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# Different Versions of Nirmala Index of Certain Chemical Structures

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***Abstract:*** *Recently, a novel degree based topological index was introduced, the so called Nirmala index. In this paper, we compute the Nirmala index, second, third, fourth and neighborhood Nirmala indices for some important chemical structures such as chloroquine, hdroxychloroquine and remdesivir.*

**Keywords:** *Nirmala index, second, third, fourth and neighborhood Nirmala indices, chemical structure.*

**Mathematics Subject Classification:** 05*C*05, 05*C*07, *05C12*, *05C35*, *05C90*.

## I. Introduction

Let $G$ be a finite, simple, connected graph with vertex set $V(G)$ and edge set $E(G)$. Let $d_G(u)$ be the degree of a vertex $u$ in a graph $G$. Let $s(u)$ denote the sum of the degrees of all vertices adjacent to vertex $u$. For undefined terms and notations, we refer [1].

Chemical Graph Theory is branch of Mathematical Chemistry which has an important effect on the development of Chemical Sciences. A molecular graph is a graph such that its vertices correspond to the atoms and the edges to the bonds. Topological indices are useful for establishing correlation between the structure of a molecular compound and its physicochemical properties. Numerous topological indices [2] have been considered in Theoretical Chemistry and have found some applications, especially in QSPR/QSAR research, see [3, 4].

In [5], Kulli introduced the Nirmala index of a graph and defined it as

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

Recently, some Nirmala indices were studied, for example, in [6, 7, 8, 9, 10, 11].

The second, third, fourth and neighborhood Nirmala indices of the molecular graph were introduced by Kulli in [12] and they are defined as follows:

The second Nirmala index of a molecular graph $G$ is defined as

$$N_2(G)=\sum_{uv\in E(G)}\sqrt{n(u)+n(v)}$$

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 $G$.

The third Nirmala index of a molecular graph $G$ is defined as

$$N_3(G)=\sum_{uv\in E(G)}\sqrt{m(u)+m(v)}$$

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 $G$.

The fourth Nirmala index of a molecular graph $G$ is defined as

$$N_4(G)=\sum_{uv\in E(G)}\sqrt{\varepsilon(u)+\varepsilon(v)}$$

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

The neighborhood Nirmala index of a molecular graph $G$ is defined as

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

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

Recently, some new versions of topological indices were studied, for example, in [ 13, 14, 15, 16, 17, 18, 19].

In this study, we compute the different types of the Nirmala indices of some significant molecular structures of drugs such as chloroquine, hydroxychloroquine, remdesivir. For molecular structures, see [ 20, 21].

## II. Results for chloroquine

Chloroquine is an antiviral compound (drug) which was discovered in 1934 by H.Andersag. This drug is medication primarily used to prevent and treat malaria.

Let $G_1$ be the chemical structure of chloroquine. This structure has 21 atoms and 23 bonds, see Figure 1.

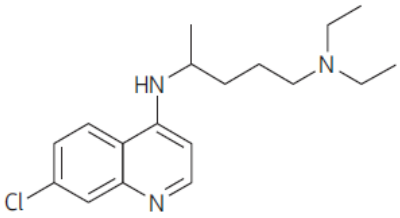


**Figure 1. Chemical structure of chloroquine**

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

**Table 1. Bond 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 bonds | 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 bonds | 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 bonds | 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 bonds | 1 | 3 | 3 | 4 | 5 | |
| | (11,12) | (12,13) | | | | |
| | 4 | 3 | | | | |
| $s(u), s(v) \setminus uv \in E(G_1)$ | | | | | | |
| Number of bonds | (2,4) | (3,5) | (4,5) | (4,6) | (5,5) | |
| | 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 different versions of Nirmala indices of chloroquine.

