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Research Paper

Nirmala leap indices of some chemical drugs against Covid-19

Bhairaba Kumar Majhi[1], Veerabhadrappa Kulli[2], Ismail Naci Cangul[3,*]

[1]Department of Mathematics, School of Applied Sciences, Centurion University of Technology and Management, Odisha, India, Bolangir Campus, 767001

[2]Department of Mathematics, Gulbarga University, Gulbarga 585106, India

[3]Department of Mathematics, Bursa Uludag University, 16059 Bursa, Turkey

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Dedicated to Prof. Alireza Ashrafi

Abstract. In Chemical Graph Theory, several degree based topological indices were introduced and studied since 1947. Some of these have important applications in chemistry while some only have nice mathematical properties. In this paper, we introduce the Nirmala leap index and modified Nirmala leap index, their polynomials and compute these indices for some important nanostructures which appeared in nanoscience, especially used as a treatment alternative against Covid-19 in many countries.

Keywords: Nirmala leap index, modified Nirmala leap exponential, nanostructure
Mathematics Subject Classification (2010): Primary 05C90; Secondary 92E10.

1 Introduction

In Chemical Graph Theory, topological indices of molecular graphs play a very well-known important role and chemical properties of drugs can be studied by such indices. Several degree based indices of a graph appeared in the literature, see [8], and have found some

*Corresponding author (*Email address*: cangul@uludag.edu.tr)
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applications, especially in QSPR/QSAR studies, see [2,4].

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 edges incident to u. The number of edges in a shortest path connecting any two vertices u and v of G is the distance between these two vertices u and v and denoted by $d(u,v)$. For a positive integer k and $v \in V(G)$, the k-th open neighborhood of v in G is defined as $N_k(v/G) = \{u \in V(G) : \ d(u,v) = k\}$. The k-distance degree of v in G is the number of k-neighbors of v in G and denoted by $d_k(v)$, see [15]. Any undefined terminologies and notations may be found in [7].

Kulli, in [9], introduced the Nirmala index of a graph G as

$$N(G) = \sum_{uv \in E(G)} [d_2(u) + d_2(v)]^{1/2}.$$

Recently, some types of Nirmala indices were studied, for example, in [3,10,12]. We introduce the Nirmala leap index of a graph G and it is defined as

$$NL(G) = \sum_{uv \in E(G)} [d_2(u) + d_2(v)]^{1/2}.$$

Recently, some leap indices were studied, for example, in [5,11].

Considering the Nirmala leap index, we introduce the Nirmala leap exponential of a graph G defined by

$$NL(G,x) = \sum_{uv \in E(G)} x^{\sqrt{d_2(u)+d_2(v)}}.$$

We define the modified Nirmala leap index of a graph G as

$$^{m}NL(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d_2(u) + d_2(v)}}.$$

Considering the modified Nirmala leap index, we proposed the modified Nirmala leap exponential of a graph G and defined it by

$$^{m}NL(G,x) = \sum_{uv \in E(G)} x^{\frac{1}{\sqrt{d_2(u)+d_2(v)}}}.$$

In this paper, the Nirmala leap index, modified Nirmala leap exponential of some recently popularized molecular structures such as chloroquine, hydroxychloroquine, remdesivir are computed. For more on the chemical drugs, see [1,6,13,14].

