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Investigating neighborhood Gourava indices using Neighborhood M-Polynomial in some drug structures

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Abstract

Studying the structure of molecular graphs of drugs, especially drugs effective in treating Covid-19, is practical and essential. Gourava indices have critical applications in chemistry; they have a high correlation with entropy and acentric factor. In this article, first, neighborhood Gourava indices are introduced. Then the mathematical relationship between NM-polynomial and neighborhood Gourava indices are obtained. Using NM-polynomial, neighborhood Gourava indices are computed for the molecular graphs of Dexamethasone, Chloroquine, Hydroxychloroquine, and Remedsivir.

Keywords: Neighborhood Gourava indices, Neighborhood Hyper Gourava indices, Molecular graph, NM-Polynomials, Antiviral drugs.

2020 MSC: 05C90, 92E10, 05C07, 92E20, 82D80.

1. Introduction

The chemical graph of a molecule is obtained by assuming its atoms as vertices and its chemical bonds as edges. Graph theory provides various valuable tools for chemists, including topological indices. The topological index shows some of the properties of the molecule. It is one of the practical tools for studying the structure and properties of a molecule, such as boiling point, evaporation heat, surface tension, vapour, pressure, etc. In a molecular graph, the topological index is expressed as an actual number, and this number is attributed to the graphs, uniform with that molecule. Despite the availability of various vaccines, COVID-19 still causes illness and has no definitive cure. Scientists have tested existing antiviral agents such as Dexamethasone, Chloroquine, Hydroxychloroquine, and Remedsivir and found a positive effect on patient recovery. The antiviral drug Chloroquine was discovered in 1934 by Andersag and is used to prevent and treat malaria. Hydroxychloroquine is also an antiviral drug with antiviral activity very similar to Chloroquine and has been used to treat several viral diseases, including HIV, systemic lupus erythematosus, and rheumatoid arthritis [11]. Mondal et al., using NM-Polynomials, calculated some topological indices based on the total degree of the neighborhood for some antiviral drugs [19]. Also, V.R. Kulli calculated Revan indices for some antiviral medicines [11]. Ghods et al. studied Revan polynomials on copper structure [4].

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It is essential to study the structure of molecular graphs of the above drugs. The results may help find more vital medicines and vaccines to treat of COVID-19. Considering M-polynomials for calculating degree-based indices, Neighborhood M-polynomials were introduced to make it easier to calculate topological indices based on neighborhood degree [20]. Neighborhood M-polynomial is effective in retrieving topological indices based on the sum of neighborhood degrees that predict different physical, chemical, and biological properties of the investigated materials. Recently, some neighborhood indices have been studied [2, 6, 8, 9, 10, 12, 13, 14, 16, 17, 20, 21]. In this article, neighborhood Gourava indices and neighborhood Hyper Gourava indices are calculated for some important pharmaceutical structures that are effective in treating Covid-19, and the results are expressed.

2. PRELIMINARIES

This section provides some definitions needed. Suppose G = (V, E) is a simple and connected graph. We represent the set of edges with E(G) and the number of edges with $|E(G)|$ and the collection of vertices with V(G) and the number of vertices with $|V(G)|$. We denote the degree of vertex u by d_u and if there is an edge between two vertices u, v, denote by $uv \in E(G)$.
Zagreb indices were found to be helpful for the calculation of the aggregate π -electron energy of the particles inside particular rough articulations [5]. Definition
2.1: The first and second Zagreb indices are defined as follows [5]:

$$M_1(H) = \sum_{uv \in E(H)} d_u + d_v,$$
$$M_2(H) = \sum_{uv \in E(H)} d_u . d_v.$$

Gourava indices have essential applications in chemistry. The first Gourava index has a high correlation with entropy (correlation coefficient 0.9644924) and the second Gourava index has a high correlation with the acentric factor (correlation coefficient 0.962243) [3]. Definition 2.2: The first and second Gourava index for graph G is defined as [7]:

$$GO_1(G) = \sum_{uv \in E(G)} [(d_u + d_v) + (d_u . d_v)],$$
$$GO_2(G) = \sum_{uv \in E(G)} [(d_u + d_v)(d_u . d_v)].$$

The following relationship exists between Zagreb indices and Gourava indices:

$$GO_1(G) = M_1(G) + M_2(G), \; GO_2(G) = M_1(G).M_2(G).$$

Aruvi et al. studied the second Gourava index for some graph products [1]. Keerthi et al. also investigated Gourava indices for some chemical structures such as benzenoid, hexagonal parallelogram nanotube and zigzag-edge coronoid fused with starphene nanotube [15]. Motivated by the definitions of Gourava indices and their applications, the neighborhood Gourava indices are defined as follows. Definition 2.3: The first and second neighborhood Gourava index for graph G is defined as:

$$NGO_1(G) = \sum_{uv \in E(G)} [(s_u + s_v) + (s_u . s_v)],$$
$$NGO_2(G) = \sum_{uv \in E(G)} [(s_u + s_v)(s_u . s_v)].$$

where S_u denote the degree sum of all vertices of G that are adjacent to u.

3. Main results

In this section, First, neighborhood Gourava indices and hyper neighborhood Gourava indices are obtained using the neighborhood M-polynomial. Then molecular graphs of Dexamethasone, Chloroquine, Hydroxychloroquine, and Remedsivir are examined, and the relevant results are stated.

