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Research Article

Application of Topological Indices of Tenofovir Chemical Structures for the Cure of HIV/AIDS Patients

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Abstract: Human immune deficiency virus (HIV), a retrovirus, is the main reason for acquired immune deficiency syndrome (AIDS), and one of the prime social and medical problems at the present time. Approximately around 100 million citizens all over the world are suffering from HIV virus and around 50 million citizens are dead. This virus expanded rapidly all over the world. Unfortunately, there is no medicine, drug or vaccine is identified to treat this virus. Scientists have recognised the effectiveness of already existing anti-viral drugs to cure and control the HIV virus. Some of them are Tri-POC Tenofovir Dimer, Tenofovir Disproxil and Tenofovir Alafenamide.Topological indices- mathematical elucidations for a molecule can be created by an algorithm and can be applied to its representation. To generate various biological and physicochemical properties of chemical compounds, topological indices are used. In the current study, by using polynomial approach, for the above mentioned antiviral drugs, certain neighbourhood sum& degree based topological indices have been studied. The outcomes achieved can support the invention of new medicine for the cure of AIDS. In the present study, we establish some topological properties of Tenofovir dimer, Tenofovir disproxil and alafenamide used to inhibit the outbreak of AIDS. We compute some topological indices (general indices (Randic and harmonic), Zagreb index (1^{st}, 2^{nd}, 3^{rd}, second modified, Redefined $3^{rd}$and Augmented), Forgotten index, Systematic division index and Inverse sum indices for these three chemical structures. In Medical Science, topological index calculation defines the topological index related to molecular structure and its corresponding biological, medical, pharmaceutical, and chemical properties of the medicines. From last twenty to thirty years the world is fronting the danger of identifying cure for AIDS. Nearly 10 million people are getting affected with this disease every year. In order to cure this malicious disease antiviral drugs, in form of anti-metabolites, hormones and alkylating agents are used. As per numerous examinations conducted with their chemical structures, it revealed that there is a association between the characteristic features of these anti-viral medicines, drugs and alkane's viz.enthalpy, melting point and boiling point. In this current study, numerous topological indices have been defined on few of the above mentioned drugs so as to assist the scientists to identify the chemical reactions and physical & chemical characteristics and biological activities that are related with them. Hence, the topological indices study on the molecular structure of the medicines, drugs chemical compounds, can constitute for absence of laboratory research which provides a notional origin for the production of chemical materials and drugs. In the present study, we analysed the Tenofovir family chemicals which is extensively used in antiviral medicines and drugs invention. Eleven topological indices are analysed using multi-order polynomials and these results can be used in medicine and pharmaceutical experiments thus paving the new way for new drug invention for AIDS.

Keywords: Tenofovir Dimer, Tenofovir Disproxil, Tenofovir Alafenamide, HIV/AIDS, M-polynomial, Molecular Graph and Topological Index.

1. Introduction

AIDS first diagnosed in Kenya in 1984. It is spreading quickly several countries worldwide. As the 15 April 2020, there were more than 19 lakhs 75 thousand confirmed cases and more than 1 lakh 25 thousand deaths worldwide (as per Wikipedia). The number of AIDS cases and deaths are still on the rise. At present, there is no drug and no vaccine available for the treatment and prevention of AIDS. Therefore there is urgent need to identify effective and safe drug and vaccine to treat this disease. Tenofovir is a medication used to treat HIV. It is taken in combination with other antiretroviral drugs.We considered three antiviral compounds (agents) such as Tenofovir dimer, Tenofovir disproxil and Tenofovir alafenamide. Tenofovir family medicines can be used for HIV cure in patients who are at high risk.

In Medical Science, molecular structure topological indices and the respective pharmaceutical, chemical, medical and biological properties of drugs is studied for topological index calculation .A molecular structure is a graph whose edges relate to the bonds and vertices relate to the atoms. The study of molecular structures is a continuous focus in Chemical Graph Theory, which better understands the molecular structure of a molecule. In 1972 dual degree based topological indices were studied.

Chemical graph theory is a branch of analytical chemistry that deals with the chemical graphs and chemical system. This theory defines topological indices on antiviral medicines. In present research article, Tenofovir family drugs are analysed and certain topological indices are well-defined on many antiviral drugs in order to regulate the chemical reactions and physical characteristics that are related with them based on the degree based calculations,

certain topological indices are well-defined on many antiviral drugs in order to regulate the chemical reactions and physical characteristics that are related with these chemicals. These topological indices are the most vital features to investigate the physical and chemical characteristics of the chosen Tenofovir compound structures. Distance, mixed, Degree, matching and eigen value are the five varied types of the topological indices. Work degree based topological indices are identified on the anticancer medicines. In the chemical compound graph, vertices denoted elements and bonds that join them represent edges. Hence, these anticancer drugs are identified as the chemical compounds that define the before defined topological indices.

In chemistry (theoretical) drugs and medicines are signified as molecular graphs. An atom is represented by vertex and each edge signifies bond between them. These molecular graphs considered are simple graphs with multiple edges and no cycle formation.

In the current technological development era, pharmaceutical and chemical techniques have been quickly developed, there by a great number of crystalline compounds, new medicines, and nano material arise each year. In order to define the chemical properties of these new compounds and drugs will require many chemical experiments, thus increasing the topics to be analysed by the pharmaceutical and chemical researchers. The molecule structure's topological index is a non-empirical numerical quantity that quantifies the structure (molecule) and its diverging arrangement. It means these indices can be considered as a total functions which draws the molecular structure to an actual number and is considered as molecule descriptor underneath analysis.

Zagreb index, PI index, harmonic index, Connectivity and Wiener indices were applied in chemical engineering for analysing the interactions between the molecular structure and the possible physic-chemical properties and characteristics. In chemistry (theoretical)drugs, chemical compounds and medicines are articulated as (molecular) graphs where vertex (molecular structure) and covalent bonds between the two atoms are considered as edges. The used terminologies and notations but not clearly defined can be identified in. To test the properties of drugs and compounds degree based indices introduced and extensively utilised in pharmacy and chemical engineering. Li and Liu analysed the tree structures by applying the first three minimum general Randic indices and described the equivalent external trees. Bollobas and Erdos presented the general Randic index which is defined as $Rk\ (G) = \sum e{=}u\mathrm{V}\ (d\ (u)\ d\ (\mathrm{V}))$ with (u) as the degree of vertex and $k$as real number.Liu and Gutman computed the general Randic index, the ordinary index & modified Zagreb index and their distinctive conditions.

2. Methodology

The present work mainly focuses algebraic polynomials approach on the topological indices of certain antiviral medicine structures to treat HIV/AIDS. The chemical structures of Tenofovir dimer, Tenofovir disproxil and alafenamide are collected. Since hydrogen atom(vertices) make no impact to graph isomorphism, hydrogen suppressed molecular graphs are analysed. Degree counting method, analytical techniques, and graph theoretical software are used to formulate the results. By utilising the separations, NM-polynomial &M-polynomials closed forms are extracted. The three dimensional polynomial surface is plotted using software Maple 2015.Using NM-polynomial and M-polynomial, neighbourhood degree-based and degree sum based indices are calculated with the help of mathematical operators, and Table two. Based on neighbourhood degree and degree sum of end vertices, edge separation forms of hydrogen removed molecular graph of Tenofovir family compounds are created. The results are plotted and compared using MATLAB 2017.

Table 2A.