**Theorem 1.** Let $G_1$ be the chemical structure of chloroquine. Then
(i) $N(G_1) = 49.195962658.$
(ii) $N_2(G_1) = 103.300885925.$
(iii) $N_3(G_1) = 106.352305337.$
(iv) $N_4(G_1) = 102.261724644.$
(v) $NN(G_1) = 73.807920156.$

**Proof:** By using the definitions and cardinalities of the bond partition of $G_1$, we deduce

(i) $$N(G_1)=\sum_{uv\in E(G_1)}\sqrt{d(u)+d(v)}$$

$$=(1+2)^{\frac{1}{2}}2+(1+3)^{\frac{1}{2}}2+(2+2)^{\frac{1}{2}}5+(2+3)^{\frac{1}{2}}12+(3+3)^{\frac{1}{2}}2$$

$$=2\sqrt{3}+14+12\sqrt{5}+2\sqrt{6}.$$

After simplification, we get the desired result.

(ii) $$N_2(G_1)=\sum_{uv\in E(G_1)}\sqrt{n(u)+n(v)}$$

$$=(1+19)^{\frac{1}{2}}2+(1+20)^{\frac{1}{2}}4+(2+18)^{\frac{1}{2}}2+(3+17)^{\frac{1}{2}}4+(4+16)^{\frac{1}{2}}$$

$$+(5+15)^{\frac{1}{2}}4+(6+14)^{\frac{1}{2}}+(7+13)^{\frac{1}{2}}3+(9+11)^{\frac{1}{2}}+(10+10)^{\frac{1}{2}}$$

$$=19\sqrt{20}+4\sqrt{21}.$$

After simplification, we get the desired result.

(iii) $$N_3(G_1)=\sum_{uv\in E(G_1)}\sqrt{m(u)+m(v)}$$

$$=(1+21)^{\frac{1}{2}}2+(1+22)^{\frac{1}{2}}4+(2+19)^{\frac{1}{2}}2+(3+18)^{\frac{1}{2}}4+(4+17)^{\frac{1}{2}}+(5+15)^{\frac{1}{2}}3$$

$$+(5+16)^{\frac{1}{2}}+(6+15)^{\frac{1}{2}}+(7+14)^{\frac{1}{2}}2+(8+13)^{\frac{1}{2}}+(9+13)^{\frac{1}{2}}+(10+12)^{\frac{1}{2}}$$

$$=4\sqrt{22}+4\sqrt{23}+12\sqrt{21}+3\sqrt{20}.$$

After simplification, we get the desired result.

(iv) $$N_4(G_1)=\sum_{uv\in E(G_1)}\sqrt{\varepsilon(u)+\varepsilon(v)}$$

$$=(7+7)^{\frac{1}{2}}+(8+7)^{\frac{1}{2}}3+(8+9)^{\frac{1}{2}}3+(9+10)^{\frac{1}{2}}4+(10+11)^{\frac{1}{2}}5$$

$$+(11+12)^{\frac{1}{2}}4+(12+13)^{\frac{1}{2}}3$$

$$=\sqrt{14}+3\sqrt{15}+3\sqrt{17}+4\sqrt{19}+5\sqrt{21}+4\sqrt{23}+15.$$

After simplification, we get the desired result.

(v) $$NN(G_1)=\sum_{uv\in E(G_1)}\sqrt{s(u)+s(v)}$$

$$=(2+4)^{\frac{1}{2}}2+(3+5)^{\frac{1}{2}}2+(4+5)^{\frac{1}{2}}4+(4+6)^{\frac{1}{2}}2+(5+5)^{\frac{1}{2}}3$$

$$+(5+6)^{\frac{1}{2}}3+(5+7)^{\frac{1}{2}}2+(5+8)^{\frac{1}{2}}+(6+7)^{\frac{1}{2}}2+(7+8)^{\frac{1}{2}}2$$

$$=2\sqrt{6}+2\sqrt{8}+12+5\sqrt{10}+3\sqrt{11}+2\sqrt{12}+3\sqrt{13}+2\sqrt{15}.$$

After simplification, we get the desired result.

## III. Results for hydroxychloroquine

Hydroxychloroquine is another antiviral compound (drug) which has antiviral activity very similar to that of chloroquine. These compounds have been repurposed for the treatment of a number of other conditions including HIV, systemic lupus erythmatosus and rheumatoid arthritis .

