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Examination of Four Antiviral Drugs by Studying Their Polynomials and Topological Indices

Setareh Javame, Masoud Ghods*

Department of Applied Mathematics, Semnan University, Semnan, 35131-19111, Iran

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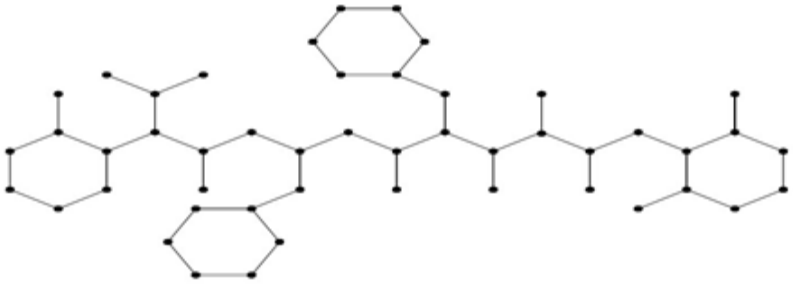
ABSTRACT

To fight against viral diseases, in addition to prevent the spread of the disease, it is necessary to discover suitable antiviral agents to save as many lives as possible. Therefore, it seems important to develop new and effective vaccines. An efficient way to find effective drugs or vaccines is to answer whether they effectively treat the viral disease of interest. In this article, M-polynomial, NM-polynomial, and some topological indices are investigated for Lopinavir, Azithromycin, Favipiravir, and Oseltamivir, which are considered as the efficient COVID-19 antiviral drugs, and they can be used as a guide to discover more efficient drugs to battle against COVID-19. Also, in addition to calculate the topological indices, M-polynomial and NM-polynomial were plotted and compared as well as they were used to calculate the topological indices.

GRAPHICAL ABSTRACT



* Corresponding author: Masoud Ghods
✉ E-mail: mghods@semnan.ac.ir

Introduction

The availability of licensed vaccines alone is insufficient to prevent COVID-19 deaths, as they should be produced on a large and cost-effective scale. They should be easily accessible to the public in suburban and rural areas, and of course, this process takes time. Until this stage is reached, it is essential to save as many lives as possible, people infected, besides preventing the spread of the disease. No specific medication is available for coronavirus. Therefore, it is essential to discover suitable antiviral agents [1]. An efficient way to find the effective drugs available is to answer whether they effectively treat the viral disease we concern.

So far, the effectiveness of various antiviral drugs in the therapy of COVID-19 patients has been investigated [2, 3].

One of the effective drugs is Lopinavir (ABT-378) which is an antiretroviral drug. It is used against HIV infections as a fixed-dose combination with ritonavir [4]. It has been previously used to treat acute respiratory syndrome- coronavirus iteration in hospitals [5].

According to FDA, another antiviral drug is Azithromycin, sold under the brand name *Zithromax*. Combining this drug and hydroxychloroquine (HCQ) has been significantly more effective against the virus [6].

The third effective antiviral drug is Favipiravir (T-705), which clinical trials have shown to effectively counteract ribonucleic acid-dependent RNA polymerase (RNA) in RNA viruses [3].

Lastly, Oseltamivir (GS-4104) sold under the brand name *Tamiflu* has been used for symptomatic patients with COVID-19 [7].

In recent years, scientists have begun to determine the properties of drugs by using mathematical methods and discover new drugs by using this method [8].

Therefore, by calculating the topological indices of molecular, pharmaceuticals, scientists, and pharmacologists can correctly identify defects in the properties of medicines according to the definition of the topological index in medical and chemical experiments. Hence, the topological index calculation methods are very appropriate tools that can be used, especially in developing countries; because without using chemical testing hardware, pharmacologists can have medical information on drugs [9].

For a molecular graph G, we denote vertex set with V(G), edge set E(G), the maximum degree Δ, and the minimum degree δ. Topological indices are numerical values related to a chemical structure that describes the correlation of chemical structure with different physical properties and chemical reactions with applications in theoretical medicine to test the drugs' properties [10].

So far, graph polynomials have been studied in mathematical chemistry. For instance, valuable results have been obtained about M- polynomials in chemical networks.

The results are used by researchers to find an effective relationship between chemical compounds and their chemical and bioactive properties.

In graph G= (V, E), M-polynomial is defined as [11]

$$M(G,x,y)=\sum_{\delta\le l,k\le\Delta} m_{l,k}x^l y^k, \qquad (1)$$

Where, $m_{\{l,k\}}=E_{\{L,K\}}$

Table 1 relates seven topological indices with M-polynomial [12].

Here, $D_X\big(f(x,y)\big)=\frac{\delta(f(x,y))}{\delta_x}$,

$$D_y(f(x,y))=y\frac{\delta(f(x,y))}{\delta y},$$

$$J\big(f(x,y)\big)=f(x,x), and\ S_X=\int_0^X \frac{f(t,y)}{t}dt,$$

In graph G= (V, E), NM -polynomial is defined as [13]:

$$NM(G,x,y)=\sum_{\delta\le l,k\le\Delta} \chi_{l,k}x^l y^k, \qquad (2)$$

Where, $X_{l,k}$is the total count of edges $ab\,\epsilon E(G)$ such that $\{\delta_a,\delta_b\}=\{l,k\}$

Table 2 relates four topological indices with NM-polynomial [13].

