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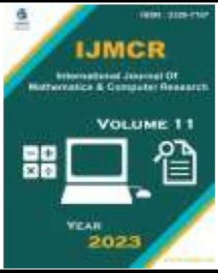

Nirmala Indices of Certain Antiviral Drugs

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ABSTRACT
In this paper, we compute the Nirmala index and its corresponding exponential of chloroquine, hydroxychloroquine and remdesivir. Also we determine the inverse Nirmal indices of chloroquine, hydroxychloroquine and remdesivir.

KEYWORDS: Nirmala index, inverse Nirmala indices, chemical drug.

I. INTRODUCTION

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. We refer [1], for other undefined notations and terminologies.

In 1972 [2], two degree based topological indices were introduced and studied. We consider three antiviral compounds (agents) such as chloroquine, hydroxychloroquine and remdesivir. In the field of Medical Science, concerning the definition of the graphical index on the molecular structure and corresponding medical, chemical, biological, pharmaceutical properties of drugs can be studied for the graphical index calculation. A molecular structure is a graph whose vertices correspond to the atoms and edges to the bonds. Studying molecular structures is a constant focus in Chemical Graph Theory: an effort to better understand molecular structure of a molecule.

The Nirmala index was introduced by Kulli in [3] and defined it as

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

The Nirmala exponential of a graph G [3] is defined as

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

In [4], the first and second inverse Nirmala indices of G were introduced and they are defined as

$$IN_1(G) = \sum_{uv \in E(G)} \left[\frac{1}{d(u)} + \frac{1}{d(v)}\right]^{\frac{1}{2}}.$$

$$IN_2(G) = \sum_{uv \in E(G)} \left[\frac{1}{d(u)} + \frac{1}{d(v)}\right]^{-\frac{1}{2}}.$$

Recently, some Nirmala indices were studied, for example, in [5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24].

In this paper, we compute the Nirmala index, inverse Nirmala indices for some chemical drugs.

In this paper, the Nirmala index and its corresponding exponential of chloroquine, hydroxychloroquine and rendesivir are computed

II. RESULTS AND DISCUSSION: CHLOROQUINE

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

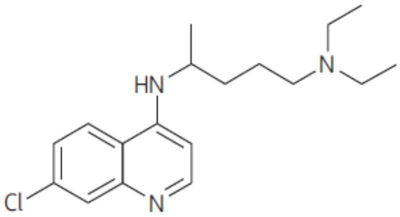

Figure 1. Graph of chloroquine

The edge set $E(G)$ can be divided into 5 partitions of end vertices of each edge as given in Table 1.

Table 1. Edge partition of *G*

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

We compute the Nirmala index of the molecular graph of chloroquine.

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

$$N(G) = 49.1958.$$

Proof: Using definition and Table 1, we have

$$N(G) = \sum_{uv \in E(G)} \sqrt{d(u)+d(v)}$$
$$= 2\sqrt{1+2} + 2\sqrt{1+3} + 5\sqrt{2+2} + 12\sqrt{2+3} + 2\sqrt{3+3}$$
$$= 2\sqrt{3} + 4 + 10 + 12\sqrt{5} + 2\sqrt{6}$$
$$= 49.1958$$

In Theorem 2, we determine the Nirmala exponential of the molecular graph of chloroquine.

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

$$N(G,x) = 2x^{\sqrt{3}} + 7x^2 + 12x^{\sqrt{5}} + 2x^{\sqrt{6}}.$$

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

$$N(G,x) = \sum_{uv \in E(G)} x^{\sqrt{d(u)+d(v)}}$$
$$= 2x^{\sqrt{1+2}} + 2x^{\sqrt{1+3}} + 5x^{\sqrt{2+2}} + 12x^{\sqrt{2+3}} + 2x^{\sqrt{3+3}}$$
$$= 2x^{\sqrt{3}} + 2x^2 + 5x^2 + 12x^{\sqrt{5}} + 2x^{\sqrt{6}}$$
$$= 2x^{\sqrt{3}} + 7x^2 + 12x^{\sqrt{5}} + 2x^{\sqrt{6}}.$$

