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Downhill Nirmala Alpha Gourava Indices of Chloroquine, Hydroxychloroquine and Remdesivir

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ARTICLE INFO	ABSTRACT
Published Online: 02 June 2025 **Corresponding Author:** V.R.Kulli	In this study, we introduce the downhill Nirmala alpha Gourava and modified downhill Nirmala alpha Gourava indices and their corresponding exponentials of a graph. Furthermore, we compute these indices for certain chemical drugs such as chloroquine, hydroxychloroquine and remdesivir.

KEYWORDS: downhill Nirmala alpha Gourava index, modified downhill Nirmala alpha Gourava index, drug.

I. INTRODUCTION

In this study, G denotes a finite, simple, connected graph, $V(G)$ and $E(G)$ denote the vertex set and edge set of G. The degree $d_G(u)$ of a vertex u is the number of vertices adjacent to u. Any undefined terminologies and notations may be found in [1].

A topological index is a numerical parameter mathematically derived from the graph structure. In Chemical Graph Theory, concerning the definition of the topological index on the molecular graph and concerning chemical properties of drugs can be studied by the graph index calculation. Several topological indices have been considered in Theoretical Chemistry and many topological indices were defined by using vertex degree concept [2]. The Zagreb, Nirmala, Gourava, Sombor, Revan, delta indices are the most degree based topological indices in Chemical Graph Theory, see [3-41]. Topological indices have their applications in various disciplines in Science and Technology [42-44].

A u-v path P in G is a sequence of vertices in G, starting with u and ending at v, such that consecutive vertices in P are adjacent, and no vertex is repeated. A path $\pi = v_1, v_2, \ldots v_{k+1}$ in G is a downhill path if for every i, $1 \le i \le k$, $d_G(v_i) \ge d_G(v_{i+1})$.

A vertex v is downhill dominates a vertex u if there exists a downhill path originated from u to v. The downhill neighborhood of a vertex v is denoted by $N_{dn}(v)$ and defined as: $N_{dn}(v) = \{u: v \text{ downhill dominates } u\}$. The downhill degree $d_{dn}(v)$ of a vertex v is the number of downhill neighbors of v [45].

The Nirmala alpha Gourava index [46] was defined as

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

Motivated by the definition of Nirmala alpha Gourava index, we introduce the downhill Nirmala alpha Gourava index of a graph and it is defined as

$$DWNG(G) = \sum_{uv \in E(G)} \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2 + d_{dn}(u)d_{dn}(v)}.$$

Considering the downhill Nirmala alpha Gourava index, we introduce the downhill Nirmala alpha Gourava exponential of a graph G and defined it as

$$DWNG(G,x) = \sum_{uv \in E(G)} x^{\sqrt{d_{dn}(u)^2 + d_{dn}(v)^2 + d_{dn}(u)d_{dn}(v)}}.$$

We define the modified downhill Nirmala alpha Gourava index of a graph G as

$$^{m}DWNG(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_{dn}(u)^2 + d_{dn}(v)^2 + d_{dn}(u)d_{dn}(v)}}.$$

Considering the modified downhill Nirmala alpha Gourava index, we introduce the modified downhill Nirmala alpha Gourava exponential of a graph G and defined it as

$$^{m}DWNG(G,x)=\sum_{uv\in E(G)} x^{\frac{1}{\sqrt{d_{dn}(u)^2+d_{dn}(v)^2+d_{dn}(u)d_{dn}(v)}}}.$$

Recently, some downhill indices were studied in [47-53].

In this paper, the downhill Nirmala alpha Gourava index, modified downhill Nirmala alpha Gourava index and their corresponding exponentials of certain chemical drugs are computed.

II. RESULTS FOR SOME STANDARD GRAPHS

Proposition 1. Let G be r-regular with n vertices and $r\geq 2$. Then

$$DWNG(G)=\frac{nr\sqrt{3}(n-1)}{2}.$$

Proof: Let G be an r-regular graph with n vertices and $r \geq 2$ and $\frac{nr}{2}$ edges. Then $d_{dn}(v)=n-1$ for every v in G. We obtain

$$DWNG(G)$$
$$=\sum_{uv\in E(G)}\sqrt{d_{dn}(u)^2+d_{dn}(v)^2+d_{dn}(u)d_{dn}(v)}.$$
$$=\frac{nr}{2}\sqrt{(n-1)^2+(n-1)^2+(n-1)^2}$$
$$=\frac{nr\sqrt{3}(n-1)}{2}$$

Corollary 1.1. Let C_n be a cycle with $n\geq 3$ vertices. Then

$$DWNG(C_n)=\sqrt{3}n(n-1).$$

Corollary 1.2. Let K_n be a complete graph with $n\geq 3$ vertices. Then

$$DWNG(K_n)=\frac{\sqrt{3}n(n-1)^2}{2}.$$

Proposition 2. Let P_n be a path with $n\geq 3$ vertices. Then

$$DWNG(P_n)=(n-1)\left(\sqrt{3}n+2-3\sqrt{3}\right).$$

Proof: Let P_n be a path with $n\geq 3$ vertices. Clearly, P_n has two types of edges based on the downhill degree of end vertices of each edge as follows:

$E_1 = \{uv$ □$E(G)|\ d_{dn}(u)=0,\ d_{dn}(v) = n-1\}$, $|E_1| = 2$.

$E_2 = \{uv$ □$E(G)|\ d_{dn}(u)= d_{dn}(v) = n-1\}$, $|E_2| = n-3$.

Then

$$DWNG(P_n)$$
$$=\sum_{uv\in E(P_n)}\sqrt{d_{dn}(u)^2+d_{dn}(v)^2+d_{dn}(u)d_{dn}(v)}$$
$$=2\sqrt{0^2+(n-1)^2+0(n-1)}$$
$$+(n-3)\sqrt{(n-1)^2+(n-1)^2+(n-1)^2}$$
$$=(n-1)\left(\sqrt{3}n+2-3\sqrt{3}\right)$$

Proposition 3. Let $K_{m,n}$ be a complete bipartite graph with $m< n$. Then

$$DWNG(K_{m,n})=mn^2.$$

Proof. Let $K_{m,n}$ be a complete bipartite graph with $m< n$. There are $m+n$ vertices and mn edges. Clearly, $K_{m,n}$ has one type of edges based on the downhill degree of end vertices of each edge as follows:

$E_1 = \{uv \in E(K_{m,n})|\ d_{dn}(u)=0,\ d_{dn}(v) = n\}$, $|E_1| = mn$.