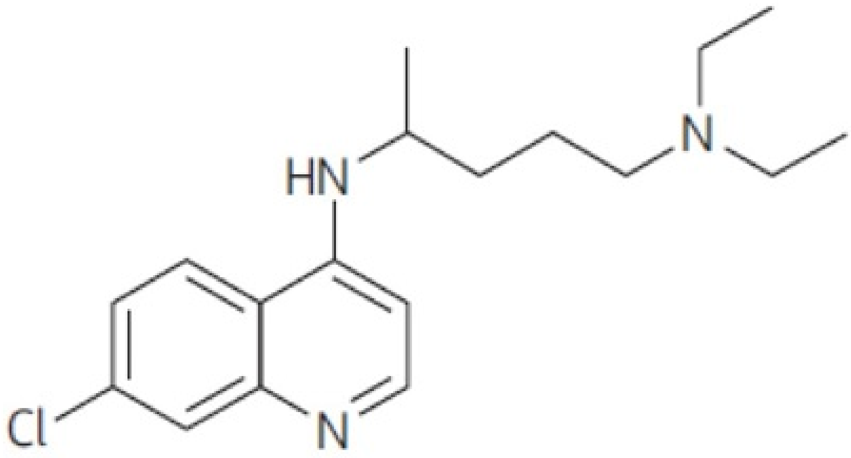

Figure 1. Chemical structure of chloroquine.

2 Results and discussion: chloroquine

Chloroquine is an antiviral compound (drug) which was discovered in 1934 by H. Andersag. This drug is primarily used to prevent and treat malaria. Let G_1 be the chemical structure of chloroquine. This structure has 21 vertices and 23 edges, see Figure 1.

In the above structure, we obtain that the set of edges $(d_2(u), d_2(v))$ for $uv \in E(G_1)$ has 9 types of edge partitions:

Table 1. Edge partition of chloroquine.

$(d_2(u), d_2(v)) : uv \in E(G_1)$	(1,2)	(2,2)	(2,3)	(2,4)	(3,3)
Number of edges:	2	2	8	1	2

$(d_2(u), d_2(v)) : uv \in E(G_1)$	(3,4)	(3,5)	(4,4)	(4,5)
Number of edges:	3	1	2	2

We calculate the Nirmala leap index and its exponential of chloroquine as follows:

Theorem 2.1. *Let G_1 be the chemical structure of chloroquine. Then*

$$(i) NL(G_1) = 6\sqrt{2} + 2\sqrt{3} + 8\sqrt{5} + 3\sqrt{6} + 3\sqrt{7} + 10,$$
$$(ii) NL(G_1, x) = 2x^{\sqrt{3}} + 2x^2 + 8x^{\sqrt{5}} + 3x^{\sqrt{6}} + 3x^{\sqrt{7}} + 3x^{2\sqrt{2}} + 2x^3.$$

Proof. By using the definitions of the indices and edge partition of G_1, we deduce

$$\begin{aligned}(i) NL(G_1) &= \textstyle\sum_{uv \in E(G_1)} [d_2(u) + d_2(v)]^{1/2} \\ &= 2(1+2)^{1/2} + 2(2+2)^{1/2} + 8(2+3)^{1/2} + (2+4)^{1/2} + 2(3+3)^{1/2} \\ &\quad +3(3+4)^{1/2} + (3+5)^{1/2} + 2(4+4)^{1/2} + 2(4+5)^{1/2}.\end{aligned}$$

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

$$
\begin{aligned}
(ii)NL(G_1,x) &= \textstyle\sum_{uv\in E(G_1)} x^{\sqrt{d_2(u)+d_2(v)}}\\
&= 2x^{(1+2)^{1/2}} + 2x^{(2+2)^{1/2}} + 8x^{(2+3)^{1/2}} + x^{(2+4)^{1/2}} + 2x^{(3+3)^{1/2}}\\
&+3x^{(3+4)^{1/2}} + x^{(3+5)^{1/2}} + 2x^{(4+4)^{1/2}} + 2x^{(4+5)^{1/2}}.
\end{aligned}
$$

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

We next compute the modified Nirmala leap index and its exponential of chloroquine as follows:

Theorem 2.2. *Let G_1 be the chemical structure of chloroquine. Then*

$$
\begin{aligned}
&(i)^m NL(G_1) = \tfrac{3}{2\sqrt{2}} + \tfrac{2}{\sqrt{3}} + \tfrac{8}{\sqrt{5}} + \tfrac{3}{\sqrt{6}} + \tfrac{3}{\sqrt{7}} + \tfrac{5}{3}.\\
&(ii)^m NL(G_1,x) = 2x^{\frac{1}{\sqrt{3}}} + 2x^{\frac{1}{2}} + 8x^{\frac{1}{\sqrt{5}}} + 3x^{\frac{1}{\sqrt{6}}} + 3x^{\frac{1}{\sqrt{7}}} + 3x^{\frac{1}{2\sqrt{2}}} + 2x^{\frac{1}{3}}.
\end{aligned}
$$