Table 1: The relationship between seven topological indices and M-polynomial

Topological index	Derivation from M(G,x,y)
M_1	$(D_x + D_y)(M(G,x,y))\,\vert_{x=y=1}$
M_2	$(D_xD_y)(M(G,x,y))\,\vert_{x=y=1}$
F	$(D_x^2 + D_y^2)(M(G,x,y))\,\vert_{x=y=1}$
H	$2S_xJ(M(G,x,y))\,\vert_{x=y=1}$
SK	$(D_x + D_y)/2)(M(G,x,y))\,\vert_{x=y=1}$
SK_1	$(D_xD_y)/2)(M(G,x,y))\,\vert_{x=y=1}$
SK_2	$((D_x^2)/4J)(M(G,x,y))\,\vert_{x=y=1}$

Table 2: The relationship between four topological indices and NM-polynomial

Topological index	Derivation from NM(G,x,y)
M_1^*	$(D_x + D_y)(NM(G,x,y))\vert_{x=y=1}$
M_2^*	$(D_xD_y)(NM(G,x,y))\vert_{x=y=1}$
F_N^*	$(D^2{}_x + D^2{}_y)(NM(G,x,y))\vert_{x=y=1}$
NH	$2S_xJ(NM(G,x,y))\vert_{x=y=1}$

Recently Gutman introduced the Sombor index as follows [14]:

$$SO(G) = \sum_{a,b\in E(G)} \sqrt{d_G{}^2(a) + d_G{}^2(b)} \qquad (3)$$

The goal of this article is to consider M-polynomial, NM-polynomial, and some derived topological indices of the antiviral drugs Lopinavir, Azithromycin, Favipiravir, and Oseltamivir. The obtained results are shown on the graphical .representations

Results and Discussion

Lopinavir

The molecular graph of Lopinavir is displayed in Figure 1 [11].

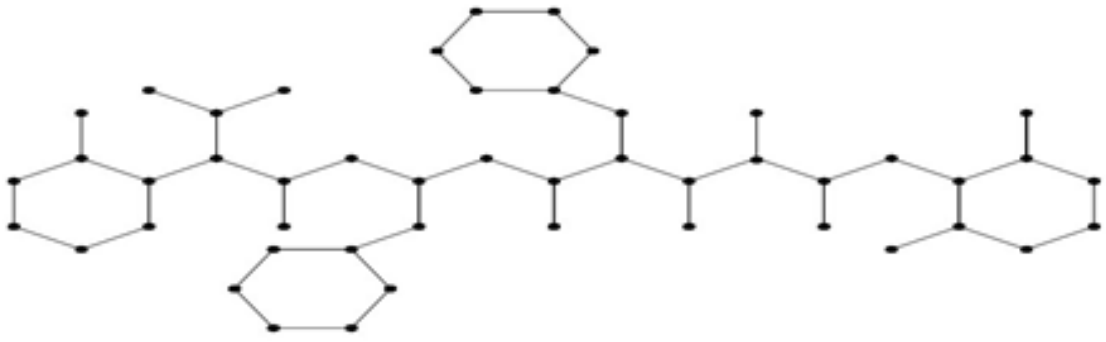


Figure 1: Molecular graph of Lopinavir

Theorem 1. Consider G be a graph structure of Lopinavir. For M- polynomial and NM- polynomial of Lopinavir, we have:

$$i)\, M(G, x, y) = 14xy^2 + 8xy^3 + 7x^3y^3 + 20x^2y^3 \quad (4)$$

$$ii)\, NM(G, x, y) = x^8y^9 + x^6y^9 + x^5y^9 + 3x^6y^8 + 2x^5y^8 + 3x^6y^7 + 7x^6y^6 + 7x^5y^6 + 4x^3y^6 + x^2y^6 + 2x^5y^5 + 7x^4y^5 + 3x^3y^5 + 5x^4y^4 + x^2y^4 \quad (5)$$

Proof

i) The graph structure of Lopinavir has 49 edges (Figure 1). According to its molecular structure, it is clear that its edge partition, Table 3 is as follows:

$$e_1 = \{(d_a, d_b) \mid ab \in E(G), d_a = 1, d_b = 2\},$$
$$e_2 = \{(d_a, d_b) \mid ab \in E(G), d_a = 1, d_b = 3\}$$
$$e_3 = \{(d_a, d_b) \mid ab \in E(G), d_a = 3, d_b = 3\},$$
$$e_4 = \{(d_a, d_b) \mid ab \in E(G), d_a = 2, d_b = 3\}$$

Table 3: Edge type of Lopinavir (ABT-378)

Edge type	e_1	e_2	e_3	e_4
Number of edges	14	8	7	20

From Equation (1), we have:

$$M(G, x, y) = \sum_{\delta \le l \le k \le \Delta} m_{l,k} x^l y^k$$
$$= m_{1,2}x^1y^2 + m_{1,3}x^1y^3 + m_{3,3}x^3y^3 + m_{2,3}x^2y^3$$
$$= 14xy^2 + 8xy^3 + 7x^3y^3 + 20x^2y^3.$$

ii) Suppose G be a graph structure of Lopinavir. According to its graph structure, by using neighbourhood degree sum of end vertices for the edge partition in this case, Table 4 is presented as follows:

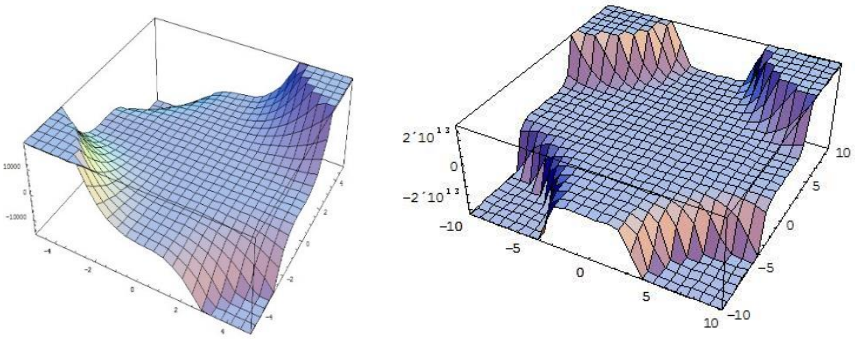
Table 4: Lopinavir edge type based on neighborhood degree sum of end vertices

Edge type based on NM	e_1^*	e_2^*	e_3^*	e_4^*	e_5^*	e_6^*	e_7^*	e_8^*	e_9^*	e_{10}^*	e_{11}^*	e_{12}^*	e_{13}^*	e_{14}^*	e_{15}^*
Number of edges	1	1	1	3	2	3	7	7	4	1	2	7	3	5	1

$$NM(G, x, y) = \sum_{\delta \le l, k \le \Delta} \chi_{l,k} x^l y^k = \chi_{8,9}x^8y^9 + \chi_{6,9}x^6y^9 + \chi_{5,9}x^5y^9 + \chi_{6,8}x^6y^8 + \chi_{5,8}x^5y^8 + \chi_{6,7}x^6y^7 + \chi_{6,6}x^6y^6 + \chi_{5,6}x^5y^6 + \chi_{3,6}x^3y^6 + \chi_{2,6}x^2y^6 + \chi_{5,5}x^5y^5 + \chi_{4,5}x^4y^5 + \chi_{3,5}x^3y^5 + \chi_{4,4}x^4y^4 + \chi_{2,4}x^2y^4.$$

The M-polynomial and NM-polynomial of Lopinavir are indicated in Figure 2.

The molecular graph of azithromycin is illustrated Figure 3 [15].



(a) (b)

Figure 2: (a) Lopinavir M-polynomial, (b) Lopinavir NM-polynomial

$i) M_1(G) = 216,$

$ii) M_2(G) = 235,$

$iii)\ F(G) = 536,$

$iv) H(G) = 23.66,$

$v) SK(G) = 108,$

$vi) SK_1(G) = 117.5,$

$vii) SK_2(G) = 251.5,$

$ix) M^*_1(G) = 511,$

$x) M^*_2(G) = 1390,$

$xi) F_N^*(G) = 2921,$

$xii) NH(G) = 9.6276.$

Proof. By using Tables 1 and 2 and Equations (4) and (5) ,we have:

$$D_x(M(G,x,y)) = 14xy^2 + 8xy^3 + 21x^3y^3 + 40x^2y^3,$$

$$D_y(M(G,x,y)) = 28xy^2 + 24xy^3 + 21x^3y^3 + 60x^2y^3,$$

$$D_xD_y(M(G,x,y)) = 28xy^2 + 24xy^3 + 63x^3y^3 + 120x^2y^3,$$

$$D^2_x(M(G,x,y)) = 14xy^2 + 8xy^3 + 63x^3y^3 + 80x^2y^3,$$

$$D^2_y(M(G,x,y)) = 56xy^2 + 72xy^3 + 63x^3y^3 + 240x^2y^3,$$

$$J(M(x,y)) = 14x^3 + 8x^4 + 20x^5 + 7x^6,$$

$$S_xJ(M(x,y)) = \int_0^x \frac{14t^3 + 8t^4 + 20t^5 + 7t^6}{t}\,dt = 14\frac{x^3}{3} + 8\frac{x^4}{4} + 20\frac{x^5}{5} + 7\frac{x^6}{6},$$

$$D^2(x)J(M(x,y)) = 126x^3 + 128x^4 + 500x^5 + 252x^6,$$

$$D_x(NM(G,x,y)) = 8x^8y^9 + 6x^6y^9 + 5x^5y^9 + 18x^6y^8 + 10x^5y^8 + 18x^6y^7 + 42x^6y^6 + 35x^5y^6 + 12x^3y^6 + 2x^2y^6 + 10x^5y^5 + 28x^4y^5 + 9x^3y^5 + 20x^4y^4 + 2x^2y^4.$$