Then

$$DWNG(K_{m,n})$$
$$=\sum_{uv\in E(K_{m,n})}\sqrt{d_{dn}(u)^2+d_{dn}(v)^2+d_{dn}(u)d_{dn}(v)}$$
$$=mn\sqrt{0^2+n^2+0n}=mn^2.$$

III. RESULTS FOR WHEEL GRAPHS

Let W_n be a wheel with $n+1$vertices and $2n$ edges, $n\geq 4$. Then there are two types of edges based on the downhill degree of end vertices of each edge as follows:

$E_1 = \{uv \in E(W_n)\ |\ d_{dn}(u) = n,\ d_{dn}(v) = n-1\}$,

$E_2 = \{uv \in E(W_n)\ |\ d_{dn}(u) = d_{dn}(v) = n-1\}$,

$|E_2| = n$.

Theorem 1. Let W_n be a wheel with $n+1$vertices and $2n$ edges, $n\geq 4$. Then

$$DWNG(W_n)=n\sqrt{3n^2-3n+1}+\sqrt{3}n(n-1).$$

Proof. We deduce

$$DWNG(W_n)$$
$$=\sum_{uv\in E(W_n)}\sqrt{d_{dn}(u)^2+d_{dn}(v)^2+d_{dn}(u)d_{dn}(v)}$$
$$=n\sqrt{n^2+(n-1)^2+n(n-1)}$$
$$+n\sqrt{(n-1)^2+(n-1)^2+(n-1)^2}$$
$$=n\sqrt{3n^2-3n+1}+\sqrt{3}n(n-1).$$

Theorem 2. Let W_n be a wheel with $n+1$vertices and $2n$ edges, $n\geq 4$. Then

$$DWNG(W_n, x) = nx^{\sqrt{3n^2-3n+1}} + nx^{\sqrt{3}(n-1)}.$$

Proof. We obtain

$$DWNG(G,x) = \sum_{uv\in E(G)} x^{\sqrt{d_{dn}(u)^2+d_{dn}(v)^2+d_{dn}(u)d_{dn}(v)}}$$

$$= nx^{\sqrt{n^2+(n-1)^2+n(n-1)}} + nx^{\sqrt{(n-1)^2+(n-1)^2+(n-1)^2}}$$

$$= nx^{\sqrt{3n^2-3n+1}} + nx^{\sqrt{3}(n-1)}.$$

Theorem 3. Let W_n be a wheel with n+1vertices and 2n edges, n≥4. Then

$$^{m}DWSO(W_n) = \frac{n}{\sqrt{3n^2-3n+1}} + \frac{n}{\sqrt{3}(n-1)}.$$

Proof. We deduce

$$^{m}DWNG(G)$$

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

$$= \frac{n}{\sqrt{n^2+(n-1)^2+n(n-1)}}$$

$$+ \frac{n}{\sqrt{(n-1)^2+(n-1)^2+(n-1)^2}}$$

$$= \frac{n}{\sqrt{3n^2-3n+1}} + \frac{n}{\sqrt{3}(n-1)}$$

Theorem 4. Let W_n be a wheel with n+1vertices and 2n edges, n≥4. Then

$$^{m}DWSO(W_n, x) = nx^{\frac{1}{\sqrt{2n^2-2n+1}}} + nx^{\frac{1}{\sqrt{2}(n-1)}}.$$

Proof. We obtain

$$^{m}DWSO(W_n, x) = \sum_{uv\in E(W_n)} x^{\frac{1}{\sqrt{d_{dn}(u)^2+d_{dn}(v)^2}}}$$

$$= nx^{\frac{1}{\sqrt{n^2+(n-1)^2}}} + nx^{\frac{1}{\sqrt{(n-1)^2+(n-1)^2}}}$$

$$= nx^{\frac{1}{\sqrt{2n^2-2n+1}}} + nx^{\frac{1}{\sqrt{2}(n-1)}}.$$

IV. RESULTS AND DISCUSSION: 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 be the chemical structure of chloroquine. This structure has 21 vertices and 23 edges, see Figure 1.

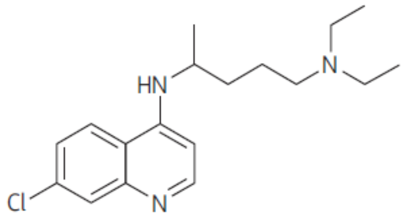

Figure 1. Chemical structure of chloroquine

From Figure 1, we obtain that $\{(d_{dn}(u), d_{dn}(v)) \setminus uv \in E(G)\}$ has 13 edge set partitions.

Table 1. Edge set partitions of chloroquine

$d_{dn}(u), d_{dn}(v) \setminus uv \in E(G)$	(9,9)	(2,9)	(1,9)	(2,7)	(1,7)	(2,5)	(1,4)	(2,2)	(1,1)	(0,9)	(0,5)	(0,4)	(0,1)
Number of edges	2	2	1	1	2	1	1	4	1	2	2	2	2

We calculate the downhill Nirmala alpha Gourava index of chloroquine as follows.

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

$$DWNG(G) = 27\sqrt{3} + 2\sqrt{103} + \sqrt{91} + \sqrt{67}$$
$$+2\sqrt{57} + \sqrt{39} + \sqrt{21} + 38.$$

Proof: We deduce

$$DWNG(G) = \sum_{uv\in E(G)} \sqrt{d_{dn}(u)^2+d_{dn}(v)^2+d_{dn}(u)d_{dn}(v)}$$
$$= 2\sqrt{9^2+9^2+9\times 9} + 2\sqrt{2^2+9^2+2\times 9}$$
$$+1\sqrt{1^2+9^2+1\times 9} + 1\sqrt{2^2+7^2+2\times 7} + 2\sqrt{1^2+7^2+1\times 7}$$
$$+1\sqrt{2^2+5^2+2\times 5} + 1\sqrt{1^2+4^2+1\times 4} + 4\sqrt{2^2+2^2+2\times 2}$$
$$+1\sqrt{1^2+1^2+1\times 1} + 2\sqrt{0^2+9^2+0\times 9} + 2\sqrt{0^2+5^2+0\times 5}$$
$$+2\sqrt{0^2+4^2+0\times 4} + 2\sqrt{0^2+1^2+0\times 1}.$$

By simplifying the above equation, we get the desired result.

