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HDR Degree Bassed Indices and M_{hr}-Polynomial for the Treatment of COVID-19

Ammar Alsinai [1,*], Hanan Ahmed [2], Anwar Alwardi [3], Soner Nandappa D. [1]

[1] Department of Studies in Mathematics University of Mysore, Manasagangotri, India; aliammar1985@gmail.com (A.A.); ndsoner@yahoo.co.in (N.D.S.);
[2] Department of Mathematics University of Mysore, India; hananahmed1a@gmail.com (H.A.);
[3] Department of Mathematics, University of Aden, Yemen; a_Alwardi@hotmail.com (A.A.);
[4] Department of Studies in Mathematics University of Mysore, Manasagangotri, India;
* Correspondence: aliiammar1985@gmail.com (A.A.);

Scopus Author ID 57222957516

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Abstract: In this research work, We introduce topological indices, namely as an HDR version of Modified Zagreb topological index (HDRM*), HDR version of Modified forgotten topological index (HDRF*), and HDR version of hyper Zagreb index (HDRHM*). Then the relatively study depends on the structure-property regression analysis to test and compute the chemical applicability of these indices to predict the physicochemical properties of octane isomers. Also, we show these HDR indices have well degeneracy properties compared to other degree-based topological indices. Also, We defined and computed the M_{hr}-polynomial of the newly indices and applied it on COVID-19 treatments. Also, we discussed some mathematical properties of HDR indices.

Keywords: $d_{hr}(v)$ degree ; HDR topological indices; Mhr-polynomial; Chloroquine; hydrocinchonine; remdesivir; COVID-19.

1. Introduction

A molecular graph is an undirected labeled graph G = (V, E) that shows the structural and functional properties. The set of vertices V of G encodes atoms, and the edges E encodes the adjacency relationship between atoms in the molecule. The corresponding chemical element labels each vertex (for example, C = Carbon, H = Hydrogen), and each edge is labeled by its type of covalent bond single -, double =, triple, aromatic [1]. In a molecular graph, nodes and edges correspond to the atoms and chemical bonds of the compound, respectively. Let G be a chemical graph containing V(G) and E(G) as vertex and edge sets. The degree of a vertex v on a graph G, denoted by $d_G(v)$, is the total number of edges associated with v [2]. In chemical graph theory, topological indices play a leading role in quantitative structure-property relationships and quantitative structure-activity relationship modeling [3].

Topological indices are numeric values that are graph invariant. A real-valued mapping considering graphs as arguments is a consistent graph if it gives the same value to isomorphic graphs. The order (number of vertices) and size (number of edges) of a graph are examples of two graphs' invariants. In chemical graph theory, the graph invariants are named topological indices. The beginning of the emergence of topological was initiated when the eminent chemist Wiener found the first topological index, known as the Wiener index[2].

In 1947 for searching boiling points of alkanes, one of the topological indices invented at the initial stage is the so-called Zagreb index, first presented by [4,5]. They investigated how the total energy of $\pi-$ electron depends on the structure of molecules, and it was discussed in detail.

The first Zagreb indices $M_1(G)$ [6] for a molecular graph G is defined as follows:

$$M_1(G) = \sum_{v\in V(G)} d^2(v) = \sum_{uv\in E(G)} [d(v) + d(u)].$$

The first leap Zagreb index[7] is defined as

$$LM *_1 (G) = \sum_{uv\in E(G)} d_2^2(v) .$$

The new visitation first leap Zagreb index[8] is defined as

$$LM *_1 (G) = \sum_{uv\in E(G)} [d_2(v) + d_2(u)].$$

The first leap hyper-Zagreb index [8] is defined as

$$LM_1(G) = \sum_{uv\in E(G)} [d_2(v) + d_2(u)]^2 .$$

Introduced the forgotten topological indiex [9] is defined as

$$F(G) = \sum_{v\in V(G)} d^3(v) = \sum_{uv\in E(G)} [d^2(v) + d^2(u)]$$

In The leap forgotten topological index was defined as

$$LF(G) = \sum_{uv\in E(G)} [d_2^2(v) + d_2^2(v)]^2$$

For more discussion on these indices, interested readers have referred to the papers [10-17].

Scientists tested some of the available antiviral agents that positively contributed to reducing the recovery time for people infected with COVID-19 from 15 days to 11 days. Among these compounds, hydroxychloroquine, remdesivir, chloroquine, and the drug remdesivir has received emergency approval from the Food and Drug Administration as the first drug to relieve symptoms of COVID-19. It has contributed positively to this matter.

V.R. Kulli [18] calculated the Revan Indices for some of the antiviral drugs, and there is also much research through which the properties of chemical compounds have been calculated for medicines that are used to alleviate the symptoms of Covid for more discussion on these indices, interested readers have referred to the papers [19-28].

In this paper, we introduce HDR of Zagreb index modified forgotten index and Hyper HDR of modified Zagreb index. Also, we check the chemical applicability of these indices. We find the correlation coefficients of these new indices and some well-established indices with acentric factor and entropy for octane isomers. Also, we calculate these introduced indices of some of the antiviral agent's Chloroquine, Hydroxychloroquine, Remdesivir. Also, the M_{hr}-polynomial is introduced, and a surface representation of the M_{hr}-polynomial has been depicted. And we discuss some mathematical properties of these newly introduced indices.

