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QSPR ANALYSIS OF CERTAIN ANTI-HIV DRUGS

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Abstract: A broad spectrum of advanced medications appears yearly following the accelerated evolution of the chemical and pharmaceutical industry. In this paper, various degree-based and neighborhood degree sum-based topological indices of some anti-HIV drugs are explored applying the M-polynomial and NM-polynomial formulations. Moreover, QSPR analysis is carried out for the topological indices with regard to the physico-chemical properties of the anti-HIV drugs. The activity of nucleoside and non-nucleoside reverse transcriptase inhibitors is implemented as in drug configuration to manifest the significance of topological indices in the medicinal world. The procured outcomes affirm that topological indices being studied reflect effective correlation in accordance to physical and chemical properties of the anti-HIV drugs and consequently can assist in development of advanced and promising pharmaceutical for HIV medication.

Keywords and Phrases: Anti-HIV drug, Topological Index, M-Polynomial, NM-Polynomial, QSPR.

2020 Mathematics Subject Classification: 05C09, 05C90, 05C92.

1. Introduction

In this period of significant scientific progression, there has been a huge evolution in chemical, pharmaceutical, medical and biological techniques and hence a considerable proportion of new nanostructures, crystal compounds as well as medicines develop with each passing year. The molecular traits of these materials and drugs can be defined by numerous techniques consequently enhancing certainly the laborious assignments of various scientific and pharmaceutical researchers. In chemical based analysis, a strong relation of the topology of molecular structures with respect to their physico-chemical natures, and organic-biologic traits such as enthalpy of vaporization, molar refractivity, stability and virulency of drugs was revealed. Acquired immunodeficiency syndrome (AIDS) is a persistent, inherently hazardous ailment generated due to human immunodeficiency virus (HIV). By harming defence mechanism of the body, HIV intervenes with individual's capability to combat infection and disease. This is such a dangerous ailment that it has taken lives of millions of people by now and is persisting to be a threat for the survival of the affected population. According to the data provided by the World Health Organization(WHO), approximately around 480000 to 1.0 million people died on grounds linked with HIV and about 1.0 to 2.0 million people got diseased with HIV in the past year, 2020. There has been a rapid increase in the transmission of this virus. Alarmingly, no drug or vaccine has been completely recognised yet to administer this virus. However, by means of some appropriate medications, the virus can be dominated to some extent. In this regard, certain topological descriptors of the tenofovir chemical structures used in the treatment of HIV have been determined in [29]. Researchers have approved the use and efficacy of some pre-existing medicines to control and manage the deadly virus. These include the nucleoside and non-nucleoside reverse transcriptase inhibitors. Topology of a molecule is fundamentally a non numerical mathematical unit. Numerous measurable characteristics of molecule are often revealed in the form of specific numerals. For relating the molecular topology to any real chemical attribute, the conversion of the relevant details embedded into chemical structure to some numeric value becomes so vital which ultimately paves the way for the emergence of topological indices. Thus, the topological index of a molecular graph is contemplated as a non-empiric numeric quantity that ascertains framework of the molecule along with the diverging sequence. It means that these topological indices are referred to be functions which maps the chemical structure to some real value.
Wiener index is one of the earliest and extensively explored molecular descriptors [30]. It has been found that Randić index has numerous implementations in chemical and therapeutic domains [10, 24]. Works on another descriptor termed harmonic

index have also been carried out [31]. Since then, a huge category of molecular descriptors have come into picture and lot of activities have been achieved in this aspect of exploration of the indices of molecular networks. The First and Second Zagreb Indices are the widely known graph invariants defined by Gutman to specify π-electron energy of the molecules [11, 12]. The second modified zagreb index is one among the various reformulations of the zagreb indices [15]. In [25], the zagreb indices were reviewed and the redefined third zagreb index emerges out of such works. Many works on another invariant namely, the forgotten topological index have also been carried out [6]. A lot of work has been done on the symmetric division deg index [9] and relation between inverse sum indeg index with the other descriptors have also been established in [20]. B.Furtula et al. [5] initiated the study of a new descriptor, augmented zagreb index which ultimately paved way for further research on the descriptor [3].
In order to suppress the rigorous work of finding the descriptors for certain molecular graphs, the approach of algebraic polynomials comes into existence which facilitates the process. Polynomials for both degree and distance based indices have been determined. In the paper by Deutsch and Klavzar [4], a polynomial called the M-polynomial was introduced which played a very pivotal role in the determination of the degree-based indices. Studies have been conducted regarding the finding of certain molecular descriptors of some molecular networks and compounds applying the approach of polynomials [13, 27].
Here, algebraic polynomial approach is utilised to generate the physical and chemical properties for molecular compounds. The paper implements the application of two nucleoside reverse transcriptase inhibitors (NRTIs) and two non-nucleoside reverse transcriptase inhibitors (NNRTIs) for controlling HIV levels in blood. Abacavir [1] and Lamivudine [22] belong to the group of drugs termed as nucleoside reverse transcriptase inhibitors while Efavirenz [23] and Doravirine [26] is in the class of medications called NNRTIs. Some topological characteristics of the stated anti-HIV drugs [2] have also been determined.

For the computation of topological indices, a chemical compound needs to amend itself to a molecular graph such that the atoms of the molecule correspond to vertices and the atomic links are depicted to be the edges. For a molecular graph $\mathscr{G} = (\mathscr{V}, \mathscr{E})$, $\mathscr{V}(\mathscr{G})$ represents the vertex set and $\mathscr{E}(\mathscr{G})$ represents the edge set. $|\mathscr{V}(\mathscr{G})|$ and $|\mathscr{E}(\mathscr{G})|$ denotes the cardinality of the vertex and edge sets of the graph, $\mathscr{G}$ respectively. Let $\mathfrak{d}(\mathfrak{v})$ denote the degree of vertex $\mathfrak{v}$ in $\mathscr{G}$ and $\mathfrak{e} = \mathfrak{v}\mathfrak{u}$ is the edge joining the vertex $\mathfrak{v}$ with vertex $\mathfrak{u}$. We have considered $W_{(i,j)}$ as the set of all edges of graph, $\mathscr{G}$ having the corresponding degrees of end vertices $i, j \geq 1$, i.e., $W_{(i,j)} = \{\mathfrak{v}\mathfrak{u} \in \mathscr{E}(\mathscr{G}) : \mathfrak{d}(\mathfrak{v}) = i, \mathfrak{d}(\mathfrak{u}) = j\}$. Let $w_{(i,j)}$ be the number of edges in

$W_{(i,j)}$. The M-Polynomial of $\mathscr{G}$ can be determined by:

$$M(\mathscr{G};x,y)=\sum_{i\leq j} w_{ij}(\mathscr{G})x^i y^j \tag{1}$$

Diverse physico-chemical characteristics can be anticipated with dominant validity and precision by the neighborhood degree sum-based indices [16, 17, 19]. Let $\mathfrak{nd}(\mathfrak{v})$ represent the sum of degrees of neighboring vertices of $\mathfrak{v}$ in $\mathscr{G}$. Here, $W^*_{(i,j)}$ is considered to be the set of all edges of graph, $\mathscr{G}$ having the corresponding neighborhood degree sum of end vertices $i,j\geq 1$, i.e., $W^*_{(i,j)}=\{\mathfrak{vu}\in\mathscr{E}(\mathscr{G}):\mathfrak{nd}(\mathfrak{v})=i,\mathfrak{nd}(\mathfrak{u})=j\}$ and $w^*_{(i,j)}$ be the number of edges in $W^*_{(i,j)}$. A quite similar polynomial is defined on the basis of neighborhood degree sum of the vertices of corresponding edges called the NM-Polynomial which can be determined as:

$$NM(\mathscr{G};x,y)=\sum_{i\leq j} w^*_{ij}(\mathscr{G})x^i y^j \tag{2}$$

Interpretation of the topological indices regarding anti-cancer drugs have also been explored [7, 28]. Also, topological indices have been utilised for the prediction of several QSPR/QSAR analysis in various medicinal domains [8]. In the recent covid-19 pandemic, some observations on the application of topological indices in the improvisation of drugs have been recognised [14, 18].