Proof. Applying the definitions and edge partition of G_1, we conclude

$$
\begin{aligned}
(i)^m NL(G_1) &= \textstyle\sum_{uv\in E(G_1)} \frac{1}{\sqrt{d_2(u)+d_2(v)}}\\
&= 2(1+2)^{-1/2} + 2(2+2)^{-1/2} + 8(2+3)^{-1/2} + (2+4)^{-1/2}\\
&+2(3+3)^{-1/2} + 3(3+4)^{-1/2} + (3+5)^{-1/2} + 2(4+4)^{-1/2}\\
&+2(4+5)^{-1/2}.
\end{aligned}
$$

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

$$
\begin{aligned}
(ii)^m NL(G_1,x) &= \textstyle\sum_{uv\in E(G_1)} x^{\frac{1}{\sqrt{d_2(u)+d_2(v)}}}\\
&= 2x^{(1+2)^{-1/2}} + 2x^{(2+2)^{-1/2}} + 8x^{(2+3)^{-1/2}} + x^{(2+4)^{-1/2}}\\
&+2x^{(3+3)^{-1/2}} + 3x^{(3+4)^{-1/2}} + x^{(3+5)^{-1/2}} + 2x^{(4+4)^{-1/2}}\\
&+2x^{(4+5)^{-1/2}}.
\end{aligned}
$$

Simplification gives the required result. □

3 Results and discussion: hydroxychloroquine

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

In the above graph, we see that the edges $(d_2(u), d_2(v))$ where $uv \in E(G_2)$ has 11 edge set partitions as given in Table 2.

We now compute the Nirmala leap index and its exponential for hydroxychloroquine as follows:

Theorem 3.1. *Let G_2 be the chemical structure of hydroxychloroquine. Then*

$$
\begin{aligned}
&(i)NL(G_2) = 7\sqrt{2} + \sqrt{3} + 8\sqrt{5} + 3\sqrt{6} + 3\sqrt{7} + 12,\\
&(ii)NL(G_2,x) = x^{\sqrt{2}} + x^{\sqrt{3}} + 3x^2 + 8x^{\sqrt{5}} + 3x^{\sqrt{6}} + 3x^{\sqrt{7}} + 3x^{2\sqrt{2}} + 2x^3.
\end{aligned}
$$

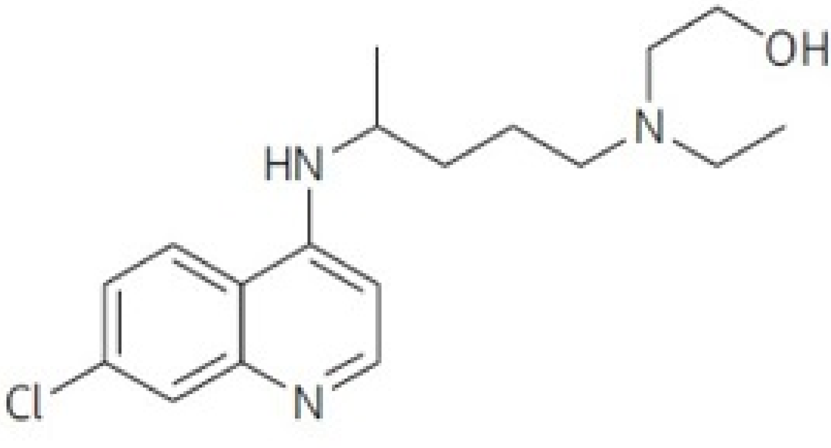

Figure 2. Chemical structure of hydroxychloroquine.