Theorem 3.1. Let $NM(G;x,y)$ be the NM-Polynomial for graph G. Then the first Neighborhood Gourava index is computed as,

$$NGO_1(G) = [(D_x + D_y + D_xD_y)(NM(G;x,y))]|_{(x,y)=(1,1)} .$$

Proof.

$$(D_x + D_y + D_xD_y)\,NM(G;x,y) = (D_x + D_y + D_xD_y) \sum_{\delta\leqslant i\leqslant j\leqslant \Delta} \chi_{ij}(G)x^iy^j$$
$$= \sum_{\delta\leqslant i\leqslant j\leqslant \Delta} (i)\chi_{ij}(G)x^iy^j + \sum_{\delta\leqslant i\leqslant j\leqslant \Delta} (j)\chi_{ij}(G)x^iy^j + \sum_{\delta\leqslant i\leqslant j\leqslant \Delta} (ij)\chi_{ij}(G)x^iy^j.$$

$$(D_x + D_y + D_xD_y)\,NM(G;x,y)|_{(x,y)=(1,1)} = \sum_{\delta\leqslant i\leqslant j\leqslant \Delta} (i+j+ij)\chi_{ij}(G),$$
$$= \sum_{uv\in E(G)} [(s_u+s_v)+(s_u.s_v)].$$

Hence,

$$NGO_1\ (G) = [(D_x + D_y + D_xD_y)(NM(G;x,y))]_{(x,y)=(1,1)} = \sum_{uv\in E(G)} [(s_u+s_v)+(s_u.s_v)].$$

□

Theorem 3.2. Let $NM(G;x,y)$ be the NM-Polynomial for graph G. Then the second Neighborhood Gourava index is computed as,

$$NGO_2(G) = [D_xD_y(D_x + D_y)NM(G;x,y)]|_{(x,y)=(1,1)}.$$

Proof.

$$(D_x + D_y)\,NM(G;x,y) = (D_x + D_y) \sum_{\delta\leqslant i\leqslant j\leqslant \Delta} \chi_{ij}(G)x^iy^j$$
$$= \sum_{\delta\leqslant i\leqslant j\leqslant \Delta} (i)\chi_{ij}(G)x^iy^j + \sum_{\delta\leqslant i\leqslant j\leqslant \Delta} (j)\chi_{ij}(G)x^iy^j = \sum_{\delta\leqslant i\leqslant j\leqslant \Delta} (i+j)\chi_{ij}(G)x^iy^j.$$

$$(D_xD_y)((D_x + D_y)NM(G;x,y)) = (D_xD_y) \sum_{\delta\leqslant i\leqslant j\leqslant \Delta} (i+j)\chi_{ij}(G)x^iy^j = \sum_{\delta\leqslant i\leqslant j\leqslant \Delta} (ij)(i+j)\chi_{ij}(G)x^iy^j.$$

$$[D_xD_y(D_x + D_y)NM(G;x,y)]|_{(x,y)=(1,1)} = \sum_{\delta\leqslant i\leqslant j\leqslant \Delta} (ij)(i+j)\chi_{ij}(G) = \sum_{uv\in E(G)} (s_u.s_v)(s_u+s_v).$$

Hence,

$$NGO_2(G) = [D_xD_y(D_x + D_y)NM(G;x,y)]|_{(x,y)=(1,1)} = \sum_{uv\in E(G)} [(s_u+s_v)(s_u.s_v)].$$

□

Theorem 3.3. Let $NM(G;x,y)$ be the NM-Polynomial for graph G. Then the first Hyper Neighborhood Gourava index is calculated as,

$$HNGO_1(G) = [(D_x^2 + D_y^2 + 2D_xD_y + D_x^2D_y^2 + 2D_x^2D_x + 2D_xD_y^2)NM(G;x,y)]\big|_{(x,y)=(1,1)}.$$

Proof.

$$\begin{aligned}[(s_u + s_v) + (s_u.s_v)]^2 &= (s_u + s_v)^2 + (s_u.s_v)^2 + 2(s_u + s_v)(s_u.s_v)\\ &= s_u^2 + s_v^2 + 2s_us_v + s_u^2s_v^2 + 2s_u^2s_v + 2s_us_v^2.\end{aligned}$$

Now we have,

$$HNGO_1(G) = \sum_{uv\in E(G)} [(s_u+s_v) + (s_u.s_v)]^2 = \sum_{uv\in E(G)} (s_u^2 + s_v^2 + 2s_us_v + s_u^2s_v^2 + 2s_u^2s_v + 2s_us_v^2),$$

Hence,

$$\begin{aligned}HNGO_1(G) &= [(D_x^2 + D_y^2 + 2D_xD_y + D_x^2D_y^2 + 2D_x^2D_y + 2D_xD_y^2)NM(G;x,y)]\big|_{(x,y)=(1,1)}\\ &= \sum_{uv\in E(G)} [(s_u+s_v)(s_u.s_v)]^2.\end{aligned}$$

□

Theorem 3.4. Let $NM(G;x,y)$ be the NM-Polynomial for graph G. Then the second Hyper Neighborhood Gourava index is calculated as,

$$HNGO_2(G) = [(D_x^4D_y^2 + 2D_x^3D_y^3 + D_x^2D_y^4)NM(G;x,y)]\big|_{(x,y)=(1,1)}.$$

Proof.

$$[(s_u + s_v)(s_u.s_v)]^2 = (s_u + s_v)^2(s_u.s_v)^2 = (s_u^2 + s_v^2 + 2s_us_v)s_u^2s_v^2 = s_u^4s_v^2 + s_u^2s_v^4 + 2s_u^3s_v^3,$$

Now we have,

$$HNGO_2(G) = \sum_{uv\in E(G)} [(s_u+s_v)(s_u.s_v)]^2 = \sum_{uv\in E(G)} (s_u^4s_v^2 + s_u^2s_v^4 + 2s_u^3s_v^3),$$

Hence,

$$HNGO_2(G) = [(D_x^4D_y^2 + 2D_x^3D_y^3 + D_x^2D_y^4)NM(G;x,y)]\big|_{(x,y)=(1,1)} = \sum_{uv\in E(G)} [(s_u+s_v)(s_u.s_v)]^2.$$

□

According to the results of the above theorems, Table 1 is obtained to calculate neighborhood Gourava indices and Hyper neighborhood Gourava indices using NM-polynomial.

