Graph Polynomial Approach for Some Molecules in H1N1 Antiviral Drugs

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Abstract

This study explores the potential of topological indices for oseltamivir and zanamivir, two common antiviral drugs. Topological indices are numerical descriptors of a molecule's structure, often used in drug discovery to predict various physical and chemical properties. We will calculate several polynomial-based indices for these drugs and analyse their relationship with their known physicochemical properties using linear regression. This analysis can provide insights into how a drug's structure influences its behaviour.

Keywords: Topological index, degree (of vertex), Chemical graph theory, Drug design
AMS Subject classication: 05C07, 05C09, 05C92

1. Introduction

The fight against infectious diseases remains a major focus in healthcare research. In 2009, a novel influenza A virus subtype, H1N1 (A/H1N1), emerged. This unique combination of influenza genes, never seen before in humans or animals, first infected a person in California and rapidly spread globally. The virus can cause serious respiratory illness. Extensive research efforts led to the development of vaccines to stop the spread, and antiviral medications like adamantanes (amantadine and rimantadine) and neuraminidase inhibitors (oseltamivir, zanamivir, and peramivir) are now used worldwide to treat influenza in humans.

The fact that both antiviral medications are routinely used as monotherapies has led to the emergence of influenza viruses that are resistant to both treatment groups [1, 2]. Because of this, only neuraminidase inhibitors (oseltamivir and zanamivir) are now recommended for treating influenza [3]. Oseltamivir and zanamivir can be used in combination treatment because of how differently they attach to the neuraminidase active site. It's improbable that viruses have zanamivir and oseltamivir resistance. Therefore, combining these two drugs in therapy is a good way to beat resistance.

Although it is used to treat influenza A and B virus infections, zanamivir appears to have few benefits in otherwise healthy people. However, it does not reduce the risk of asymptomatic flu. The diagnostic uncertainty, the possibility of viral strain resistance, the likelihood of side effects, and the expense of zanamivir exceed the meagre advantages it offers for prevention and treatment of healthy individuals [4]. A medication called oseltamivir is used to treat and prevent influenza brought on by the influenza A and B viruses. The World Health Organisation has classified it as a necessary medication. The WHO advises against it for seriously ill patients who have been admitted to the hospital and are experiencing a severe illness brought on by a known or suspected influenza virus infection.

Zanamivir is an antiviral medication used to treat and prevent influenza (the flu) caused by influenza A and B viruses. It is a neuraminidase inhibitor, which works by blocking the neuraminidase enzyme of the influenza virus. This enzyme is essential for the release of new virus particles from infected cells. By blocking neuraminidase, zanamivir prevents the spread of the virus and helps to shorten the duration of flu symptoms.

Figure 1

Zanamivir is available as a powder for inhalation. It is typically inhaled twice a day for 5 days to treat the flu, or once a day for 10 or 28 days to prevent the flu. Zanamivir is not a substitute for the flu vaccine. The flu vaccine is the best way to prevent the flu. However, zanamivir may be an option for people who cannot get the flu vaccine or who are sick with the flu.

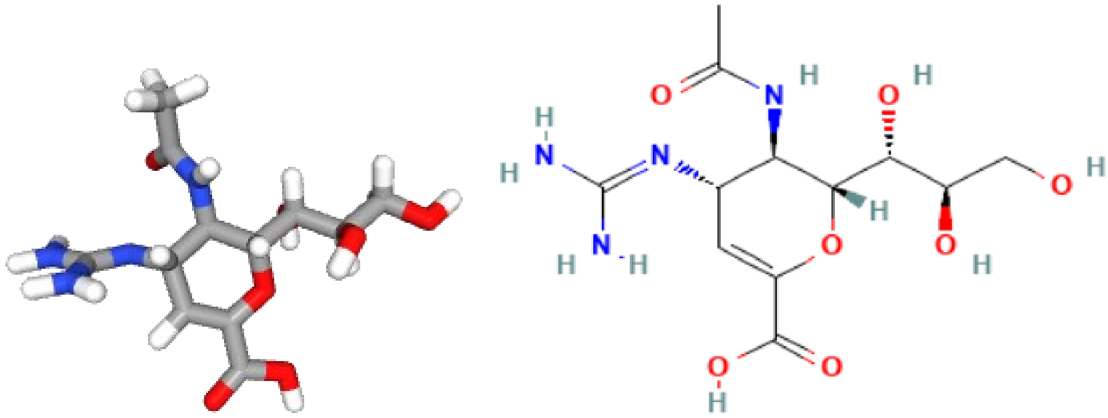

Figure 2. Structure of Zanamivir $C_{12}H_{20}N_4O_7$.