We calculate the downhill Nirmala alpha Gourava exponential of chloroquine as follows.

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

$$DWNG(G,x)=2x^{9\sqrt{3}}+2x^{\sqrt{103}}+1x^{\sqrt{91}}+1x^{\sqrt{67}}+2x^{\sqrt{57}}+1x^{\sqrt{39}}+1x^{\sqrt{21}}+4x^{2\sqrt{3}}+1x^{\sqrt{3}}+2x^{9}+2x^{5}+2x^{4}+2x^{1}.$$

Proof: We deduce

$$DWNG(G,x)=\sum_{uv\in E(G)} x^{\sqrt{d_{dn}(u)^2+d_{dn}(v)^2+d_{dn}(u)d_{dn}(v)}}$$
$$=2x^{\sqrt{9^2+9^2+9\times9}}+2x^{\sqrt{2^2+9^2+2\times9}}+1x^{\sqrt{1^2+9^2+1\times9}}+1x^{\sqrt{2^2+7^2+2\times7}}+2x^{\sqrt{1^2+7^2+1\times7}}+1x^{\sqrt{2^2+5^2+2\times5}}+1x^{\sqrt{1^2+4^2+1\times4}}+4x^{\sqrt{2^2+2^2+2\times2}}+1x^{\sqrt{1^2+1^2+1\times1}}+2x^{\sqrt{0^2+9^2+0\times9}}+2x^{\sqrt{0^2+5^2+0\times5}}+2x^{\sqrt{0^2+4^2+0\times4}}+2x^{\sqrt{0^2+1^2+0\times1}}.$$

By simplifying the above equation, we obtain the desired result.

We compute the modified downhill Nirmala alpha Gourava index of chloroquine as follows.

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

$${}^{m}DWNG(G)=\frac{2}{9\sqrt{3}}+\frac{2}{\sqrt{103}}+\frac{1}{\sqrt{91}}+\frac{1}{\sqrt{67}}+\frac{2}{\sqrt{57}}+\frac{1}{\sqrt{39}}+\frac{1}{\sqrt{21}}+\frac{4}{2\sqrt{3}}+\frac{1}{\sqrt{3}}+\frac{2}{9}+\frac{2}{5}+\frac{2}{4}+\frac{2}{1}.$$

Proof: We derive

$${}^{m}DWNG(G)=$$
$$=\sum_{uv\in E(G)}\frac{1}{\sqrt{d_{dn}(u)^2+d_{dn}(v)^2+d_{dn}(u)d_{dn}(v)}}$$
$$=\frac{2}{\sqrt{9^2+9^2+9\times9}}+\frac{2}{\sqrt{2^2+9^2+2\times9}}+\frac{1}{\sqrt{1^2+9^2+1\times9}}+\frac{1}{\sqrt{2^2+7^2+2\times7}}+\frac{2}{\sqrt{1^2+7^2+1\times7}}+\frac{1}{\sqrt{2^2+5^2+2\times5}}+\frac{1}{\sqrt{1^2+4^2+1\times4}}+\frac{4}{\sqrt{2^2+2^2+2\times2}}+\frac{1}{\sqrt{1^2+1^2+1\times1}}+\frac{2}{\sqrt{0^2+9^2+0\times9}}+\frac{2}{\sqrt{0^2+5^2+0\times5}}+\frac{2}{\sqrt{0^2+4^2+0\times4}}+\frac{2}{\sqrt{0^2+1^2+0\times1}}.$$

By simplifying the above equation, we get the required result.

We compute the modified downhill Nirmala alpha Gourava exponential of chloroquine as follows.

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

$${}^{m}DWNG(G,x)=2x^{\frac{1}{9\sqrt{3}}}+2x^{\frac{1}{\sqrt{103}}}+1x^{\frac{1}{\sqrt{91}}}+1x^{\frac{1}{\sqrt{67}}}+2x^{\frac{1}{\sqrt{57}}}+1x^{\frac{1}{\sqrt{39}}}+1x^{\frac{1}{\sqrt{21}}}+4x^{\frac{1}{2\sqrt{3}}}+1x^{\frac{1}{\sqrt{3}}}+2x^{\frac{1}{9}}+2x^{\frac{1}{5}}+2x^{\frac{1}{4}}+2x^{1}.$$

Proof: We derive

$${}^{m}DWNG(G,x)=\sum_{uv\in E(G)} x^{\frac{1}{\sqrt{d_{dn}(u)^2+d_{dn}(v)^2+d_{dn}(u)d_{dn}(v)}}}$$
$$=2x^{\frac{1}{\sqrt{9^2+9^2+9\times9}}}+2x^{\frac{1}{\sqrt{2^2+9^2+2\times9}}}+1x^{\frac{1}{\sqrt{1^2+9^2+1\times9}}}+1x^{\frac{1}{\sqrt{2^2+7^2+2\times7}}}+2x^{\frac{1}{\sqrt{1^2+7^2+1\times7}}}+1x^{\frac{1}{\sqrt{2^2+5^2+2\times5}}}+1x^{\frac{1}{\sqrt{1^2+4^2+1\times4}}}+4x^{\frac{1}{\sqrt{2^2+2^2+2\times2}}}+1x^{\frac{1}{\sqrt{1^2+1^2+1\times1}}}+2x^{\frac{1}{\sqrt{0^2+9^2+0\times9}}}+2x^{\frac{1}{\sqrt{0^2+5^2+0\times5}}}+2x^{\frac{1}{\sqrt{0^2+4^2+0\times4}}}+2x^{\frac{1}{\sqrt{0^2+1^2+0\times1}}}.$$

After simplification, we obtain the desired result.