Topological Index	Resulting from M(G)
1. 1st Zagreb Index (M_1)	$(D_x + D_y)\ (M(G))_{x=y=1}$
2. 2nd Zagreb Index (M_2)	$(D_x.D_y)\ (M(G))_{x=y=1}$
3. Forgotten Index (F)	$(D^2{}_x + D^2{}_y)\ (M(G))_{x=y=1}$
4. 2nd Modified Zagreb Index	$(I_x.I_y)\ (M(G))_{x=y=1}$
5. General Randic Index	$(D^\alpha{}_x D^\alpha{}_y)\ (M(G))_{x=y=1}$
6. Redefined 3rd Zagreb Index($ReZG_3$)	$D_xD_y(D_x + D_y)\ (M(G))_{x=y=1}$
7. Symmetric division index (SDD)	$(D_xI_y + I_xD_y)\ (M(G))_{x=y=1}$
8. Harmonic Index(H)	$2\ I_x\ J\ (M(G))_{x=y=1}$
9. Inverse Sum Index (I)	$I_x\ J\ D_xD_y\ (M(G))_{x=y=1}$
10. Augmented Zagreb Index(A)	$I^3{}_xQ_{-2}JD^3{}_xD^3{}_y(M(G))_{x=y=1}$
11. General Randic Index (RR_α)	$(I^\alpha{}_xI^\alpha{}_y)\ (M(G))_{x=y=1}$

Table 2B.

Topological Index	Resulting from M(G)
1. 1st Zagreb Index (M'_1)	$(D_x + D_y)\ (NM(G))_{x=y=1}$

2. 2nd Zagreb Index (M^*_2)	$(D_x.D_y)\ (NM(G))_{x=y=1}$
3. Forgotten Index (F^*_N)	$(D^2{}_x + D^2{}_y)\ (NM(G))_{x=y=1}$
4. 2nd Modified Zagreb Index ($^{nm}M_2$)	$(I_x.I_y)\ (NM(G))_{x=y=1}$
5. General Randic Index (NR_α)	$(D^\alpha{}_x D^\alpha{}_y)\ (NM(G))_{x=y=1}$
6. Redefined 3rd Zagreb Index(ND_3)	$D_xD_y(D_x + D_y)\ (NM(G))_{x=y=1}$
7. Symmetric division index (ND_5)	$(D_xI_y + I_xD_y)\ (NM(G))_{x=y=1}$
8. Harmonic Index(NH)	$2\ I_x\ J\ (NM(G))_{x=y=1}$
9. Inverse Sum Index (NI)	$I_x\ J\ D_xD_y\ (NM(G))_{x=y=1}$
10. Augmented Zagreb Index(S)	$I^3{}_x Q_{-2} J D^3{}_x D^3{}_y (NM(G))_{x=y=1}$
11. General Randic Index (NRR_α)	$(I^\alpha{}_x I^\alpha{}_y)\ (NM(G))_{x=y=1}$

Where, $D_x\big(M(G)\big) = x\frac{\partial(M(G))}{\partial x}; D_y\big(M(G)\big) = y\frac{\partial(M(G))}{\partial y}; I_x\big(M(G)\big) = \int_0^x \frac{M(t,y)}{t}dt;\ I_y\big(M(G)\big) = \int_0^y \frac{M(x,t)}{t}dt; J\big(M(G)\big) = M(x,x); Q_\alpha\big(M(G)\big) = x^\alpha M(G)$

3. Chemical Structures

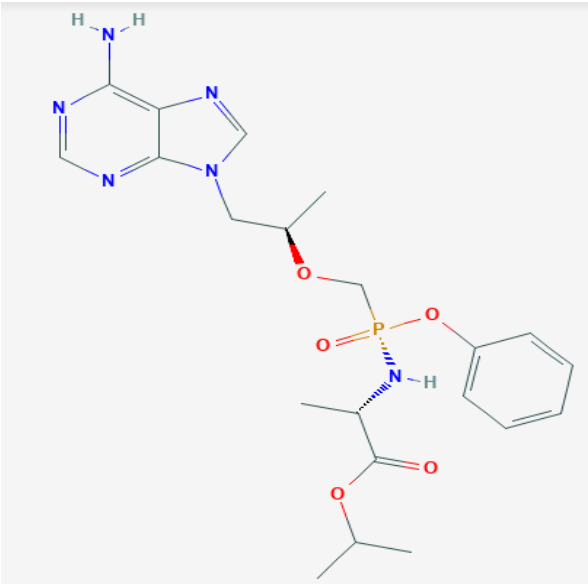


Figure 1. Alafenamide Chemical Structure

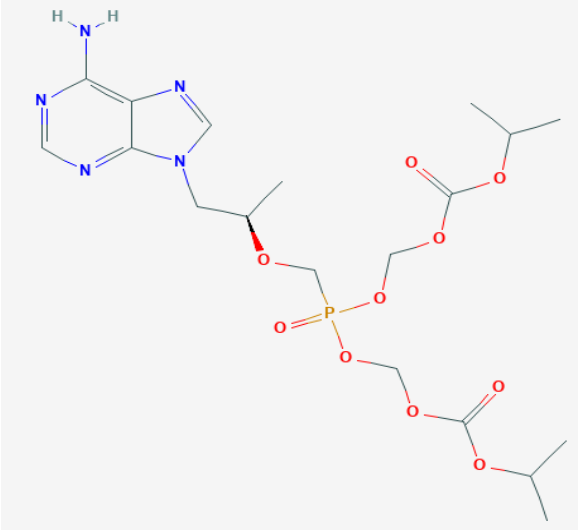


Figure 2. Disoproxil Chemical Structure

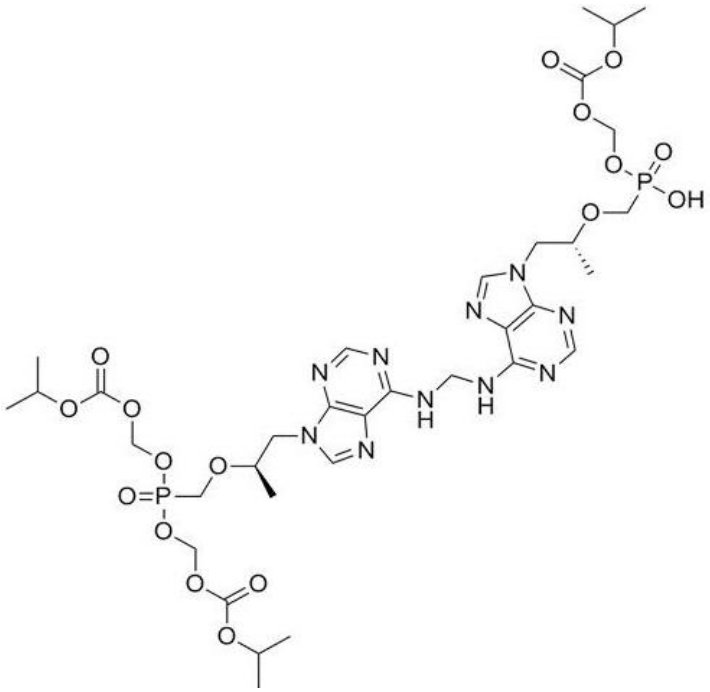


Figure 3. Tri-POC Tenofovir Dimer Chemical structure

4. Computations and Discussions

In this section, main theorems and results are presented. Multiplicative-Polynomial M (G) and Non-Multiplicative-polynomial NM (G) of the molecular graph of Tenofovir alafenamide, Tenofovir disoproxil and Tri-POC Tenofovir dimer in the following theorems.