Table 2. Edge set partitions of hydroxychloroquine.

$(d_2(u), d_2(v)) : uv \in E(G_2)$	(1,1)	(1,2)	(1,3)	(2,2)	(2,3)	(2,4)
Number of edges:	1	1	1	2	8	1

$(d_2(u), d_2(v)) : uv \in E(G_2)$	(3,3)	(3,4)	(3,5)	(4,4)	(4,5)
Number of edges:	2	3	1	2	2

Proof. Applying the definitions and edge partition of G_2, we deduce that

$$\begin{aligned}(i)NL(G_2) &= \textstyle\sum_{uv\in E(G_2)}[d_2(u)+d_2(v)]^{1/2}\\ &= (1+1)^{1/2}+(1+2)^{1/2}+(1+3)^{1/2}+2(2+2)^{1/2}+8(2+3)^{1/2}\\ &\quad +(2+4)^{1/2}+2(3+3)^{1/2}+3(3+4)^{1/2}+(3+5)^{1/2}+2(4+4)^{1/2}\\ &\quad +2(4+5)^{1/2}.\end{aligned}$$

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

$$\begin{aligned}(ii)NL(G_2,x) &= \textstyle\sum_{uv\in E(G_2)} x^{\sqrt{d_2(u)+d_2(v)}}\\ &= x^{(1+1)^{1/2}}+x^{(1+2)^{1/2}}+x^{(1+3)^{1/2}}+2x^{(2+2)^{1/2}}+8x^{(2+3)^{1/2}}\\ &\quad +x^{(2+4)^{1/2}}+2x^{(3+3)^{1/2}}+3x^{(3+4)^{1/2}}+x^{(3+5)^{1/2}}+2x^{(4+4)^{1/2}}\\ &\quad +2x^{(4+5)^{1/2}}.\end{aligned}$$

After simplifying, we obtain the desired result. □

Now, we similarly compute the modified Nirmala leap index and its exponential of hydroxychloroquine as follows:

Theorem 3.2. *Let G_2 be the chemical structure of hydroxychloroquine. Then*

$$(i)^{m}NL(G_2) = \sqrt{2} + \tfrac{1}{\sqrt{3}} + \tfrac{8}{\sqrt{5}} + \tfrac{3}{\sqrt{6}} + \tfrac{3}{\sqrt{7}} + \tfrac{1}{2\sqrt{2}} + \tfrac{13}{6}.$$
$$(ii)^{m}NL(G_2,x) = x^{\frac{1}{\sqrt{2}}} + x^{\frac{1}{\sqrt{3}}} + 3\sqrt{x} + 8x^{\frac{1}{\sqrt{5}}} + 3x^{\frac{1}{\sqrt{6}}} + 3x^{\frac{1}{\sqrt{7}}} + 3x^{\frac{1}{2\sqrt{2}}} + 2x^{\frac{1}{3}}.$$

Proof. By using the definitions and edge partitions of G_2, we deduce

$$\begin{aligned}(i)^{m}NL(G_2) &= \textstyle\sum_{uv\in E(G_2)} \frac{1}{\sqrt{d_2(u)+d_2(v)}}\\ &= (1+1)^{-1/2} + (1+2)^{-1/2} + (1+3)^{-1/2} + 2(2+2)^{-1/2}\\ &+8(2+3)^{-1/2} + (2+4)^{-1/2} + 2(3+3)^{-1/2} + 3(3+4)^{-1/2}\\ &+(3+5)^{-1/2} + 2(4+4)^{-1/2} + 2(4+5)^{-1/2}.\end{aligned}$$

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

$$\begin{aligned}(ii)^{m}NL(G_2,x) &= \textstyle\sum_{uv\in E(G_2)} x^{\frac{1}{\sqrt{d_2(u)+d_2(v)}}}\\ &= x^{(1+1)^{-1/2}} + x^{(1+2)^{-1/2}} + x^{(1+3)^{-1/2}} + 2x^{(2+2)^{-1/2}}\\ &+8x^{(2+3)^{-1/2}} + x^{(2+4)^{-1/2}} + 2x^{(3+3)^{-1/2}} + 3x^{(3+4)^{-1/2}}\\ &+x^{(3+5)^{-1/2}} + 2x^{(4+4)^{-1/2}} + 2x^{(4+5)^{-1/2}}.\end{aligned}$$

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

4 Results and discussion: remdesivir

Let G_3 be used to denote the the molecular graph of remdesivir. This graph has 41 vertices and 44 edges, see Figure 3.