Theorem 3.5. Let D be the molecular graph of Dexamethasone. Then the neighborhood M-Polynomial of D is computed as,

$$\begin{aligned}NM(D;\,x,\,y) = {} & x^2y^4 + x^3y^5 + 2x^3y^7 + x^4y^7 + 3x^4y^{10} + x^4y^{11} + 2x^5y^5 + 3x^5y^6 + x^5y^8 + 2x^5y^9\\ & + x^6y^8 + 2x^6y^{10} + x^7y^7 + 2x^7y^{10} + x^7y^{11} + x^8y^{10} + x^9y^9 + x^9y^{10} + x^9y^{11} + x^{10}y^{10} + x^{10}y^{11}.\end{aligned}$$

Proof. By using the relations in Table 2 and placing them in definition 2.2, the proof is complete. □

Table 2 shows the types and number of edges in the molecular graph of Dexamethasone.

Table 1: Derivation of neighborhood Gourava indices from NM-polynomial.

Topological Index	Derivation from NM(G; x, y)
First Neighborhood Gourava	$[(D_x + D_y + D_xD_y)(NM(G;x,y))]\|_{(x,y)=(1,1)}$
Second Neighborhood Gourava	$[D_xD_y(D_x + D_y)NM(G;x,y)]\|_{(x,y)=(1,1)}$.
First Hyper Neighborhood Gourava	$[(D_x^2 + D_y^2 + 2D_xD_y + D_x^2D_y^2 + 2D_x^2D_x + 2D_xD_y^2)NM(G;x,y)]\|_{(x,y)=(1,1)}$
Second Hyper Neighborhood Gourava	$[(D_x^4D_y^2 + 2D_x^3D_y^3 + D_x^2D_y^4)NM(G;x,y)]\|_{(x,y)=(1,1)}$

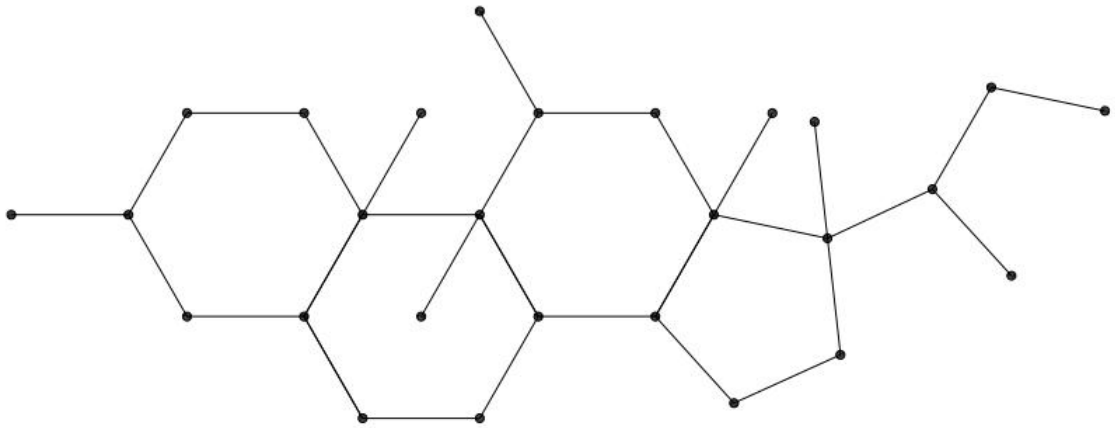

Figure 1: shows the behavior of the NM-polynomial of Dexamethasone.

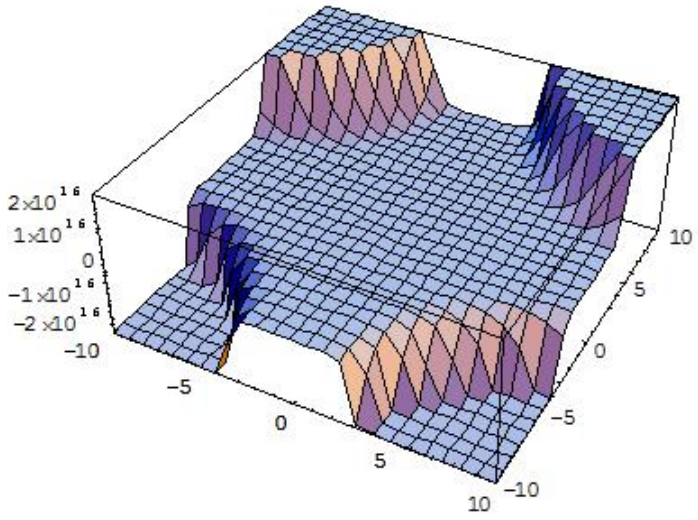

Figure 2: shows the behavior of the NM-polynomial of Dexamethasone.

Table 2: Edge types and number of edges in the molecular graph of Dexamethasone.

$(S_u, S_v)\backslash\ uv \in E(D)$	(2,4)	(3,5)	(3,7)	(4,7)	(4,10)	(4,11)	(5,5)
Number of edges	1	1	2	1	3	1	2
$(S_u, S_v)\backslash\ uv \in E(D)$	(5,6)	(5,8)	(5,9)	(6,8)	(6,10)	(7,7)	(7,10)
Number of edges	3	1	2	1	2	1	2
$(S_u, S_v)\backslash\ uv \in E(D)$	(7,11)	(8,10)	(9,9)	(9,10)	(9,11)	(10,10)	(10,11)
Number of edges	1	1	1	1	1	1	1

Theorem 3.6. Let D be the molecular graph of Dexamethasone. Then the neighborhood Gourava indices and Hyper neighborhood Gourava indices are computed as,

1. $NGO_1(D) = 1945$,
2. $NGO_2(D) = 24448$,
3. $HNGO_1(D) = 153013$,
4. $HNGO_1(D) = 30990608$.