Theorem 3. Let G be the molecular graph of chloroquine. Then

$$IN_1(G) = 22.3463$$

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

$$IN_1(G) = \sum_{uv \in E(G)} \left[\frac{1}{d(u)} + \frac{1}{d(v)}\right]^{\frac{1}{2}}$$
$$= 2\left[\frac{1}{1}+\frac{1}{2}\right]^{\frac{1}{2}} + 2\left[\frac{1}{1}+\frac{1}{3}\right]^{\frac{1}{2}} + 5\left[\frac{1}{2}+\frac{1}{2}\right]^{\frac{1}{2}} + 12\left[\frac{1}{2}+\frac{1}{3}\right]^{\frac{1}{2}} + 2\left[\frac{1}{3}+\frac{1}{3}\right]^{\frac{1}{2}}$$
$$= 2\sqrt{\frac{3}{2}} + 2\sqrt{\frac{4}{3}} + 5 + 12\sqrt{\frac{5}{6}} + 2\sqrt{\frac{2}{3}}$$
$$= 22.3463$$

Theorem 4. Let G be the molecular graph of chloroquine. Then

$$IN_2(G) = 23.9598$$

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

$$IN_2(G) = \sum_{uv \in E(G)} \left[\frac{1}{d(u)} + \frac{1}{d(v)}\right]^{-\frac{1}{2}}$$
$$= 2\left[\frac{1}{1}+\frac{1}{2}\right]^{-\frac{1}{2}} + 2\left[\frac{1}{1}+\frac{1}{3}\right]^{-\frac{1}{2}} + 5\left[\frac{1}{2}+\frac{1}{2}\right]^{-\frac{1}{2}} + 12\left[\frac{1}{2}+\frac{1}{3}\right]^{-\frac{1}{2}} + 2\left[\frac{1}{3}+\frac{1}{3}\right]^{-\frac{1}{2}}$$
$$= 2\sqrt{\frac{2}{3}} + 2\sqrt{\frac{3}{4}} + 5 + 12\sqrt{\frac{6}{5}} + 2\sqrt{\frac{3}{2}}$$
$$= 23.9598$$

III. RESULTS AND DISCUSSION: HYDROXYCHLOROQUINE

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

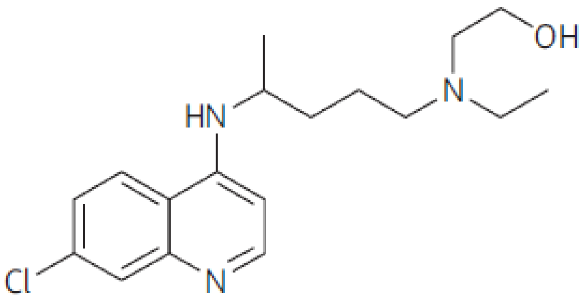

Figure 2. Graph of hydroxychloroquine

The edge set of H can be divided into five partitions of end vertices of each edge as given in Table 2.

Table 2. Edge partition of *H*

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

In the following theorem, we determine the Nirmala index of the molecular graph of hydroxychloroquine.

Theorem 5. Let H be the molecular graph of hydroxychloroquine. Then

$$N(H) = 51.1958$$

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

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

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

$$= 2\sqrt{3} + 4 + 12 + 12\sqrt{5} + 2\sqrt{6}$$

$$= 2\sqrt{3} + 16 + 12\sqrt{5} + 2\sqrt{6}$$

$$= 51.1958$$

In the next theorem, we compute the Nirmala exponential of the molecular graph of hydroxychloroquine.

Theorem 6. Let H be the molecular graph of hydroxychloroquine. Then

$$N(H,x) = 2x^{\sqrt{3}} + 8x^2 + 12x^{\sqrt{5}} + 2x^{\sqrt{6}}.$$

Proof: Using definition and using Table 2, we have

$$N(H,x) = \sum_{uv\in E(H)} x^{\sqrt{d(u)+d(v)}}$$

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

$$= 2x^{\sqrt{3}} + 2x^2 + 6x^2 + 12x^{\sqrt{5}} + 2x^{\sqrt{6}}$$

$$= 2x^{\sqrt{3}} + 8x^2 + 12x^{\sqrt{5}} + 2x^{\sqrt{6}}.$$

Theorem 7. Let H be the molecular graph of chloroquine. Then

$$IN_1(H) = 23.3463$$

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

$$IN_1(H) = \sum_{uv\in E(G)} \left[\frac{1}{d(u)} + \frac{1}{d(v)}\right]^{\frac{1}{2}}$$