In the above graph, we obtain that $(d_2(u),d_2(v))$ with $uv \in E(G_3)$ has 13 edge partitions as listed in Table 3.

Table 3. Edge partitions of remdesivir.

$(d_2(u),d_2(v)):\ uv \in E(G_3)$	(1,2)	(2,2)	(2,3)	(2,4)	(2,5)	(3,3)	(3,4)
Number of edges:	2	3	10	1	1	7	3

$(d_2(u),d_2(v)):\ uv \in E(G_3)$	(3,5)	(3,6)	(4,4)	(4,5)	(5,5)	(5.6)
Number of edges:	8	1	1	2	3	2

We calculate the Nirmala leap index and its exponential of remdesivir as follows:

Theorem 4.1. *Let G_3 be the chemical graph of remdesivir. Then*

$$(i)NL(G_3) = 18\sqrt{2} + 2\sqrt{3} + 10\sqrt{5} + 8\sqrt{6} + 4\sqrt{7} + 3\sqrt{10} + 2\sqrt{11} + 15$$
$$(ii)NL(G_3,x) = 9x^{2\sqrt{2}} + 2x^{\sqrt{3}} + 10x^{\sqrt{5}} + 8x^{\sqrt{6}} + 4x^{\sqrt{7}} + 3x^{\sqrt{10}} + 2x^{\sqrt{11}} + 3x^{2} + 3x^{3}.$$

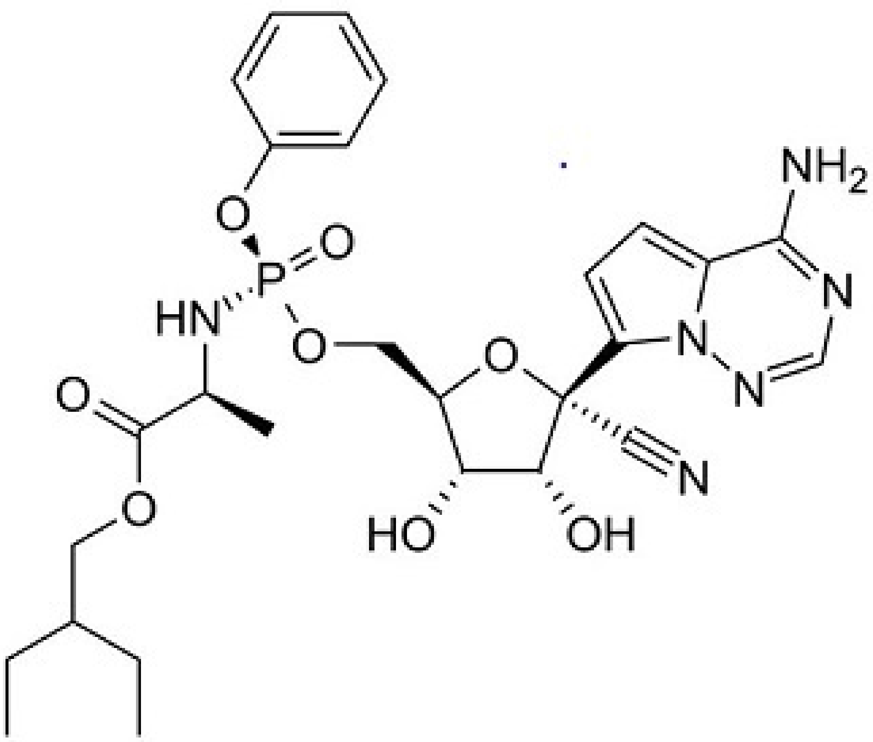

Figure 3. Chemical structure of remdesivir.