Proof. Applying the relations of Table 1 to Theorem 3.5, we have:

1. $NGO_1(D) = [(D_x + D_y + D_xD_y)(NM(D;x,y))]|_{(x,y)=(1,1)}$
$= [(2+4)+(2\times 4)] + [(3+5)+(3\times 5)] + 2[(3+7)+(3\times 7)] + [(4+7)+(4\times 7)]$
$+3[(4+10)+(4\times 10)] + [(4+11)+(4\times 11)] + 2[(5+5)+(5\times 5)] + 3[(5+6)+(5\times 6)]$
$+[(5+8)+(5\times 8)] + 2[(5+9)+(5\times 9)] + [(6+8)+(6\times 8)] + 2[(6+10)+(6\times 10)]$
$+[(7+7)+(7\times 7)] + 2[(7+10)+(7\times 10)] + [(7+11)+(7\times 11)] + [(8+10)+(8\times 10)]$
$+[(9+9)+(9\times 9)] + [(9+10)+(9\times 10)] + [(9+11)+(9\times 11)] + [(10+10)+(10\times 10)]$
$+[(10+11)+(10\times 11)] = 1945$,
2. $NGO_2(D) = [D_xD_y(D_x + D_y)NM(D;x,y)]|_{(x,y)=(1,1)}$
$= [(2+4).(2\times 4)] + [(3+5).(3\times 5)] + 2[(3+7).(3\times 7)] + [(4+7).(4\times 7)]$
$+3[(4+10).(4\times 10)] + [(4+11).(4\times 11)] + 2[(5+5).(5\times 5)] + 3[(5+6).(5\times 6)]$
$+[(5+8).(5\times 8)] + 2[(5+9).(5\times 9)] + [(6+8).(6\times 8)] + 2[(6+10).(6\times 10)]$
$+[(7+7).(7\times 7)] + 2[(7+10).(7\times 10)] + [(7+11).(7\times 11)] + [(8+10).(8\times 10)]$
$+[(9+9).(9\times 9)] + [(9+10).(9\times 10)] + [(9+11).(9\times 11)] + [(10+10).(10\times 10)]$
$+[(10+11).(10\times 11)] = 24448$,

3. $HNGO_1(D) = [(D_x^2 + D_y^2 + 2D_xD_y + D_x^2D_y^2 + 2D_x^2D_x + 2D_xD_y^2)NM(D;x,y)]\big|_{(x,y)=(1,1)}$
$= [(2+4)+(2\times 4)]^2 + [(3+5)+(3\times 5)]^2 + 2[(3+7)+(3\times 7)]^2 + [(4+7)+(4\times 7)]^2$
$+3[(4+10)+(4\times 10)]^2 + [(4+11)+(4\times 11)]^2 + 2[(5+5)+(5\times 5)]^2 + 3[(5+6)+(5\times 6)]^2$
$+[(5+8)+(5\times 8)]^2 + 2[(5+9)+(5\times 9)]^2 + [(6+8)+(6\times 8)]^2 + 2[(6+10)+(6\times 10)]^2$
$+[(7+7)+(7\times 7)]^2 + 2[(7+10)+(7\times 10)]^2 + [(7+11)+(7\times 11)]^2 + [(8+10)+(8\times 10)]^2$
$+[(9+9)+(9\times 9)]^2 + [(9+10)+(9\times 10)]^2 + [(9+11)+(9\times 11)]^2 + [(10+10)+(10\times 10)]^2$
$+[(10+11)+(10\times 11)]^2 = 153013$,

4. $HNGO_2(D) = [(D_x^4D_y^2 + 2D_x^3D_y^3 + D_x^2D_y^4)NM(D;x,y)]\big|_{(x,y)=(1,1)}$
$= [(2+4).(2\times 4)]^2 + [(3+5).(3\times 5)]^2 + 2[(3+7).(3\times 7)]^2 + [(4+7).(4\times 7)]^2$
$+3[(4+10).(4\times 10)]^2 + [(4+11).(4\times 11)]^2 + 2[(5+5).(5\times 5)]^2 + 3[(5+6).(5\times 6)]^2$
$+[(5+8).(5\times 8)]^2 + 2[(5+9).(5\times 9)]^2 + [(6+8).(6\times 8)]^2 + 2[(6+10).(6\times 10)]^2$
$+[(7+7).(7\times 7)]^2 + 2[(7+10).(7\times 10)]^2 + [(7+11).(7\times 11)]^2 + [(8+10).(8\times 10)]^2$
$+[(9+9).(9\times 9)]^2 + [(9+10).(9\times 10)]^2 + [(9+11).(9\times 11)]^2 + [(10+10).(10\times 10)]^2$
$+[(10+11).(10\times 11)]^2 = 30990608$.

□

Figure 3 shows the molecular graph of Chloroquine.

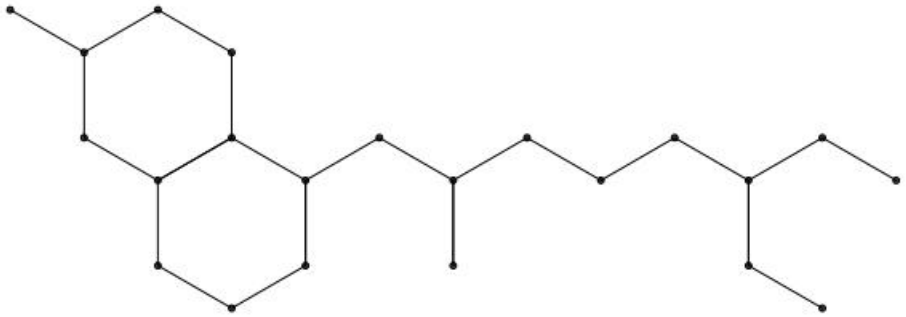

Figure 3: Chloroquine 2D molecular graph.