$$D_y(NM(G,x,y)) = 9x^8y^9 + 9x^6y^9 + 9x^5y^9 + 24x^6y^8 + 16x^5y^8 + 21x^6y^7 + 42x^6y^6 + 42x^5y^6 + 24x^3y^6 + 6x^2y^6 + 10x^5y^5 + 35x^4y^5 + 15x^3y^5 + 20x^4y^4 + 4x^2y^4.$$

$$D_xD_y(NM(G,x,y)) = 72x^8y^9 + 54x^6y^9 + 45x^5y^9 + 144x^6y^8 + 80x^5y^8 + 126x^6y^7 + 252x^6y^6 + 210x^5y^6 + 72x^3y^6 + 12x^2y^6 + 50x^5y^5 + 140x^4y^5 + 45x^3y^5 + 80x^4y^4 + 8x^2y^4$$

$$D^2_x(NM(G,x,y)) = 64x^8y^9 + 36x^6y^9 + 25x^5y^9 + 108x^6y^8 + 50x^5y^8 + 108x^6y^7 + 252x^6y^6$$

$$+175x^5y^6+36x^3y^6+4x^2y^6+50x^5y^5+112x^4y^5+27x^3y^5+80x^4y^4+4x^2y^4.$$

$$D^2{}_y(NM(G,x,y))=81x^8y^9+81x^6y^9+81x^5y^9+192x^6y^8+128x^5y^8+147x^6y^7+252x^6y^6$$
$$+252x^5y^6+144x^3y^6+36x^2y^6+50x^5y^5+175x^4y^5+75x^3y^5+80x^4y^4+16x^2y^4.$$

$$J(NM(x,y))=x^{17}+x^{15}+4x^{14}+7x^{13}+7x^{12}+7x^{11}+2x^{10}+16x^9+4x^8+x^6,$$

$$S_xJ(NM(x,y))=\int_0^x\frac{t^{17}+t^{15}+4t^{14}+7t^{13}+7t^{12}+7t^{11}+2t^{10}+16t^9+4t^8+t^6}{t}dt$$

$$=\frac{x^{17}}{17}+\frac{x^{15}}{15}+4\frac{x^{14}}{14}+7\frac{x^{13}}{13}+7\frac{x^{12}}{12}+7\frac{x^{11}}{11}+2\frac{x^{10}}{10}+16\frac{x^{19}}{9}+4\frac{x^8}{8}+\frac{x^6}{6}.$$

$$i)M_1(G)=(D_x+D_y)(M(G,x,y))|_{x=y=1}=216,$$

$$ii)\ M_2(G)=\left(D_xD_y\right)\left(M(G,x,y)\right)\Big|_{x=y=1}=235$$

$$iii)F(G)=(D^2{}_x+D^2{}_y)(M(G,x,y))|_{x=y=1}=536,$$

$$iv)H(G)=2S_xJ(M(G,x,y))|_{x=y=1}=\frac{28}{3}+4+8+\frac{14}{6}=23.66,$$

$$v)SK(G)=\frac{1}{2}(D_x+D_y)(M(G,x,y))|_{x=y=1}=108,$$

$$vi)SK_1(G)=\frac{1}{2}(D_xD_y)(M(G,x,y))|_{x=y=1}=117.5,$$

$$vii)\ SK_2(G)=\frac{1}{4}(D_X^2)/J\left(M(G,x,y)\right)\Big|_{x=y=1}=\frac{126}{4}+\frac{128}{4}+\frac{500}{4}+\frac{252}{4}=251.5,$$

$$ix)M^*{}_1(G)=(D_x+D_y)(NM(G,x,y))|_{x=y=1}=511,$$

$$x)M^*{}_2(G)=(D_xD_y)(NM(G,x,y))|_{x=y=1}=1390,$$

$$xi)F^*{}_N(G)=(D^2{}_x+D^2{}_y)(M(G,x,y))|_{x=y=1}=2921,$$

$$xii)NH(G)=2S_xJ(NM(G,x,y))|_{x=y=1}=9.6276.$$

Also, we have:

$$i)M_1(G)=\sum_{ab\in E(G)}d_G(a)+d_G(b)=\sum_{ab\in e_1}d_G(a)+d_G(b)+\sum_{ab\in e_2}d_G(a)+d_G(b)$$
$$+\sum_{ab\in e_3}d_G(a)+d_G(b)+\sum_{ab\in e_4}d_G(a)+d_G(b)$$
$$=14(1+2)+8(1+3)+7(3+3)+20(2+3)=216,$$

$$ii)\ M_2(G)=\sum_{ab\in E(G)}d_G(a)d_G(b)=\sum_{ab\in e_1}d_G(a)d_G(b)+\sum_{ab\in e_2}d_G(a)d_G(b)$$

$$+\sum_{ab\in e_3}d_G(a)d_G(b)+\sum_{ab\in e_4}d_G(a)d_G(b)$$
$$=4(1\times2)+8(1\times3)+7(3\times3)+20(2\times3)=235,$$

$$iii)\ F(G) = \sum_{ab\in E(G)} {d^2}_G(a) + d^2(b) = \sum_{ab\in e_1} {d^2}_G(a) + {d^2}_G(b) + \sum_{ab\in e_2} {d^2}_G(a) + {d^2}_G(b)$$