2. Methodology

Our paper primarily focuses on determining the molecular descriptors of some anti-HIV therapeutic molecular compounds by algebraic polynomial approach. We utilise Chemsketch for plotting the molecular graphs of efavirenz, abacavir, lamivudine and doravirine. The hydrogen suppressed molecular graphs are taken into consideration as nodes interpreting hydrogen don't possess any impact on isomorphism of graphs. Computations on edge partition procedures, graph analytic mechanisms, logical approaches with degree calculations are applied in the findings.

In the beginning, based on degree and neighborhood degree sum of end vertices of the hydrogen eliminated molecular graph of the stated compounds, some sequences of edge partitions are constructed. Using those separation patterns, the M-polynomial and NM-polynomial formulation is acquired.

Here, $D_x(h(x,y))=x\frac{\partial(h(x,y))}{\partial x}$, $D_y(h(x,y))=y\frac{\partial(h(x,y))}{\partial y}$,
$S_x(h(x,y))=\int_0^x \frac{h(t,y)}{t}dt$, $S_y(h(x,y))=\int_0^y \frac{h(x,t)}{t}dt$, $Jh(x,y)=h(x,x)$,
$Q_k h(x,y)=x^k h(x,y)$, where $h(x,y)=M(\mathscr{G};x,y)$ for degree based topological indices and $h(x,y)=NM(\mathscr{G};x,y)$ for neighborhood degree sum-based indices.

Topological Indices	**Determination from $\mathbf{h(x,y) = M(\mathscr{G}; x, y)}$**
First Zagreb Index, $M_1(\mathscr{G})$	$(D_x + D_y)[h(x,y)]\|_{x=y=1}$
Second Zagreb Index, $M_2(\mathscr{G})$	$(D_xD_y)[h(x,y)]\|_{x=y=1}$
Second Modified Zagreb Index, $mM_2(\mathscr{G})$	$(S_xS_y)[h(x,y)]\|_{x=y=1}$
Redefined Third Zagreb Index, $ReZG_3(\mathscr{G})$	$D_xD_y(D_x + D_y)[h(x,y)]\|_{x=y=1}$
Forgotten Index, $F(\mathscr{G})$	$(D_x^2 + D_y^2)[h(x,y)]\|_{x=y=1}$
Randić Index, $R_\alpha(\mathscr{G})$	$(D_x^\alpha D_y^\alpha)[h(x,y)]\|_{x=y=1}$
Inverse Randić Index, $RR_\alpha(\mathscr{G})$	$(S_x^\alpha S_y^\alpha)[h(x,y)]\|_{x=y=1}$
Symmetric Division Deg Index, $SDD(\mathscr{G})$	$(S_yD_x + S_xD_y)[h(x,y)]\|_{x=y=1}$
Harmonic Index, $H(\mathscr{G})$	$(2S_xJ)[h(x,y)]\|_{x=y=1}$
Inverse Sum Indeg Index, $I(\mathscr{G})$	$(S_xJD_xD_y)[h(x,y)]\|_{x=y=1}$
Augmented Zagreb Index, $A(\mathscr{G})$	$(S_x^3Q_{-2}JD_x^3D_y^3)[h(x,y)]\|_{x=y=1}$

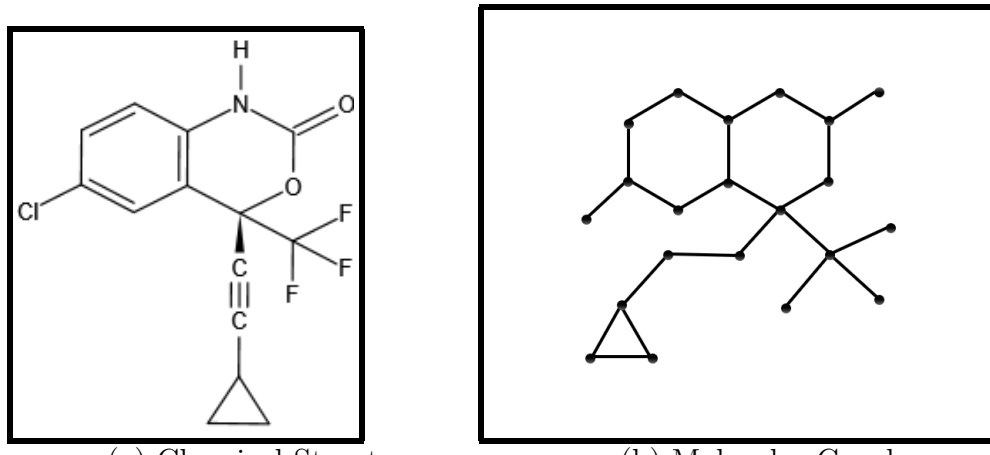
Table 1: Formulation of topological index from M-Polynomial

Topological Indices	**Determination from $\mathbf{h(x,y) = NM(\mathscr{G}; x, y)}$**
Third version Zagreb Index, $NM_1(\mathscr{G})$	$(D_x + D_y)[h(x,y)]\|_{x=y=1}$
Neighborhood Second Zagreb Index, $NM_2(\mathscr{G})$	$(D_xD_y)[h(x,y)]\|_{x=y=1}$
Neighborhood Second Modified Zagreb Index, $NmM_2(\mathscr{G})$	$(S_xS_y)[h(x,y)]\|_{x=y=1}$
Third NDe Index, $ND_3(\mathscr{G})$	$D_xD_y(D_x + D_y)[h(x,y)]\|_{x=y=1}$
Neighborhood Forgotten Index, $NF(\mathscr{G})$	$(D_x^2 + D_y^2)[h(x,y)]\|_{x=y=1}$
Neighborhood Randic Index, $NR_\alpha(\mathscr{G})$	$(D_x^\alpha D_y^\alpha)[h(x,y)]\|_{x=y=1}$
Neighborhood Inverse Randic Index, $NRR_\alpha(\mathscr{G})$	$(S_x^\alpha S_y^\alpha)[h(x,y)]\|_{x=y=1}$
Fifth NDe Index, $ND_5(\mathscr{G})$	$(S_yD_x + S_xD_y)[h(x,y)]\|_{x=y=1}$
Neighborhood Harmonic Index, $NH(\mathscr{G})$	$(2S_xJ)[h(x,y)]\|_{x=y=1}$
Neighborhood Inverse Sum Index, $NI(\mathscr{G})$	$(S_xJD_xD_y)[h(x,y)]\|_{x=y=1}$
Sanskruti Index, $S(\mathscr{G})$	$(S_x^3Q_{-2}JD_x^3D_y^3)[h(x,y)]\|_{x=y=1}$

Table 2: Formulation of topological index from NM-Polynomial

Theorem 1. *If Z represents molecular graph of Efavirenz;*

$$\begin{aligned} M(Z;x,y) &= 2xy^3 + 3x^2y^2 + 3xy^4 + 10x^2y^3 + 2x^2y^4 + x^3y^3 + x^3y^4 + x^4y^4 \\ NM(Z;x,y) &= 2x^3y^5 + 3x^5y^5 + 6x^5y^6 + 3x^4y^7 + 2x^5y^7 + x^6y^7 + x^6y^9 + x^7y^9 \\ &\quad + x^6y^{11} + 2x^7y^{11} + x^9y^{11} \end{aligned}$$



(a) Chemical Structure (b) Molecular Graph

Figure 1: Efavirenz

Proof. Let Z depict molecular graph of Efavirenz having 23 edges. By the molecular structure of Efavirenz, edge set of Z is partitioned in 8 categories based on the degree of the end vertices for corresponding edges. From the figure (1), $w_{(13)} = 2$, $w_{(22)} = 3$, $w_{(14)} = 3$, $w_{(23)} = 10$, $w_{(24)} = 2$, $w_{(33)} = 1$, $w_{(34)} = 1$, $w_{(44)} = 1$. Following equation (1), we get M-polynomial of Z :

$$\begin{aligned} M(Z;x,y) &= \sum_{i\leq j} w_{ij}(Z)x^iy^j \\ &= w_{13}xy^3 + w_{22}x^2y^2 + w_{14}xy^4 + w_{23}x^2y^3 + w_{24}x^2y^4 + w_{33}x^3y^3 \\ &\quad + w_{34}x^3y^4 + w_{44}x^4y^4 \end{aligned}$$