Proof. By using the definitions and edge partitions of G_3, we deduce that

$$\begin{aligned}(i) NL(G_3) &= \textstyle\sum_{uv\in E(G_3)} [d_2(u)+d_2(v)]^{1/2} \\ &= 2(1+2)^{1/2} + 3(2+2)^{1/2} + 10(2+3)^{1/2} + (2+4)^{1/2} + (2+5)^{1/2} \\ &+7(3+3)^{1/2} + 3(3+4)^{1/2} + 8(3+5)^{1/2} + (3+6)^{1/2} + (4+4)^{1/2} \\ &+2(4+5)^{1/2} + 3(5+5)^{1/2} + 2(5+6)^{1/2}.\end{aligned}$$

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

$$\begin{aligned}(ii) NL(G_3,x) &= \textstyle\sum_{uv\in E(G_3)} x^{\sqrt{d_2(u)+d_2(v)}} \\ &= 2x^{(1+2)^{1/2}} + 3x^{(2+2)^{1/2}} + 10x^{(2+3)^{1/2}} + x^{(2+4)^{1/2}} + x^{(2+5)^{1/2}} \\ &+7x^{(3+3)^{1/2}} + 3x^{(3+4)^{1/2}} + 8x^{(3+5)^{1/2}} + x^{(3+6)^{1/2}} + x^{(4+4)^{1/2}} \\ &+2x^{(4+5)^{1/2}} + 3x^{(5+5)^{1/2}} + 2x^{(5+6)^{1/2}}.\end{aligned}$$

Simplification gives the desired result. □

Now, we compute the modified Nirmala leap index and its exponential of remdesivir as follows:

Theorem 4.2. *Let G_3 be the chemical graph of remdesivir. Then*

$(i)\, {}^mNL(G_3) = \frac{2}{\sqrt{3}} + \frac{9}{2\sqrt{2}} + \frac{10}{\sqrt{5}} + \frac{8}{\sqrt{6}} + \frac{4}{\sqrt{7}} + \frac{3}{\sqrt{10}} + \frac{2}{\sqrt{11}} + \frac{5}{2}.$

$(ii)\, {}^mNL(G_3,x) = 2x^{\frac{1}{\sqrt{3}}} + 3\sqrt{x} + 10x^{\frac{1}{\sqrt{5}}} + 8x^{\frac{1}{2\sqrt{6}}} + 4x^{\frac{1}{\sqrt{7}}} + 9x^{\frac{1}{2\sqrt{2}}} + 3x^{\frac{1}{3}} + 3x^{\frac{1}{\sqrt{10}}} + 2x^{\frac{1}{\sqrt{11}}}.$

Proof. Similarly, we get

$$
\begin{aligned}
(i)^m NL(G_3) &= \textstyle\sum_{uv\in E(G_3)} \frac{1}{\sqrt{d_2(u)+d_2(v)}}\\
&= 2(1+2)^{-1/2} + 3(2+2)^{-1/2} + 10(2+3)^{-1/2} + (2+4)^{-1/2}\\
&+(2+5)^{-1/2} + 7(3+3)^{-1/2} + 3(3+4)^{-1/2} + 8(3+5)^{-1/2}\\
&+(3+6)^{-1/2} + (4+4)^{-1/2} + 2(4+5)^{-1/2} + 3(5+5)^{-1/2}\\
&+2(5+6)^{-1/2}.
\end{aligned}
$$

The result is deduced similarly.