Oseltamivir, sold under the brand name Tamiflu, is an antiviral medication used to treat and prevent influenza A and B, viruses that cause the flu.

Figure 3

Many medical organizations recommend it in people who have complications or are at high risk of complications within 48 hours of first symptoms of infection. They recommend it to prevent infection in those at high risk, but not the general population. The Centers for Disease Control and Prevention (CDC) recommends that clinicians use their discretion to treat those at lower risk who present within 48 hours of first symptoms of infection.

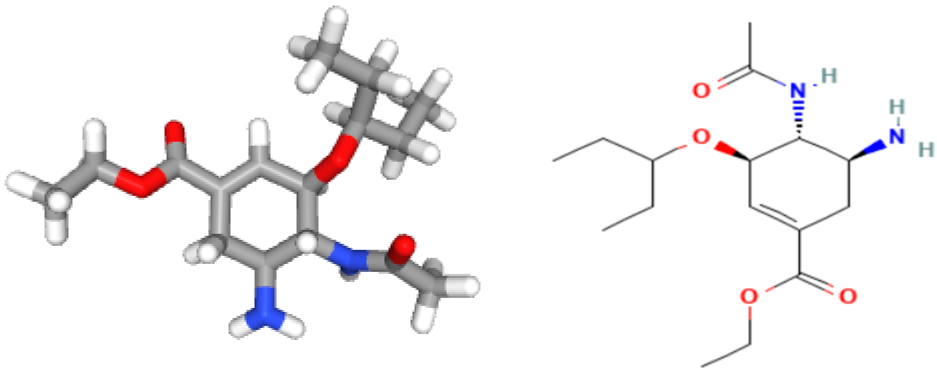

Figure 4. Structure of Oseltamivir $C_{16}H_{28}N_2O_4$

Here's how oseltamivir works:

- It is a neuraminidase inhibitor, a competitive inhibitor of influenza's neuraminidase enzyme.
- The enzyme cleaves the sialic acid which is found on glycoproteins on the surface of human cells that helps new virions to exit the cell, preventing new viral particles from being released.

Key points about Oseltamivir:

- It can shorten the duration of flu symptoms by 1-2 days.
- It may also help reduce the severity of symptoms.
- Oseltamivir is most effective when taken within 48 hours of the first symptoms of the flu.
- It is available in capsule and liquid forms.
- Oseltamivir is not a substitute for the flu vaccine. The flu vaccine is the best way to prevent the flu.

It is important to talk to your doctor about oseltamivir to see if it is right for you. They can also advise on the dosage and potential side effects.

2. Method and Analysis

Let G = (V, E) denote a graph with set of vertices V and two element subsets of V, known as the edges forming E. The degree of a vertex u is the number of vertices at distance one denoted as $d(u)$. In the literature, a number of graph polynomials were introduced, and some of them proved to be beneficial in Biology and Chemistry. Graph polynomials are functions of isomorphism-invariant graphs. Usually, they are polynomials with integer coefficients in one or two variables. Various applications of degree-based TDs were studied by many researchers in [2, 3, 8, 9, 12, 13, 16, and 17].