Theorem 1: Figure 1 is the molecular graph of Tenofovir alafenamide. For this graph we have,

$$M(G) = 6xy^3 + xy^4 + 8x^2y^2 + 13x^2y^3 + 3x^2y^4 + 4x^3y^3$$
$$NM(G) = 2x^3y^4 + x^3y^5 + 3x^3y^6 + 2x^4y^4 + 4x^4y^5 + x^4y^6 + x^4y^7 + 3x^5y^5 + 4x^5y^6 + x^5y^7 + 2x^5y^8 + 2x^6y^6 + 4x^6y^7 + x^6y^8 + 2x^7y^7 + x^7y^8 + x^8y^8$$

Proof: The molecular graph has 35 number of edges. Let $\rho_{(i,j)}$be the number of edges. From the Tenofovir alafenamide molecular structure, $\rho_{(1,3)} = 6, \rho_{(2,3)} = 13, \rho_{(2,2)} = 8, \rho_{(3,3)} = 4, \rho_{(2,4)} = 3,$ and $\rho_{(1,4)} = 1.0$.

The M-polynomial of G can be result anted as

$$M(G) = \sum_{i \le j}^{\cdot} . \rho_{(i,j)} x^i y^j$$
$$= \rho_{(1,3)} xy^3 + \rho_{(1,4)} xy^4 + \rho_{(2,2)} x^2y^2 + \rho_{(2,3)} x^2y^3 + \rho_{(2,4)} x^2y^4 + \rho_{(3,3)} x^3y^3.$$

Substituting the $\rho_{(i,j)}$values,

$$M(G) = 6xy^3 + xy^4 + 8x^2y^2 + 13x^2y^3 + 3x^2y^4 + 4x^3y^3$$

Let P^* be the edges set with neighbourhood degree sum of end vertices (i, j) and $\rho^*_{(I,j)}$ be the number of edges in$P^*_{(I,j)}$. From the Tenofovir alafenamide molecular structure, it can be observed that, $\rho^*_{(3,6)} = 3, \rho^*_{(3,5)} = 1, \rho^*_{(3,4)} = 2, \rho^*_{(5,5)} = 3, \rho^*_{(5,8)} = 2, \rho^*_{(5,7)} = 1, \rho^*_{(6,7)} = 4, \rho^*_{(6,5)} = 4, \rho^*_{(6,6)} = 2, \rho^*_{6,4)} = 1, \rho^*_{(4,5)} = 4, \rho^*_{(4,4)} = 2, \rho^*_{(8,8)} = 1, \rho^*_{(8,7)} = 1, \rho^*_{(6,8)} = 1, \rho^*_{(7,7)} = 2, \rho^*_{(4,7)} = 1.$

From second equation, NM-Polynomial can be derived as below:

$$\mathrm{NM(G)} = \sum_{i\le j}^{\cdot} .\rho^{*}_{(i,j)} x^i y^j$$
$$= \rho^{*}_{(3,4)}x^3y^4 + \rho^{*}_{(3,5)}x^3y^5 + \rho^{*}_{(3,6)}x^3y^6 + \rho^{*}_{(4,4)}x^4y^4 + \rho^{*}_{(4,5)}x^4y^5 + \rho^{*}_{(4,6)}x^4y^6$$
$$+ \rho^{*}_{(4,7)}x^4y^7 + \rho^{*}_{(5,5)}x^5y^5 + \rho^{*}_{(5,6)}x^5y^6 + \rho^{*}_{(5,7)}x^5y^7 + \rho^{*}_{(5,8)}x^5y^8 + \rho^{*}_{(6,6)}x^6y^6$$
$$+ \rho^{*}_{(6,7)}x^6y^7 + \rho^{*}_{(6,8)}x^6y^8 + \rho^{*}_{(7,7)}x^7y^7 + \rho^{*}_{(7,8)}x^7y^8 + \rho^{*}_{(8,8)}x^8y^8.$$

After substituting the $\rho^{*}_{(i,j)}$ values,

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

From the above polynomials, we can compute some-degree based and neighbourhood degree some based topological indices of the Tenofovir alafenamide molecular structure in the following theorems.

Theorem 2: Figure 1 is the molecular graph of Tenofovir alafenamide. For this graph we have,

1. $\mathrm{M_1(G)} = 168, \mathrm{M_1}^{1}(\mathrm{G}) = 383,$
2. $\mathrm{M_2(G)} = 192, \mathrm{M_2}^{*}(\mathrm{G}) = 1073,$
3. $\mathrm{F(G)} = 442, \mathrm{F_N}^{*}(\mathrm{G}) = 2231,$
4. $^{\mathrm{m}}\mathrm{M_2(G)} = 7.236, {}^{\mathrm{nm}}\mathrm{M_2(G)} = 1.38,$
5. $R_\alpha(\mathrm{G}) = 4(9)^\alpha + 3(8)^\alpha + 13(6)^\alpha + 8(4)^\alpha + (4)^\alpha + 6(3)^\alpha,$ $\mathrm{NR}_\alpha(\mathrm{G}) = (64)^\alpha + (56)^\alpha + 2(49)^\alpha + (48)^\alpha + 4(42)^\alpha + 2(36)^\alpha$
$+ 2(40)^\alpha + (35)^\alpha + 4(30)^\alpha + 3(25)^\alpha + (28)^\alpha + (24)^\alpha$
$+ 4(20)^\alpha + 2(16)^\alpha + 3(18)^\alpha + (15)^\alpha + 2(12)^\alpha,$
6. $ReZG_3(G) = 970, ND_3(G) = 12784,$
7. $SDD(G) = 83.92, ND_5(G) = 73.52,$
8. $H(G) = 14.93, NH(G) = 6.69,$
9. $I(G) = 38.9, NI(G) = 93.7,11.$
10. $A(G) = 260.182, S(G) = 1352.96,$
11. $\mathrm{RR}_\alpha\mathrm{M(G)} = (\frac{4}{9^\alpha} + \frac{3}{8^\alpha} + \frac{13}{6^\alpha} + \frac{8}{4^\alpha} + \frac{1}{4^\alpha} + \frac{6}{3^\alpha})$, $\mathrm{NRR}_\alpha(\mathrm{NM(G)} = \frac{1}{(64)^\alpha} + \frac{1}{(56)^\alpha} + \frac{2}{(49)^\alpha} + \frac{3}{(18)^\alpha} + \frac{1}{(15)^\alpha} + \frac{2}{(12)^\alpha} + \frac{1}{(48)^\alpha} + \frac{4}{(42)^\alpha} + \frac{2}{(36)^\alpha} + \frac{1}{(28)^\alpha} + \frac{1}{(24)^\alpha} + \frac{4}{(20)^\alpha} + \frac{2}{(16)^\alpha} + \frac{2}{(40)^\alpha} + \frac{1}{(35)^\alpha} + \frac{4}{(30)^\alpha} + \frac{3}{(25)^\alpha}.$

Proof: Initially we will calculate the degree-based indices.