Substituting the values of w_{ij}, we get;

$$M(Z;x,y) = 2xy^3 + 3x^2y^2 + 3xy^4 + 10x^2y^3 + 2x^2y^4 + x^3y^3 + x^3y^4 + x^4y^4$$

Based on the sum of neighborhood vertex degree, edge set of Z is partitioned in 11 categories as: $w^*_{(35)} = 2, w^*_{(55)} = 3, w^*_{(47)} = 3, w^*_{(56)} = 6, w^*_{(57)} = 2, w^*_{(67)} = 1, w^*_{(69)} =$

$1, w^*_{(79)} = 1, w^*_{(6,11)} = 1, w^*_{(7,11)} = 2, w^*_{(9,11)} = 1$. Following equation (2), we get the NM-polynomial of Z as:

$$\begin{aligned} NM(Z;x,y) &= \sum_{i\leq j} w^*_{ij}(Z)x^i y^j \\ &= w^*_{(35)}x^3y^5 + w^*_{(55)}x^5y^5 + w^*_{(47)}x^4y^7 + w^*_{(56)}x^5y^6 + w^*_{(57)}x^5y^7 \\ &\quad + w^*_{(67)}x^6y^7 + w^*_{(69)}x^6y^9 + w^*_{(79)}x^7y^9 + w^*_{(6,11)}x^6y^{11} \\ &\quad + w^*_{(7,11)}x^7y^{11} + w^*_{(9,11)}x^9y^{11} \end{aligned}$$

Substituting the values of w^*_{ij}, we get;

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

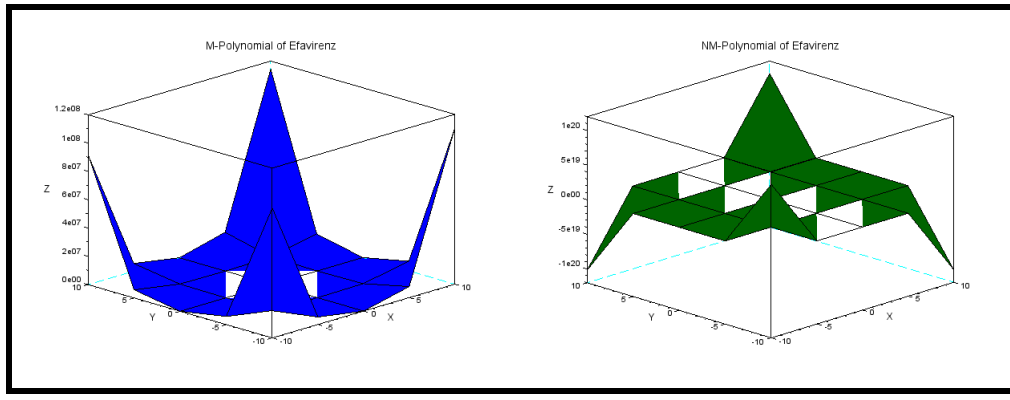


Figure 2: Representation of M & NM Polynomial for Efavirenz

Theorem 2. *If Z represents molecular graph of Efavirenz;*

1. $M_1(Z) = 118,\ NM_1(Z) = 286$
2. $M_2(Z) = 143,\ NM_2(Z) = 917$
3. $mM_2(Z) = 4.3403,\ NmM_2(Z) = 0.7270$
4. $ReZG_3(Z) = 4.3403,\ ND_3(Z) = 12972$
5. $F(Z) = 340,\ NF(Z) = 1958$

6. $R_\alpha(Z) = 2(3)^\alpha + 3(2)^{2\alpha} + 3(4)^\alpha + 10(2)^\alpha(3)^\alpha + 2(2)^{3\alpha} + (3)^{2\alpha} + (3)^\alpha(4)^\alpha + (4)^{2\alpha}$,

$NR_\alpha(Z) = 2(3)^\alpha(5)^\alpha + 3(5)^{2\alpha} + 3(4)^\alpha(7)^\alpha + 6(5)^\alpha(6)^\alpha + 2(5)^\alpha(7)^\alpha + (6)^\alpha(7)^\alpha + (6)^\alpha(9)^\alpha + (7)^\alpha(9)^\alpha + (6)^\alpha(11)^\alpha + 2(7)^\alpha(11)^\alpha + (9)^\alpha(11)^\alpha$

7. $RR_\alpha(Z) = \frac{2}{(3)^\alpha} + \frac{3}{(2)^{2\alpha}} + \frac{3}{(4)^\alpha} + \frac{10}{(2)^\alpha(3)^\alpha} + \frac{2}{(2)^\alpha(4)^\alpha} + \frac{1}{(3)^{2\alpha}} + \frac{1}{(3)^\alpha(4)^\alpha} + \frac{1}{(4)^{2\alpha}}$,

$NRR_\alpha(Z) = \frac{2}{(3)^\alpha(5)^\alpha} + \frac{3}{(5)^{2\alpha}} + \frac{3}{(4)^\alpha(7)^\alpha} + \frac{6}{(5)^\alpha(6)^\alpha} + \frac{2}{(5)^\alpha(7)^\alpha} + \frac{1}{(6)^\alpha(7)^\alpha} + \frac{1}{(6)^\alpha(9)^\alpha} + \frac{1}{(7)^\alpha(9)^\alpha} + \frac{1}{(6)^\alpha(11)^\alpha} + \frac{2}{(7)^\alpha(11)^\alpha} + \frac{1}{(9)^\alpha(11)^\alpha}$

8. $SDD(Z) = 58.1667$, $ND_5(Z) = 49.0149$

9. $H(Z) = 9.2357$, $NH(Z) = 3.9217$

10. $I(Z) = 26.781$, $NI(Z) = 69.2395$

11. $A(Z) = 178.0387$, $S(Z) = 1214.0486$

Proof. Here for computation of degree based indices, we have,
$M(Z;x,y) = h(x,y) = 2xy^3 + 3x^2y^2 + 3xy^4 + 10x^2y^3 + 2x^2y^4 + x^3y^3 + x^3y^4 + x^4y^4$.
Then,

$(D_x+D_y)(h(x,y)) = 8xy^3+12x^2y^2+15xy^4+50x^2y^3+12x^2y^4+6x^3y^3+7x^3y^4+8x^4y^4$

$(D_yD_x)(h(x,y)) = 6xy^3+12x^2y^2+12xy^4+60x^2y^3+16x^2y^4+9x^3y^3+12x^3y^4+16x^4y^4$

$$\begin{aligned}(D_x^2+D_y^2)(h(x,y)) &= 20xy^3 + 24x^2y^2 + 51xy^4 + 130x^2y^3 + 40x^2y^4 + 18x^3y^3 \\ &\quad + 25x^3y^4 + 32x^4y^4\\ (D_x^\alpha D_y^\alpha)(h(x,y)) &= 2(3)^\alpha xy^3 + 3(2)^{2\alpha}x^2y^2 + 3(4)^\alpha xy^4 + 10(2)^\alpha(3)^\alpha x^2y^3 \\ &\quad + 2(2)^\alpha(4)^\alpha x^2y^4 + (3)^{2\alpha}x^3y^3 + (3)^\alpha(4)^\alpha x^3y^4 + (4)^{2\alpha}x^4y^4\\ D_xD_y(D_x+D_y)(h(x,y)) &= 24xy^3 + 48x^2y^2 + 60xy^4 + 300x^2y^3 + 96x^2y^4 + 54x^3y^3 \\ &\quad + 84x^3y^4 + 128x^4y^4\end{aligned}$$

$$\begin{aligned}(S_xS_y)(h(x,y)) &= \frac{2}{3}xy^3 + \frac{3}{4}x^2y^2 + \frac{3}{4}xy^4 + \frac{5}{3}x^2y^3 + \frac{1}{4}x^2y^4 + \frac{1}{9}x^3y^3 \\ &\quad + \frac{1}{12}x^3y^4 + \frac{1}{16}x^4y^4\\ (S_x^\alpha S_y^\alpha)(h(x,y)) &= \frac{2}{3^\alpha}xy^3 + \frac{3}{2^{2\alpha}}x^2y^2 + \frac{3}{4^\alpha}xy^4 + \frac{10}{2^\alpha 3^\alpha}x^2y^3 + \frac{2}{2^\alpha 4^\alpha}x^2y^4 + \frac{1}{3^{2\alpha}}x^3y^3 \\ &\quad + \frac{1}{3^\alpha 4^\alpha}x^3y^4 + \frac{1}{4^{2\alpha}}x^4y^4\end{aligned}$$