Table 3 shows the types and number of edges in the molecular graph of Chloroquine.

Table 3: Edge types and number of edges in the molecular graph of Chloroquine.

$(S_u, S_v)\backslash\ uv \in E(D)$	(2,4)	(3,5)	(4,5)	(4,6)	(5,5)	(5,6)	(5,7)	(5,*)	(6,7)	(7,8)
Number of edges	2	2	4	2	3	3	2	1	2	2

Theorem 3.7. Let C be the molecular graph of Chloroquine. Then the neighborhood M-Polynomial of C is computed as,

$$NM(C; x, y) = 2x^2y^4 + 2x^3y^5 + 4x^4y^5 + 2x^4y^6 + 3x^5y^5 + 3x^5y^6 + 2x^5y^7 + x^5y^8 + 2x^6y^7 + 2x^7y^8.$$

Proof. By using the relations in Table 3 and placing them in definition 2.2, the proof is complete. □

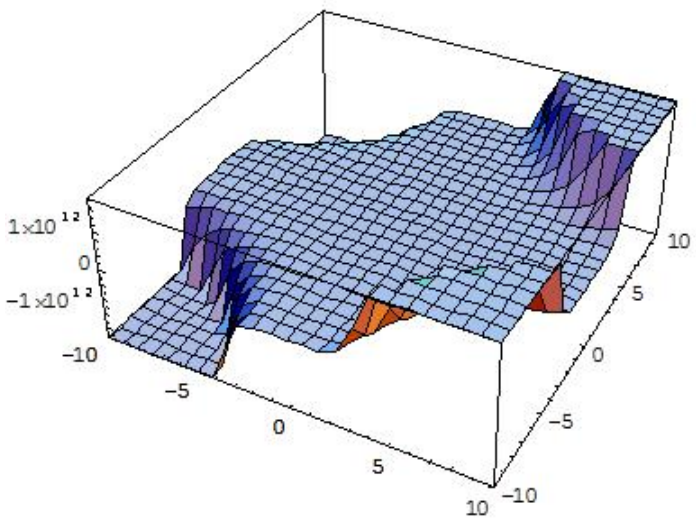

Figure 4: The behavior of the M-polynomial of the molecular graph of Chloroquine.

According to Figure 4, it can be concluded that Table 1 is suitable for calculating Gourava indices for Chloroquine because its neighborhood polynomial is positive for the values of x = 1 and y = 1.

Theorem 3.8. Suppose C be the molecular graph of Chloroquine. Then the neighborhood Gourava indices and Hyper neighborhood Gourava indices are computed as,

$$\begin{aligned}&1.\, NGO_1(C) = 885,\\ &2.\, NGO_2(C) = 7048,\\ &3.\, HNGO_1(C) = 39203,\\ &4.\, HNGO_1(C) = 3185440.\end{aligned}$$

Proof. Applying the relations of Table 1 to Theorem 3.7, we have:

$$\begin{aligned}1.\, NGO_1(C) &= [(D_x + D_y + D_xD_y)(NM(C;x,y))]|_{(x,y)=(1,1)}\\ &= 2[(2+4)+(2\times 4)] + 2[(3+5)+(3\times 5)] + 4[(4+5)+(4\times 5)] + 2[(4+6)+(4\times 6)]\\ &+3[(5+5)+(5\times 5)] + 3[(5+6)+(5\times 6)] + 2[(5+7)+(5\times 7)] + [(5+8)+(5\times 8)]\\ &+2[(6+7)+(6\times 7)] + 2[(7+8)+(7\times 8)] = 885,\end{aligned}$$

$$\begin{aligned}2.\, NGO_2(C) &= [D_xD_y(D_x + D_y)NM(C;x,y)]|_{(x,y)=(1,1)}\\ &= 2[(2+4)\times(2\times 4)] + 2[(3+5)\times(3\times 5)] + 4[(4+5)\times(4\times 5)] + 2[(4+6)\times(4\times 6)]\\ &+3[(5+5)\times(5\times 5)] + 3[(5+6)\times(5\times 6)] + 2[(5+7)+(5\times 7)]\times[(5+8)+(5\times 8)]\\ &+2[(6+7)\times(6\times 7)] + 2[(7+8)\times(7\times 8)] = 7048,\end{aligned}$$

$$\begin{aligned}3.\, HNGO_1(C) &= [(D_x^2 + D_y^2 + 2D_xD_y + D_x^2D_y^2 + 2D_x^2D_x + 2D_xD_y^2)NM(C;x,y)]\big|_{(x,y)=(1,1)}\\ &= 2[(2+4)+(2\times 4)]^2 + 2[(3+5)+(3\times 5)]^2 + 4[(4+5)+(4\times 5)]^2 + 2[(4+6)+(4\times 6)]^2\\ &+3[(5+5)+(5\times 5)]^2 + 3[(5+6)+(5\times 6)]^2 + 2[(5+7)+(5\times 7)]^2 + [(5+8)+(5\times 8)]^2\\ &+2[(6+7)+(6\times 7)]^2 + 2[(7+8)+(7\times 8)]^2 = 39203,\end{aligned}$$

$$\begin{aligned}4.\, HNGO_2(C) &= [(D_x^4D_y^2 + 2D_x^3D_y^3 + D_x^2D_y^4)NM(C;x,y)]\big|_{(x,y)=(1,1)}\\ &= 2[(2+4)\times(2\times 4)]^2 + 2[(3+5)\times(3\times 5)]^2 + 4[(4+5)\times(4\times 5)]^2 + 2[(4+6)\times(4\times 6)]^2\\ &+3[(5+5)\times(5\times 5)]^2 + 3[(5+6)\times(5\times 6)]^2 + 2[(5+7)\times(5\times 7)]^2 + [(5+8)\times(5\times 8)]^2\\ &+2[(6+7)\times(6\times 7)]^2 + 2[(7+8)\times(7\times 8)]^2 = 3185440.\end{aligned}$$

□

Figure 5 shows the molecular graph of Hydroxychloroquine.