Let us use the following notation for the rest of the paper.

$$V_i = \{v \in V(G) | d(v) = i\} \text{ And } |V_i| = n_i$$

$$m_{ij} = |E_{ij}|, \text{Where } E_{ij} = \{uv \in E(G) | d(u) = i, d(v) = j\}$$

$$\bar{m}_{ij} = |\bar{E}_{ij}|, \text{Where } \bar{E}_{ij} = \{uv \notin E(G) | d(u) = i, d(v) = j\}$$

The M-polynomial [4] of graph G is defined as

$$M(G; x, y) = \sum_{i \le j} m_{ij}(G) x^i y^j,$$

Where $m_{ij}(G), i, j \ge 1$ be the number of edges $uv \in E(G)$ such that$\{(d(u), d(v)) = (i, j)\}$

Now we concentrate for non-adjacent pair of vertices and define $\bar{M}$- Polynomial [22] like M – polynomial as follows;

$$\bar{M}(G;x,y) = \sum_{i\le j} \bar{m}_{ij}(G)x^i y^j,$$

Where $\bar{m}_{ij}(G), i,j \ge 1$ be the number of edges $uv \notin E(G)$ such that$\{(d(u),d(v)) = (i,j)\}$

Let $\delta(v)$ represent the neighbourhood degree of v in the graph G, that is, $\delta(v) = \sum_{u\in N_G(u)} d(u)$, where $N_G(u)$ being the set of adjacent vertices of u.

Let $\chi_{i,j}(G); i,j \ge 1$be the number of edges $e = uv$of G such that $\{\delta(u),\delta(v)\} = \{i,j\}$

Then the NM-Polynomial [19, 20, and 21] of graph G is defined as

$$NM(G;x,y) = \sum_{i\le j} \chi_{i,j}(G)x^i y^j.$$

3. Formulation of some TDs from polynomials

Some degree-based, some neighbourhood degree-based TDs and their association with $\bar{M}$-Polynomial and NM-Polynomial of a graph G respectively are given below in the Table 1 and 2 of form

$$D_x = x\frac{\partial\big(f(x,y)\big)}{\partial x}, D_x = y\frac{\partial\big(f(x,y)\big)}{\partial y}, S_x = \int_0^x \frac{f(t,y)}{t}dt, S_x = \int_0^y \frac{f(x,t)}{t}dt,$$

$$J(f(x,y)) = f(x,x) \ \ and \ Q_k(f(x,y)) = x^k f(x,y)$$

Table 1. Description of some degree-based descriptors

Degree- based Topological indices	**Mathematical Expression**	**Derivative $M(G,x,y)$**
First Zagreb index	$\sum_{uv\in E(G)} (d(u)+d(v))$	$(D_x + D_y)(M(G,x,y))/x = 1, y = 1.$
second Zagreb index	$\sum_{uv\in E(G)} d(u)\, d(v)$	$(D_x * D_y)(M(G,x,y))/x = 1, y = 1.$
F-index	$\sum_{uv\in E(G)} (d^2(u)+d^2(v))$	$(D^2{}_x + D^2{}_y)(M(G,x,y))/x = 1, y = 1.$
Second modified Zagreb index	$\sum_{uv\in E(G)} \frac{1}{d(u)d(v)}$	$(S_x * S_y)(M(G,x,y))/x = 1, y = 1.$
Symmetric Division index	$\sum_{uv\in E(G)} \frac{d^2(u)+d^2(v)}{d(u)d(v)}$	$(D_xS_y + S_xD_y)\big(M(G,x,y)\big)/x = 1,$ $y = 1.$
Harmonic index	$\sum_{uv\in E(G)} \frac{2}{d(u)+d(v)}$	$(2S_xJ)(M(G,x,y))/x = 1.$
Inverse sum index	$\sum_{uv\in E(G)} \frac{d(u)d(v)}{d(u)+d(v)}$	$(S_xJD_xD_y)(M(G,x,y))/x = 1.$

Augmented Zagreb index	$\sum_{uv\in E(G)} \left(\frac{d(u)d(v)}{d(u)+d(v)-2}\right)^3$	$(S_x{}^3Q_{-2}JD_x{}^3D_y{}^3)(M(G,x,y))/x=1.$