V. RESULTS AND DISCUSSION: HYDROXYCHLOROQUINE

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

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

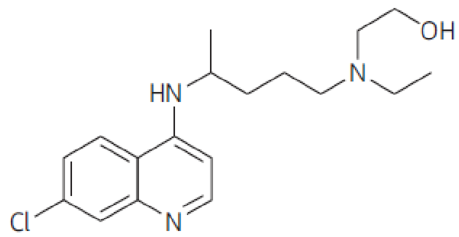

Figure 2. Chemical structure of hydroxychloroquine

From Figure 2, we obtain that $\{(d_{dn}(u), d_{dn}(v))\setminus uv\in E(H)\}$ has 14 edge set partitions.

Table 2. Edge set partitions of hydroxychloroquine

$d_{dn}(u), d_{dn}(v) \setminus uv \in E(H)$	(9,9)	(2,9)	(1,9)	(2,8)	(1,8)
Number of edges	2	2	1	2	1
	(2,5)	(1,4)	(2,2)	(1,1)	(0,9)
	1	1	5	1	2
	(0,5)	(0,4)	(0,2)	(0,1)	
	2	2	1	1	

We calculate the downhill Nirmala alpha Gourava index of hydroxychloroquine as follows.

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

$$DWNG(H)=29\sqrt{3}+2\sqrt{103}+\sqrt{91}+2\sqrt{84}+\sqrt{73}+\sqrt{39}+\sqrt{21}+39.$$

Proof: We deduce

$$DWNG(H)=\sum_{uv\in E(H)}\sqrt{d_{dn}(u)^2+d_{dn}(v)^2+d_{dn}(u)d_{dn}(v)}$$
$$=2\sqrt{9^2+9^2+9\times 9}+2\sqrt{2^2+9^2+2\times 9}+1\sqrt{1^2+9^2+1\times 9}+2\sqrt{2^2+8^2+2\times 8}+1\sqrt{1^2+8^2+1\times 8}$$
$$+1\sqrt{2^2+5^2+2\times 5}+1\sqrt{1^2+4^2+1\times 4}+5\sqrt{2^2+2^2+2\times 2}+1\sqrt{1^2+1^2+1\times 1}+2\sqrt{0^2+9^2+0\times 9}+2\sqrt{0^2+5^2+0\times 5}$$
$$+2\sqrt{0^2+4^2+0\times 4}+1\sqrt{0^2+2^2+0\times 2}+1\sqrt{0^2+1^2+0\times 1}.$$

By simplifying the above equation, we get the desired result.

We calculate the downhill Nirmala alpha Gourava exponential of hydroxychloroquine as follows.

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

$$DWNG(H,x)=2x^{9\sqrt{3}}+2x^{\sqrt{103}}+1x^{\sqrt{91}}+2x^{\sqrt{84}}+1x^{\sqrt{73}}+1x^{\sqrt{39}}+1x^{\sqrt{21}}+5x^{2\sqrt{3}}+1x^{\sqrt{3}}+2x^{9}+2x^{5}+2x^{4}+1x^{2}+1x^{1}.$$

Proof: We deduce

$$DWNG(H,x)=\sum_{uv\in E(H)}x^{\sqrt{d_{dn}(u)^2+d_{dn}(v)^2+d_{dn}(u)d_{dn}(v)}}$$
$$=2x^{\sqrt{9^2+9^2+9\times 9}}+2x^{\sqrt{2^2+9^2+2\times 9}}+1x^{\sqrt{1^2+9^2+1\times 9}}+2x^{\sqrt{2^2+8^2+2\times 8}}$$
$$+1x^{\sqrt{1^2+8^2+1\times 8}}+1x^{\sqrt{2^2+5^2+2\times 5}}+1x^{\sqrt{1^2+4^2+1\times 4}}+5x^{\sqrt{2^2+2^2+2\times 2}}$$
$$+1x^{\sqrt{1^2+1^2+1\times 1}}+2x^{\sqrt{0^2+9^2+0\times 9}}+2x^{\sqrt{0^2+5^2+0\times 5}}$$
$$+2x^{\sqrt{0^2+4^2+0\times 4}}+1x^{\sqrt{0^2+2^2+0\times 2}}+1x^{\sqrt{0^2+1^2+0\times 1}}.$$

By simplifying the above equation, we obtain the desired result.

We compute the modified downhill Nirmala alpha Gourava index of hydroxychloroquine as follows.

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

$$^{m}DWNG(H)=\frac{2}{9\sqrt{3}}+\frac{2}{\sqrt{103}}+\frac{1}{\sqrt{91}}+\frac{2}{\sqrt{84}}+\frac{1}{\sqrt{73}}+\frac{1}{\sqrt{39}}+\frac{1}{\sqrt{21}}+\frac{5}{2\sqrt{3}}+\frac{1}{\sqrt{3}}+\frac{2}{9}+\frac{2}{5}+\frac{2}{4}+\frac{1}{2}+\frac{1}{1}.$$

Proof: We derive

$$^{m}DWNG(H)=$$
$$=\sum_{uv\in E(H)}\frac{1}{\sqrt{d_{dn}(u)^2+d_{dn}(v)^2+d_{dn}(u)d_{dn}(v)}}$$
$$=\frac{2}{\sqrt{9^2+9^2+9\times 9}}+\frac{2}{\sqrt{2^2+9^2+2\times 9}}+\frac{1}{\sqrt{1^2+9^2+1\times 9}}$$
$$+\frac{2}{\sqrt{2^2+8^2+2\times 8}}+\frac{1}{\sqrt{1^2+8^2+1\times 8}}+\frac{1}{\sqrt{2^2+5^2+2\times 5}}$$
$$+\frac{1}{\sqrt{1^2+4^2+1\times 4}}+\frac{5}{\sqrt{2^2+2^2+2\times 2}}+\frac{1}{\sqrt{1^2+1^2+1\times 1}}$$
$$+\frac{2}{\sqrt{0^2+9^2+0\times 9}}+\frac{2}{\sqrt{0^2+5^2+0\times 5}}+\frac{2}{\sqrt{0^2+4^2+0\times 4}}$$
$$+\frac{1}{\sqrt{0^2+2^2+0\times 2}}+\frac{1}{\sqrt{0^2+1^2+0\times 1}}.$$

By simplifying the above equation, we get the required result.