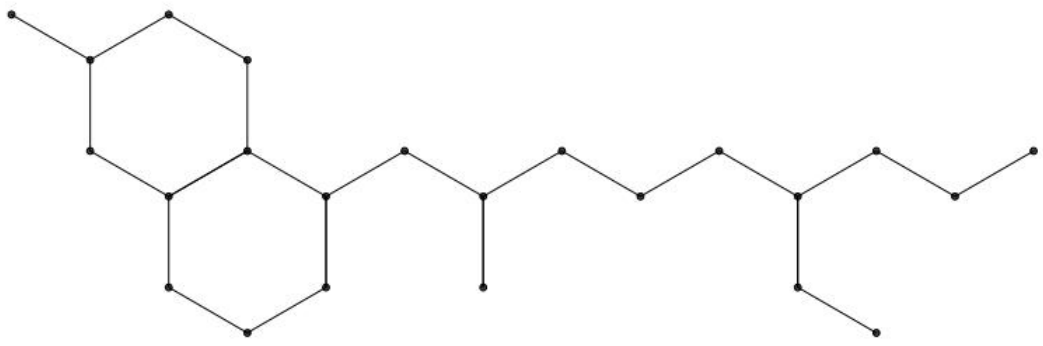

Figure 5: Hydroxychloroquine 2D molecular graph.

Table 4 shows the types and number of edges in the molecular graph of Hydroxychloroquine.

Table 4: Edge types and number of edges in the molecular graph of Hydroxychloroquine.

$(S_u, S_v)\setminus uv \in E(D)$	(2,3)	(2,4)	(3,5)	(4,5)	(4,6)	(5,5)
Number of edges	1	1	3	4	1	3
$(S_u, S_v)\setminus uv \in E(D)$	(5,6)	(5,7)	(5,8)	(6,7)	(7,8)	
Number of edges	4	2	1	2	2	

Theorem 3.9. Let H be the molecular graph of Hydroxychloroquine. Then the neighborhood M-Polynomial of H is computed as,

$$NM(H;\, x,\, y) = x^2y^3 + 2x^2y^4 + 3x^3y^5 + 4x^4y^5 + 1x^4y^6 + 3x^5y^5 + 4x^5y^6 + 2x^5y^7 + 1x^5y^8 + 2x^6y^7 + 2x^7y^8.$$

Proof. By using the relations in Table 4 and placing them in definition 2.2, the proof is complete. □

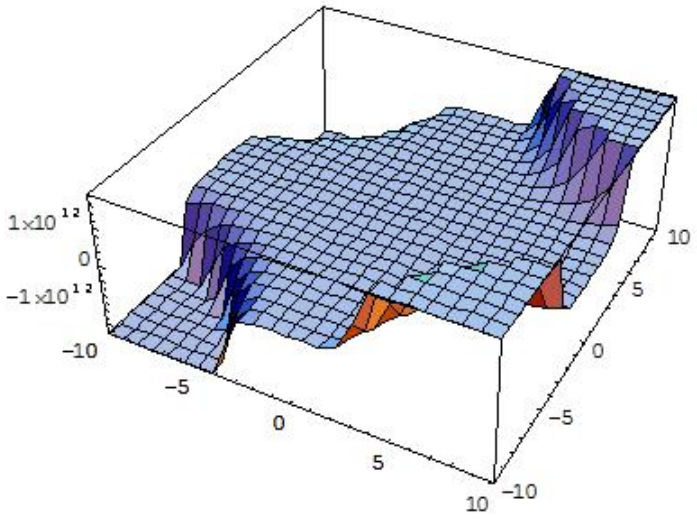

Figure 6: The behavior of the M-polynomial of the molecular graph of Hydroxychloroquine.

Theorem 3.10. Consider H to be the molecular graph of Hydroxychloroquine. Then the neighborhood Gourava indices and Hyper neighborhood Gourava indices are computed as,

1. $NGO_1(H) = 912$,
2. $NGO_2(H) = 7600$,
3. $HNGO_1(H) = 40182$,
4. $HNGO_1(H) = 3487336$.

Proof. Applying the relations of Table 1 to Theorem 3.9, we have:

$$\begin{aligned} 1.\, NGO_1(H) &= [(D_x + D_y + D_xD_y)\,(NM\,(H; x, y))]|_{(x,y)=(1,1)} \\ &= [(2+3)+(2\times 3)] + [(2+4)+(2\times 4)] + 3[(3+5)+(3\times 5)] + 4[(4+5)+(4\times 5)] \\ &+[(4+6)+(4\times 6)] + 3[(5+5)+(5\times 5)] + 4[(5+6)+(5\times 6)] + 2[(5+7)+(5\times 7)] \\ &+[(5+8)+(5\times 8)] + 2\,[(6+7)+(6\times 7)] + 2\,[(7+8)+(7\times 8)] \;\; = 912, \end{aligned}$$

$$2.\,NGO_2(H) = [D_xD_y(D_x + D_y)NM\,(H;x,y)]|_{(x,y)=(1,1)}\cdot$$
$$= [(2+3)\times(2\times3)] + [(2+4)\times(2\times4)] + 3[(3+5)\times(3\times5)] + 4[(4+5)\times(4\times5)]$$
$$+[(4+6)\times(4\times6)] + 3[(5+5)\times(5\times5)] + 4[(5+6)\times(5\times6)] + 2[(5+7)\times(5\times7)]$$
$$+[(5+8)\times(5\times8)] + 2\,[(6+7)\times(6\times7)] + 2\,[(7+8)\times(7\times8)] \;= 7600,$$