$(S_xD_y+S_yD_x)(h(x,y)) = \frac{20}{3}xy^3+6x^2y^2+\frac{51}{4}xy^4+\frac{65}{3}x^2y^3+5x^2y^4+2x^3y^3+\frac{25}{12}x^3y^4+2x^4y^4$

$(S_xJ)(h(x,y)) = \frac{5}{4}x^4+\frac{13}{5}x^5+\frac{1}{2}x^6+\frac{1}{7}x^7+\frac{1}{8}x^8$

$(S_xJD_yD_x)(h(x,y)) = \frac{9}{2}x^4+\frac{72}{5}x^5+\frac{25}{6}x^6+\frac{12}{7}x^7+2x^8$

$(S_x^3Q_{-2}JD_x^3D_y^3)(h(x,y)) = \frac{246}{8}x^2+\frac{2352}{27}x^3+\frac{1753}{64}x^4+\frac{1728}{125}x^5+\frac{4096}{216}x^6$

By using Table (1), we have;

$$\begin{aligned}
M_1(Z) &= 8xy^3+12x^2y^2+15xy^4+50x^2y^3+12x^2y^4+6x^3y^3+7x^3y^4\\
&\quad +8x^4y^4|_{x=y=1} = 118\\
M_2(Z) &= 6xy^3+12x^2y^2+12xy^4+60x^2y^3+16x^2y^4+9x^3y^3+12x^3y^4\\
&\quad +16x^4y^4|_{x=y=1} = 143\\
mM_2(Z) &= \frac{2}{3}xy^3+\frac{3}{4}x^2y^2+\frac{3}{4}xy^4+\frac{5}{3}x^2y^3+\frac{1}{4}x^2y^4+\frac{1}{9}x^3y^3+\frac{1}{12}x^3y^4\\
&\quad +\frac{1}{16}x^4y^4|_{x=y=1} = 4.3403\\
ReZG_3(Z) &= 24xy^3+48x^2y^2+60xy^4+300x^2y^3+96x^2y^4+54x^3y^3+84x^3y^4\\
&\quad +128x^4y^4|_{x=y=1} = 794\\
F(Z) &= 20xy^3+24x^2y^2+51xy^4+130x^2y^3+40x^2y^4+18x^3y^3+25x^3y^4\\
&\quad +32x^4y^4|_{x=y=1} = 340\\
R_\alpha(Z) &= 2(3)^\alpha xy^3+3(2)^{2\alpha}x^2y^2+3(4)^\alpha xy^4+10(2)^\alpha(3)^\alpha x^2y^3+2(2)^\alpha(4)^\alpha x^2y^4\\
&\quad +(3)^{2\alpha}x^3y^3+(3)^\alpha(4)^\alpha x^3y^4+(4)^{2\alpha}x^4y^4|_{x=y=1}\\
&= 2(3)^\alpha+3(2)^{2\alpha}+3(4)^\alpha+10(2)^\alpha(3)^\alpha+2(2)^{3\alpha}+(3)^{2\alpha}+(3)^\alpha(4)^\alpha+(4)^{2\alpha}\\
SDD(Z) &= \frac{20}{3}xy^3+6x^2y^2+\frac{51}{4}xy^4+\frac{65}{3}x^2y^3+5x^2y^4+2x^3y^3+\frac{25}{12}x^3y^4\\
&\quad +2x^4y^4|_{x=y=1} = 58.1667
\end{aligned}$$

$H(Z) = 2[\frac{5}{4}x^4+\frac{13}{5}x^5+\frac{1}{2}x^6+\frac{1}{7}x^7+\frac{1}{8}x^8]|_{x=y=1} = 9.2357$

$I(Z) = \frac{9}{2}x^4+\frac{72}{5}x^5+\frac{25}{6}x^6+\frac{12}{7}x^7+2x^8|_{x=y=1} = 26.781$

$A(Z) = \frac{246}{8}x^2+\frac{2352}{27}x^3+\frac{1753}{64}x^4+\frac{1728}{125}x^5+\frac{4096}{216}x^6|_{x=y=1} = 178.0387$

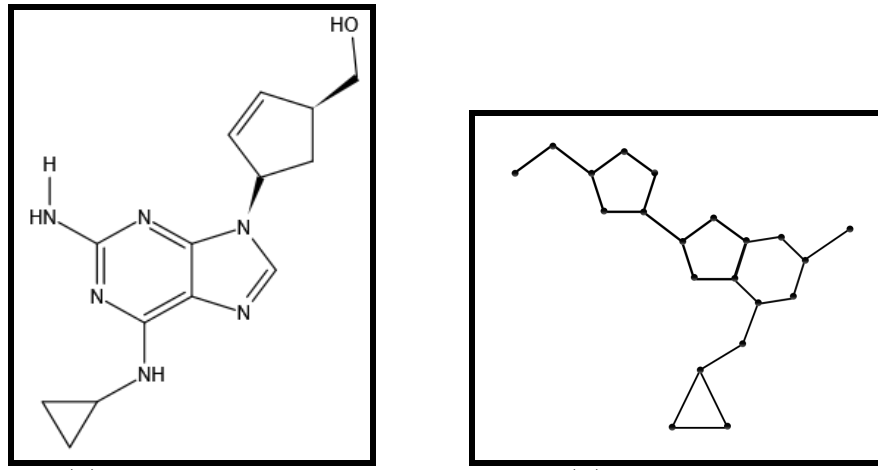
Now, we have

$$NM(Z;x,y) = 2x^3y^5 + 3x^5y^5 + 3x^4y^7 + 6x^5y^6 + 2x^5y^7 + x^6y^7 + x^6y^9 + x^7y^9 + x^6y^{11} + 2x^7y^{11} + x^9y^{11}$$

By the above equations and Table (2), the neighborhood degree sum based topological indices are obtained. Hence, this concludes our proof.

Theorem 3. *If B represents molecular graph of Abacavir;*

$$M(B;x,y) = xy^2 + xy^3 + 3x^2y^2 + 15x^2y^3 + 4x^3y^3$$
$$NM(B;x,y) = x^2y^4 + x^3y^5 + x^4y^6 + 3x^5y^5 + 5x^5y^6 + x^5y^7 + 2x^6y^6 + 2x^5y^8 + 3x^6y^7 + x^6y^8 + 2x^7y^8 + 2x^8y^8$$



(a) Chemical Structure (b)Molecular Graph

Figure 3: Abacavir

Proof. Let B depict molecular graph of Abacavir having 24 edges. By the molecular structure of Abacavir, edge set of B is partitioned in 5 categories based on the degree of the end vertices for corresponding edges. From the figure (3), $w_{(12)} = 1, w_{(13)} = 1, w_{(22)} = 3, w_{(23)} = 15$ and $w_{(33)} = 4$. Following equation (1), we get M-polynomial of B:

$$\begin{aligned} M(B;x,y) &= \sum_{i\leq j} w_{ij}(B)x^iy^j \\ &= w_{12}xy^2 + w_{13}xy^3 + w_{22}x^2y^2 + w_{23}x^2y^3 + w_{33}x^3y^3 \end{aligned}$$