2. Materials and Methods

Our main results include introducing new topological indices HDRM, HDRF, and HDRHM. Also, check the chemical applicability of these indices and find the correlation coefficients of these new indices and some well-established indices with acentric factor and

entropy for octane isomers. We made calculations of the chemical compounds used for the treatment of COVID-19 in terms of HDR topological indices, particularly chloroquine, hydroxychloroquine, remdesivir. We evaluate the M_{hr}–polynomial of these structures with 3D graphical representation using MATLAB.

3. Results and Discussion

We divide this section into three subsections with HDR topological indices, Chemical significance of HDR indices, and evaluate the M_{hr}- polynomial and computing the HDR-based topological indices of chemical compounds used for the treatment of COVID-19.

3.1. On HDR indices of the graph.

In this subsection, we present the definitions of the HDR Zagreb index, HDR modified forgotten topological index and modified Hyper HDR Zagreb index. Also, we obtain some mathematical properties and establish the formulas of the exact values of the newly introduced indices for some well-known graph classes.

3.1.1. Definition.

For a graph G, the HDR of Zagreb index, modified forgotten topological index, version modified of Hyper HDR Zagreb indices are defined as follows:

$$\mathbf{HDRM_1^*(G)} = \sum_{\mathbf{uv\in E(G)}} [\mathbf{d_{hr}(v)} + \mathbf{d_{hr}(u)}].$$

$$\mathbf{HDRHM_1^*(G)} = \sum_{\mathbf{uv\in E(G)}} [\mathbf{d_{hr}(v)} + \mathbf{d_{hr}(v)}]^{\mathbf{2}}$$

$$\mathbf{HDRF^*(G)} = \sum_{\mathbf{uv\in E(G)}} [\mathbf{d_{hr}^2(v)} + \mathbf{d_{hr}^2(u)}].$$

where $d_{hr}(v) = |\{u, v \in V(G) | d(u, v) = \lceil \frac{R}{2} \rceil\}|$ And $d(u, v)$ is the distance between the vertices u and v in V(G), and R is the radius of graph G.

3.1.2. Proposition.

Let G be a connected graph with radius R. Then if R(G)=1 $\Rightarrow d_{hr}(v) = d_1(v)$

But if $d_{hr}(v) = d_1(v) \nRightarrow$ r(G)=1. example cycle graph with n≥4.

3.1.3. Proposition.

Let G be a graph such that $G \cong C_n, K_n, K_{n,m} W_n, F_p$ .Then

$$\mathbf{HDRM_1^*(G)} = \mathbf{M_1^*(G)}, \mathbf{HDRF^*(G)} = \mathbf{F_1^*(G)}, \mathbf{HDRHM_1^*(G)} = \mathbf{HM_1^*(G)}.$$

3.1.4. Definition.

Bn,k-banana tree is a graph obtained by connecting one leaf of each of n copies of a k-star graph with a single root vertex distinct from all the stars.

Table 1. The number of edges of n,k-banana tree with n> 3.

$d_{hr}(u,v)$	No.edge
(n,n+k-3)	n
(n+k-3,1)	n
(1,k-2)	n(k-2)

Theorem 1. Let $B_{n,k}$ -banana tree with $k > 3$. Then

$$HDRM_1^*(G) = n(3n + k^2 - k - 3)$$

$$HDRF^*(G) = n(5n^2 - 2k^2 + 6nk - 16n - 5k + 11)$$

$$HDRHM_1^*(G) = n(3n^2 - 12n - 10) + k(4n^2 - 4nk - 15n + nk^2)$$

Proof. Let $B_{n,k}$ banana tree with k> 3. Therefore

by definition of $HDRM_1^*(G)$, and Table 1, we have

$$HDRM_1^*(G) = \sum_{uv\in E(G)} [d_{hr}(v) + d_{hr}(u)]$$

$$= \sum_{uv\in E_1(G)} (n + (n + k - 3) + \sum_{uv\in E_2(G)} (n + k - 3) + 1)$$

$$+ \sum_{uv\in E_3(G)} (1 + k - 2)$$

$$= n(2n + k - 3) + n(n + k - 2) + n(k - 1)(k - 2)$$

Therefore $HDRM_1^*(G) = n(3n + k^2 - k - 3)$

By definition of $HDRHM_1^*(G)$ and Table 1, we have

$$HDRHM_1^*(G) = \sum_{uv\in E(G)} [d_{hr}(v) + d_{hr}(u)]^2$$

$$= \sum_{uv\in E_1(G)} (2n + k - 3)^2 + \sum_{uv\in uv\in E_2(G)} (n + k - 2)^2 + \sum_{uv\in uv\in E_3(G)} (k - 1)^2$$

$$= n(4n^2 + k^2 + 4nk - 12n - 6k + 9) + n(n^2 + k^2 + 2nk - 4n - 4k +$$

$$+n(k - 2)(k^2 - 2k + 1)$$

Therefore $HDRHM_1^*(G) = n(5n - 2k^2 + k^3 + 6nk - 16n - 5k + 11)$

By definition of $HDRF^*(G)$ and Table1, we have

$$HDRF^*(G) = \sum_{uv\in E(G)} [d_{hr}^2(v) + d_{hr}^2(u)]$$

$$= \sum_{uv\in E_1(G)} (n^2 + (n + k - 3)^2) + \sum_{uv\in E_2(G)} (1 + (n + k - 3)^2)$$

$$+ \sum_{uv\in E_2(G)} (1 + (k - 2)^2)$$

Therefore $HDRF^*(G) = n(3\boldsymbol{n^2} - 12n - 10) + k(4\boldsymbol{n^2} - 4nk - 15n + nk^2)$.