Table 2. Description of some degree-based co-descriptors

Degree- based Topological coindices	Mathematical Expression	Derivative $\bar{M}(G,x,y)$
First Zagreb coindex	$\sum_{uv\in E(G)} (d(u)+d(v))$	$(D_x+D_y)(\ \bar{M}(G,x,y)\ )/$ $x=1, y=1.$
second Zagreb coindex	$\sum_{uv\in E(G)} d(u)\,d(v)$	$(D_x * D_y)(\bar{M}(G,x,y))/x=1,$ $y=1.$
F-coindex	$\sum_{uv\in E(G)} (d^2(u)+d^2(v))$	$(D^2{}_x+D^2{}_y)(\bar{M}(G,x,y))/$ $x=1, y=1.$
Second modified Zagreb coindex	$\sum_{uv\in E(G)} \frac{1}{d(u)d(v)}$	$(S_x * S_y)(\bar{M}(G,x,y))/x=1,$ $y=1.$
Symmetric Division coindex	$\sum_{uv\in E(G)} \frac{d^2(u)+d^2(v)}{d(u)d(v)}$	$(D_xS_y+S_xD_y)(\bar{M}(G,x,y))/$ $x=1, y=1.$
Harmonic coindex	$\sum_{uv\in E(G)} \frac{2}{d(u)+d(v)}$	$(2S_xJ)(\bar{M}(G,x,y))/x=1.$
Inverse sum coindex	$\sum_{uv\in E(G)} \frac{d(u)d(v)}{d(u)+d(v)}$	$(S_xJD_xD_y)(\bar{M}(G,x,y))/x=1.$
Augmented Zagreb coindex	$\sum_{uv\in E(G)} \left(\frac{d(u)d(v)}{d(u)+d(v)-2}\right)^3$	$(S_x{}^3Q_{-2}JD_x{}^3D_y{}^3)(\bar{M}(G,x,y))$ $/x=1.$

Table 3. Description of some degree-based neighbourhood descriptors

Neighbourhood degree -based topological indices	Mathematical Expression	Derivative of $NM(G_1,x,y)$
Neighbourhood First Zagreb index	$\sum_{uv\in E(G)} (\delta(u)+\delta(v))$	$(D_x+D_y)(NM(G,x,y))/x=1,$ $y=1.$
Neighbourhood second Zagreb index	$\sum_{uv\in E(G)} \delta(u)\delta(v)$	$(D_x * D_y)(NM(G,x,y))/x=1,$ $y=1.$
Neighbourhood F-index	$\sum_{uv\in E(G)} \delta^2(u)+\delta^2(v)$	$(D^2{}_x+D^2{}_y)(NM(G,x,y))/x=1,$ $y=1.$

Neighbourhood Second modified Zagreb index	$\sum_{uv\in E(G)} \frac{1}{\delta(u)\delta(v)}$	$(S_x * S_y)(NM(G,x,y)/x = 1, y = 1.$
Neighbourhood Symmetric Division index	$\sum_{uv\in E(G)} \frac{\delta^2(u)+\delta^2(v)}{\delta(u)\delta(v)}$	$(D_xS_y + S_xD_y)(NM(G,x,y))/x = 1, y = 1.$
Neighbourhood Harmonic index	$\sum_{uv\in E(G)} \frac{2}{\delta(u)+\delta(v)}$	$(2S_xJ)(NM(G,x,y))/x = 1.$
Neighbourhood Inverse sum index	$\sum_{uv\in E(G)} \frac{\delta(u)\delta(v)}{\delta(u)+\delta(v)}$	$(S_xJD_xD_y)(NM(G,x,y))/x = 1.$
Neighbourhood Augmented Zagreb index	$\sum_{uv\in E(G)} \left(\frac{\delta(u)\delta(v)}{\delta(u)+\delta(v)-2}\right)^3$	$(S_x{}^3Q_{-2}JD_x{}^3D_y{}^3)(NM(G,x,y))/ x = 1.$

Lemma 1. For a connected graph G of n vertices
Whenever$i \neq j, \bar{m}_{ij} = |\bar{E}_{ij}| = n_in_j - m_{ij}$
Whenever$i = j, \bar{m}_{ij} = |\bar{E}_{ij}| = \frac{(n_i-1)n_j}{2} - m_{ij}$