We compute the modified downhill Nirmala alpha Gourava exponential of hydroxychloroquine as follows

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

$$^{m}DWNG(H,x)=2x^{\frac{1}{9\sqrt{3}}}+2x^{\frac{1}{\sqrt{103}}}+1x^{\frac{1}{\sqrt{91}}}+2x^{\frac{1}{\sqrt{84}}}+1x^{\frac{1}{\sqrt{73}}}+1x^{\frac{1}{\sqrt{39}}}+1x^{\frac{1}{\sqrt{21}}}+5x^{\frac{1}{2\sqrt{3}}}+1x^{\frac{1}{\sqrt{3}}}+2x^{\frac{1}{9}}+2x^{\frac{1}{5}}+2x^{\frac{1}{4}}+1x^{\frac{1}{2}}+1x^{1}.$$

Proof: We derive

$$^{m}DWNG(H,x)=\sum_{uv\in E(H)}x^{\frac{1}{\sqrt{d_{dn}(u)^2+d_{dn}(v)^2+d_{dn}(u)d_{dn}(v)}}}$$
$$=2x^{\frac{1}{\sqrt{9^2+9^2+9\times 9}}}+2x^{\frac{1}{\sqrt{2^2+9^2+2\times 9}}}+1x^{\frac{1}{\sqrt{1^2+9^2+1\times 9}}}+2x^{\frac{1}{\sqrt{2^2+8^2+2\times 8}}}$$
$$+1x^{\frac{1}{\sqrt{1^2+8^2+1\times 8}}}+1x^{\frac{1}{\sqrt{2^2+5^2+2\times 5}}}+1x^{\frac{1}{\sqrt{1^2+4^2+1\times 4}}}+5x^{\frac{1}{\sqrt{2^2+2^2+2\times 2}}}$$
$$+1x^{\frac{1}{\sqrt{1^2+1^2+1\times 1}}}+2x^{\frac{1}{\sqrt{0^2+9^2+0\times 9}}}+2x^{\frac{1}{\sqrt{0^2+5^2+0\times 5}}}+2x^{\frac{1}{\sqrt{0^2+4^2+0\times 4}}}$$
$$+1x^{\frac{1}{\sqrt{0^2+2^2+0\times 2}}}+1x^{\frac{1}{\sqrt{0^2+1^2+0\times 1}}}$$

By simplifying the above equation, we get the required result.

After simplification, we obtain the desired result.

VI. RESULTS AND DISCUSSION: REMDESIVIR

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

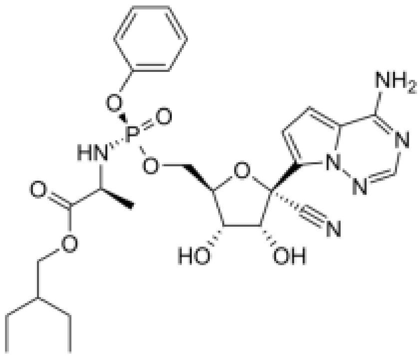

Figure 3. Chemical structure of remdesivir

From Figure 3, we obtain that $\{(d_{dn}(u), d_{dn}(v)) \setminus uv \in E(R)\}$ has 20 edge set partitions.

Table 3. Edge set partitions of remdesivir

$d_{dn}(u), d_{dn}(v)$ $\setminus uv \in E(R)$	9,19)	(7,19)	(9,9)	(2,9)	(1,9)
Number of edges	1	1	3	2	2
	(7,7)	(1,7)	(6,6)	(4,6)	(1,6)
	2	1	1	2	4
	(1,5)	(4,4)	(2,2)	(1,1)	(0,19)
	1	4	2	3	2
	(0,9)	(0,7)	(0,6)	(0,5)	(0,1)
	1	3	4	3	2

We calculate the downhill Nirmala alpha Gourava index of remdesivir as follows.

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

$$DWNG(R) = \sqrt{613} + \sqrt{543} + 70\sqrt{3} + 2\sqrt{103} + 2\sqrt{91} + \sqrt{57} + 4\sqrt{19} + 4\sqrt{43} + \sqrt{31} + 109.$$

Proof: We deduce

$$DWNG(R) = \sum_{uv \in E(R)} \sqrt{d_{dn}(u)^2 + d_{dn}(v)^2 + d_{dn}(u)d_{dn}(v)}$$
$$= 1\sqrt{9^2 + 19^2 + 9\times19} + 1\sqrt{7^2 + 19^2 + 7\times19}$$
$$+3\sqrt{9^2 + 9^2 + 9\times9} + 2\sqrt{2^2 + 9^2 + 2\times9} + 2\sqrt{1^2 + 9^2 + 1\times9}$$
$$+2\sqrt{7^2 + 7^2 + 7\times7} + 1\sqrt{1^2 + 7^2 + 1\times7} + 1\sqrt{6^2 + 6^2 + 6\times6}$$
$$+2\sqrt{4^2 + 6^2 + 4\times6} + 4\sqrt{1^2 + 6^2 + 1\times6} + 1\sqrt{1^2 + 5^2 + 1\times5}$$
$$+4\sqrt{4^2 + 4^2 + 4\times4} + 2\sqrt{2^2 + 2^2 + 2\times2} + 3\sqrt{1^2 + 1^2 + 1\times1}$$
$$+2\sqrt{0^2 + 19^2 + 0\times19} + 1\sqrt{0^2 + 9^2 + 0\times9}$$
$$+3\sqrt{0^2 + 7^2 + 0\times7} + 4\sqrt{0^2 + 6^2 + 0\times6}$$
$$+3\sqrt{0^2 + 5^2 + 0\times5} + 2\sqrt{0^2 + 1^2 + 0\times1}.$$

By simplifying the above equation, we get the desired result.

We calculate the downhill Nirmala alpha Gourava exponential of remdesivir as follows.