3.2. Chemical significance HDR indices.

In this subsection, We present the Chemical significance of HDR indices, clarify their quality compared to other indices, and the possibility of their application in the study of chemical compounds.

The chemical applicability of topological indices can be evaluated by regression analysis IAMC (International Academy of Mathematical Chemistry). IAMC (International Academy of Mathematical Chemistry). Then Eighteen octane isomers are helpful for such investigation since the number of the structural isomers of octane is large Eighteen enough to create the statistical perfection faithful.[9].

Furtula *et al*. [9] showed that F and M_1 yield correlation greater than (0.96) with acentric factor octane isomers. Also, a simple linear model $(M_1 + \lambda F)$, where λ is disparate from -20 to 20 is designed to improve the predictive ability of these indices. De *et al.* [12]. Computed that the correlation coefficient of F-coindex for octane isomers in the case of the logarithm of the octanol-water partition coefficient (P) is 0.966. In a recent work [2], the application possibilities of various graph irregularity indices for predicting physicochemical properties are described. We find the correlation of different physiochemical properties with $HDRM_1^*$, $HDRHM_1^*$ and HDRF $*$of octane isomers and good results are obtained in case acentric factor (Acent Fac.) and entropy (S) which are shown in Table 2. The correlations of acentric factor and entropy with some well-known degree-based topological indices are also investigated in Table 4. The results are also shown graphically in Figure 1. The data of octane isomers (Table 2) are collected from Sourav. Thus the HDR introduced indices can help to predict the acentric factor with powerful accuracy.

Table 2. Experimental values of the acentric factor, entropy (S), and the corresponding values of $HDRM_1^*, HDRHM_1^*, HDRF^*$.

Molecule name	Acent Fac.	S	$HDRM_1^*(G)$	$HDRHM_1^*(G)$	$HDRF^*(G)$
n-octane	0.397898	111.6	22	38	74
2-methly heptane	0.377916	109.84	24	48	88
3-methly heptane	0.371002	111.26	26	44	104
4- methly heptane	0.371504	109.32	26	58	106
3-ethyl hexane	0.362472	109.43	26	66	124
2,2-dimethy1 hexane	0.339426	109.42	28	74	122
2,3dimethy1 hexane	0.348247	108.02	30	72	138
2,4-dimethy1 hexane	0.344223	106.98	28	68	120
2,5-dimethy1 hexane	0.35683	105.72	26	58	104
3,3-dimethy1 hexane	0.322596	104.74	32	83	156
3,4-dimethy1 hexane	0.340345	106.59	32	80	154
2-methy1-3- ethy1 pentane	0.332433	106.06	30	74	135
3-methy1-3- enty1 pentane	0.306899	101.48	32	92	160
2,2,3-trimethy1 pentane	0.300816	101.31	34	104	174
2,2,4-trimethy1 pentane	0.30537	104.09	34	104	168
2,3,3- trimethy1 pentane	0.293177	102.06	34	104	176
2,3,4- trimethy1 pentane	0.317422	102.39	32	86	152
2,2,3,3- tetramethy1 butane	0.255294	93.06	38	134	202

Table 3. Correlation coefficient of $HDRM_1^*, HDRHM_1^*, HDRF^*$ with acentric factor and entropies.

	$HDRM_1^*(G)$	$HDRHM_1^*(G)$	$HDRF^*(G)$
Acent Fac	*-0.9656*	-0.981	-0.9617
S	-0.8674	-0.925	-0.8585

Table 4. Correlation coefficient of $HDRM_1^*, HDRHM_1^*, HDRF^*$ with acentric factor and entropies.

	$LM_1^*(G)$	$F(G)$	$F_N(G)$	$HLM_1^*(G)$	$LF^*(G)$
Acent Fac	-0.9438	-0.96505	-0.97547	-0.9464	-0.9789
S	-0.8981	-0.9527	-0.93146	-0.89	-0.9211