Let $G_2$ be the chemical structure of hydroxychloroquine. This structure has 22 vertices and 24 edges, see Figure 2.

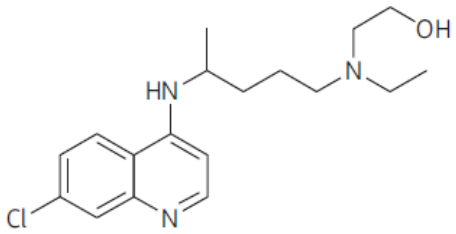


**Figure 2. Chemical structure of hydroxychloroquine**

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

**Table 2. Bond 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 bonds | 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 bonds | 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 bonds | 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 bonds | 3 | 2 | 3 | 4 | 6 | |
| | (12,13) | (13,14) | | | | |
| | 4 | 2 | | | | |
| $s(u), s(v) \setminus uv \in E(G_2)$ | | | | | | |
| Number of bonds | (2,3) | (2,4) | (3,5) | (4,5) | (4,6) | (5,5) |
| | 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 different versions of Nirmala indices of hydroxychloroquine.

**Theorem 2.** Let $G_2$ be the chemical structure of hudroxychloroquine. Then
(i) $N(G_2) = 51.1958968307.$
(ii) $N_2(G_2) = 110.413176938.$
(iii) $N_3(G_2) = 113.607791762.$
(iv) $N_4(G_2) = 110.439454886.$
(v) $NN(G_2) = 76.5772726457.$

**Proof:** By using the definitions and cardinalities of the bond partitions of $G_2$, we deduce

(i) $$N(G_2) = \sum_{uv \in E(G_2)} \sqrt{d(u) + d(v)}$$

$$= (1+2)^{\frac{1}{2}} 2 + (1+3)^{\frac{1}{2}} 2 + (2+2)^{\frac{1}{2}} 6 + (2+3)^{\frac{1}{2}} 12 + (3+3)^{\frac{1}{2}} 2$$

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

After simplification, we get the desired result.

(ii) $$N_2(G_2) = \sum_{uv \in E(G_2)} \sqrt{n(u) + n(v)}$$

$$= (1+20)^{\frac{1}{2}} 2 + (1+21)^{\frac{1}{2}} 4 + (2+19)^{\frac{1}{2}} 3 + (3+18)^{\frac{1}{2}} 4 + (5+16)^{\frac{1}{2}} 4$$
$$+ (6+15)^{\frac{1}{2}} 3 + (7+14)^{\frac{1}{2}} 2 + (10+11)^{\frac{1}{2}} + (8+13)^{\frac{1}{2}}$$
$$= 20\sqrt{21} + 4\sqrt{22}.$$

After simplification, we get the desired result.

(iii) $$N_3(G_2) = \sum_{uv \in E(G_2)} \sqrt{m(u) + m(v)}$$

$$= (1+22)^{\frac{1}{2}} 2 + (1+23)^{\frac{1}{2}} 4 + (2+20)^{\frac{1}{2}} 2 + (2+21)^{\frac{1}{2}} + (3+19)^{\frac{1}{2}} 4 + (5+16)^{\frac{1}{2}} 3$$
$$+ (5+17)^{\frac{1}{2}} + (6+16)^{\frac{1}{2}} + (7+15)^{\frac{1}{2}} + (8+14)^{\frac{1}{2}} 3 + (10+13)^{\frac{1}{2}} + (11+12)^{\frac{1}{2}}$$
$$= 5\sqrt{23} + 4\sqrt{24} + 12\sqrt{22} + 3\sqrt{21}.$$

After simplification, we get the desired result.

(iv) $$N_4(G_2) = \sum_{uv \in E(G_2)} \sqrt{\varepsilon(u) + \varepsilon(v)}$$

$$= (7+8)^{\frac{1}{2}} 3 + (8+9)^{\frac{1}{2}} 2 + (9+10)^{\frac{1}{2}} 3 + (10+11)^{\frac{1}{2}} 4 + (11+12)^{\frac{1}{2}} 6$$
$$+ (12+13)^{\frac{1}{2}} 4 + (13+14)^{\frac{1}{2}} 2$$
$$= 3\sqrt{15} + 2\sqrt{17} + 3\sqrt{19} + 4\sqrt{21} + 6\sqrt{23} + 20 + 2\sqrt{27}.$$

After simplification, we get the desired result.