Let $M(G) = 6xy^3 + xy^4 + 8x^2y^2 + 13x^2y^3 + 3x^2y^4 + 4x^3y^3$. From this,

$(D_x + D_y)\mathrm{M(G)} = xy^2(24x^2y + 18xy^2 + 65xy + 32x + 5y^2 + 24y),$
$D_xD_yM(G) = 2xy^2(18x^2y + 12xy^2 + 39xy + 16x + 2y^2 + 9y),$
$\left(D_x{}^2 + D_y{}^2\right)M(G) = xy^2(72x^2y + 60xy^2 + 169xy + 64x + 17y^2 + 60y),$
$\left(\mathrm{I}_x I_y\right)M(G) = \frac{4}{9}x^3y^3 + x^2\left(\frac{3}{8}y^4 + \frac{13}{6}y^3 + 2y^2\right) + x\left(\frac{1}{4}y^4 + 2y^3\right),$
$D_xD_y\left(D_x + D_y\right)M(G) = 2xy^2(108x^2y + 72xy^2 + 195xy + 64x + 10y^2 + 36y),$
$\left(D_xI_y + \mathrm{I}_xD_y\right)M(G) = \frac{1}{12}[xy^2(96x^2y + 90xy^2 + 338xy + 192x + 51y^2 + 240y)],$
$D_x{}^{\alpha}D_y{}^{\alpha}M(G) = 4(9^\alpha)x^3y^3 + 3(8^\alpha)x^2y^4 + 13(6^\alpha)x^2y^3 + 8(4^\alpha)x^2y^2 + (4^\alpha)xy^4 + 6(3^\alpha)xy^3,$
$2\mathrm{I}_xJ\left(M(G)\right) = \frac{7}{15}x^4(5x^2 + 12x + 15)$
$\mathrm{I}_xJD_xD_yM(G) = \frac{1}{10}x^4(100x^2 + 64x + 125)$
$I_x{}^3Q_{-2}JD_x{}^3D_y{}^3M(G) = \frac{x^2(30051x^2 + 45952x + 36396)}{432}$

From Table no 2A and 2B,

$\mathrm{M_1(G)} = xy^2(24x^2y + 18xy^2 + 65xy + 32x + 5y^2 + 24y)_{x=y=1} = 168.$
$\mathrm{M_2(G)} = [2xy^2(18x^2y + 12xy^2 + 39xy + 16x + 2y^2 + 9y)]_{\mathrm{x=y=1}} = 192$

$$F(G) = [xy^2(72x^2y + 60xy^2 + 169xy + 64x + 17y^2 + 60y)]_{x=y=1} = 442.$$

$$^{n}M_2(G) = [\frac{4}{9}x^3y^3 + x^2(\frac{3}{8}y^4 + \frac{13}{6}y^3 + 2y^2) + x(\frac{1}{4}y^4 + 2y^3)]_{x=y=}1 = 7.236$$

$$ReZG_3(G) = [2xy^2(108x^2y + 72xy^2 + 195xy + 64x + 10y^2 + 36y)]_{x=y=1} = 970$$

$$SDD(G) = [\frac{1}{12}[xy^2(108x^2y + 72xy^2 + 195xy + 64x + 10y^2 + 36y)]]_{x=y=1} = 83.91.$$

$$H(G) = [\frac{7}{15}x^4(5x^2 + 12x + 15)]_{x=y=1} = 14.93.$$

$$I(G) = [\frac{1}{10}x^4(100x^2 + 64x + 125)]_{x=y=1} = 38.9$$

$$A(G) = [\frac{x^2(30051x^2 + 45952x + 36396)}{432}]_{x=y=1} = 260.18$$

$$RR_\alpha M(G) = (\frac{4}{9^\alpha}x^3y^3 + \frac{3}{8^\alpha}x^2y^4 + \frac{13}{6^\alpha}x^2y^3 + \frac{8}{4^\alpha}x^2y^2 + \frac{1}{4^\alpha}xy^4 + \frac{6}{3^\alpha}xy^3)_{x=y=1}$$
$$= (\frac{4}{9^\alpha} + \frac{3}{8^\alpha} + \frac{13}{6^\alpha} + \frac{8}{4^\alpha} + \frac{1}{4^\alpha} + \frac{6}{3^\alpha})$$

For neighbourhood indices degree sum-based indices, we consider $NM(G) = 2x^3y^4 + x^3y^5 + 3x^3y^6 + 2x^4y^4 + 4x^4y^5 + x^4y^6 + x^4y^7 + 3x^5y^5 + 4x^5y^6 + x^5y^7 + 2x^5y^8 + 2x^6y^6 + 4x^6y^7 + x^6y^8 + 2x^7y^7 + x^7y^8 + x^8y^8$. Later, applying the above operations and table 2A and 2B values, one can easily obtain the neighbourhood degree sum-based indices. This completes the proof.

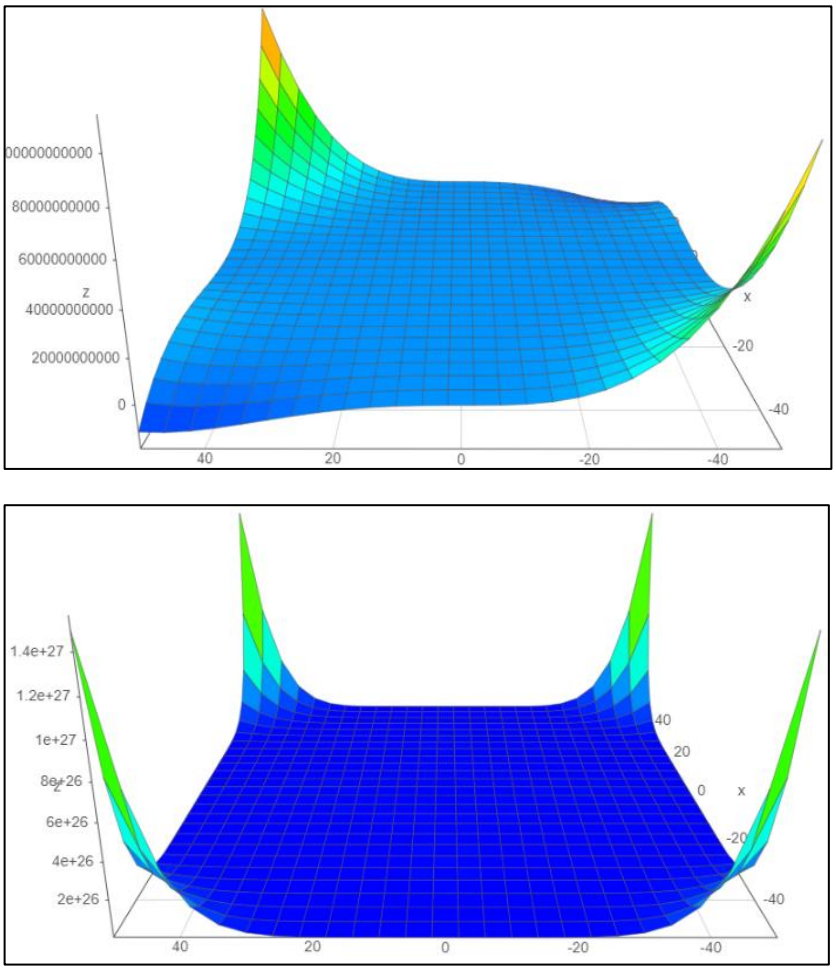


Figure 4. M-Polynomial (a) & NM-polynomial (b) of Tenofovir alafenamide.