Substituting the values of w_{ij}, we get;

$$M(B;x,y) = xy^2 + xy^3 + 3x^2y^2 + 15x^2y^3 + 4x^3y^3$$

Based on the sum of the neighborhood vertex degree, edge set of B is partitioned in 12 categories as: $w^*_{(24)} = 1, w^*_{(35)} = 1, w^*_{(46)} = 1, w^*_{(55)} = 3, w^*_{(56)} = 5, w^*_{(57)} = 1, w^*_{(66)} = 2, w^*_{(58)} = 2, w^*_{(67)} = 3, w^*_{(68)} = 1, w^*_{(78)} = 2, w^*_{(88)} = 2$. Following equation (2), we get the NM-polynomial of B as:

$$\begin{aligned} NM(B;x,y) &= \sum_{i\leq j} w^*_{ij}(B)x^iy^j \\ &= w^*_{(24)}x^2y^4 + w^*_{(35)}x^3y^5 + w^*_{(46)}x^4y^6 + w^*_{(55)}x^5y^5 + w^*_{(56)}x^5y^6 \\ &\quad + w^*_{(57)}x^5y^7 + w^*_{(66)}x^6y^6 + w^*_{(58)}x^5y^8 + w^*_{(67)}x^6y^7 + w^*_{(68)}x^6y^8 \\ &\quad + w^*_{(78)}x^7y^8 + w^*_{(88)}x^8y^8 \end{aligned}$$

Substituting the values of w^*_{ij}, we get;

$$\begin{aligned} NM(B;x,y) = x^2y^4 + x^3y^5 + x^4y^6 + 3x^5y^5 + 5x^5y^6 + x^5y^7 + 2x^6y^6 + 2x^5y^8 \\ + 3x^6y^7 + x^6y^8 + 2x^7y^8 + 2x^8y^8 \end{aligned}$$

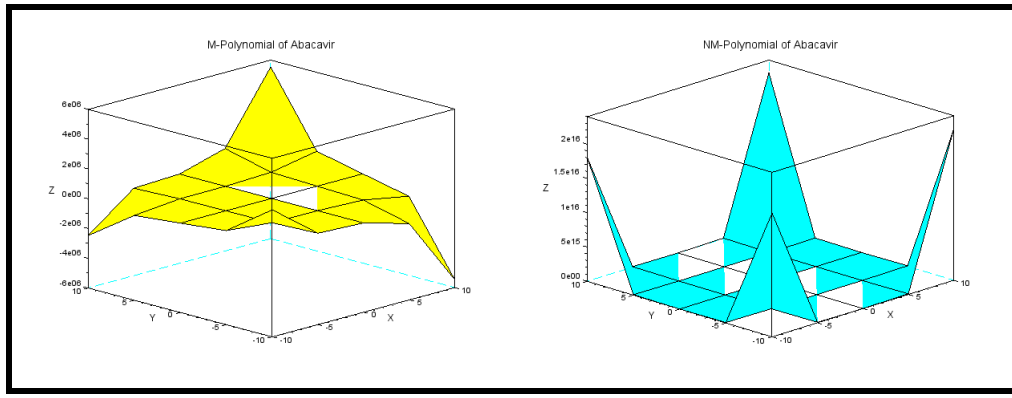


Figure 4: Representation of M & NM Polynomial for Abacavir

Theorem 4. *If B represents molecular graph of Abacavir;*

1. $M_1(B) = 118,\ NM_1(B) = 286$
2. $M_2(B) = 143,\ NM_2(B) = 873$

3. $mM_2(B) = 4.5278$, $NmM_2(B) = 0.8134$

4. $ReZG_3(B) = 732$, $ND_3(B) = 11170$

5. $F(B) = 306$, $NF(B) = 1794$

6. $R_\alpha(B) = (2)^\alpha + (3)^\alpha + 3(2)^{2\alpha} + 15(2)^\alpha(3)^\alpha + 4(3)^{2\alpha}$,

$$NR_\alpha(B) = (2)^\alpha(4)^\alpha + (3)^\alpha(5)^\alpha + (4)^\alpha(6)^\alpha + 3(5)^{2\alpha} + 5(5)^\alpha(6)^\alpha + 2(6)^{2\alpha} + (5)^\alpha(7)^\alpha + 2(5)^\alpha(8)^\alpha + 3(6)^\alpha(7)^\alpha + (6)^\alpha(8)^\alpha + 2(7)^\alpha(8)^\alpha + 2(8)^{2\alpha}$$

7. $RR_\alpha(B) = \frac{1}{(2)^\alpha} + \frac{1}{(3)^\alpha} + \frac{3}{(2)^{2\alpha}} + \frac{15}{(2)^\alpha(3)^\alpha} + \frac{4}{(3)^{2\alpha}}$,

$$NRR_\alpha(B) = \frac{1}{(2)^\alpha(4)^\alpha} + \frac{1}{(3)^\alpha(5)^\alpha} + \frac{1}{(4)^\alpha(6)^\alpha} + \frac{3}{(5)^{2\alpha}} + \frac{5}{(5)^\alpha(6)^\alpha} + \frac{2}{(6)^{2\alpha}} + \frac{1}{(5)^\alpha(7)^\alpha} + \frac{2}{(5)^\alpha(8)^\alpha} + \frac{3}{(6)^\alpha(7)^\alpha} + \frac{1}{(6)^\alpha(8)^\alpha} + \frac{2}{(7)^\alpha(8)^\alpha} + \frac{2}{(8)^{2\alpha}}$$

8. $SDD(B) = 52.3333$, $ND_5(B) = 49.8548$

9. $H(B) = 10$, $NH(B) = 4.2212$

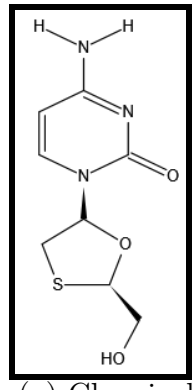
10. $I(B) = 28.4167$, $NI(B) = 70.4028$

11. $A(B) = 200.9375$, $S(B) = 1141.6444$

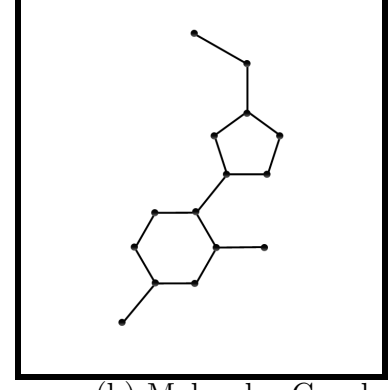
Theorem 5. *If L represents molecular graph of Lamivudine;*

$$M(L; x, y) = xy^2 + 2xy^3 + 2x^2y^2 + 9x^2y^3 + 2x^3y^3$$

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



(a) Chemical Structure



(b) Molecular Graph

Figure 5: Lamivudine

Proof. Let L depict the molecular graph of Lamivudine having 16 edges. By the molecular structure of Lamivudine, edge set of L is partitioned in 5 categories based on the degree of the end vertices for corresponding edges. From the figure (5), $w_{(12)} = 1, w_{(13)} = 2, w_{(22)} = 2, w_{(23)} = 9$ and $w_{(33)} = 2$. Following equation (1), we get M-polynomial of L:

$$\begin{aligned} M(L;x,y) &= \sum_{i\leq j} w_{ij}(L)x^i y^j \\ &= w_{12}xy^2 + w_{13}xy^3 + w_{22}x^2y^2 + w_{23}x^2y^3 + w_{33}x^3y^3 \end{aligned}$$