(v) $$NN(G_2) = \sum_{uv \in E(G_2)} \sqrt{s(u) + s(v)}$$

$$= (2+3)^{\frac{1}{2}} + (2+4)^{\frac{1}{2}} + (3+5)^{\frac{1}{2}} 3 + (4+5)^{\frac{1}{2}} 4 + (4+6)^{\frac{1}{2}} + (5+5)^{\frac{1}{2}} 3$$
$$+ (5+6)^{\frac{1}{2}} 4 + (5+7)^{\frac{1}{2}} 2 + (5+8)^{\frac{1}{2}} + (6+7)^{\frac{1}{2}} 2 + (7+8)^{\frac{1}{2}} 2$$
$$= \sqrt{5} + \sqrt{6} + 3\sqrt{8} + 12 + 4\sqrt{10} + 4\sqrt{11} + 2\sqrt{12} + 3\sqrt{13} + 2\sqrt{15}.$$

After simplification, we get the desired result.

## IV. Results for remdesivir

Remdesivir is an antiviral drug which was developed by the biopharmaceutical company Gilead Sciences. Let $G_3$ be the molecular graph of remdesivir. This graph has 41 vertices and 44 edges.

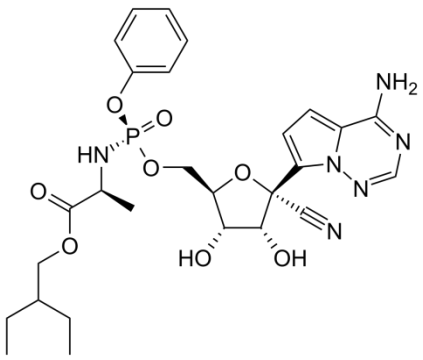


**Figure 3. Chemical structure of remdesivir**

**Table 3. Bond set partitions of remdesivir**

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| $d(u), d(v)\backslash uv \in E(G_3)$ | (1,2) | (1, 3) | (1, 4) | (2, 2) | (2, 3) | (2, 4) | (3, 3) | (3, 4) |
| Number of bonds | 2 | 5 | 2 | 9 | 14 | 4 | 6 | 2 |
| $n(u), n(v)\backslash uv \in E(G_3)$ | (1,6) | (1,34) | (1,38) | (1,39) | (2,37) | (3,12) | (3,23) | (3,36) |
| Number of bonds | 1 | 1 | 2 | 9 | 8 | 1 | 1 | 2 |
| | (4,32) | (4,33) | (4,34) | (4,35) | (5,34) | (6,32) | (6,33) | (8,31) |
| | 1 | 1 | 1 | 1 | 2 | 1 | 2 | 1 |
| | (9,30) | (10,29) | (11,28) | (12,24) | (13,24) | (13,25) | (17,22) | (18,21) |
| | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| | (19,20) | | | | | | | |
| | 1 | | | | | | | |
| $m(u),m(v)\backslash uv \in E(G_3)$ | (1,42) | (1,43) | (2,8) | (2,32) | (2,40) | (2,41) | (3,39) | (4,15) |
| Number of bonds | 2 | 9 | 1 | 1 | 2 | 6 | 2 | 1 |
| | (4,39) | (4,26) | (5,37) | (5,38) | (6,35) | (6,37) | (7,36) | (8,35) |
| | 1 | 1 | 2 | 1 | 1 | 2 | 1 | 2 |
| | (10,33) | (11,32) | (15,27) | (16,26) | (16,27) | (20,23) | (21,22) | |
| | 1 | 2 | 1 | 1 | 1 | 1 | 2 | |
| $\varepsilon(u),\varepsilon(v)\backslash uv \in E(G_3)$ | (9,10) | (10,11) | (11,12) | (12,13) | (13,13) | (13,14) | (14,15) | (15,16) |
| Number of bonds | 2 | 4 | 4 | 7 | 1 | 7 | 5 | 4 |
| | (16,16) | (16,17) | (17,18) | | | | | |
| | 1 | 4 | 5 | | | | | |
| $s(u),s(v)\backslash uv \in E(G_3)$ | (2,4) | (3,6) | (3,7) | (3,8) | (4,4) | (4,5) | (4,6) | (4,7) |
| Number of bonds | 2 | 3 | 1 | 1 | 2 | 4 | 2 | 1 |
| | (4,9) | (5,5) | (5,6) | (5,7) | (5,8) | (5,9) | (6,6) | (6,7) |
| | 1 | 2 | 6 | 1 | 2 | 1 | 1 | 3 |
| | (6,8) | (7,7) | (7,8) | (7,9) | (8,8) | (8,9) | (9,9) | |
| | 1 | 4 | 1 | 1 | 1 | 2 | 1 | |