Theorem 3: Figure 2 is the molecular graph of Tenofovir disoproxil. For this graph we have,

$$M(G) = 8xy^3 + xy^4 + 8x^2y^2 + 13x^2y^3 + 3x^2y^4 + 3x^3y^3$$
$$NM(G) = 3x^3y^4 + 4x^3y^5 + x^3y^6 + 4x^4y^5 + x^4y^7 + 4x^5y^5 + 5x^5y^6 + 3x^5y^7 + 4x^6y^7 + 2x^6y^9 + x^7y^9 + 4x^4y^6$$

Proof: The molecular graph has 35 number of edges. Let $\rho_{(i,j)}$be the number of edges. From the Tenofovir disoproxil molecular structure, $\rho_{(1,3)} = 8, \rho_{(2,3)} = 13, \rho_{(2,2)} = 8, \rho_{(3,3)} = 3, \rho_{(2,4)} = 3,$ and $\rho_{(1,4)} = 1.$

The M-polynomial of G can be result anted as

$$M(G) = \sum_{i \le j} . \rho_{(i,j)} x^i y^j$$
$$= \rho_{(1,3)} xy^3 + \rho_{(1,4)} xy^4 + \rho_{(2,2)} x^2 y^2$$
$$+ \rho_{(2,3)} x^2 y^3 + \rho_{(2,4)} x^2 y^4 + \rho_{(3,3)} x^3 y^3.$$

Substituting the $\rho_{(i,j)}$values,

$$M(G) = 8xy^3 + xy^4 + 8x^2y^2 + 13x^2y^3 + 3x^2y^4 + 3x^3y^3$$

Let P^* be the set of all edges with neighbourhood degree sum of end vertices i, j. Let $\rho^*_{(I,j)}$ be the number of edges in $P^*_{(I,j)}$. From the Tenofovir disoproxil molecular structure, it can be observed that, $\rho^*_{(3,4)} = 3, \rho^*_{(3,5)} = 4, \rho^*_{(3,6)} = 1, \rho^*_{(4,5)} = 4, \rho^*_{(4,6)} = 4, \rho^*_{(4,7)} = 1, \rho^*_{(5,5)} = 4, \rho^*_{(5,6)} = 5, \rho^*_{(5,7)} = 3, \rho^*_{(6,7)} = 4, \rho^*_{(6,9)} = 2, \rho^*_{(7,9)} = 1,$

From second equation, NM-Polynomial can be derived as below:

$$NM(G) = \sum_{i \le j} . \rho^*_{(i,j)} x^i y^j$$
$$= \rho^*_{(3,4)} x^3 y^4 + \rho^*_{(3,5)} x^3 y^5 + \rho^*_{(3,6)} x^3 y^6 + \rho^*_{(4,5)} x^4 y^5 + \rho^*_{(4,6)} x^4 y^6 + \rho^*_{(4,7)} x^4 y^7$$
$$+ \rho^*_{(5,5)} x^5 y^5 + \rho_{(5,6)} x^5 y^6 + \rho_{(5,7)} x^5 y^7 + \rho^*_{(6,7)} x^6 y^7 + \rho^*_{(6,9)} x^6 y^9 + \rho^*_{(7,9)} x^7 y^9.$$

After substituting the $\rho^*_{(i,j)}$ values,

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

From the above polynomials, we can compute some-degree based and neighbourhood degree some based topological indices of the Tenofovir disoproxil molecular structure in the following theorems.

Theorem 4: Let G be the molecular graph of Tenofovir disoproxil. For this graph we have,

1. $M_1(G) = 170, {M_1}^1(G) = 378,$
2. $M_2(G) = 189,\ {M_2}^*(G) = 1012,$
3. $F(G) = 444,\ {F_N}^*(G) = 2124,$
4. ${}^{m}M_2(G) = 7.78,\ {}^{nm}M_2(G) = 1.535,$
5. $R_\alpha(G) = 3(9)^\alpha + 3(8)^\alpha + 13(6)^\alpha + 8(4)^\alpha + (4)^\alpha + 8(3)^\alpha;\ NR_\alpha(G) = (63)^\alpha + 2(54)^\alpha + 4(42)^\alpha + 3(35)^\alpha + 5(30)^\alpha + 4(25)^\alpha + (28)^\alpha + 4(24)^\alpha + 4(20)^\alpha + (18)^\alpha + 4(15)^\alpha + 3(12)^\alpha,$
6. $ReZG_3(G) = 940, ND_3(G) = 11604,$
7. $SDD(G) = 88.58, ND_5(G) = 76,$
8. $H(G) = 15.6, NH(G) = 7.166,$
9. $I(G) = 38.9, NI(G) = 92.124,$
10. $A(G) = 255.54, S(G) = 1245.38,$
11. $RR_\alpha M(G) = (\frac{3}{9^\alpha} + \frac{3}{8^\alpha} + \frac{13}{6^\alpha} + \frac{8}{4^\alpha} + \frac{1}{4^\alpha} + \frac{8}{3^\alpha});\quad NRR_\alpha(NM(G)) = \frac{1}{(63)^\alpha} + \frac{1}{(18)^\alpha} + \frac{4}{(15)^\alpha} + \frac{3}{(12)^\alpha} + \frac{1}{(28)^\alpha} + \frac{4}{(24)^\alpha} + \frac{4}{(20)^\alpha} + \frac{3}{(25)^\alpha} + \frac{5}{(30)^\alpha} + \frac{4}{(25)^\alpha} + \frac{2}{(54)^\alpha} + \frac{4}{(42)^\alpha}$

Proof: Initially we will calculate the degree-based indices.

Let $M(G) = 8xy^3 + xy^4 + 8x^2y^2 + 13x^2y^3 + 3x^2y^4 + 3x^3y^3.$

From this,

$(D_x + D_y)\mathrm{M(G)} = xy^2(18x^2y + 18xy^2 + 65xy + 32x + 5y^2 + 24y)$,

$D_xD_yM(G) = xy^2(27x^2y + 24xy^2 + 78xy + 32x + 4y^2 + 24y)$,

$\left(D_x{}^2 + D_y{}^2\right)M(G) = xy^2(54x^2y + 60xy^2 + 169xy + 64x + 17y^2 + 80y)$,

$\left(\mathrm{I}_x I_y\right)M(G) = \frac{1}{9}x^3y^3 + x^2\left(\frac{3}{8}y^4 + \frac{13}{6}y^3 + 2y^2\right) + x\left(\frac{1}{4}y^4 + \frac{8}{3}y^3\right)$,

$D_xD_y\left(D_x + D_y\right)M(G) = 2xy^2(81x^2y + 72xy^2 + 195xy + 64x + 10y^2 + 48y)$,

$\left(D_xI_y + \mathrm{I}_xD_y\right)M(G) = \frac{1}{12}[xy^2(72x^2y + 90xy^2 + 338xy + 192x + 51y^2 + 320y)]$,

$D_x{}^{\alpha}D_y{}^{\alpha}M(G) = 3(9^{\alpha})x^3y^3 + 3(8^{\alpha})x^2y^4 + 13(6^{\alpha})x^2y^3 + 8(4^{\alpha})x^2y^2 + (4^{\alpha})xy^4 + 8(3^{\alpha})xy^3$,

$2\mathrm{I}_xJ\left(M(G)\right) = 2x^4\left(x^2 + \frac{14}{5}x + 4\right)$

$\mathrm{I}_xJD_xD_yM(G) = \frac{1}{10}x^4(85x^2 + 164x + 140)$

$I_x{}^3Q_{-2}JD_x{}^3D_y{}^3M(G) = x^2[\frac{3723}{64}x^2 + \frac{2872}{27}x + 91]$