Substituting the values of w_{ij}, we get;

$$M(L;x,y) = xy^2 + 2xy^3 + 2x^2y^2 + 9x^2y^3 + 2x^3y^3$$

Based on the sum of the neighborhood vertex degree, edge set of L is partitioned in 12 categories as: $w^*_{(24)} = 1, w^*_{(35)} = 1, w^*_{(36)} = 1, w^*_{(46)} = 1, w^*_{(55)} = 3, w^*_{(56)} = 2, w^*_{(57)} = 1, w^*_{(66)} = 2, w^*_{(58)} = 1, w^*_{(67)} = 1, w^*_{(68)} = 1$ and $w^*_{(78)} = 1$.
Following equation (2), we get the NM-polynomial of L:

$$\begin{aligned} NM(L;x,y) &= \sum_{i\leq j} w^*_{ij}(L)x^i y^j \\ &= w^*_{(24)}x^2y^4 + w^*_{(35)}x^3y^5 + w^*_{(36)}x^3y^6 + w^*_{(46)}x^4y^6 + w^*_{(55)}x^5y^5 \\ &\quad + w^*_{(56)}x^5y^6 + w^*_{(57)}x^5y^7 + w^*_{(66)}x^6y^6 + w^*_{(58)}x^5y^8 + w^*_{(67)}x^6y^7 \\ &\quad + w^*_{(68)}x^6y^8 + w^*_{(78)}x^7y^8 \end{aligned}$$

Substituting the values of w^*_{ij}, we get;

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

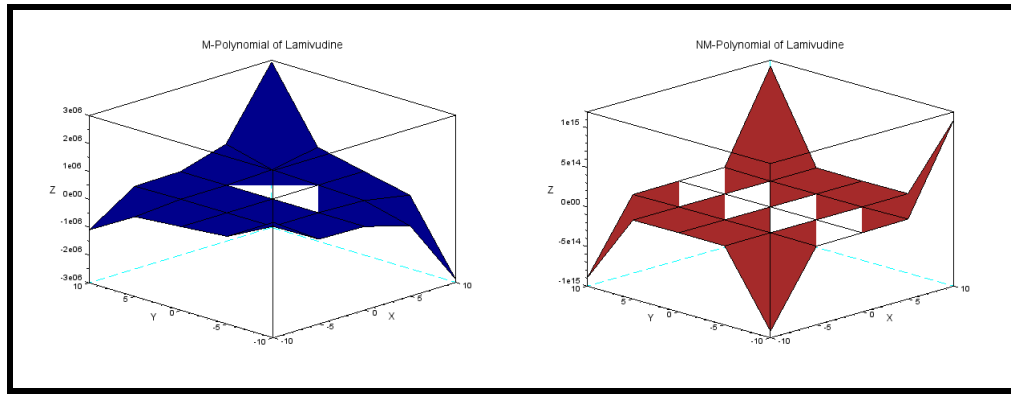


Figure 6: Representation of M & NM Polynomial for Lamivudine

Theorem 6. *If L represents molecular graph of Lamivudine;*

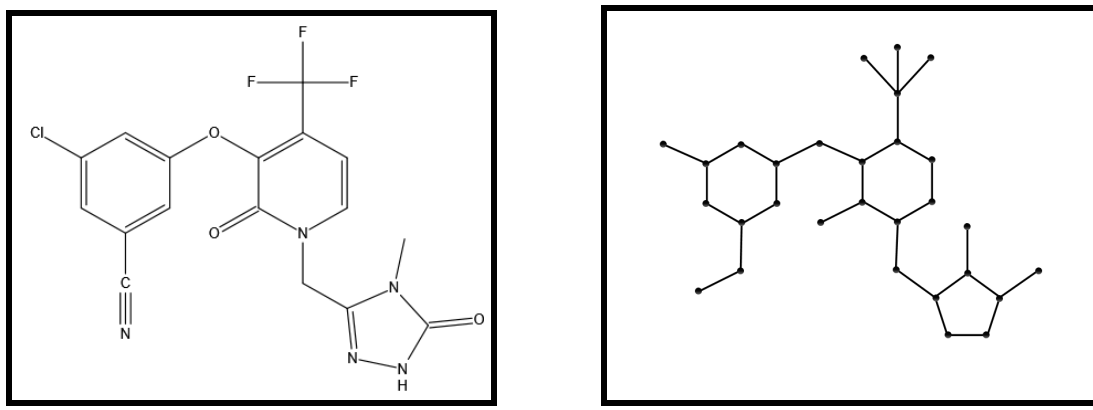
1. $M_1(L) = 76,\ NM_1(L) = 176$
2. $M_2(L) = 88,\ NM_2(L) = 493$
3. $mM_2(L) = 3.3889,\ NmM_2(L) = 0.6472$
4. $ReZG_3(L) = 440,\ ND_3(L) = 5842$
5. $F(L) = 194,\ NF(L) = 1028$
6. $R_\alpha(L) = (2)^\alpha + 2(3)^\alpha + 2(2)^{2\alpha} + 9(2)^\alpha(3)^\alpha + 2(3)^{2\alpha}$,

   $NR_\alpha(L) = (2)^\alpha(4)^\alpha + (3)^\alpha(5)^\alpha + (3)^\alpha(6)^\alpha + (4)^\alpha(6)^\alpha + 3(5)^{2\alpha} + 2(5)^\alpha(6)^\alpha + (5)^\alpha(7)^\alpha + 2(6)^{2\alpha} + (5)^\alpha(8)^\alpha + (6)^\alpha(7)^\alpha + (6)^\alpha(8)^\alpha + (7)^\alpha(8)^\alpha$
7. $RR_\alpha(L) = \frac{1}{(2)^\alpha} + \frac{2}{(3)^\alpha} + \frac{2}{(2)^{2\alpha}} + \frac{9}{(2)^\alpha(3)^\alpha} + \frac{2}{(3)^{2\alpha}}$,

   $NRR_\alpha(L) = \frac{1}{(2)^\alpha(4)^\alpha} + \frac{1}{(3)^\alpha(5)^\alpha} + \frac{1}{(3)^\alpha(6)^\alpha} + \frac{1}{(4)^\alpha(6)^\alpha} + \frac{3}{(5)^{2\alpha}} + \frac{2}{(5)^\alpha(6)^\alpha} + \frac{1}{(5)^\alpha(7)^\alpha} + \frac{2}{(6)^{2\alpha}} + \frac{1}{(5)^\alpha(8)^\alpha} + \frac{1}{(6)^\alpha(7)^\alpha} + \frac{1}{(6)^\alpha(8)^\alpha} + \frac{1}{(7)^\alpha(8)^\alpha}$
8. $SDD(L) = 36.6667,\ ND_5(L) = 33.9643$
9. $H(L) = 6.9333,\ NH(L) = 3.0531$
10. $I(L) = 17.9667,\ NI(L) = 42.9491$
11. $A(L) = 125.53125,\ S(L) = 617.1237$

Theorem 7. *If D represents molecular graph of Doravirine;*

$$\begin{aligned} M(D;x,y) &= xy^2 + 4xy^3 + 2x^2y^2 + 3xy^4 + 15x^2y^3 + 5x^3y^3 + x^3y^4 \\ NM(D;x,y) &= x^2y^4 + x^3y^5 + x^3y^6 + 2x^3y^7 + 4x^4y^6 + 2x^5y^5 + 3x^5y^6 + 2x^5y^7 \\ &\quad + 5x^6y^6 + 3x^6y^7 + x^5y^9 + x^6y^8 + 2x^7y^7 + x^6y^9 + x^7y^8 + x^8y^9 \end{aligned}$$



(a) Chemical Structure (b) Molecular Graph

Figure 7: Doravirine

Proof. If D represent molecular graph of Doravirine having 31 edges. By the molecular structure of Doravirine, edge set of D is partitioned in 7 categories based on the degree of the end vertices for corresponding edges. From the figure 7, $w_{(12)} = 1, w_{(13)} = 4, w_{(14)} = 3, w_{(22)} = 2, w_{(23)} = 15, w_{(33)} = 5$ and $w_{(34)} = 1$. Following equation (1), we get M-polynomial of D:

$$\begin{aligned} M(D;x,y) &= \sum_{i\leq j} w_{ij}(D)x^iy^j \\ &= w_{12}xy^2 + w_{13}xy^3 + w_{14}xy^4 + w_{22}x^2y^2 + w_{23}x^2y^3 + w_{33}x^3y^3 + w_{34}x^3y^4 \end{aligned}$$