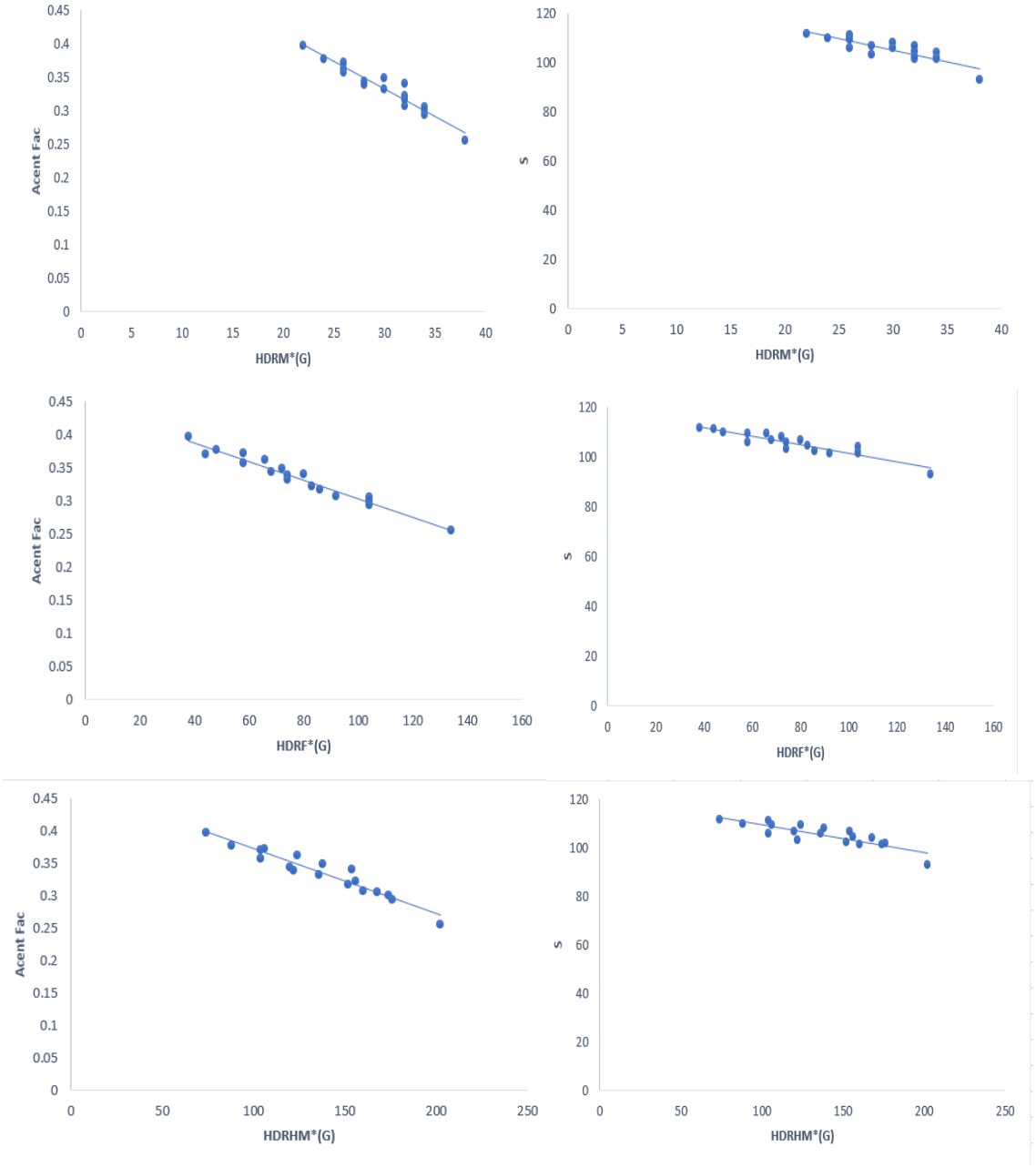

Figure 1. Correlation of acentric factor and entropy (S) with the newly introduced indices for octane isomers.

Table 5. Correlation coefficient of $HDRM_1^*, HDRHM_1^*, HDRF^*$ with with some other indices.

	$HDRM_1^*$	$HDRHM_1^*$	$HDRF^*$	LM_1^*	LF^*	F_n	HLM_1^*
$HDRM_1^*$	1						
$HDRHM_1^*$	0.9656	1					
$HDRF^*$	0.9894	0.9713	1				
LM_1^*	0.9413	0.9241	0.9432	1			
LF^*	0.9558	0.9754	0.9661	0.9662	1		
F_N	0.9487	0.9585	0.9573	0.9868	0.9809	1	
HLM_1^*	0.9262	0.9275	0.941	0.9937	0.9667	0.9929	1

3.3. Evalute the M_{hr}- polynomial and computing the HDR-based topological indices of chemical compounds used for the treatment of COVID-19.

In this subsection, we present the definitions of the M_{hr}- polynomial and computing the HDR-based topological indices of chemical compounds used for the treatment of COVID-19. Also, We evaluate the M_{hr}- polynomial of these structures with 3D graphical representation using MATLAB.

3.3.1. Definition.

Let the edge partition of the graph G be defined as:

$$M_{hr}(i,j)(G) = \{uv \in E(G): d_{hr}(u) = i, \text{and } j\}.$$

The Maximum degree $\Delta_{hr}(G)$ is defined as $\Delta_{hr} = max\{ d_{hr}(v): v \in V(G)\}$.

The minimum degree $\delta_{hr}(G)$ is defined as $\delta_{hr} = min\{d_{hr}(v): v \in V(G)\}$.

3.3.2. *Definition.*

Let G be graph and

$M_{hr}(i,j)(G), i,j \geq 1$, be the number of edge e=vu of G such that $\{d_{hr}(u); d_{hr}(v)\} = \{i,j\}$. $Let\ M_{hr}(i,j) = |M_{hr}(i,j)|$. We introduce the M_{hr} −polynomial of a graph as

$$M_{hr}(G,x,y) = \sum_{\delta_{hr} \leq i \leq j \leq \Delta_{hr}} M_{hr}(i,j)x^i y^j.$$

3.3.2. Chloroquine.

Let G be a molecular graph of Chloroquine, as shown in Figure2. The graph G has 23 edges and 22 vertices.

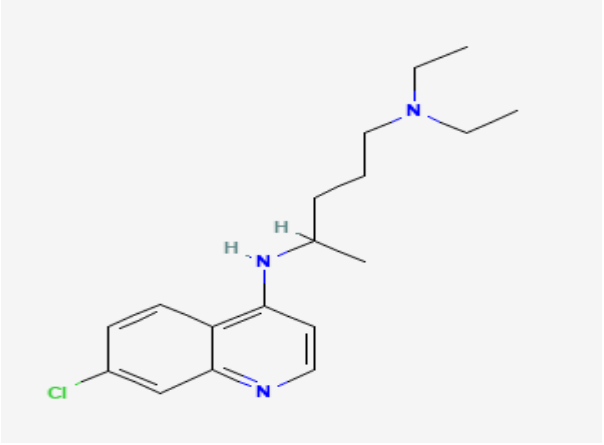

Figure 2. Molecular graph of chloroquine with 22 vertices and 23 edges.