$$3.\,HNGO_1(H) = [(D_x^2 + D_y^2 + 2D_xD_y + D_x^2D_y^2 + 2D_x^2D_x + 2D_xD_y^2)NM\,(H;x,y)]\big|_{(x,y)=(1,1)}$$
$$= [(2+3)+(2\times3)]^2 + [(2+4)+(2\times4)]^2 + 3[(3+5)+(3\times5)]^2 + 4[(4+5)+(4\times5)]^2$$
$$+[(4+6)+(4\times6)]^2 + 3[(5+5)+(5\times5)]^2 + 4[(5+6)+(5\times6)]^2 + 2[(5+7)+(5\times7)]^2$$
$$+[(5+8)+(5\times8)]^2 + 2\,[(6+7)+(6\times7)]^2 + 2\,[(7+8)+(7\times8)]^2 \;= 40182,$$

$$4.\,HNGO_2(H) = [(D_x^4D_y^2 + 2D_x^3D_y^3 + D_x^2D_y^4)NM\,(H;x,y)]\big|_{(x,y)=(1,1)}$$
$$= [(2+3)\times(2\times3)]^2 + [(2+4)\times(2\times4)]^2 + 3[(3+5)\times(3\times5)]^2 + 4[(4+5)\times(4\times5)]^2$$
$$+[(4+6)\times(4\times6)]^2 + 3[(5+5)\times(5\times5)]^2 + 4[(5+6)\times(5\times6)]^2 + 2[(5+7)\times(5\times7)]^2$$
$$+[(5+8)\times(5\times8)]^2 + 2\,[(6+7)\times(6\times7)]^2 + 2\,[(7+8)\times(7\times8)]^2 \;= 3487336.$$

□

Figure 7 shows the molecular graph of Remdesivir. This graph has 41 atoms and 44 bonds.

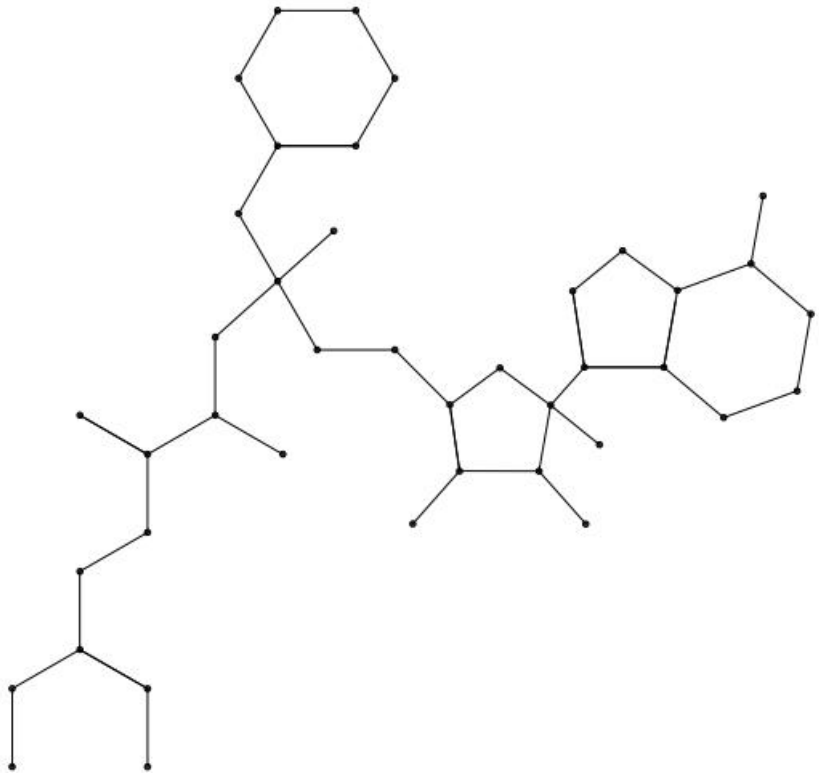

Figure 7: Remdesivir molecular graph.

Table 5 shows the types and number of edges in the molecular graph of Remdesivir.

Theorem 3.11. Let R be the molecular graph of Remdesivir. Then the neighborhood M-Polynomial of R is computed as,

$$NM(R;\,x,\,y) = 2x^4y^6 + x^4y^7 + x^4y^9 + 2x^5y^5 + 6x^5y^6 + x^5y^7 + 2x^5y^8 + x^5y^9$$
$$+1x^6y^6 + 3x^6y^7 + x^6y^8 + 4x^7y^7 + x^7y^8 + x^7y^9 + x^8y^8 + 2x^8y^9 + x^9y^9.$$

Proof. By using the relations in Table 5 and placing them in definition 2.2, the proof is complete. □

Table 5: Edge types and number of edges in the molecular graph of Remdesivir.

$(S_u, S_v)\setminus uv \in E(D)$	(2,4)	(3,6)	(3,7)	(3,8)	(4,4)	(4,5)
Number of edges	2	3	1	1	2	4
$(S_u, S_v)\setminus uv \in E(D)$	(4,6)	(4,7)	(4,9)	(5,5)	(5,6)	(5,7)
Number of edges	2	1	1	2	6	1
$(S_u, S_v)\setminus uv \in E(D)$	(5,8)	(5,9)	(6,6)	(6,7)	(6,8)	(7,7)
Number of edges	2	1	1	3	1	4
$(S_u, S_v)\setminus uv \in E(D)$	(7,8)	(7,9)	(8,8)	(8,9)	(9,9)	
Number of edges	1	1	1	2	1	

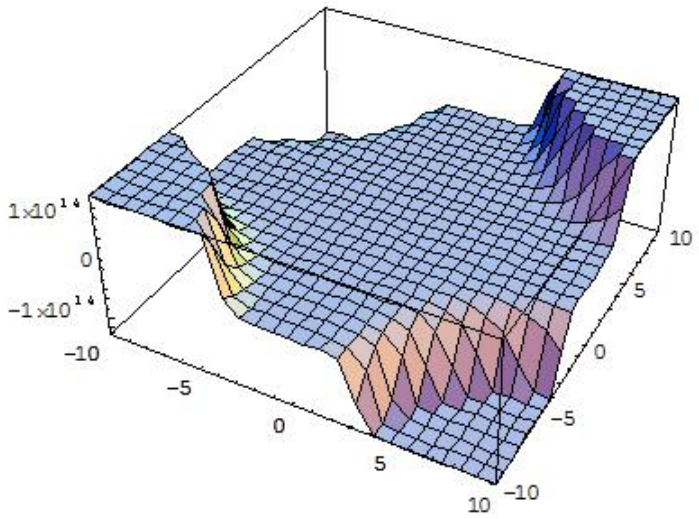

Figure 8: The behavior of the M-polynomial of the molecular graph of Remdesivir.