$$= 14(1+4) + 8(1+9) + 7(9+9) + 20(4+9) = 536,$$

$$iv)\ H(G) = \sum_{ab\in E(G)} \frac{2}{d_G(a)+d_G(b)} = \sum_{ab\in e_1} \frac{1}{d_G(a)+d_G(b)} + \sum_{ab\in e_1} \frac{1}{d_G(a)+d_G(b)}$$

$$+ \sum_{ab\in e_3} \frac{1}{d_G(a)+d_G(b)} + \sum_{ab\in e_4} \frac{1}{d_G(a)+d_G(b)}$$

$$28(\frac{1}{1+2}) + 16(\frac{1}{1+3}) + 14(\frac{1}{3+3}) + 40(\frac{1}{2+3}) = 23.66,$$

$$v)SK(G) = \sum_{ab\in E(G)} \frac{d_G(a)+d_G(b)}{2} = \sum_{ab\in e_1} \frac{d_G(a)+d_G(b)}{2} + \sum_{ab\in e_2} \frac{d_G(a)+d_G(b)}{2}$$

$$+ \sum_{ab\in e_3} \frac{d_G(a)+d_G(b)}{2} + \sum_{ab\in e_4} \frac{d_G(a)+d_G(b)}{2}$$

$$= 14(\frac{1+2}{2}) + 8(\frac{1+3}{2}) + 7(\frac{3+3}{2}) + 20(\frac{2+3}{2}) = 108,$$

$$vi)SK_1(G) = \sum_{ab\in E(G)} \frac{d_G(a)d_G(b)}{2} = \sum_{ab\in e_1} \frac{d_G(a)d_G(b)}{2} + \sum_{ab\in e_2} \frac{d_G(a)d_G(b)}{2}$$

$$+ \sum_{ab\in e_3} \frac{d_G(a)d_G(b)}{2} + \sum_{ab\in e_4} \frac{d_G(a)d_G(b)}{2}$$

$$= 14(\frac{1\times 2}{2}) + 8(\frac{1\times 3}{2}) + 7(\frac{3\times 3}{2}) + 20(\frac{2\times 3}{2}) = 117.5,$$

$$vii)SK_2(G) = \sum_{ab\in E(G)} (\frac{d_G(a)+d_G(b)}{2})^2 = \sum_{ab\in e_1} (\frac{d_G(a)+d_G(b)}{2})^2 + \sum_{ab\in e_2} (\frac{d_G(a)+d_G(b)}{2})^2$$

$$+ \sum_{ab\in e_3} (\frac{d_G(a)+d_G(b)}{2})^2 + \sum_{ab\in e_4} (\frac{d_G(a)+d_G(b)}{2})^2$$

$$= 14(\frac{1+2}{2})^2 + 8(\frac{1+3}{2})^2 + 7(\frac{3+3}{2})^2 + 20(\frac{2+3}{2})^2 = 251.5,$$

$$viii)SO(G) = \sum_{ab\in E(G_1)} \sqrt{{d^2}_G(a) + {d^2}_G(b)} = \sum_{ab\in e_1} \sqrt{{d^2}_G(a) + {d^2}_G(b)} + \sum_{ab\in e_2} \sqrt{{d^2}_G(a) + {d^2}_G(b)}$$

$$+ \sum_{ab\in e_3} \sqrt{{d^2}_G(a) + {d^2}_G(b)} + \sum_{ab\in e_4} \sqrt{{d^2}_G(a) + {d^2}_G(b)}$$

$$= 14(\sqrt{1+4}) + 8(\sqrt{1+4}) + 7(\sqrt{9+9}) + 20(\sqrt{4+9}) = 151.003005824, \square$$

Azithromycin

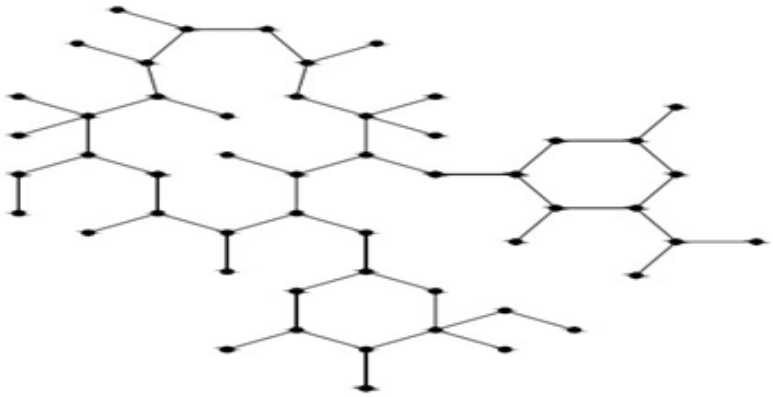


Figure 3: Molecular graph of Azithromycin

Theorem 3. Suppose G be a graph structure corresponding to Azithromycin. M-polynomial and NM-polynomial of Azithromycin are:

$$i) M(G,x,y) = 13xy^3 + 15x^2y^3 + 2xy^2 + 7x^3y^3 + 7xy^4 + 5x^4y^3 + 5x^2y^4 + x^4y^4,$$