Table 6. The number of edges of chloroquine using $d_{hr}(v)$ degree.

$M_{hr}(i,j)$	$M_{hr}(2,3)$	$M_{hr}(3,4)$	$M_{hr}(3,5)$	$M_{hr}(3,3)$	$M_{hr}(4,4)$	$M_{hr}(1,2)$	$M_{hr}(1,1)$
no.edge	2	7	5	2	2	3	2

Theorem 2. Let G be a molecular graph of Chloroquine. Then

$M_{hr}(G,x,y) = 2xy + 3x\,y^2 + 2x^2y^3 + 2x^3y^3 + 7x^3y^4 + 2x^4y^4 + 5x^3y^5$.

Proof. Let G a molecular graph of chloroquine as in Figure 2. Then from Table 6 and Definition 3.3.2, we get

$$M_{hr}(G,x,y) = \sum_{\delta_{hr} \leq i \leq j \leq \Delta_{hr}} M_{hr}(i,j)x^i y^j$$

$$= M_{hr}(1,1)xy + M_{hr}(1,2)xy^2 + M_{hr}(2,3)x^2y^3 + M_{hr}(3,3)x^3y^3$$

$$+ M_{hr}(3,4)x^3x^4 + M_{hr}(4,4)x^4y^4 + M_{hr}(4,5)x^4y^5$$

$$= 2xy + 3x\,y^2 + 2x^2y^3 + 2x^3y^3 + 7x^3y^4 + 2x^4y^4 + 5x^3y^5$$

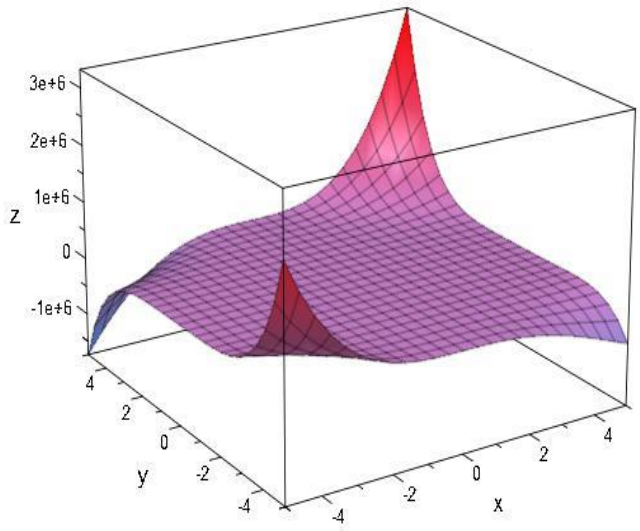

Figure 3. M_{hr} −polynomial of chloroquine.

Theorem 3. Let G be a molecular graph of Chloroquine. Then

$$HDRM_1^*(G) = 140, HDRHM_1^*(G) = 948, DHRF^*(G) = 490$$

Proof**.** Let G a molecular graph of chloroquine as in Figure 2. Then from Table 6 and Definition 3.1.1, we get

$$\mathrm{HDRM}_1^*(\mathrm{G}) = \sum_{uv\in E(G)} [d_{hr}(v) + d_{hr}(u)] = 10 + 49 + 40 + 12 + 16 + 9 + 4 = 140.$$

$$\mathrm{HDRHM}_1^*(\mathrm{G}) = \sum_{uv\in E(G)} [d_{hr}^2(v) + d_{hr}^2(v)]^2 = 50 + 343 + 320 + 72 + 128 + 27 + 8 = 948.$$

$$\mathrm{HDRF}^*(\mathrm{G}) = \sum_{uv\in E(G)} [d_{hr}^2(v) + d_{hr}^2(u)] = 26 + 175 + 170 + 36 + 64 + 15 + 4 = 490.$$

3.3.3. Hydroxychloroquine.

Let G be a molecular graph of hydroxychloroquine, as shown in Figure 4. The graph G has 24 edges and 23 vertices.

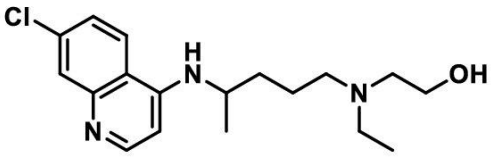

Figure 4. Molecular graph of hydroxychloroquine with 23 vertices and 24 edges.

Table 7. The number of edges of hydroxychloroquine using $d_{hr}(v)$ degree.

$M_{hr}(i,j)$	$M_{hr}(2,3)$	$M_{hr}(3,3)$	$M_{hr}(3,4)$	$M_{hr}(3,5)$	$M_{hr}(4,4)$
no.edge	1	3	7	5	2
$M_{hr}(i,j)$	.	$M_{hr}(1,3)$	$M_{hr}(1,2)$	$M_{hr}(2,2)$	$M_{hr}(1,1)$
no. edge	.	1	2	2	1

Theorem 4. Let G be a molecular graph of Hydroxychloroquine. Then

$M_{hr}(G,x,y) = xy + 2x\,y^2 + xy^3 + 2x^2y^2 + x^2y^3 + 3x^3y^3 + 7x^3y^4 + 5x^3y^5 + 2x^4y^4$.