In the following theorem, we compute the different versions of Nirmala indices of remdesivir.

**Theorem 3.** Let $G_3$ be the chemical structure of remdesivir. Then

(i) $N(G_3) = 91.0275893051.$

(ii) $N_2(G_3) = 266.993550868.$

(iii) $N_3(G_3) = 281.041297659.$

(iv) $N_4(G_3) = 230.115898471.$

(v) $NN(G_3) = 149.273510847.$

**Proof:** By using the definitions and cardinalities of the bond partitions of $G_3$, we deduce

(i) $$N(G_3) = \sum_{uv \in E(G_3)} \sqrt{d(u)+d(v)}$$

$$= (1+2)^{\frac{1}{2}}2 + (1+3)^{\frac{1}{2}}5 + (1+4)^{\frac{1}{2}}2 + (2+2)^{\frac{1}{2}}9 + (2+3)^{\frac{1}{2}}14 + (2+4)^{\frac{1}{2}}4$$

$$+ (3+3)^{\frac{1}{2}}6 + (3+4)^{\frac{1}{2}}2$$

$$= 2\sqrt{3} + 22 + 16\sqrt{5} + 10\sqrt{6} + 2\sqrt{7}.$$

After simplification, we get the desired result.

(ii) $$N_2(G_3) = \sum_{uv \in E(G_3)} \sqrt{n(u)+n(v)}$$

$$= (1+6)^{\frac{1}{2}} + (1+34)^{\frac{1}{2}} + (1+38)^{\frac{1}{2}}2 + (1+39)^{\frac{1}{2}}9 + (2+37)^{\frac{1}{2}}8 + (3+12)^{\frac{1}{2}} + (3+23)^{\frac{1}{2}}$$

$$+ (3+36)^{\frac{1}{2}}2 + (4+32)^{\frac{1}{2}} + (4+33)^{\frac{1}{2}} + (4+34)^{\frac{1}{2}} + (4+35)^{\frac{1}{2}} + (5+34)^{\frac{1}{2}}2 + (6+32)^{\frac{1}{2}}$$

$$+(6+33)^{\frac{1}{2}}2+(8+31)^{\frac{1}{2}}+(9+30)^{\frac{1}{2}}+(10+29)^{\frac{1}{2}}+(11+28)^{\frac{1}{2}}+(12+24)^{\frac{1}{2}}+(13+24)^{\frac{1}{2}}$$
$$+(13+25)^{\frac{1}{2}}+(17+22)^{\frac{1}{2}}+(18+21)^{\frac{1}{2}}+(19+20)^{\frac{1}{2}}$$
$$=\sqrt{7}+\sqrt{35}+\sqrt{15}+\sqrt{26}+2\sqrt{36}+2\sqrt{37}+3\sqrt{38}+24\sqrt{39}+9\sqrt{40}.$$

After simplification, we get the desired result.