Theorem 1. Let G_1 be a molecular graph of Zanamivir. Then

(i) $M(G_1: x,y) = 7xy^3 + xy^2 + 11x^2y^3 + 3x^3y^3$

(ii) $\overline{M}(G_1,x,y) = 57xy^3 + 47xy^2 + 37x^2y^3 + 25x^3y^3$

(iii) $NM(G_1,x,y) = x^2y^4 + 4x^3y^4 + 3x^3y^5 + 4x^4y^6 + 3x^5y^6 + x^5y^8 + x^6y^8 + 2x^6y^7 + 2x^4y^5 + x^7y^8$

Proof. From the structure of the molecular graphG_1, one can obtain that $|V(G_1)| = 22$ and $|E(G_1)| = 22$.

(i) The edge set of G_1 may be categorizes into three following categorizes on the degree of vertices edge partitions:

$$m_{13} = |E_{13}| = 7, m_{12} = |E_{12}| = 1, m_{23} = |E_{23}| = 11, m_{33} = |E_{33}| = 3$$

By the definition of M - Polynomial,

$$M(G_1; x,y) = \sum_{i\leq j} m_{ij}\, x^iy^j$$
$$= m_{12}xy^2 + m_{13}xy^3 + m_{23}x^2y^3 + m_{33}x^3y^3$$
$$= xy^2 + 7xy^3 + 11x^2y^3 + 3x^3y^3.$$

(ii) The vertex set can be partition into subsets, namely $|V_1| = 8$, $|V_2| = 6$, $|V_3| = 8$

Using lemma 1, we obtain

$$\overline{m}_{12} = n_1n_2 - m_{12} = 47$$
$$\overline{m}_{13} = n_1n_3 - m_{13} = 57$$
$$\overline{m}_{23} = n_2n_3 - m_{23} = 37$$
$$\overline{m}_{33} = \left\{\frac{(n_3-1)n_3}{2}\right\} - m_{33} = 25$$

By the definition of $\bar{M}$- Polynomial,

$$\overline{M}(G_1;x,y) = \sum_{i\le j} \overline{m_{ij}}\, x^i y^j$$
$$= \overline{m_{13}}xy^3 + \overline{m_{12}}xy^2 + \overline{m_{23}}x^2y^3 + \overline{m_{33}}x^3y^3$$
$$= 57xy^3 + 47xy^2 + 37x^2y^3 + 25x^3y^3.$$

(iii) χ_{ij} denote the set of all edges with neighbourhood degree sum of end vertices i and j from the construction of the graph G_1, we obtain $\upsilon_{ij} = |\chi_{ij}| = 22$, $\upsilon_{24} = |\chi_{24}| = 1$, $\upsilon_{34} = |\chi_{34}| = 4$, $\upsilon_{35} = |\chi_{35}| = 3$, $\upsilon_{46} = |\chi_{46}| = 4$, $\upsilon_{56} = |\chi_{56}| = 3$, $\upsilon_{58} = |\chi_{58}| = 1$, $\upsilon_{68} = |\chi_{68}| = 1$, $\upsilon_{67} = |\chi_{67}| = 2$, $\upsilon_{45} = |\chi_{45}| = 2$, $\upsilon_{78} = |\chi_{78}| = 1$.

Hence from the definition of NM Polynomial we obtain

$$NM(G_1,x,y) = \sum_{i\le j} \upsilon_{ij}\, x^i y^j$$
$$= \upsilon_{24}x^2y^4 + \upsilon_{34}x^3y^4 + \upsilon_{35}x^3y^5 + \upsilon_{46}x^4y^6 + \upsilon_{56}x^5y^6$$
$$+\upsilon_{58}x^5y^8 + \upsilon_{68}x^6y^8 + \upsilon_{67}x^6y^7 + \upsilon_{45}x^4y^5 + \upsilon_{78}x^7y^8.$$

$$NM(G_1{:}\,x,y) = x^2y^4 + 4x^3y^4 + 3x^3y^5 + 4x^4y^6 + 3x^5y^6 + x^5y^8$$
$$+x^6y^8 + 2x^6y^7 + 2x^4y^5 + x^7y^8.$$