Proof. Let G a molecular graph of hydroxychloroquine as in Figure 4. Then from Table 7 and Definition 3.3.2, we get

$$M_{hr}(G,x,y) = \sum_{\delta_{hr}\le i\le j\le \Delta_{hr}} M_{hr}(i,j)x^i\, y^j$$
$$= M_{hr}(1,1)xy + M_{hr}(1,2)xy^2 + M_{hr}(1,3)xy^3 + M_{hr}(2,2)x^2y^2$$
$$+ M_{hr}(2,3)x^2x^3 + M_{hr}(3,3)x^3y^3 + M_{hr}(3,4)x^3y^4$$
$$+M_{hr}(3,5)x^3y^5 + M_{hr}(4,4)x^4y^4$$
$$= xy + 2x\, y^2 + xy^3 + 2x^2y^2 + x^2y^3 + 3x^3y^3 + 7x^3y^4 + 5x^3y^5 + 2x^4y^4.$$

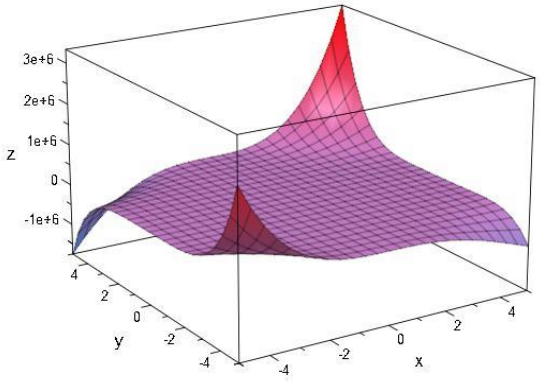

Figure 5. M_{hr} −polynomial of hydroxychloroquine.

Theorem 5. Let G be a molecular graph of hydroxychloroquine. Then

$$HDRM_1^*(G) = 148, HDRHM_1^*(G) = 994, DHRF^*(G) = 516$$

Proof**.** Let G a molecular graph of hydroxychloroquine as in Figure 4. Then from Table 7 and Definition 3.1.1, we get

$$HDRM_1^*(G) = \sum_{uv\in E(G)} [d_{hr}(v) + d_{hr}(u)] = 5 + 18 + 49 + 40 + 16 + 4 + 6 + 8 + 2$$
$$= 148.$$
$$HDRHM_1^*(G) = \sum_{uv\in E(G)} [d_{hr}(v) + d_{hr}(u)]^2$$
$$= 25 + 108 + 343 + 320 + 128 + 16 + 18 + 32 + 4 = 994.$$
$$HDRF^*(G) = \sum_{uv\in E(G)} [d_{hr}^2(v) + d_{hr}^2(u)]$$
$$= 13 + 54 + 175 + 170 + 64 + 10 + 10 + 18 + 2 = 516.$$

3.3.3. Redeliver.

Let G be a molecular graph of remdesivir, as shown in Figure 6. The graph G has 44 edges and 41 vertices.

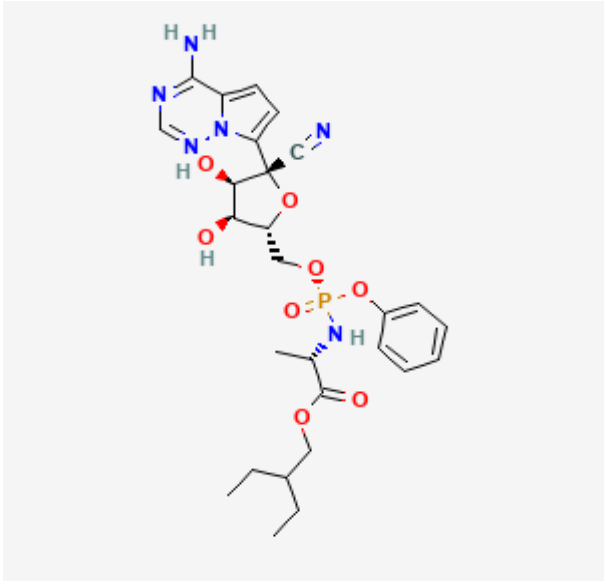

Figure 6. Molecular graph of remdesivir with 41 vertices and 44 edges.

Table 8. The number of edges of remdesivir using $d_{hr}(v)$ degree.

$M_{hr}(i,j)$	$M_{hr}(1,2)$	$M_{hr}(1,3)$	$M_{hr}(2,2)$	$M_{hr}(2,3)$	$M_{hr}(3,3)$	$M_{hr}(3,5)$
no.edge	*7*	*5*	*2*	*8*	*4*	*3*
$M_{hr}(i,j)$	$M_{hr}(3,4)$	$M_{hr}(4,5)$	$M_{hr}(5,5)$	$M_{hr}(5,6)$	$M_{hr}(5,7)$	$M_{hr}(6,7)$
no.edge	*4*	*4*	*3*	*2*	*1*	*1*

Theorem 6. Let G be a molecular graph of Remdesivir. Then

$M_{hr}(G,x,y) = 7xy^2 + 5xy^3 + 2x^2y^2 + 8x^2y^3 + 4x^3y^3 + 3x^3y^5 + 4x^3y^4 + 4x^4y^5 + 3x^5y^5 + 2x^5y^6 + x^5y^7 + x^6y^7.$

Proof. Let G a molecular graph of remdesivir as in Figure 6. Then from Table 8 and Definition 3.3.2, we get

$$M_{hr}(G,x,y) = \sum_{\delta_{hr} \le i \le j \le \Delta_{hr}} M_{hr}(i,j)x^i y^j$$

$$= M_{hr}(1,2)xy^2 + M_{hr}(1,3)\,xy^3 + M_{hr}(2,2)x^2y^2 + M_{hr}(2,3)x^2y^3 + M_{hr}(3,3)x^3y^3 + M_{hr}(3,5)\,x^3y^5 + M_{hr}(3,4)x^3y^4 + M_{hr}(4,5)x^4y^5 + M_{hr}(5,5)x^5y^5 + M_{hr}(5,6)\,x^5y^6 + M_{hr}(5,7)x^5y^7 + M_{hr}(6,7)x^6y^7.$$