Theorem 3.12. Let R be the molecular graph of Remdesivir. Then the neighborhood Gourava indices and Hyper neighborhood Gourava indices are computed as,

$$\begin{aligned}
&1.\, NGO_1(R) = 1718,\\
&2.\, NGO_2(R) = 18090,\\
&3.\, HNGO_1(R) = 104502,\\
&4.\, HNGO_1(R) = 13628884.
\end{aligned}$$

Proof. Applying the relations of Table 1 to Theorem 3.11, we have:

$$\begin{aligned}
1.\, NGO_1(R) &= [(D_x + D_y + D_xD_y)\,(NM\,(H; x, y))]|_{(x,y)=(1,1)}\\
&= 2[(4+6)+(4\times 6)] + [(4+7)+(7\times 4)] + [(4+9)+(4\times 9)] + 2[(5+5)+(5\times 5)]\\
&+6[(5+6)+(5\times 6)] + [(5+7)+(5\times 7)] + 2[(5+8)+(5\times 8)] + [(5+9)+(5\times 9)]\\
&+[(6+6)+(6\times 6)] + 3\,[(6+7)+(6\times 7)] + [(6+8)+(6\times 8)] + 4\,[(7+7)+(7\times 7)]\\
&+[(7+8)+(7\times 8)] + [(7+9)+(7\times 9)] + [(8+8)+(8\times 8)] + 2\,[(8+9)+(8\times 9)]\\
&+[(9+9)+(9\times 9)] = 1718,
\end{aligned}$$

$$2.\ NGO_2(R) = [D_x D_y (D_x + D_y) NM(r; x, y)]|_{(x,y)=(1,1)}$$
$$= 2[(4+6)\times(4\times6)] + [(4+7)\times(7\times4)] + [(4+9)\times(4\times9)] + 2[(5+5)\times(5\times5)]$$
$$+6[(5+6)\times(5\times6)] + [(5+7)\times(5\times7)] + 2[(5+8)\times(5\times8)] + [(5+9)\times(5\times9)]$$
$$+[(6+6)\times(6\times6)] + 3[(6+7)\times(6\times7)] + [(6+8)\times(6\times8)] + 4[(7+7)\times(7\times7)]$$
$$+[(7+8)\times(7\times8)] + [(7+9)\times(7\times9)] + [(8+8)\times(8\times8)] + 2[(8+9)\times(8\times9)]$$
$$+[(9+9)\times(9\times9)] = 18090,$$

$$3.\ HNGO_1(R) = [(D_x^2 + D_y^2 + 2D_xD_y + D_x^2D_y^2 + 2D_x^2D_x + 2D_xD_y^2) NM(H; x, y)]|_{(x,y)=(1,1)}$$
$$= 2[(4+6)+(4\times6)]^2 + [(4+7)+(7\times4)]^2 + [(4+9)+(4\times9)]^2 + 2[(5+5)+(5\times5)]^2$$
$$+6[(5+6)+(5\times6)]^2 + [(5+7)+(5\times7)]^2 + 2[(5+8)+(5\times8)]^2 + [(5+9)+(5\times9)]^2$$
$$+[(6+6)+(6\times6)]^2 + 3[(6+7)+(6\times7)]^2 + [(6+8)+(6\times8)]^2 + 4[(7+7)+(7\times7)]^2$$
$$+[(7+8)+(7\times8)] + [(7+9)+(7\times9)] + [(8+8)+(8\times8)] + 2[(8+9)+(8\times9)]$$
$$+[(9+9)+(9\times9)]^2 = 104502,$$

$$4.\ HNGO_2(R) = [(D_x^4D_y^2 + 2D_x^3D_y^3 + D_x^2D_y^4) NM(H; x, y)]|_{(x,y)=(1,1)}$$
$$= 2[(4+6)\times(4\times6)]^2 + [(4+7)\times(7\times4)]^2 + [(4+9)\times(4\times9)]^2 + 2[(5+5)\times(5\times5)]^2$$
$$+6[(5+6)\times(5\times6)]^2 + [(5+7)\times(5\times7)]^2 + 2[(5+8)\times(5\times8)]^2 + [(5+9)\times(5\times9)]^2$$
$$+[(6+6)\times(6\times6)]^2 + 3[(6+7)\times(6\times7)]^2 + [(6+8)\times(6\times8)]^2 + 4[(7+7)\times(7\times7)]^2$$
$$+[(7+8)\times(7\times8)]^2 + [(7+9)\times(7\times9)]^2 + [(8+8)\times(8\times8)]^2 + 2[(8+9)\times(8\times9)]^2$$
$$+[(9+9)\times(9\times9)]^2 = 13628884.$$

□

4. Conclusion

In this article, the Gourava neighborhood indices and hyper neighborhood Gourava indices were introduced and calculated for the molecular diagrams of effective drugs in some pharmaceutical structures. First, these indices were obtained using the NM-polynomial, and then they were calculated for the drug molecular graph. The results of this article can be very useful in pharmaceutical science. Calculating neighborhood Gourava indices for other molecular structures and examining their characteristics can be the subject of future research.

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