Now we present the some degree- based and Neighbourhood degree- based topological indices of molecular graph of Zanamivir using M- Polynomial, $\overline{M}$- Polynomial and NM – Polynomial. From Table 1, we obtain the following;

1. $(D_x + D_y)_{x=1,y=1} = 28xy^3 + 3xy^2 + 55x^2y^3 + 18x^3y^3|_{x=1,y=1} = 104.$
2. $(D_xD_y)_{x=1,y=1} 21xy^3 + 2xy^2 + 66x^2y^3 + 27x^3y^3|_{x=1,y=1} = 116.$
3. $(D_x{}^2 + D_y{}^2)_{x=1,y=1} = 70xy^3 + 5xy^2 + 143x^2y^3 + 54x^3y^3|_{x=1,y=1} = 272.$
4. $(S_xS_y)_{x=1,y=1} = \frac{7}{3}xy^3 + \frac{1}{2}xy^2 + \frac{11}{6}x^2y^3 + \frac{3}{9}x^3y^3|_{x=1,y=1} = 547.$
5. $(D_xS_y + D_yS_x)_{x=1,y=1} = \frac{70}{3}xy^3 + \frac{5}{2}xy^2 + \frac{143}{6}x^2y^3 + 9x^3y^3|_{x=1,y=1} = 58.6667.$
6. $(2S_xJ)_{x=1,y=1} = \frac{7}{2}x^4 + \frac{2}{3}x^3 + \frac{22}{5}x^5 + x^6|_{x=1,y=1} = 9.5667.$
7. $(S_xJD_xD_y)_{x=1,y=1} = \frac{21}{4}x^4 + \frac{2}{3}x^3 + \frac{66}{5}x^5 + \frac{27}{6}x^6|_{x=1,y=1} = 23.6167.$
8. $(S_x^3Q_{-2}JD_x^3D_y^3)_{x=1,y=1} = \frac{189}{8}x^4 + 8x^3 + \frac{2376}{27}x^5 + \frac{2178}{64}x^6|_{x=1,y=1} = 153.7969.$

Likewise, Table 2, we have the following

1. $(D_x + D_y)_{x=1,y=1} = 228xy^3 + 141xy^2 + 185x^2y^3 + 150x^3y^3|_{x=1,y=1} = 704.$
2. $(D_xD_y)_{x=1,y=1} = 171xy^3 + 94xy^2 + 222x^2y^3 + 225x^3y^3|_{x=1,y=1} = 712.$

3. $(D_x{}^2 + D_y{}^2)_{x=1,y=1} = 570xy^3 + 235xy^2 + 481x^2y^3 + 450x^3y^3|_{x=1,y=1} = 1736.$
4. $(S_xS_y)_{x=1,y=1} = \frac{57}{3}xy^3 + \frac{47}{3}xy^2 + \frac{37}{3}x^2y^3 + \frac{25}{3}x^3y^3|_{x=1,y=1} = 166.$
5. $(D_xS_y + D_yS_x)_{x=1,y=1} = 190xy^3 + \frac{235}{2}xy^2 + \frac{481}{6}x^2y^3 + \frac{450}{9}x^3y^3|_{x=1,y=1} = 437.6667$
6. $(2S_xJ)_{x=1,y=1} = \frac{114}{4}x^4 + \frac{94}{3}x^3 + \frac{74}{5}x^5 + \frac{50}{6}x^6|_{x=1,y=1} = 82.9667.$
7. $(S_xJD_xD_y)_{x=1,y=1} = \frac{171}{4}x^4 + \frac{94}{3}x^3 + \frac{222}{5}x^5 + \frac{225}{6}x^6|_{x=1,y=1} = 155.9833.$
8. $(S_x^3Q_{-2}JD_x^3D_y^3)_{x=1.y=1} = \frac{1539}{8}x^2 + 376x + 296x^3 + \frac{18225}{64}x^4|_{x=1,y=1} = 1149.6094.$