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

$$DWNG(R,x)$$
$$= 1x^{\sqrt{613}} + 1x^{\sqrt{543}} + 3x^{9\sqrt{3}} + 2x^{\sqrt{103}} + 2x^{\sqrt{91}} + 2x^{7\sqrt{3}}$$
$$+1x^{\sqrt{57}} + 1x^{6\sqrt{3}} + 2x^{2\sqrt{19}} + 4x^{\sqrt{43}} + 1x^{\sqrt{31}} + 4x^{4\sqrt{3}}$$
$$+2x^{2\sqrt{3}} + 3x^{\sqrt{3}} + 2x^{19} + 1x^{9} + 3x^{7} + 4x^{6} + 3x^{5} + 2x^{1}.$$

Proof: We deduce

$$DWNG(R,x) = \sum_{uv \in E(R)} x^{\sqrt{d_{dn}(u)^2 + d_{dn}(v)^2 + d_{dn}(u)d_{dn}(v)}}$$
$$= 1x^{\sqrt{9^2+19^2+9\times19}} + 1x^{\sqrt{7^2+19^2+7\times19}} + 3x^{\sqrt{9^2+9^2+9\times9}}$$
$$+2x^{\sqrt{2^2+9^2+2\times9}} + 2x^{\sqrt{1^2+9^2+1\times9}} + 2x^{\sqrt{7^2+7^2+7\times7}} + 1x^{\sqrt{1^2+7^2+1\times7}}$$
$$+1x^{\sqrt{6^2+6^2+6\times6}} + 2x^{\sqrt{4^2+6^2+4\times6}} + 4x^{\sqrt{1^2+6^2+1\times6}} + 1x^{\sqrt{1^2+5^2+1\times5}}$$
$$+4x^{\sqrt{4^2+4^2+4\times4}} + 2x^{\sqrt{2^2+2^2+2\times2}} + 3x^{\sqrt{1^2+1^2+1\times1}} + 2x^{\sqrt{0^2+19^2+0\times19}}$$
$$+1x^{\sqrt{0^2+9^2+0\times9}} + 3x^{\sqrt{0^2+7^2+0\times7}} + 4x^{\sqrt{0^2+6^2+0\times6}}$$
$$+3x^{\sqrt{0^2+5^2+0\times5}} + 2x^{\sqrt{0^2+1^2+0\times1}}.$$

By simplifying the above equation, we obtain the desired result.

We compute the modified downhill Nirmala alpha Gourava index of remdesivir as follows.

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

$$^{m}DWNG(R) = \frac{1}{\sqrt{613}} + \frac{1}{\sqrt{543}} + \frac{3}{9\sqrt{3}} + \frac{2}{\sqrt{103}}$$
$$+\frac{2}{\sqrt{91}} + \frac{2}{7\sqrt{3}} + \frac{1}{\sqrt{57}} + \frac{1}{6\sqrt{3}} + \frac{2}{2\sqrt{19}} + \frac{4}{\sqrt{43}} + \frac{1}{\sqrt{31}}$$
$$+\frac{4}{4\sqrt{3}} + \frac{2}{2\sqrt{3}} + \frac{3}{\sqrt{3}} + \frac{2}{19} + \frac{1}{9} + \frac{3}{7} + \frac{4}{6} + \frac{3}{5} + \frac{2}{1}.$$

Proof: We derive

$$
\begin{aligned}
&{}^{m}DWNG(R)=\\
&=\sum_{uv\in E(R)}\frac{1}{\sqrt{d_{dn}(u)^2+d_{dn}(v)^2+d_{dn}(u)d_{dn}(v)}}\\
&=\frac{1}{\sqrt{9^2+19^2+9\times 19}}+\frac{1}{\sqrt{7^2+19^2+7\times 19}}\\
&+\frac{3}{\sqrt{9^2+9^2+9\times 9}}+\frac{2}{\sqrt{2^2+9^2+2\times 9}}+\frac{2}{\sqrt{1^2+9^2+1\times 9}}\\
&+\frac{2}{\sqrt{7^2+7^2+7\times 7}}+\frac{1}{\sqrt{1^2+7^2+1\times 7}}+\frac{1}{\sqrt{6^2+6^2+6\times 6}}\\
&+\frac{2}{\sqrt{4^2+6^2+4\times 6}}+\frac{4}{\sqrt{1^2+6^2+1\times 6}}+\frac{1}{\sqrt{1^2+5^2+1\times 5}}\\
&+\frac{4}{\sqrt{4^2+4^2+4\times 4}}+\frac{2}{\sqrt{2^2+2^2+2\times 2}}+\frac{3}{\sqrt{1^2+1^2+1\times 1}}\\
&+\frac{2}{\sqrt{0^2+19^2+0\times 19}}+\frac{1}{\sqrt{0^2+9^2+0\times 9}}\\
&+\frac{3}{\sqrt{0^2+7^2+0\times 7}}+\frac{4}{\sqrt{0^2+6^2+0\times 6}}\\
&+\frac{3}{\sqrt{0^2+5^2+0\times 5}}+\frac{2}{\sqrt{0^2+1^2+0\times 1}}.
\end{aligned}
$$

By simplifying the above equation, we get the required result.

We compute the modified downhill Nirmala alpha Gourava exponential of remdesivir as follows

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

$$
\begin{aligned}
{}^{m}DWNG(R,x)&=1x^{\frac{1}{\sqrt{613}}}+1x^{\frac{1}{\sqrt{543}}}+3x^{\frac{1}{9\sqrt{3}}}+2x^{\frac{1}{\sqrt{103}}}\\
&+2x^{\frac{1}{\sqrt{91}}}+2x^{\frac{1}{7\sqrt{3}}}+1+2x^{\frac{1}{\sqrt{84}}}+1x^{\frac{1}{6\sqrt{3}}}+2x^{\frac{1}{2\sqrt{19}}}+4x^{\frac{1}{\sqrt{43}}}\\
&+1x^{\frac{1}{\sqrt{31}}}+4x^{\frac{1}{4\sqrt{3}}}+2x^{\frac{1}{2\sqrt{3}}}+3x^{\frac{1}{\sqrt{3}}}+2x^{\frac{1}{19}}+1x^{\frac{1}{9}}+3x^{\frac{1}{7}}\\
&+4x^{\frac{1}{6}}+3x^{\frac{1}{5}}+2x^{1}.
\end{aligned}
$$

