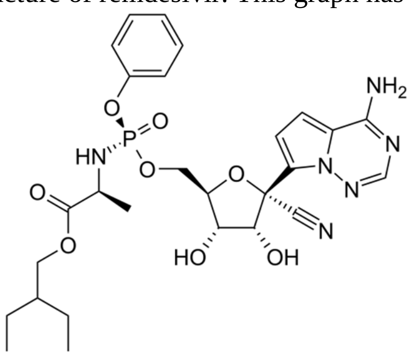

Figure 3: Structure of remdesivir

In G, the edge set of G can be divided into 8 partitions based on the degree of end vertices of each edge as follows:

$E_1 = \{uv \,\square\, E(G) \mid d_G(u) = 1, d_G(v) = 2\}$, $|E_1| = 2$,
$E_2 = \{uv \,\square\, E(G) \mid d_G(u) = 1, d_G(v) = 3\}$, $|E_2| = 5$,
$E_3 = \{uv \in E(G) \mid d_G(u) = 1, d_G(v) = 4\}$, $|E_3| = 2$,
$E_4 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 2\}$, $|E_4| = 9$,
$E_5 = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 3\}$, $|E_5| = 14$.
$E_6 = \{uv \in E(G) \mid d_G(u) = 2, d_G(v) = 4\}$, $|E_6| = 4$.
$E_7 = \{uv \in E(G) \mid d_G(u) = d_G(v) = 3\}$, $|E_7| = 6$.
$E_8 = \{uv \in E(G) \mid d_G(u) = 3, d_G(v) = 4\}$, $|E_8| = 2$.

The vertices of G are either of degree 1, 2, 3 or 4. Therefore $\Delta(G) = 4$, $\delta(G) = 1$. Thus $r_G(u) = \Delta(G) + \delta(G) - d_G(u) = 5 - d_G(u)$. In G, there are 8 types of Revan edges based on the Revan degree of end Revan vertices of each Revan edge as given in Table 3.

$r_G(u), r_G(v)\backslash uv\in E(G)$	(4, 3)	(4, 2)	(4, 1)	(3, 3)	(3, 2)	(3, 1)	(2, 2)	(2, 1)
Number of edges	2	5	2	9	14	4	6	2

Table 3: Revan edge partition of G

In the following theorem, we determine the Revan-Nirmala index of remdesivir.

Theorem 5. Let G be the molecular structure of remdesivir. Then

$$RN(G) = 2\sqrt{7} + 14\sqrt{6} + 16\sqrt{5} + 20 + 2\sqrt{3}.$$

Proof: From definition and by using Table 3, we obtain

$$RN(G) = \sum_{uv\in E(G)} \sqrt{r_G(u) + r_G(v)}$$

$$= 2\sqrt{4+3} + 5\sqrt{4+2} + 2\sqrt{4+1} + 9\sqrt{3+3} + 14\sqrt{3+2} + 4\sqrt{3+1} + 6\sqrt{2+2} + 2\sqrt{2+1}$$

$$= 2\sqrt{7} + 14\sqrt{6} + 16\sqrt{5} + 20 + 2\sqrt{3}.$$

In the next theorem, we compute the Revan-Nirmala exponential of remdesivir.

Theorem 6. Let G be the molecular structure of remdesivir. Then

$$RN(G,x) == 2x^{\sqrt{7}} + 14x^{\sqrt{6}} + 16x^{\sqrt{5}} + 10x^{2} + 2x^{\sqrt{3}}.$$

Proof: Using definition and using Table 3, we establish

$$RN(G,x) = \sum_{uv\in E(G)} x^{\sqrt{r_G(u)+r_G(v)}}$$

$$= 2x^{\sqrt{4+3}} + 5x^{\sqrt{4+2}} + 2x^{\sqrt{4+1}} + 9x^{\sqrt{3+3}} + 14x^{\sqrt{3+2}} + 4x^{\sqrt{3+1}} + 6x^{\sqrt{2+2}} + 2x^{\sqrt{2+1}}$$

$$= 2x^{\sqrt{7}} + 14x^{\sqrt{6}} + 16x^{\sqrt{5}} + 10x^{2} + 2x^{\sqrt{3}}$$

5. A property of the Revan-Nirmala index

Theorem 7. Let G be a connected graph with m edges. Then $RN(G) \le \sqrt{mR_1(G)}$.

Proof: Using the Cauchy-Schwarz inequality, we obtain

$$\left(\sum_{uv\in E(G)} \sqrt{r_G(u) + r_G(v)}\right)^2 \le \sum_{uv\in E(G)} 1 \sum_{uv\in E(G)} \left(r_G(u) + r_G(v)\right) = mR_1(G).$$

Thus $$RN(G) \le \sqrt{mR_1(G)}.$$

6. Conclusion

In this paper, we have defined the Revan-Nirmala index and Revan-Nirmala exponential of a graph. Furthermore, the Revan-Nirmala index and its corresponding exponential for chloroquine, hydroxychloroquine and remdesivir are computed.

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Authors' Contributions. All the authors contributed equally to this work.

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