$$= 2\left[\frac{1}{1}+\frac{1}{2}\right]^{\frac{1}{2}} + 2\left[\frac{1}{1}+\frac{1}{3}\right]^{\frac{1}{2}} + 6\left[\frac{1}{2}+\frac{1}{2}\right]^{\frac{1}{2}} + 12\left[\frac{1}{2}+\frac{1}{3}\right]^{\frac{1}{2}} + 2\left[\frac{1}{3}+\frac{1}{3}\right]^{\frac{1}{2}}$$

$$= 2\sqrt{\frac{3}{2}} + 2\sqrt{\frac{4}{3}} + 6 + 12\sqrt{\frac{5}{6}} + 2\sqrt{\frac{2}{3}}$$

$$= 23.3463$$

Theorem 8. Let H be the molecular graph of chloroquine. Then

$$IN_2(H) = 24.9598$$

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

$$IN_2(H) = \sum_{uv\in E(G)} \left[\frac{1}{d(u)} + \frac{1}{d(v)}\right]^{-\frac{1}{2}}$$

$$= 2\left[\frac{1}{1}+\frac{1}{2}\right]^{-\frac{1}{2}} + 2\left[\frac{1}{1}+\frac{1}{3}\right]^{-\frac{1}{2}} + 6\left[\frac{1}{2}+\frac{1}{2}\right]^{-\frac{1}{2}} + 12\left[\frac{1}{2}+\frac{1}{3}\right]^{-\frac{1}{2}} + 2\left[\frac{1}{3}+\frac{1}{3}\right]^{-\frac{1}{2}}$$

$$= 2\sqrt{\frac{2}{3}} + 2\sqrt{\frac{3}{4}} + 6 + 12\sqrt{\frac{6}{5}} + 2\sqrt{\frac{3}{2}}$$

$$= 24.9598$$

IV. RESULTS AND DISCUSSION: REMDESIVIR

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

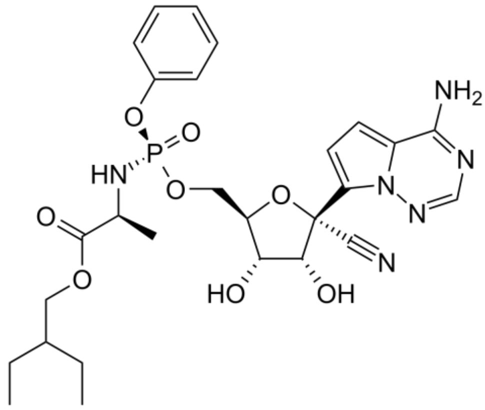

Figure 3. Graph of remdesivir

The edge set $E(R)$ can be divided into 8 partitions of end vertices of each edge as given in Table 3.

Table 3. Edge partition of *R*

$d_{hr}(u), d_{hr}(v) \setminus uv \in E(R)$	Number of edges
(1, 2)	2
(1, 3)	5
(1, 4)	2
(2, 2)	9
(2, 3)	14
(2, 4)	4
(3, 3)	6
(3, 4)	2

In Theorem 9, we determine the Nirmala index of the molecular graph of remdesivir.

Theorem 9. Let R be the molecular graph of remdesivir. Then

$$N(R) = 97.0275.$$

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

$$N(R)=\sum_{uv\in E(R)}\sqrt{d(u)+d(v)}$$
$$=2\sqrt{1+2}+5\sqrt{1+3}+2\sqrt{1+4}+9\sqrt{2+2}$$
$$+14\sqrt{2+3}+4\sqrt{2+4}+6\sqrt{3+3}+2\sqrt{3+4}$$
$$=2\sqrt{3}+10+2\sqrt{5}+18+14\sqrt{5}+4\sqrt{6}+$$
$$6\sqrt{6}+2\sqrt{7}$$
$$=2\sqrt{3}+28+16\sqrt{5}+10\sqrt{6}+2\sqrt{7}$$
$$=97.0275$$

In the next theorem, we compute the Nirmala exponential of the molecular graph of remdesivir.