$I_x{}^{\alpha}I_y{}^{\alpha}M(G) = \frac{3}{9^{\alpha}}x^3y^3 + \frac{3}{8^{\alpha}}x^2y^4 + \frac{13}{6^{\alpha}}x^2y^3 + \frac{8}{4^{\alpha}}x^2y^2 + \frac{1}{4^{\alpha}}xy^4 + \frac{8}{3^{\alpha}}xy^3$

From Table no 2A and 2B,

$\mathrm{M}_1(\mathrm{G}) = xy^2(18x^2y + 18xy^2 + 65xy + 32x + 5y^2 + 32y)_{x=y=1} = 170.$

$\mathrm{M}_2(\mathrm{G}) = [xy^2(27x^2y + 24xy^2 + 78xy + 32x + 24 + 24y)]_{\mathrm{x=y=1}} = 189$

$\mathrm{F(G)} = [xy^2(54y + 60xy^2 + 169xy + 64x + 17y^2 + 80y)]_{\mathrm{x=y=1}} = 444.$

${}^{\mathrm{n}}\mathrm{M}_2(\mathrm{G}) = [\frac{1}{3}x^3y^3 + x^2(\frac{3}{8}y^4 + \frac{13}{6}y^3 + 2y^2) + x(\frac{1}{4}y^4 + \frac{8}{3}y^3)]_{\mathrm{x=y=}}1 = 7.79$

$\mathrm{ReZG}_3(\mathrm{G}) = [2xy^2(81x^2y + 72xy^2 + 195xy + 64x + 10y^2 + 48y)]_{\mathrm{x=y=1}} = 940$

$\mathrm{SDD(G)} = [\frac{1}{12}[xy^2(72x^2y + 90xy^2 + 338xy + 192x + 51y^2 + 320y)]]_{\mathrm{x=y=1}} = 88.58.$

$\mathrm{H(G)} = [2x^4(x^2 + \frac{14}{5}x + 4)]_{\mathrm{x=y=1}} = 15.6.$

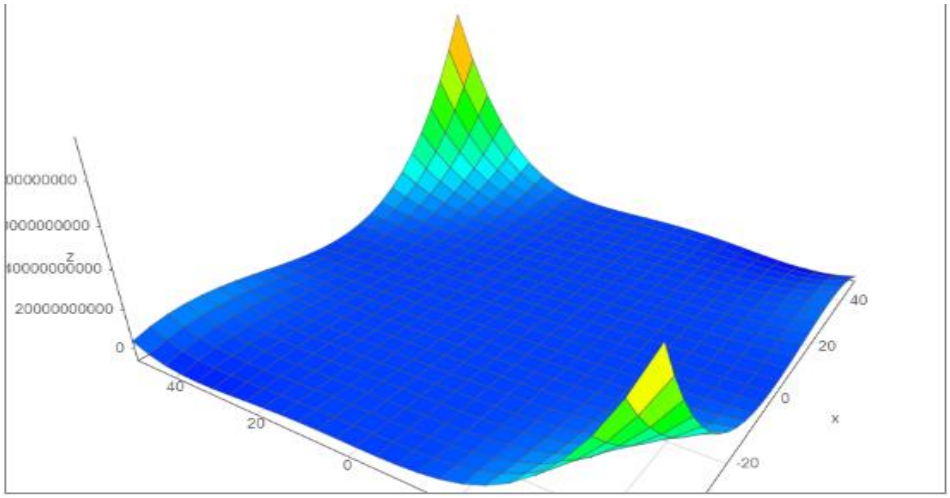
$\mathrm{I(G)} = [\frac{1}{10}x^4(85x^2 + 164x + 140)]_{\mathrm{x=y=1}} = 38.9$

$\mathrm{A(G)} = [\frac{x^2(100521x^2 + 183808x + 157248)}{1728}]_{\mathrm{x=y=1}} = 255.54$

$\mathrm{RR}_{\alpha}\mathrm{M(G)} = (\frac{3}{9^{\alpha}}x^3y^3 + \frac{3}{8^{\alpha}}x^2y^4 + \frac{13}{6^{\alpha}}x^2y^3 + \frac{8}{4^{\alpha}}x^2y^2 + \frac{1}{4^{\alpha}}xy^4 + \frac{8}{3^{\alpha}}xy^3)_{\mathrm{x=y=1}}$

$= (\frac{3}{9^{\alpha}} + \frac{3}{8^{\alpha}} + \frac{13}{6^{\alpha}} + \frac{8}{4^{\alpha}} + \frac{1}{4^{\alpha}} + \frac{8}{3^{\alpha}})$

For neighbourhood indices degree sum-based indices, we consider $NM(G) = 3x^3y^4 + 4x^3y^5 + x^3y^6 + 4x^4y^5 + 4x^4y^6$. Later, applying the above operations and table 2 values, one can easily obtain the neighbourhood degree sum-based indices. This completes the proof.



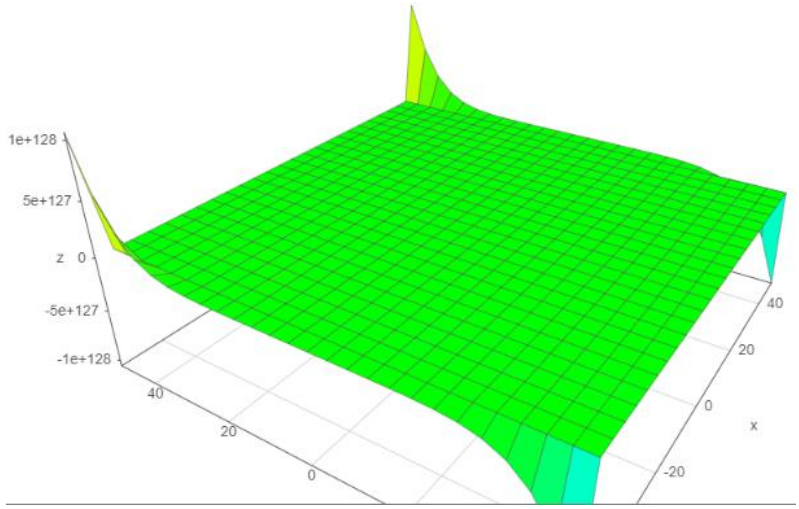


Figure 5. M-Polynomial (a) & NM-polynomial (b) of Tenofovir disoproxil

Theorem 5: Let G be the molecular graph of Tri-Poc Tenofovir dimer. For this graph we have,

$$M(G) = 11xy^3 + 3xy^4 + 15x^2y^2 + 27x^2y^3 + 5x^2y^4 + 5x^3y^3$$
$$NM(G) = 5x^3y^5 + 6x^3y^4 + x^4y^4 + 7x^4y^5 + 8x^4y^6 + x^4y^7 + 7x^5y^5 + 7x^5y^6 + 6x^5y^7 + 2x^5y^8 + 5x^6y^6 + 5x^6y^7 + x^6y^8 + 4x^7y^8 + x^8y^8$$