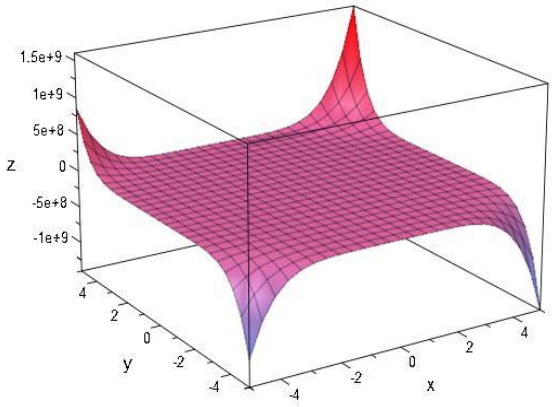

Figure 7. M_{hr} −polynomial of remdesivir.

Theorem 5. Let G be a molecular graph of remdesivir. Then

$HDRM_1^*(G) = 278, HDRHM_1^*(G) = 1965, DHRF^*(G) = 1013.$

Proof**.** Let G a molecular graph of remdesivir as in Figure 6. Then from Table 8, and Definition 3.1.1, we get

$$HDRM_1^*(G) = \sum_{uv\in E(G)} [d_{hr}(v) + d_{hr}(u)]$$
$$= 21 + 20 + 8 + 40 + 24 + 24 + 28 + 36 + 30 + 22 + 12 + 13 = 278..$$
$$HDRHM_1^*(G) = \sum_{uv\in E(G)} [d_{hr}(v) + d_{hr}(u)]^2$$
$$= 63 + 80 + 32 + 200 + 144 + 192 + 196 + 324 + 300 + 121 + 144 + 169 = 1965.$$

$HDRF^*(G) = \sum_{uv\in E(G)}[d_{hr}^2(v) + d_{hr}^2(u)] = 35 + 50 + 16 + 104 + 72 + 102 + 100 + 164 + 150 + 61 + 74 + 85 = 1013.$

4. Conclusions

In this research work, we have introduced some new topological indices, namely as an HDR version of Modified Zagreb topological index (HDRM1*), HDR version of Modified forgotten topological index (HDRF*), and HDR version of hyper Zagreb index (HDRHM*), and some mathematical properties of these topological indices are discussed. Their chemical applicability is also investigated here. These indices have a significant correlation with acentric factor and entropy in comparison with $LM_1^*(G)$, $F(G)$, $F_N(G)$, $HLM_1^*(G)$,$LF^*(G)$, shown in Table 3 and Table 4. Thus the three novel indices $HDRM_1^*$, $HDRF^*$, $HDRHM_1^*$ Deserve to be considered as applicable topological indices. We have correlated indices among themselves and with some other well-known degree-based topological indices in Table 5. From the correlation among the novel indices, it is clear that $HDRM_1^*$ and $HDRF^*$ have good quality mong three indices. Also, we calculate these introduced indices of some of the antiviral agent's Chloroquine, Hydroxychloroquine, Remdesivir. Also, the Mhr-polynomial is introduced, and a surface representation of the Mhr-polynomial has been depicted.

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Conflicts of Interest

The authors declare no conflict of interest.

References

1. Ilemo, S.N.; Barth, D.; David, D.; Quessette, F.; Weisser, M.A. Improving graphs of cycles approach to structural similarity of molecules. *PLoS ONE* **2019**, *14*, 1-25, https://doi.org/10.1371/journal.pone.0226680.
2. Mondal, S.; De, N.; Pal, A. On some new neighborhood degree based indices. *ACTA CHEMICA IASI* **2019,** *27*,31-46, https://doi.org/10.2478/achi-2019-0003.
3. Ashrafi, A.R.; Saheli, M.; Ghorbani, M. The eccentric connectivity index of nanotubes and nanotori. *J. Comput. Appl. Math* **2011**, *235*, 4561-4566, https://doi.org/10.1016/j.com.2010/30.001 .
4. Gutman, I.; Ru'ci'c, B.; Trinajesti'c, N.; Wilcox, C.F. Graph theory and molecular orbitals. XII. *The Journal of Chemical Physics* **1975**, *62* , 3399, https://doi.org/10.1063/1.430994.