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

Proof. i) The graph structure of Azithromycin has 55 edges. Its edge partition, Table 5 is as follows:

$$e_1 = \{(d_a, d_b) \mid ab \in E(G), d_a = 1, d_b = 3\},\ e_2 = \{(d_a, d_b) \mid ab \in E(G), d_a = 2, d_b = 3\}$$
$$e_3 = \{(d_a, d_b) \mid ab \in E(G), d_a = 1, d_b = 2\},\ e_4 = \{(d_a, d_b) \mid ab \in E(G), d_a = 3, d_b = 3\}$$
$$e_5 = \{(d_a, d_b) \mid ab \in E(G), d_a = 1, d_b = 4\},\ e_6 = \{(d_a, d_b) \mid ab \in E(G), d_a = 3, d_b = 4\}$$
$$e_7 = \{(d_a, d_b) \mid ab \in E(G), d_a = 2, d_b = 4\},\ e_8 = \{(d_a, d_b) \mid ab \in E(G), d_a = 4, d_b = 4\}$$

Table 5: Edge type of Azithromycin

Edge type	e_1	e_2	e_3	e_4	e_5	e_6	e_7	e_8
Number of edges	13	15	2	7	7	5	5	1

So, from Equation (1), we have:

$$M(G,x,y) = 13xy^3 + 15x^2y^3 + 2xy^2 + 7x^3y^3 + 7xy^4 + 5x^4y^3 + 5x^2y^4 + x^4y^4.$$

ii) Suppose G be the graph structure of Azithromycin. According to its graph structure, by using the edge partition based on the neighbourhood degree sum of end vertices, Table 6 is as follows:

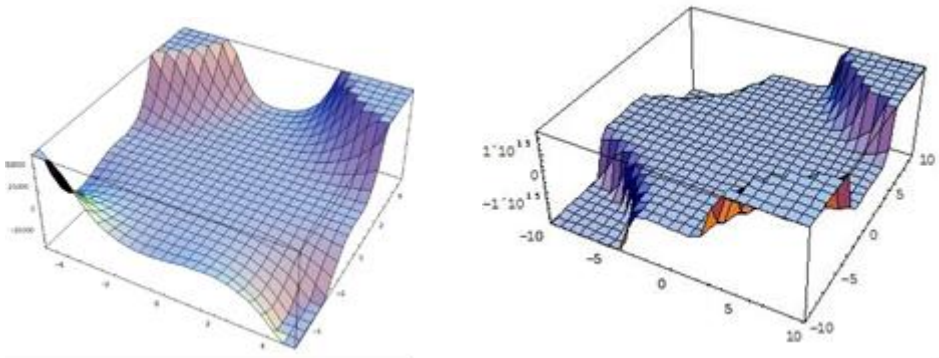
Table 6: Azithromycin edge type based on the neighborhood degree sum of end vertices

Edge type based on NM	e_1^*	e_2^*	e_3^*	e_4^*	e_5^*	e_6^*	e_7^*	e_8^*	e_9^*	e_{10}^*	e_{11}^*	e_{12}^*	e_{13}^*
Number of edges	1	1	1	1	1	1	1	1	1	3	4	3	2
Edge type based on NM	e_{14}^*	e_{15}^*	e_{16}^*	e_{17}^*	e_{18}^*	e_{19}^*	e_{20}^*	e_{21}^*	e_{22}^*	e_{23}^*	e_{24}^*	e_{25}^*	
Number of edges	6	4	2	4	1	2	4	3	3	4	1	1	

From equation (2), we have:

$$NM(G,x,y) = x^9y^{10} + x^8y^{10} + x^7y^{10} + x^4y^{10} + x^9y^9 + x^8y^9 + x^7y^9 + x^4y^9$$
$$+x^3y^9 + 3x^8y^8 + 4x^7y^8 + 3x^6y^8 + 2x^5y^8 + 6x^4y^8 + 4x^3y^8 + 2x^7y^7$$
$$+4x^6y^7 + x^5y^7 + 2x^3y^7 + 4x^6y^6 + 3x^5y^6 + 3x^3y^6 + 4x^3y^5 + x^2y^5 + x^2y^4.$$

The behaviour of M-polynomial and NM-polynomial of Azithromycin is demonstrated in Figure 4.



(a) (b)

Figure 4: (a) Azithromycin M-polynomial, (b) Azithromycin NM-polynomial

Theorem 4. Suppose G be a graph structure of Azithromycin. Then, for topological indices of Azithromycin, we have:

$i) M_1(G) = 283,$
$ii) M_2(G) = 340,$
$iii) F(G) = 837,$
$iv) H(G) = 9.75595238,$
$v) SK(G) = 141.5$
$vi) SK_1(G) = 170,$
$vii) SK_2(G) = 360.5,$
$viii) SO(G) = 186.242773,$
$ix) M_1^*(G) = 701,$
$x) M_2^*(G) = 2196,$
$xi) F_N^*(G) = 4807,$
$xii) NH(G) = 2307.25.$

Proof. The desired results are achieved by the results of Theorem 3 and Equations (1)-(3). □

Favipiravir

The molecular graph of Favipiravir is indicated Figure 5 [14].