Proof: We derive

$$
\begin{aligned}
&{}^{m}DWNG(R,x)=\sum_{uv\in E(R)}x^{\frac{1}{\sqrt{d_{dn}(u)^2+d_{dn}(v)^2+d_{dn}(u)d_{dn}(v)}}}\\
&=1x^{\frac{1}{\sqrt{9^2+19^2+9\times 19}}}+1x^{\frac{1}{\sqrt{7^2+19^2+7\times 19}}}+3x^{\frac{1}{\sqrt{9^2+9^2+9\times 9}}}\\
&+2x^{\frac{1}{\sqrt{2^2+9^2+2\times 9}}}+2x^{\frac{1}{\sqrt{1^2+9^2+1\times 9}}}+2x^{\frac{1}{\sqrt{7^2+7^2+7\times 7}}}+1x^{\frac{1}{\sqrt{1^2+7^2+1\times 7}}}\\
&+1x^{\frac{1}{\sqrt{6^2+6^2+6\times 6}}}+2x^{\frac{1}{\sqrt{4^2+6^2+4\times 6}}}+2x^{\frac{1}{\sqrt{1^2+6^2+1\times 6}}}+1x^{\frac{1}{\sqrt{1^2+5^2+1\times 5}}}\\
&+4x^{\frac{1}{\sqrt{4^2+4^2+4\times 4}}}+2x^{\frac{1}{\sqrt{2^2+2^2+2\times 2}}}+3x^{\frac{1}{\sqrt{1^2+1^2+1\times 1}}}+2x^{\frac{1}{\sqrt{0^2+19^2+0\times 19}}}\\
&+1x^{\frac{1}{\sqrt{0^2+9^2+0\times 9}}}+3x^{\frac{1}{\sqrt{0^2+7^2+0\times 7}}}+4x^{\frac{1}{\sqrt{0^2+6^2+0\times 6}}}\\
&+3x^{\frac{1}{\sqrt{0^2+5^2+0\times 5}}}+2x^{\frac{1}{\sqrt{0^2+1^2+0\times 1}}}.
\end{aligned}
$$

After simplification, we obtain the desired result.

VII. CONCLUSION

In this paper, the downhill Nirmala alpha Gourava and modified downhill Nirmala alpha Gourava indices are defined. Also these newly defined indices and their corresponding exponentials of certain chemical drugs are determined.

REFERENCES

1. V.R.Kulli, *College Graph Theory*, Vishwa International Publications, Gulbarga, India (2012).
2. V.R.Kulli, Graph indices, in *Hand Book of Research on Advanced Applications of Application Graph Theory in Modern Society*, M. Pal. S. Samanta and A. Pal, (eds.) IGI Global, USA (2019) 66-91.
3. I.Gutman and N.Trinajstic, Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons, *Chem. Phys. Let.* 17 (1972) 535-538.
4. A.H.Karim, N.E.Arif and A.M.Ramadan, The M-Polynomial and Nirmala index of certain composite graphs, *Tikrit Journal of Pure Science*, 27(3) (2022) 92-101.
5. V.R.Kulli, Reverse Nirmala index, *International Journal of Engineering Sciences and Research Technology*, 11(8) (2022) 12-19.
6. V.R.Kulli, On multiplicative inverse Nirmala indices, *Annals of Pure and Applied Mathematics*, 23(2) (2021) 57-61.
7. V.R.Kulli, Revan Nirmala index, *Annals of Pure and Applied Mathematics*, 26(1) (2022) 7-13.
8. V.R.Kulli, HDR Nirmala index, *International Journal of Mathematics and Computer Research*, 10(7) (2022) 2796-2800.
9. V.R.Kulli, Computation of E-Banhatti Nirmala indices of 1,3-Adamantane, *Annals of Pure and Applied Mathematics*, 26(2) (2022) 119-124.
10. V.R.Kulli, On multiplicative inverse Nirmala indices, *Annals of Pure and Applied Mathematics*, 23(2) (2021) 57-61.
11. V.R.Kulli, Domination Nirmala indices of graphs, *International Journal of Mathematics and Computer Research*, 11(6) (2023) 3497-3502.
12. V.R.Kulli, Multiplicative domination Nirmala indices of graphs, *International Journal of Mathematics And its Applications*, (2023).