5. Gutman, I.; Trinajesti'c, N. Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons. *Chem. Phys* **1972**, *17*, 535- 538, https://doi.org/10.1016/0009-2614(72)85099-1.
6. Gutman,I;.Das, K.C. The first Zagreb index 30 years after .*MATCH Commun. Math. Comput. Chem* **2004**, *50*, 83.
7. Naji, A. M; Soner, N.D.; Gutman, I. On leap Zagreb indices of graphs. *Commun.Comb. Optim*. **2017,** *2*, 99-117, https://doi.org/10.22049/cco.2017.25949.1059.
8. Kulli, V. R. Leap hyper Zagreb indices and their polynomials of certain graphs.*International Journal of Current Researcher in Life Scienes* **2018**,7 , 2783-2791. http://www.ijcrls.com.
9. Furtula, B.; Gutman, I. Forgotten topological index. J. *Math. Chem*. **2015**, 53, 1184-1190. https://doi.org/10.1007/s10910-015-0480-z .
10. Bharali, A.; Doley, A.; Buragohain, J. Entire forgotten topological index of graphs. *Mathematical Computation in Combinatorics and Graph Theory* **2020**, *39*, https://doi.org/10.22199/issn.0717-6279-2020-04-0064.
11. Alsinai, A.; Alwardi, A.; and Soner, N. D. On Reciprocals Leap indices of graphs. *International Journal of Analysis and Applications* **2020**, *19*, 1-19, https://doi.org/10.28924/2291-8639-19-2021-1.
12. Das, K.C.; Xu, K.; Gutman, I. On Zagreb and Harary Indices. *MATCH Commun. Math. Comput. Chem*. **2013**, *70*, 301-314.
13. Chidambaram, N.; Mohandoss, S.; Yu, X.; Zhang, X. On leap Zagreb indices of bridge and chain graphs.*AIMS mathematices* **2020**, *6*, 6521-6536, https://doi.org/10.3934/math.2020420.
14. Alsinai, A.; Alwardi, A.; Soner, N. D. On ψk-polynomial of graph. *Eurasian Chemical Communcations* **2021**, *3*, 219-226, https://doi.org/10.22034/ECC.2021.274069.1138.
15. LiuKey, H.; TangKey, Z. The hyper-Zagreb index of cacti with perfect matchings. *AKCE InternationalJournal of Graphs and Combinatorics* **2020**, *17*, 422-428, https://doi.org/10.1016/j.akcej.2019.03.022.
16. Alsinai, A.; Alwardi, A.; Soner, N. D. Topological properties of Graphene using ψ_k polynomial. *Pro-ceedings of the Jangjeon Mathematical Society* **2021**, *24*, 375 – 388, https://doi.org/10.17777/pjms2021.24.375.
17. Reti, T.; Sharafdini, R.; Dregelyi-Kiss, A.; Haghbin, H. Graph irregularity indices used as molecular descriptors in QSPR studies. *MATCH Commun. Math. Comput. Chem* **2018**, *79*, 509-524, https://scholar.google.com/citations?view_op=view_citation&hl=en&user=d7Tm_bwAAAAJ&citation_for_view=d7Tm_bwAAAAJ:uLbwQdceFCQC.
18. Kulli, V.R. Revan Indices of Chloroquine, Hydroxychloroquine, Remdesivir: Research Advances for the treatment of COVID-19. *Int. J. Eng. Sci. Technol.* **2020**, *9*, 73-74, https://doi.org/10.5281/zenodo.3828871.
19. Matečića I.X.; Šikanjićb, P.R.; Lewisb, A.P. The potential of forgotten and hidden Zagreb historical cemeteries in the design of 'dark' tourist experiences. *Journal of Heritage Tourism* **2021,** *16*, 450-468, https://doi.org/10.1080/1743873X.2020.1864384.
20. Afzal, F.; Afzal, D.; Baig, A.Q.; Farahani, M.R.; Cancan, M.; Ediz, E.The first and second Zagreb polynomial and the forgotten polynomial of Cm×Cn. *Eurasian Chemical Communications* **2020**, *2*,12, https://doi.org/10.22034/ECC.2020.256293.1097.
21. Schrezenmeier, E.; Dörner, T. Mechanisms of action of hydroxychloroquine and chloroquine: implications for rheumatology. *Nature Reviews Rheumatology* **2020**, *16*, 155-166, https://doi.org/10.1038/s41584-020-0372-x .
22. Wang, M.; Cao, R.; Zhang, L.; Yang, X.; Liu, J.; Xu, M.; Shi, Z.; Hu, Z.; Zhong, W.; Xiao, G. Remdesivir and chloroquine effectively inhibit the recently emerged novel coronavirus (2019-nCoV) in vitro. *Cell Research* **2020**, *30*, 269-271, https://doi.org/10.1038/s41422-020-0282-0.
23. Mondal, S.; De, N.; Pal, A. Topological Indices of Some Chemical Structures Applied for the Treatment of COVID-19 Patients. *Polycyclic Aromatic Compounds* **2020**, https://doi.org/10.1080/10406638.2020.1770306.
24. Wang, M.; Cao, R.; Zhang, L.; Yang, X.; Liu, J.; Xu, M.; Shi, Z.; Hu, Z.; Zhong, W.; Xiao, G. Remdesivir and chloroquine effectively inhibit the recently emerged novel coronavirus (2019-nCoV) in vitro. *Cell Research* **2020**, *30*, 269-271, https://doi.org/10.1038/s41422-020-0282-0.
25. Mondal, S.; De, N.; Pal, A. Topological Properties of Networks Using M-Polynomial Approach. *Konuralp J. Math*. **2020**, *8*, 97-105.
26. Ahmed, H.; Salestina, R.M; Alwardi, A.; Soner, N.D. Forgotten domination, hyper domination and modified forgotten domination indices of graphs, *Journal of Discrete Mathematical Sciences and Cryptography* **2021**, 24, 353-368, https://doi.org/10.1080/09720529.2021.1885805.
27. Liu, J.B.; Zhao, J.; He, H.; Shao, Z. Valency-Based Topological Descriptors and Structural Property of the Generalized Sierpinski Networks. *J. Stat. Phys.* **2019**, *177*, 1131-1147, https://doi.org/10.1007/s10955-019-02412-2.
28. Afzal, F.; Hussain, S.; Afzal, D.; Razaq, S. Some new degree based topological indices via M-polynomial. *Journal of Information and Optimization Sciences* **2020**, *41*, 1061-1076, https://doi.org/10.1080/02522667.2020.1744307.