Proof: Let G be the molecular graph and has 66 number of edges. Let $P_{(i,j)}$ be the set of edges with degree of end vertices i,j. Let $\rho_{(i,j)}$be the number of edges in $P_{(i,j)}$. From the Tenofovir dimer molecular structure, it can be observed that $\rho_{(1,3)} = 11, \rho_{(2,2)} = 15, \rho_{(2,3)} = 27, \rho_{(3,3)} = 5, \rho_{(2,4)} = 5,$ and $\rho_{(1,4)} = 3.$ Let P^* be the set of all edges with neighbourhood degree sum of end vertices i, j. Let $\rho^*_{(I,j)}$ be the number of edges in $P^*_{(I,j)}$. From the Tri-Poc tenofovir dimer molecular structure, it can be observed that,

$$\rho^*_{(3,5)} = 5, \rho^*_{(4,3)} = 6, \rho^*_{(4,4)} = 1, \rho^*_{(4,5)} = 7, \rho^*_{(4,6)} = 8, \rho^*_{(4,7)} = 1, \rho^*_{(5,5)} = 7, \rho^*_{(5,6)} = 7, \rho^*_{(5,7)} = 6, \rho^*_{(5,8)} = 2, \rho^*_{(6,6)} = 5, \rho^*_{(6,8)} = 1, \rho^*_{(6,7)} = 5, \rho^*_{(7,8)} = 4, \rho^*_{(8,8)} = 1.$$

From second equation, NM-Polynomial can be derived as below:

$$\mathrm{NM(G)} = \sum_{i \le j} . \rho^*_{(i,j)} x^i y^j$$
$$= \rho^*_{(3,5)} x^3y^5 + \rho^*_{(3,4)} x^3y^4 + \rho^*_{(4,4)} x^4y^4 + \rho^*_{(4,5)} x^4y^5 + \rho^*_{(4,6)} x^4y^6 + \rho^*_{(4,7)} x^4y^7 + \rho^*_{(5,5)} x^5y^5 + \rho_{(5,6)} x^5y^6 + \rho_{(5,7)} x^5y^7 + \rho^*_{(5,8)} x^5y^8 + \rho^*_{(6,6)} x^6y^6 + \rho^*_{(6,7)} x^6y^7 + \rho^*_{(6,8)} x^6y^8 + \rho^*_{(7,8)} x^7y^8 + \rho^*_{(8,8)} x^8y^8$$

After substituting the $\rho^*_{(i,j)}$ values,

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

From the above polynomials, we can compute some-degree based and neighbourhood degree some based topological indices of the Tri-Poc Tenofovir dimer molecular structure in the following theorems.

Theorem 6: Let G be the molecular graph of Tri-Poc Tenofovir dimer. For this graph we have,

1. $\mathrm{M_1(G)} = 314, \mathrm{M_1}^1\mathrm{(G)} = 704,$
2. $\mathrm{M_2(G)} = 352, \mathrm{M_2}^*\mathrm{(G)} = 1924,$
3. $\mathrm{F(G)} = 822, \mathrm{F_N}^*\mathrm{(G)} = 3984,$
4. ${}^{\mathrm{m}}\mathrm{M_2(G)} = 13.84, {}^{\mathrm{nm}}\mathrm{M_2(G)} = 2.715,$
5. $R_\alpha(\mathrm{G}) = 5(9)^\alpha + 5(8)^\alpha + 27(6)^\alpha + 15(4)^\alpha + 3(4)^\alpha + 11(3)^\alpha;$ $NR_\alpha(\mathrm{G}) = (64)^\alpha + 4(56)^\alpha + (48)^\alpha + 5(42)^\alpha + 5(36)^\alpha + 2(40)^\alpha$

$+6\,(35)^{\alpha}+7(30)^{\alpha}+7(25)^{\alpha}+(28)^{\alpha}+8(24)^{\alpha}+7(20)^{\alpha}+(16)^{\alpha}+5(15)^{\alpha}+6(12)^{\alpha}$

6. $ReZG_3(G)=1752, ND_3(G)=22286,$
7. $SDD(G)=160.416, ND_5(G)=137.48,$
8. $H(G)=28.33, NH(G)=12.9358,$
9. $I(G)=72.2, NI(G)=172.73,$
10. $A(G)=477.189, S(G)=2406.57.$

. $\mathrm{RR}_{\alpha}\big(\mathrm{M(G)}\big)=\frac{5}{9^{\alpha}}+\frac{5}{8^{\alpha}}+\frac{27}{6^{\alpha}}+\frac{15}{4^{\alpha}}+\frac{3}{4^{\alpha}}+\frac{11}{3^{\alpha}}$; $\mathrm{NRR}_{\alpha}(\mathrm{G})=\frac{4}{(56)^{\alpha}}+\frac{1}{(64)^{\alpha}}+\frac{5}{(15)^{\alpha}}+\frac{6}{(12)^{\alpha}}+\frac{1}{(48)^{\alpha}}+\frac{5}{(42)^{\alpha}}+\frac{5}{(36)^{\alpha}}+\frac{1}{(28)^{\alpha}}+\frac{8}{(24)^{\alpha}}+\frac{7}{(20)^{\alpha}}+\frac{1}{(16)^{\alpha}}+\frac{2}{(40)^{\alpha}}+\frac{6}{(35)^{\alpha}}+\frac{7}{(30)^{\alpha}}+\frac{7}{(25)^{\alpha}}$.

Proof: Initially we will calculate the degree-based indices.

Let$M(G)=11xy^3+3xy^4+15x^2y^2+27x^2y^3+5x^2y^4+5x^3y^3$. From this,

$(D_x+D_y)\mathrm{M(G)}=xy^2(30x^2y+30xy^2+135xy+60x+15y^2+44y),$

$D_xD_yM(G)=xy^2(45x^2y+40xy^2+162xy+60x+12y^2+33y),$

$\big({D_x}^2+{D_y}^2\big)M(G)=xy^2(90x^2y+100xy^2+351xy+120x+51y^2+110y),$

$\big(\mathrm{I}_x I_y\big)M(G)=\frac{5}{9}x^3y^3+x^2\left(\frac{5}{8}y^4+\frac{9}{2}y^3+\frac{15}{4}y^2\right)+x\left(\frac{3}{4}y^4+\frac{11}{3}y^3\right),$

$D_xD_y\big(D_x+D_y\big)M(G)=6xy^2(45x^2y+40xy^2+135xy+40x+10y^2+22y),$

$\big(D_xI_y+\mathrm{I}_xD_y\big)M(G)=\frac{1}{12}[xy^2(120x^2y+150xy^2+702xy+360x+153y^2+440y)],$

${D_x}^{\alpha}{D_y}^{\alpha}M(G)=5(9^{\alpha})x^3y^3+5(8^{\alpha})x^2y^4+27(6^{\alpha})x^2y^3+15(4^{\alpha})x^2y^2+3(4^{\alpha})xy^4+11(3^{\alpha})xy^3,$

$2\mathrm{I}_xJ\big(M(G)\big)=\frac{1}{3}x^4(10x^2+36x+39)$

$\mathrm{I}_xJD_xD_yM(G)=\frac{1}{60}x^4(850x^2+2088x+1395)$

${I_x}^3Q_{-2}J{D_x}^3{D_y}^3M(G)=\frac{1}{576}x^2[55845x^2+128512x+90504]$

${I_x}^{\alpha}{I_y}^{\alpha}M(G)=\frac{5}{9^{\alpha}}x^3y^3+\frac{5}{8^{\alpha}}x^2y^4+\frac{27}{6^{\alpha}}x^2y^3+\frac{15}{4^{\alpha}}x^2y^2+\frac{3}{4^{\alpha}}xy^4+\frac{11}{3^{\alpha}}xy^3$

From Table no 2A and 2B,

$\mathrm{M}_1(\mathrm{G})=xy^2(30x^2y+30xy^2+135xy+60x+15y^2+44y)_{x=y=1}=314.$

$\mathrm{M}_2(\mathrm{G})=[xy^2(45x^2y+40xy^2+162xy+60x+12y^2+33y)]_{\mathrm{x=y=1}}=352$