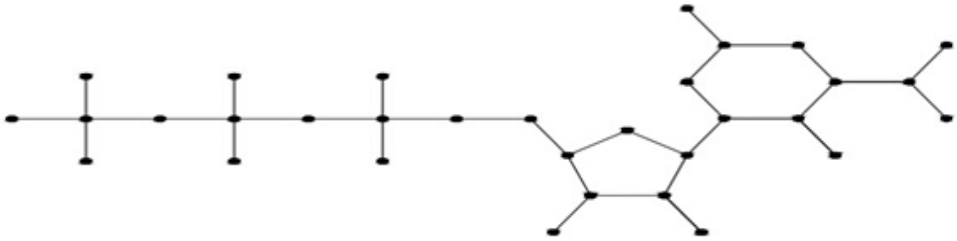


Figure 5: Molecular graph of Favipiravir

Theorem 5. Consider G be a graph structure of Favipiravir. Then, M- polynomial and NM-polynomial of Favipiravir are obtained as the following equation:

$$i) M(G,x,y) = 7xy^4 + 5x^2y^4 + 7x^2y^3 + 6xy^3 + 6x^3y^3 + x^2y^2$$
$$ii) NM(G,x,y) = x^8y^8 + 9x^6y^8 + 2x^5y^8 + x^7y^7 + 2x^6y^7 + x^5y^7 + x^3y^7 + x^6y^6 + 3x^5y^6 + 4x^4y^6 + 2x^3y^6 + 3x^4y^5 + 3x^3y^5$$

Proof.

i) As can be seen in Figure 5, the graph structure of Favipiravir has 32 edges. it is clear that its edge partition of this molecular structure is obtained as follows:

$$e_1 = \{(d_a, d_b) \mid ab \in E(G), d_a = 1, d_b = 4\},\ e_2 = \{(d_a, d_b) \mid ab \in E(G), d_a = 2, d_b = 4\}$$
$$e_3 = \{(d_a, d_b) \mid ab \in E(G), d_a = 2, d_b = 3\},\ e_4 = \{(d_a, d_b) \mid ab \in E(G), d_a = 1, d_b = 3\}$$
$$e_5 = \{(d_a, d_b) \mid ab \in E(G), d_a = 3, d_b = 3\},\ e_6 = \{(d_a, d_b) \mid ab \in E(G), d_a = 2, d_b = 2\}$$

Table 7: Edge type of Favipiravir

Edge type	e_1	e_2	e_3	e_4	e_5	e_6
Number of edges	7	5	7	6	6	1

So, we have:

$$M(G,x,y)=7xy^4+5x^2y^4+7x^2y^3+6xy^3+6x^3y^3+x^2y^2$$

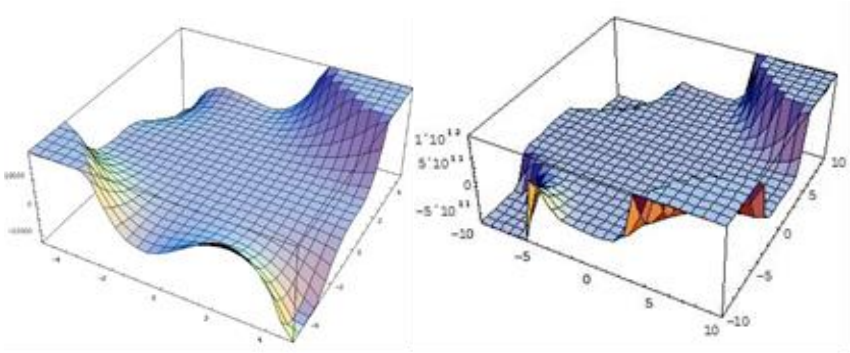
ii) From Table 8, we have:

Table 8: Favipiravir edge type based on neighborhood degree sum of end vertices

Edge type based on NM	e_1^*	e_2^*	e_3^*	e_4^*	e_5^*	e_6^*	e_7^*	e_8^*	e_9^*	e_{10}^*	e_{11}^*	e_{12}^*	e_{13}^*
Number of edges	1	9	2	1	2	1	1	1	3	4	2	3	3

$$NM(G,x,y)=x^8y^8+9x^6y^8+2x^5y^8+x^7y^7+2x^6y^7+x^5y^7+x^3y^7+x^6y^6+3x^5y^6+4x^4y^6+2x^3y^6+3x^4y^5+3x^3y^5.$$

The behaviour of M-polynomial NM-polynomial of Favipiravir is depicted in Figure 6.



(a) (b)

Figure 6: (a) Favipiravir M-polynomial (b) Favipiravir NM-polynomial

Theorem 6. Consider G be the graph structure of Favipiravir. Then,

$i)M_1(G)=164,$

$ii)M_2(G)=186,$

$iii)F(G)=486,$

$iv)H(G)=9.9666,$

$v)SK(G)=82$

$vi)SK_1(G)=93,$

$vii)SK_2(G)=169.5,$

$viii)SO(G)=123.719215,$

$ix)M_1^*(G)=384,$

$x)M_2^*(G)=1128,$

$xi)F_N^*(G)=2384,$

$xii)NH(G)=2.9544.$

Proof. Similar to proof of Theorem 2 the desired results were achieved.