Substituting the values of w_{ij}, we get;

$$M(D;x,y) = xy^2 + 4xy^3 + 2x^2y^2 + 3xy^4 + 15x^2y^3 + 5x^3y^3 + x^3y^4$$

Based on the sum of the neighborhood vertex degree, edge set of D is partitioned in 16 categories as: $w^*_{(24)} = 1, w^*_{(35)} = 1, w^*_{(36)} = 1, w^*_{(37)} = 2, w^*_{(46)} = 4, w^*_{(55)} = 2, w^*_{(56)} = 3, w^*_{(57)} = 2, w^*_{(66)} = 5, w^*_{(67)} = 3, w^*_{(59)} = 1, w^*_{(68)} = 1, w^*_{(77)} = 2, w^*_{(69)} =$

$1, w^*_{(78)} = 1$ and $w^*_{(89)} = 1$.
Following equation (2), we get NM-polynomial of D:

$$\begin{aligned} NM(D;x,y) &= \sum_{i\leq j} w^*_{ij}(D)x^i y^j \\ &= w^*_{(24)}x^2y^4 + w^*_{(35)}x^3y^5 + w^*_{(36)}x^3y^6 + w^*_{(37)}x^3y^7 + w^*_{(46)}x^4y^6 + \\ &\quad w^*_{(55)}x^5y^5 + w^*_{(56)}x^5y^6 + w^*_{(57)}x^5y^7 + w^*_{(66)}x^6y^6 + w^*_{(67)}x^6y^7 + \\ &\quad w^*_{(59)}x^5y^9 + w^*_{(68)}x^6y^8 + w^*_{(77)}x^7y^7 + w^*_{(69)}x^6y^9 + \\ &\quad w^*_{(78)}x^7y^8 + w^*_{(89)}x^8y^9 \end{aligned}$$

Substituting the values of w^*_{ij}, we get;

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

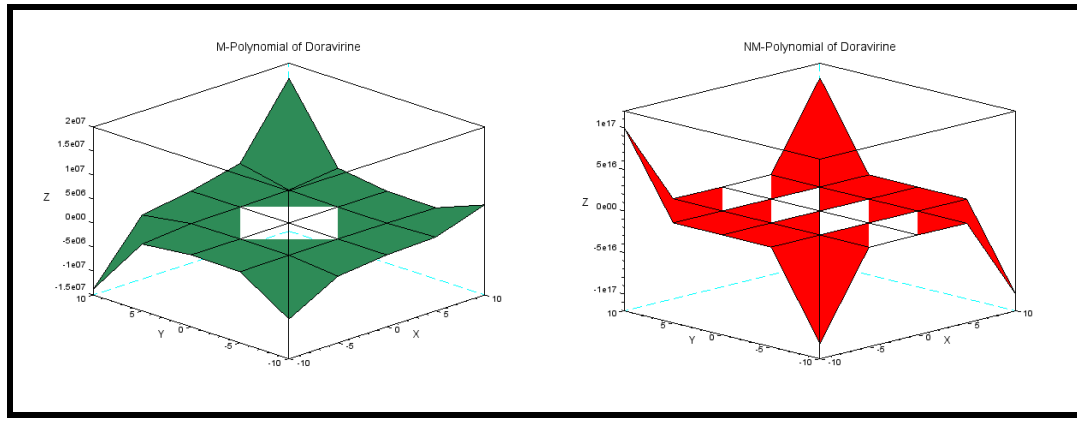


Figure 8: Representation of M & NM Polynomial for Doravirine

Theorem 8. *If D represents molecular graph of Doravirine;*

1. $M_1(D) = 154,\ NM_1(D) = 362$
2. $M_2(D) = 181,\ NM_2(D) = 1068$
3. $mM_2(D) = 6.2222,\ NmM_2(D) = 1.0907$
4. $ReZG_3(D) = 950,\ ND_3(D) = 13386$

5. $F(D) = 422$, $NF(D) = 2246$

6. $R_\alpha(D) = (2)^\alpha + 4(3)^\alpha + 3(4)^\alpha + 2(2)^{2\alpha} + 15(2)^\alpha(3)^\alpha + 5(3)^{2\alpha} + (3)^\alpha(4)^\alpha$,

   $NR_\alpha(D) = (2)^\alpha(4)^\alpha + (3)^\alpha(5)^\alpha + (3)^\alpha(6)^\alpha + 2(3)^\alpha(7)^\alpha + 4(4)^\alpha(6)^\alpha + 2(5)^{2\alpha}$
   $+3(5)^\alpha(6)^\alpha + 2(5)^\alpha(7)^\alpha + 5(6)^{2\alpha} + 3(6)^\alpha(7)^\alpha + (5)^\alpha(9)^\alpha$
   $+(6)^\alpha(8)^\alpha + 2(7)^{2\alpha} + (6)^\alpha(9)^\alpha + (7)^\alpha(8)^\alpha + (8)^\alpha(9)^\alpha$

7. $RR_\alpha(D) = \frac{1}{(2)^\alpha} + \frac{4}{(3)^\alpha} + \frac{3}{(4)^\alpha} + \frac{2}{(2)^{2\alpha}} + \frac{15}{(2)^\alpha(3)^\alpha} + \frac{5}{(3)^{2\alpha}} + \frac{1}{(3)^\alpha(4)^\alpha}$,

   $NRR_\alpha(D) = \frac{1}{(2)^\alpha(4)^\alpha} + \frac{1}{(3)^\alpha(5)^\alpha} + \frac{1}{(3)^\alpha(6)^\alpha} + \frac{2}{(3)^\alpha(7)^\alpha} + \frac{4}{(4)^\alpha(6)^\alpha} + \frac{2}{(5)^{2\alpha}} + \frac{3}{(5)^\alpha(6)^\alpha}$
   $+\frac{2}{(5)^\alpha(7)^\alpha} + \frac{5}{(6)^{2\alpha}} + \frac{3}{(6)^\alpha(7)^\alpha} + \frac{1}{(5)^\alpha(9)^\alpha} + \frac{1}{(6)^\alpha(8)^\alpha} + \frac{2}{(7)^{2\alpha}} + \frac{1}{(6)^\alpha(9)^\alpha}$
   $+\frac{1}{(7)^\alpha(8)^\alpha} + \frac{1}{(8)^\alpha(9)^\alpha}$

8. $SDD(D) = 77.1667$, $ND_5(D) = 66.4944$

9. $H(D) = 12.8190$, $NH(D) = 5.5350$

10. $I(D) = 35.281$, $NI(D) = 87.9273$

11. $A(D) = 235.3882$, $S(D) = 1358.0711$

3. QSPR analysis of related anti-HIV drugs

This section demonstrates the quantitative structure property relationship (QSPR) connecting several specified graph invariants with some physico-chemical drug attributes. The potency of the descriptors is investigated by such analysis. Some topological indices are represented with few physico-chemical properties such as molar volume(MV), polarizability(P), molar refraction(MR) and complexity of anti HIV drugs. The values for the respective physico-chemical properties, were acquired from ChemSpider as shown in Table (3). Table (4) enlists the calculated degree-based topological indices of related medication. The correlation coefficient (r) values for the drug characteristics are expressed with specified degree-based topological index in the Table (5). Also, the correlation of Harmonic index with Molar Refractivity and Polarizability is depicted in figure (9).