Theorem 10. Let R be the molecular graph of remdesivir. Then

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

Proof: Using definition and Table 3, we have

$$N(\mathrm{R},x)=\sum_{uv\in E(R)}x^{\sqrt{d(u)+d(v)}}$$
$$=2x^{\sqrt{1+2}}+5x^{\sqrt{1+3}}+2x^{\sqrt{1+4}}+9x^{\sqrt{2+2}}$$
$$+14x^{\sqrt{2+3}}+4x^{\sqrt{2+4}}+6x^{\sqrt{3+3}}+2x^{\sqrt{3+4}}$$
$$=2x^{\sqrt{3}}+5x^{2}+2x^{\sqrt{5}}+9x^{2}$$
$$+14x^{\sqrt{5}}+4x^{\sqrt{6}}+6x^{\sqrt{6}}+2x^{\sqrt{7}}$$
$$=2x^{\sqrt{3}}+14x^{2}+16x^{\sqrt{5}}+10x^{\sqrt{6}}+2x^{\sqrt{7}}.$$

Theorem 11. Let R be the molecular graph of chloroquine. Then

$$IN_1(R)=42.1298$$

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

$$IN_1(R)=\sum_{uv\in E(G)}\left[\frac{1}{d(u)}+\frac{1}{d(v)}\right]^{\frac{1}{2}}$$
$$=2\left[\frac{1}{1}+\frac{1}{2}\right]^{\frac{1}{2}}+5\left[\frac{1}{1}+\frac{1}{3}\right]^{\frac{1}{2}}+2\left[\frac{1}{1}+\frac{1}{4}\right]^{\frac{1}{2}}+9\left[\frac{1}{2}+\frac{1}{2}\right]^{\frac{1}{2}}+$$
$$14\left[\frac{1}{2}+\frac{1}{3}\right]^{\frac{1}{2}}+4\left[\frac{1}{2}+\frac{1}{4}\right]^{\frac{1}{2}}+6\left[\frac{1}{3}+\frac{1}{3}\right]^{\frac{1}{2}}+2\left[\frac{1}{3}+\frac{1}{4}\right]^{\frac{1}{2}}$$
$$=2\sqrt{\frac{3}{2}}+5\sqrt{\frac{4}{3}}+2\sqrt{\frac{5}{4}}+9+14\sqrt{\frac{5}{6}}+4\sqrt{\frac{3}{4}}+6\sqrt{\frac{2}{3}}+2\sqrt{\frac{7}{12}}$$
$$=42.1298$$

Theorem 12. Let R be the molecular graph of chloroquine. Then

$$IN_2(R)==46.674$$

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

$$IN_2(R)=\sum_{uv\in E(G)}\left[\frac{1}{d(u)}+\frac{1}{d(v)}\right]^{-\frac{1}{2}}$$
$$=2\left[\frac{1}{1}+\frac{1}{2}\right]^{-\frac{1}{2}}+5\left[\frac{1}{1}+\frac{1}{3}\right]^{-\frac{1}{2}}+2\left[\frac{1}{1}+\frac{1}{4}\right]^{-\frac{1}{2}}+9\left[\frac{1}{2}+\frac{1}{2}\right]^{-\frac{1}{2}}+$$
$$14\left[\frac{1}{2}+\frac{1}{3}\right]^{-\frac{1}{2}}+4\left[\frac{1}{2}+\frac{1}{4}\right]^{-\frac{1}{2}}+6\left[\frac{1}{3}+\frac{1}{3}\right]^{-\frac{1}{2}}+2\left[\frac{1}{3}+\frac{1}{4}\right]^{-\frac{1}{2}}$$
$$=2\sqrt{\frac{2}{3}}+5\sqrt{\frac{3}{4}}+2\sqrt{\frac{4}{5}}+9+14\sqrt{\frac{6}{5}}+4\sqrt{\frac{4}{3}}+6\sqrt{\frac{3}{2}}+2\sqrt{\frac{12}{7}}$$
$$=46.674$$

V. CONCLUSION

In this paper, a novel invariant is considered which is the Nirmala index. The Nirmala index and its corresponding exponential for chloroquine, hydroxychloroquine, remdesivir are determined.

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