Finally from Table 3, we obtain the value of following neighbourhood degree- based indices

1. $(D_x + D_y)_{x=1,y=1`} = 6x^2y^4 + 28x^3y^4 + 24x^3y^5 + 40x^4y^6 + 33x^5y^6 + 13x^5y^8 + 14x^6y^8 + 26x^6y^7 + 18x^4y^5 + 15x^7y^8|_{x=1,y=1} = 217.$
2. $(D_xD_y)_{x=1,y=1} = 8x^2y^4 + 48x^3y^4 + 45x^3y^5 + 96x^4y^6 + 90x^5y^6 + 40x^5y^8 + 48x^6y^8 + 84x^6y^7 + 40x^4y^5 + 56x^7y^8|_{x=1,y=1} = 555.$
3. $(D_x{}^2 + D_y{}^2)_{x=1,y=1} = 64x^2y^4 + 576x^3y^4 + 675x^3y^5 + 2304x^4y^6 + 2700\,x^5y^6 + 1600x^5y^8 + 2304x^6y^8 + 3528x^6y^7 + 800x^4y^5 + 3136x^7y^8|_{x=1,y=1} = 17687.$
4. $(S_xS_y)_{x=1,y=1} = \frac{1}{8}x^2y^4 + \frac{1}{3}x^3y^4 + \frac{1}{5}x^3y^5 + \frac{1}{6}x^4y^6 + \frac{1}{10}x^5y^6 + \frac{1}{40}x^5y^8 + \frac{1}{48}x^6y^8 + \frac{1}{21}x^6y^7 + \frac{1}{10}x^4y^5 + \frac{1}{56}x^7y^8|_{x=1,y=1} = 1.1363.$
5. $(D_xS_y + D_yS_x)_{x=1,y=1} = \frac{20}{8}x^2y^4 + \frac{100}{12}x^3y^4 + \frac{102}{15}x^3y^5 + \frac{208}{24}x^4y^6 + \frac{183}{30}x^5y^6 + \frac{89}{40}x^5y^8 + \frac{100}{48}x^6y^8 + \frac{156}{42}x^6y^7 + \frac{82}{20}x^4y^5 + x^7y^8|_{x=1,y=1} = 46.5405$
6. $(2S_xJ)_{x=1,y=1} = \frac{2}{6}x^6 + \frac{4}{7}x^7 + \frac{3}{8}x^8 + \frac{4}{10}x^{10} + \frac{3}{11}x^{11} + \frac{1}{13}x^{13} + \frac{1}{14}x^{14} + \frac{2}{13}x^{13} + \frac{2}{9}x^9 + \frac{1}{15}x^{15}|_{x=1,y=1} = 2.5436.$
7. $(S_xJD_xD_y)_{x=1,y=1} = \frac{8}{6}x^6 + \frac{48}{7}x^7 + \frac{45}{8}x^8 + \frac{96}{10}x^{10} + \frac{90}{11}x^{11} + \frac{40}{13}x^{13} + \frac{48}{14}x^{14}$

$$+\frac{84}{13}x^{13}+\frac{40}{9}x^{9}+\frac{56}{15}x^{15}|_{x=1,y=1}=52.7421.$$

8. $$\left(S_x^3Q_{-2}JD_x^3D_y^3\right)_{x=1,y=1}=8x^4+\frac{6912}{125}x^5+\frac{10125}{216}x^6+\frac{55296}{512}x^8+\frac{81000}{729}x^9+\frac{64000}{1331}x^{11}+\frac{110592}{1728}x^{12}+\frac{148176}{1331}x^{11}+\frac{16000}{343}x^7+\frac{175616}{2197}x^{13}|_{x=1,y=1}=679.2748.$$

Theorem 2. Let G_2 be a molecular graph of Oseltamivir. Then

(i) $M(G_2,x,y)=3xy^2+4xy^3+11x^2y^3+x^2y^2+3x^3y^3$

(ii) $\overline{M}(G_2,x,y)=53xy^2+45xy^3+45x^2y^3+25x^2y^2+18x^3y^3$

(iii) $NM(G_2,x,y)=2x^2y^4+x^2y^3+2x^3y^4+x^3y^5+3x^4y^6+x^5y^6+2x^6y^6+5x^6y^7+x^7y^8+2x^3y^6+2x^6y^8$