Drugs	Molar Refractivity	Polarizability	Molar Volume	Complexity
Efavirenz	68.4	27.1	205.3	519
Abacavir	75.8	30.1	167.7	414
Lamivudine	54.1	21.5	132.2	331
Doravirine	96.8	38.4	271.9	860

Table 3: Anti-HIV Drugs with its physico-chemical properties

Drugs	M_1	M_2	mM_2	$ReZG_3$	F	SDD	H	I	A	$R_{-1/2}$
Efavirenz	118	143	4.3403	794	340	58.1667	9.2357	26.781	178.0387	9.8163
Abacavir	118	143	4.5278	732	306	52.3333	10	28.4167	200.9375	10.24151
Lamivudine	76	88	3.3889	440	194	36.6667	6.9333	17.9667	125.53125	7.20271
Doravirine	154	181	6.2222	950	422	77.1667	12.819	35.28095	235.3882	13.59557

Table 4: Anti-HIV Drugs with degree based topological indices

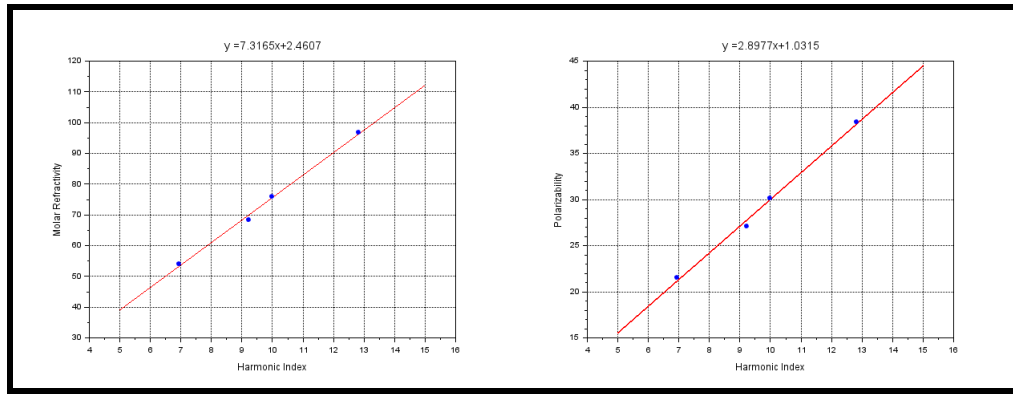


Figure 9: Correlation of Harmonic Index with Molar Refractivity (MR) & Polarizability (P)

Index	**Molar Refractivity**	**Polarizability**	**Molar Volume**	**Complexity**
M_1	0.972129506	0.971123533	0.945098257	0.910371282
M_2	0.957465679	0.956327334	0.927528749	0.880404514
mM_2	0.991821732	0.991531889	0.947345112	0.957968124
$ReZG_3$	0.915590076	0.913891224	0.934342951	0.869530394
F	0.929800155	0.928154125	0.964222958	0.912841539
SDD	0.949958741	0.948607412	0.988567507	0.962809767
H	0.997981516	0.997710137	0.921138319	0.91564938
I	0.979410828	0.978735795	0.911495437	0.879516045
A	0.974851642	0.974562943	0.859506443	0.830148932
$R_{-1/2}$	0.994150477	0.993665	0.944644028	0.937917431

Table 5: The correlation values between the degree based topological indices with the anti-HIV drug properties

From the Table (5), it is to be noted:

- Harmonic Index shows strong correlation with Molar Refractivity ($R^2 = 0.9960$) and Polarizability ($R^2 = 0.9954$).

- Symmetric division deg index shows good correlation with Molar Volume ($R^2 = 0.9773$) and Complexity ($R^2 = 0.9270$).

Now, we see that Table (6) records the evaluated neighborhood degree sum-based descriptors. Table (7) consists of correlated values of physico-chemical characteristics for anti-HIV medicines with neighborhood degree sum-based topological index. Further, the correlation of Fifth NDe index with Molar Volume and Complexity is depicted in figure (10).

- Neighborhood Harmonic Index values a strong correlation with Molar Refractivity ($R^2 = 0.9971$) and Polarizability ($R^2 = 0.9967$).

- Fifth NDe Index shows good correlation with Molar Volume ($R^2 = 0.9070$) and Complexity ($R^2 = 0.8734$).

Drugs	NM_1	NM_2	NmM_2	ND_3	NF	ND_5	NH	NI	S	$NR_{-1/2}$
Efavirenz	286	917	0.727	12972	1958	49.0149	3.9217	69.2395	1214.0486	3.5445
Abacavir	286	873	0.8134	11170	1794	49.8548	4.2212	70.4028	1141.6444	4.2718
Lamivudine	176	493	0.6472	5842	1028	33.9643	3.0531	42.9491	617.1237	3.1095
Doravirine	362	1068	1.0907	13386	2246	66.4944	5.535	87.9273	1358.0711	5.6491

Table 6: Anti-HIV Drugs with neighborhood degree sum based topological indices

Index	Molar Refractivity	Polarizability	Molar Volume	Complexity
NM_1	0.957465679	0.956327334	0.927528749	0.880404514
NM_2	0.898410861	0.896743504	0.894692313	0.818865754
NmM_2	0.981632831	0.982061783	0.892701109	0.93225984
ND_3	0.788997817	0.786586792	0.840436719	0.732840592
NF	0.885308454	0.883435818	0.905470209	0.826630068
ND_5	0.986696879	0.985959224	0.952340895	0.934583488
NH	0.998557994	0.998371678	0.928600573	0.933338554
NI	0.959505269	0.958454261	0.918330368	0.871690697
S	0.864337599	0.862490132	0.866003348	0.77764876
$NR_{-(1/2)}$	0.984926224	0.985599247	0.858066374	0.895243117

Table 7: The correlation values between the neighborhood degree sum-based topological indices with the anti-HIV drug properties

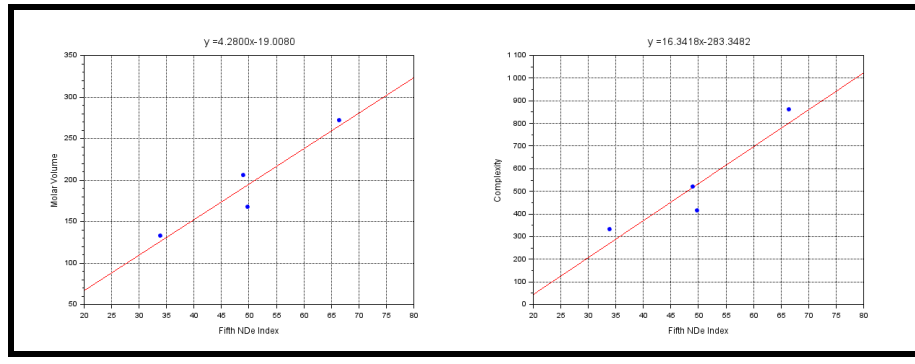


Figure 10: Correlation of ND_5 with Molar Volume & Complexity

The noted observations on the correlation reveal the utility of molecular descriptors for the physico-chemical properties of the specified anti-HIV pharmaceuticals during QSPR model. Chiefly, harmonic index and neighborhood harmonic index reflect strong positive correlation for Molar refractivity and Polarizability. Similar case holds for the symmetric division deg index and the fifth ND_e index. Hence, we can assert possibly that the studied descriptors are inherent units for QSPR inspection of drugs.

4. Conclusion

In medicinal discipline, every characteristic of a chemical graph is crucial to acquire an advanced drug and the process can be facilitated by the proper analysis of topological indices. Interpretation of M-polynomial and NM-polynomial for the mentioned pharmaceuticals are formulated on exploring the arrangement of the molecular compounds. The expression of the above polynomials aided in the determination of various degree-based as well as neighborhood degree sum-based molecular descriptors. Some strong correlations are also obtained between the descriptors and the physico-chemical properties for specified medications.

Accordingly, this paper analyses various favourable anti-HIV drugs in particular Efavirenz, Abacavir, Lamivudine and Doravirine. These medications play a vital role in antiretroviral therapy. Doravirine has highest value for all the specified topological indices out of all the above stated drugs. Clinically, defiance in opposition to Doravirine based antiretroviral therapies is anticipated to be limited. Pharmaceutical details on Doravirine along the prominence on drug persistence is found in [21]. These findings may be beneficial for recognising the efficacy of the mentioned anti-HIV therapeutic agents and treatment patterns of the ailment.

The action of nucleoside and non-nucleoside reverse transcriptase inhibitors is utilised for presenting drug implementation that lowers the HIV levels in blood by means of graph invariants. The proposed outcomes procured in this paper have favourable angles towards the designing of advanced and improvised anti-HIV drugs.

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