Oseltamivir

In Figure 7, molecular graph of Oseltamivir can be seen [17].

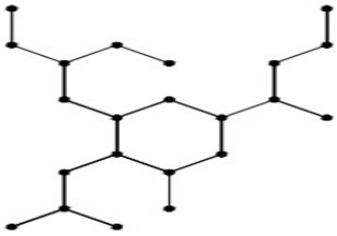


Figure 7: Molecular graph of Oseltamivir

Theorem 7. Suppose G be the graph structure of Oseltamivir. Then, for M- polynomial and NM-polynomial of Oseltamivir, we have:

$$i) M(G,x,y) = 11x^2y^3 + 3xy^2 + 4xy^3 + 3x^3y^3 + x^2y^2,$$

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

Proof.

i) By using Figure 7, the graph structure of Oseltamivir has 22 edges, and the edge partition is as follows:

$e_1 = \{(d_a, d_b) \mid ab \in E(G), d_a = 2, d_b = 3\}$, $e_2 = \{(d_a, d_b) \mid ab \in E(G), d_a = 1, d_b = 2\}$

$e_3 = \{(d_a, d_b) \mid ab \in E(G), d_a = 1, d_b = 3\}$, $e_4 = \{(d_a, d_b) \mid ab \in E(G), d_a = 3, d_b = 3\}$

$e_5 = \{(d_a, d_b) \mid ab \in E(G), d_a = 2, d_b = 2\}$.

Table 9: Edge type of Oseltamivir

Edge type	e_1	e_2	e_3	e_4	e_5
Number of edges	11	3	4	3	1

So, by using Equation (1) we have:

$M(G,x,y) = 11x^2y^3 + 3xy^2 + 4xy^3 + 3x^3y^3 + x^2y^2$ ii) We have:

Table 10: Oseltamivir edge type based on the neighborhood degree sum of end vertices

Edge type based on NM	e_1^*	e_2^*	e_3^*	e_4^*	e_5^*	e_6^*	e_7^*	e_8^*	e_9^*	e_{10}^*	e_{11}^*	e_{12}^*
Number of edges	1	1	1	5	1	2	3	1	2	2	2	1

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

The behaviour of M-polynomial and NM-polynomial of Oseltamivir is displayed in Figure 8. The behaviour of M-polynomial and NM-polynomial of Oseltamivir is displayed in Figure 8

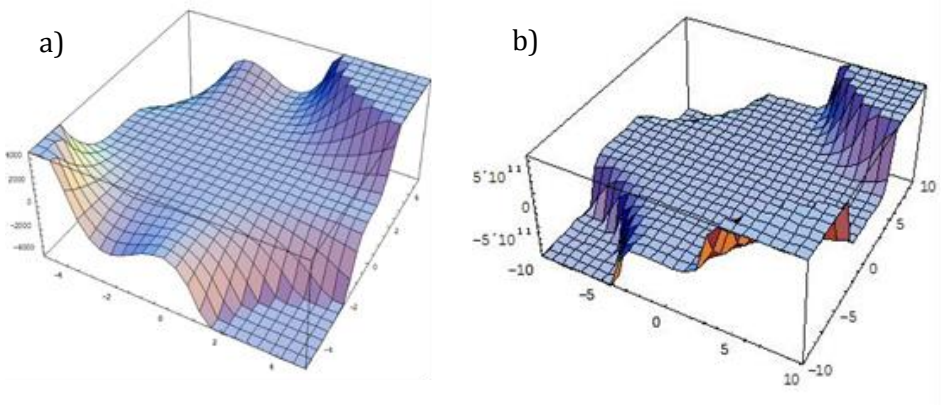


Figure 8: (a) Oseltamivir M-polynomial, (b) Oseltamivir NM-polynomial

Theorem 8. Consider G be the graph structure of Oseltamivir. Then,

$i)M_1(G)=102,$

$ii)M_2(G)=115,$

$iii)F(G)=260,$

$iv)H(G)=4.95,$

$v)SK(G)=51,$

$vi)SK_1(G)=87.5,$

$vii)SK_2(G)=73.7463007,$

$ix)M_1^*(G)=202,$

$x)M_2^*(G)=560,$

$xi)F_N^*(G)=1182,$

$xii)NH(G)=3.93664114.$

Proof. The desired results were achieved by the results of Theorem 7 and Equations 1-3.

Conclusion

In this article, by using degree-based indices, some drug structures were applied for improving the condition of COVID-19 patients. It includes Lopinavir, Azithromycin, Favipiravir, and Oseltamivir. The M-polynomial and the NM-polynomial of those structures were evaluated. In addition, the graphical representations of the results are presented in Figures 2, 4, 6, and 8. Secondly, some effective topological indices were computed. The findings of this study could be helpful in discovering new and more effective drugs and vaccines to battle the coronavirus.

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Authors' contributions

All authors contributed to data analysis, drafting, and revising of the paper and agreed to be responsible for all the aspects of this work.

Conflict of Interest

We have no conflicts of interest to disclose.

ORCID

Setareh Javame
https://orcid.org/0000-0001-5519-2300
Masoud Ghods
https://orcid.org/0000-0002-5006-5107

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