$\mathrm{F(G)}=[xy^2(90x^2y+100xy^2+351xy+120x+51y^2+110y)]_{\mathrm{x=y=1}}=822.$

${}^{n}\mathrm{M}_2(\mathrm{G})=[\frac{5}{9}x^3y^3+x^2(\frac{5}{8}y^4+\frac{9}{2}y^3+\frac{15}{4}y^2)+x(\frac{3}{4}y^4+\frac{11}{3}y^3)]_{\mathrm{x=y=1}}=13.84$

$R_{\alpha}(G)=[5(9)^{\alpha}x^3y^3+5(8)^{\alpha}x^2y^4+27(6)^{\alpha}x^2y^3+15(4)^{\alpha}x^2y^2+3(4)^{\alpha}xy^4+11(3)^{\alpha}\mathrm{xy}^3]_{x=y=1}$

$=5(9)^{\alpha}+5(8)^{\alpha}+27(6)^{\alpha}+15(4)^{\alpha}+3(4)^{\alpha}+11(3)^{\alpha}$

$\mathrm{ReZG_3(G)}=[6xy^2(45x^2y+40xy^2+135xy+40x+10y^2+22y)]_{\mathrm{x=y=1}}=1752$

$\mathrm{SDD(G)}=[\frac{1}{12}[xy^2(120x^2y+150xy^2+702xy+360x+153y^2+440y)]]_{\mathrm{x=y=1}}=160.41$

$\mathrm{H(G)}=[\frac{1}{3}x^4(10x^2+36x+39)]_{\mathrm{x=y=1}}=28.33.$

$\mathrm{I(G)}=[\frac{1}{60}x^4(850x^2+2088x+1395)]_{\mathrm{x=y=1}}=72.21$

$\mathrm{A(G)}=[\frac{x^2(55845x^2+128512x+90504)}{576}]_{\mathrm{x=y=1}}=477.189$

$\mathrm{RR}_{\alpha}\big(\mathrm{M(G)}\big)=[\Big(\frac{5}{9^{\alpha}}x^3y^3+\frac{5}{8^{\alpha}}x^2y^4+\frac{27}{6^{\alpha}}x^2y^3+\frac{15}{4^{\alpha}}x^2y^2+\frac{3}{4^{\alpha}}xy^4+\frac{11}{3^{\alpha}}xy^3\Big)]_{\mathrm{x=y=1}}$

$=\frac{5}{9^{\alpha}}+\frac{5}{8^{\alpha}}+\frac{27}{6^{\alpha}}+\frac{15}{4^{\alpha}}+\frac{3}{4^{\alpha}}+\frac{11}{3^{\alpha}}$

For neighbourhood indices degree sum-based indices, consider$NM(G)$. Later, applying the above operations and table 2 values, one can easily obtain the neighbourhood degree sum-based indices. This concludes the proof.

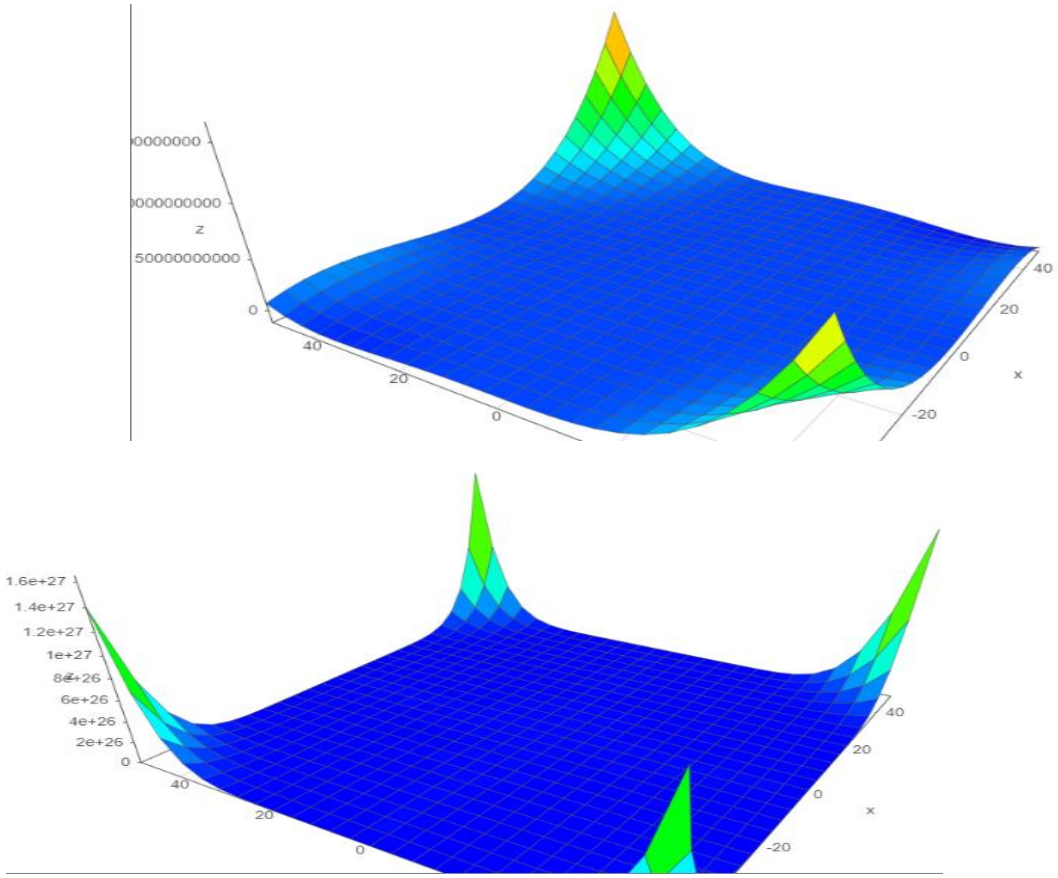


Figure 6. M-Polynomial (a) & NM-polynomial (b) of Tri-Poc Tenofovir dimer

5. Conclusion

In the presenter search paper, certain topological properties of Tenofovir molecular structures that are utilized to stop the occurrence and transmission of AIDS are studied and certain neighbourhood-based and certain degree-based indices are computed.Tri-POC tenofovir Dimer, Tenofovir Disproxil and Tenofovir alafenamide chemical structures are used for indices calculation. At first, with graphical representations, the researcher evaluated the Multiplicative polynomials and Non-Multiplicative polynomials of the Tenofovir structures. Based on resulted polynomial expressions, topological indices are computed for the respective structures. Using topological indices, scientists can predict various properties (i.e., boiling point (B.P), enthalpy and entropy). In this study, the expressions of some topological indices of Tri-POC tenofovir Dimer, Tenofovir Disproxil and Tenofovir Alafenamide have been determined. In Medical Science, medical, chemical, pharmaceutical and biological, properties of molecular structure are necessary for drug design and are studied by the topological index calculation. These calculations may be utilised in inventing new medicines, vaccines and drugs for the cure and prevention of AIDS/HIV. This paper mainly focuses on the numerical examination of topological indices for the tenofovir family molecular structure. The researcher presented the exact expression of several important indices based on edge dividing approaches including general indices (Randic and harmonic) , Systematic division index, Zagreb index (1^{st}, 2^{nd}, 3^{rd}, second modified, Redefined $3^{rd}$and Augmented), Forgotten index, Inverse sum indices, general sum connectivity. The results may prove the favourable presentation visions in chemical and pharmacy engineering.

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