(iii) $$N_3(G_3)=\sum_{uv\in E(G_3)}\sqrt{m(u)+m(v)}$$
$$=(1+42)^{\frac{1}{2}}2+(1+43)^{\frac{1}{2}}9+(2+8)^{\frac{1}{2}}+(2+32)^{\frac{1}{2}}+(2+40)^{\frac{1}{2}}2+(2+41)^{\frac{1}{2}}6+(3+39)^{\frac{1}{2}}2$$
$$+(4+15)^{\frac{1}{2}}+(4+39)^{\frac{1}{2}}+(4+26)^{\frac{1}{2}}+(5+37)^{\frac{1}{2}}2+(5+38)^{\frac{1}{2}}+(6+35)^{\frac{1}{2}}+(6+37)^{\frac{1}{2}}2$$
$$+(7+36)^{\frac{1}{2}}+(8+35)^{\frac{1}{2}}2+(10+33)^{\frac{1}{2}}+(11+32)^{\frac{1}{2}}2+(15+27)^{\frac{1}{2}}$$
$$+(16+26)^{\frac{1}{2}}+(16+27)^{\frac{1}{2}}+(20+23)^{\frac{1}{2}}+(21+22)^{\frac{1}{2}}2$$
$$=\sqrt{10}+\sqrt{19}+\sqrt{30}+\sqrt{34}+\sqrt{41}+8\sqrt{42}+22\sqrt{43}+9\sqrt{44}.$$

After simplification, we get the desired result.

(iv) $$N_4(G_3)=\sum_{uv\in E(G_3)}\sqrt{\varepsilon(u)+\varepsilon(v)}$$
$$=(9+10)^{\frac{1}{2}}2+(10+11)^{\frac{1}{2}}4+(11+12)^{\frac{1}{2}}4+(12+13)^{\frac{1}{2}}7+(13+13)^{\frac{1}{2}}+(13+14)^{\frac{1}{2}}7$$
$$+(14+15)^{\frac{1}{2}}5+(15+16)^{\frac{1}{2}}4+(16+16)^{\frac{1}{2}}+(16+17)^{\frac{1}{2}}4+(17+18)^{\frac{1}{2}}5$$
$$=2\sqrt{19}+4\sqrt{21}+4\sqrt{23}+7\sqrt{25}+\sqrt{26}+7\sqrt{27}+5\sqrt{29}+4\sqrt{31}+\sqrt{32}+4\sqrt{33}+5\sqrt{35}.$$

After simplification, we get the desired result.

(v) $$NN(G_3)=\sum_{uv\in E(G_3)}\sqrt{s(u)+s(v)}$$
$$=(2+4)^{\frac{1}{2}}2+(3+6)^{\frac{1}{2}}3+(3+7)^{\frac{1}{2}}+(3+8)^{\frac{1}{2}}+(4+4)^{\frac{1}{2}}2+(4+5)^{\frac{1}{2}}4+(4+6)^{\frac{1}{2}}2$$
$$+(4+7)^{\frac{1}{2}}+(4+9)^{\frac{1}{2}}+(5+5)^{\frac{1}{2}}2+(5+6)^{\frac{1}{2}}6+(5+7)^{\frac{1}{2}}+(5+8)^{\frac{1}{2}}2+(5+9)^{\frac{1}{2}}+(6+6)^{\frac{1}{2}}$$
$$+(6+7)^{\frac{1}{2}}3+(6+8)^{\frac{1}{2}}+(7+7)^{\frac{1}{2}}4+(7+8)^{\frac{1}{2}}+(7+9)^{\frac{1}{2}}+(8+8)^{\frac{1}{2}}+(8+9)^{\frac{1}{2}}2+(9+9)^{\frac{1}{2}}$$
$$=29+2\sqrt{6}+2\sqrt{8}+5\sqrt{10}+8\sqrt{11}+2\sqrt{12}+6\sqrt{13}+6\sqrt{14}+\sqrt{15}+2\sqrt{17}+\sqrt{18}.$$

After simplification, we get the desired result.

## V. Conclusion

In this study, we have computed the different types of Nirmala indices of some important chemical structures of drugs which are applied to test the chemical, medical and pharmaceutical characteristics.

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