$$
\begin{aligned}
(ii)^m NL(G_3, x) &= \textstyle\sum_{uv\in E(G_3)} x^{\frac{1}{\sqrt{d_2(u)+d_2(v)}}}\\
&= 2x^{(1+2)^{-1/2}} + 3x^{(2+2)^{-1/2}} + 10x^{(2+3)^{-1/2}} + x^{(2+4)^{-1/2}}\\
&+x^{(2+5)^{-1/2}} + 7x^{(3+3)^{-1/2}} + 3x^{(3+4)^{-1/2}} + 8x^{(3+5)^{-1/2}}\\
&+x^{(3+6)^{-1/2}} + x^{(4+4)^{-1/2}} + 2x^{(4+5)^{-1/2}} + 3x^{(5+5)^{-1/2}}\\
&+2x^{(5+6)^{-1/2}}.
\end{aligned}
$$

By simplifying, the result is deduced. □

5 Conclusion

Topological graph indices which number more that 3000 in chemical databases are important tools in Mathematics and in Molecular Chemistry. Some of them are defined and have many nice arithmetical properties and some have important applications when we consider each molecule as a grpah modeling this molecule. Studying on the modeling graph, we obtain mathematical values that help us to calculate, or at least estimate some chemical and physicochemical properties of the molecule. Therefore, each graph index has its importance, solely in Mathematics, or also in Chemistry. In this study, we have introduced the Nirmala leap and modified Nirmala leap indices of a graph. Furthermore, we have determined the Nirmala leap and modified Nirmala leap indices of some recent chemical drugs such as chloroquine, hydroxychloroquine and remdesivir. More applications of these indices are expected in QSAR and QSPR studies.

References

[1] B. Chaluvaraju, A. B. Shaikh, Different versions of atom bond connectivity indices of some molecular structures: Applied for the treatment of Covid-19, Polycycl. Aromat. Compd. 42(6) (2022) 3748–3761.

[2] M. V. Diudea (ed.), QSPR-QSAR studies by Molecular Descriptors, NOVA, New York, 2001.

[3] I. Gutman, V. R. Kulli, Nirmala energy, Open J. Discret. Appl. Math. 4(2) (2021) 11–16.

[4] I. Gutman, O. E. Polansky, Mathematical Concepts in Organic Chemistry, Springer, Berlin, 1986.

[5] I. Gutman, Z. Shao, Z. Li, S. Wang, P. Wu, Leap Zagreb indices of trees and unicyclic graphs, Commun. Comb. Optim. 3(2) (2018) 179-194.

[6] N. Kansal, P. Garg, O. Singh, Temperature based topological indices and OSPR Analysis of Covid-19 drugs, Polycycl. Aromat. Compd. (2022) 1–22.

[7] V. R. Kulli, College Graph Theory, Vishwa International Publications, Gulbarga, India, 2012.
[8] V. R. Kulli, Graph Indices, in Hand Book of Research on Advanced Applications of Graph Theory in Modern Society, M. Pal. S. Samanta, A. Pal, (eds.) IGI Global, USA (2020) 66–91.
[9] V. R. Kulli, Nirmala index, Int. J. Math. Trend. Tech. 67(3) (2021) 8–12.
[10] V. R. Kulli, I. Gutman, On some mathematical properties of Nirmala index, Annal. Pure Appl. Math. 23(2) (2021) 93–99.
[11] V. R. Kulli, N. Harish, B. Chaluvaraju, Sombor leap indices of some chemical drugs, Res. Rev. Int. J. Multidiscip. 7(10) (2022) 158–166.
[12] V. R. Kulli, V. Lokesha, Nirupadi K, Computation of inverse Nirmala indices of certain nanostructures, Int. J. Math. Comb. 2 (2021) 32–39.
[13] V. R. Kulli, Revan indices of chloroquine, hydroxychloroquine, remdesimir: Research Advances for the treatment of Covid-19, Int. J. Eng. Res. Technol. 9(5) (2020) 73–84.
[14] A. Mahboob, G. Muhiuddin, I. Siddique, S. M. Alam, A view of Banhatti and Revan indices of chemical graphs, J. Math. 10 (2022) 1-10.
[15] A. Naji, N. D. Soner, I. Gutman, On leap Zagreb indices of graphs, Commun. Comb. Optim. 2 (2017) 99–117.

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