13. V.R.Kulli, Irregularity domination Nirmala and domination Sombor indices of certain drugs, *International Journal of Mathematical Archive*, 14(8) (2023) 1-7.
14. V.R.Kulli, Edge versions of Sombor and Nirmala indices of some nanotubes and nanotori, *International Journal of Mathematics and Computer Research*, 11(3) (2023) 3305-3310.
15. V.R.Kulli, Gourava Nirmala indices of certain nanostructures, *International Journal of Mathematical Archive*, 14(2) (2023) 1-9.
16. N.K.Raut and G.K.Sanap, On Nirmala indices of carbon nanocone C4[2], *IOSR Journal of Mathematics*, 18(4) (2022) 10-15.
17. N.F.Yalcin, Bounds on Nirmala energy of graphs, *Acta Univ. Sapientiae Informatica*, 14(2) (2022) 302-315.
18. G.N.Adithya, N.D.Soner and M.Kirankumar, Gourava indices for Jahangir graph and phase transfer catalyst, *Journal of Emerging Technologies and Innovative Research*, 10(6) (2023) f394-f399.
19. M.Aruvi, J.M.Joseph and E.Ramganesh, The second Gourava index of some graph products, *Advances in Mathematics: Scientific Journal*, 9(12) (2020) 10241-10249.
20. V.R.Kulli, Gourava domination indices of graphs, *International Journal of Mathematics and Computer Research*, 11(8) (2023) 3680-3684. DOI:10.47191/ijmcr/v11i8.08.
21. V.R.Kulli, On hyper Gourava domination indices, *International Journal of Engineering Sciences & Research Technology*, 12(10) (2023) 12-20. DOI: 10.5281/zenodo.10036777.
22. I.Gutman and V.R.Kulli, Estimating the Gourava Sombor index, *Ser. A: Appl. Math. Inform. And Mech.* 16(1) (2024) 47-52.
23. V.R.Kulli, On alpha and gamma Gourava indices, *International Journal of Mathematics and Computer Research*, 12(4) (2024) 4139-4144. DOI:10.47191/ijmcr/v12i4.04.
24. V.R.Kulli, Nirmala alpha Gourava and modified Nirmala alpha Gourava indices of certain dendrimers, *International Journal of Mathematics and Computer Research*, 12(5) (2024) 4256-4263. DOI:10.47191/ijmcr/v12i5.10.
25. V.R.Kulli, Elliptic Revan Sombor index and its exponential of certain networks, *International Journal of Mathematics and Computer Research*, 12(2) (2024) 4055-4061. DOI:10.47191/ijmcr/v12i2.08.
26. B.K.Majhi, V.R.Kulli and I.N.Cangul, Revan indices and their polynomials of square snake graphs, *Montes Taurus J. Pure Appl. Math.* 6(1) (2024) 12-17.
27. V.R.Kulli, Modified elliptic Revan index of two families of nanotubes, *Annals of Pure and Applied Mathematics*, 29(2), (2024) 103-107.
28. V.R.Kulli, Revan Kepler Banhatti and modified Revan Kepler Banhatti indices of certain nanotubes, *Annals of Pure and Applied Mathematics*, 30(2), (2024) 129-136.
29. I.Gutman, V.R.Kulli and I.Redzepovic, Irregularity Sombor, index, *Bull. Acad. Serbe. Sci. Arts (Cl. Sci. Math. Natur.)* 156 (2023) 31-37.
30. V.R.Kulli, ve-Degree Sombor indices of certain networks, *International Journal of Mathematics Trends and Technology*, 68(9) (2022) 5-10.
31. V.R.Kulli, Euler Sombor Banhatti indices, *International Journal of Engineering Sciences & Research Technology*, 13(6) (2024) 12-45.
32. V.R.Kulli, Modified elliptic Sombor index and its exponential of a graph, *International Journal of Mathematics and Computer Research*, 12 (1) (2024)3949-3954..
33. V.R.Kulli, Reverse elliptic Sombor and modified reverse elliptic Sombor indices, *International Journal of Mathematical Archive*, 15(1) (2024) 1-7.
34. V.R. Kulli, Multiplicative elliptic Sombor and multiplicative modified elliptic Sombor indices, *Annals of Pure and Applied Mathematics*, 29(1) (2024) 19-23.
35. V.R.Kulli, δ-Banhatti, hyper δ-Banhatti indices and their polynomials of certain networks, *International Journal of Engineering Sciences and Research Technology*, 10(3) (2021) 1-8.
36. V.R.Kulli, Delta atom bond connectivity indices of certain networks, *International Journal of Mathematics and its Applications*, 11(4) (2023) 89-98.
37. V.R.Kulli, On delta harmonic and multiplicative delta harmonic indices of some nanostructures, *International Journal of Mathematics and Statistics Invention*, 11(5) (2023) 38-45.
38. B.K.Majhi, V.R.Kulli and I.N.Cangul, Sum connectivity delta Banhatti and product connectivity delta Banhatti indices of certain nanotubes, *Montes Taurus J. Pure Appl. Math.* 5(2) (2023) 89-97.
39. V.R.Kulli, Delta geometric-arithmetic and delta arithmetic-geometric indices of certain nanotubes, *International Journal of Mathematics and its Applications*, 12(1) (2024) 43-51.
40. V.R.Kulli, Elliptic delta and modified elliptic delta indices of certain networks, *International Journal of Mathematics and its Applications*, 12(2) (2024) 104-116.
41. V.R.Kulli, Delta Kepler Banhatti indices of certain nanostructures, *International Journal of Mathematical Archive*, 16(2) (2025) 5-13.

42. M.V.Diudea (ed.) *QSPR/QSAR Studies by Molecular Descriptors*, NOVA New York, (2001).
43. I.Gutman and O.E.Polansky, *Mathematical Concepts in Organic Chemistry*, Springer, Berlin (1986).
44. S.Wagner and H.Wang, *Introduction Chemical Graph Theory,* Boca Raton, CRC Press, (2018).
45. B.Al-Ahmadi, A.Saleh and W.Al-Shammakh, Downhill Zagreb topological indices of graphs, *International Journal of Analysis and Applications*, 19(2) (2021) 205-227.
46. V.R.Kulli, Nirmala alpha Gourava and modified Nirmala alpha Gourava indices of certain dendrimers, *International Journal of Mathematics and Computer Research*, 12 (5) (2024) 4256-4263.
47. B.Al-Ahmadi, A.Saleh and W.Al-Shammakh, Downhill Zagreb topological indices and Mdn-Polynomial of some chemical structures applied to the treatment of COVID-19 patients, *Open Journal of Applied Sciences*, 11(4) (2021) 395-413.
48. B.Al-Ahmadi, A.Saleh and W.Al-Shammakh, Downhill Zagreb polynomials of graphs, *Research & Reviews: Discrete Mathematical Structures*, 7 (2020) 15-26.
49. V.R.Kulli, Downhill Nirmala indices of graphs, *International Journal of Mathematics and Computer Research*, 13(4) (2025) 5126-5131.
50. V.R.Kulli, Downhill Sombor modified downhill Sombor indices of graphs, *Annals of Pure and Applied Mathematics,* 31(2) (2025) 107-112.
51. V.R.Kulli, Harmonic downhill indices of graphs, *Journal of Mathematics and Informatics*, 28 (2025) 33-37.
52. V.R.Kulli, Downhill product connectivity indices of graphs, *International Journal of Mathematics and Computer Research*, 13(5) (2025) 5223-5226.
53. V.R.Kulli, Hyper downhill indices and their polynomials of certain chemical drugs, *International Journal of Engineering Sciences & Research Technology*, 14(40 92025) 23-30. DOI: 10.5281/zenodo.15424878.