Proof. From the structure of the molecular graphG_2, one can obtain that $|V(G_2)|=22$ and $|E(G_2)|=22$.
The edge set of G_2 may be categorizes into three following categorizes on the degree of vertices edge partitions:
$m_{13}=|E_{13}|=4$,$m_{12}=|E_{12}|=3$,$m_{23}=|E_{23}|=11$, $m_{22}=|E_{22}|=1$, $m_{33}=|E_{33}|=3$.
By the definition of M - Polynomial,

$$M(G_2;x,y)=\sum_{i\le j} m_{ij}\,x^iy^j$$
$$M(G_2;x,y)=m_{12}xy^2+m_{13}xy^3+m_{23}x^2y^3+m_{22}x^2y^2+m_{33}x^3y^3$$
$$M(G_2;x,y)=xy^2+7xy^3+11x^2y^3+x^2y^2+3x^3y^3$$

The vertex set can be partition into subsets, namely $|V_1|=7$, $|V_2|=8$, $|V_3|=7$.
Using Lemma 1, we obtain

$$\overline{m}_{12}=n_1n_2-m_{12}=53$$
$$\overline{m}_{13}=n_1n_3-m_{13}=45$$
$$\overline{m}_{23}=n_2n_3-m_{23}=45$$
$$\overline{m}_{22}=\left\{\frac{(n_2-1)n_2}{2}\right\}-m_{22}=27$$
$$\overline{m}_{33}=\left\{\frac{(n_3-1)n_3}{2}\right\}-m_{33}=18$$

By the definition of $\bar{M}$- Polynomial,

$$\overline{M}(G_1;x,y)=\sum_{i\le j}\overline{m_{ij}}\,x^iy^j$$
$$\overline{M}(G_1;x,y)=\overline{m_{13}}xy^3+\overline{m_{12}}xy^2+\overline{m_{23}}x^2y^3+\overline{m_{22}}x^2y^2+\overline{m_{33}}x^3y^3$$
$$\overline{M}(G_1;x,y)=53xy^2+45xy^3+45x^2y^3+25x^2y^2+18x^3y^3$$

χ_{ij} denote the set of all edges with neighbourhood degree sum of end vertices *i* and *j* from the construction of the graphG_2, we obtain $\upsilon_{ij}=|\chi_{ij}|=22$, $\upsilon_{24}=|\chi_{24}|=$

$2, \upsilon_{23} = |\chi_{23}| = 1, \upsilon_{34} = |\chi_{34}| = 2, \upsilon_{35} = |\chi_{35}| = 1, \upsilon_{46} = |\chi_{46}| = 3, \upsilon_{56} = |\chi_{56}| = 1, \upsilon_{66} = |\chi_{66}| = 2, \upsilon_{67} = |\chi_{67}| = 5,\ \upsilon_{78} = |\chi_{78}| = 1, \upsilon_{36} = |\chi_{36}| = 2, \upsilon_{68} = |\chi_{68}| = 2.$

Hence from the definition of NM- Polynomial we obtain

$$NM(G_1, x, y) = \sum_{i \le j} \upsilon_{ij}\, x^i y^j$$

$$NM(G_1, x, y) = \upsilon_{24}x^2y^4 + \upsilon_{34}x^3y^4 + \upsilon_{35}x^3y^5 + \upsilon_{46}x^4y^6 + \upsilon_{56}x^5y^6 + \upsilon_{58}x^5y^8 + \upsilon_{68}x^6y^8 + \upsilon_{67}x^6y^7 + \upsilon_{45}x^4y^5 + \upsilon_{78}x^7y^8.$$

$$NM(G_1 : x, y) = x^2y^4 + 4x^3y^4 + 3x^3y^5 + 4x^4y^6 + 3x^5y^6 + x^5y^8 + x^6y^8 + 2x^6y^7 + 2x^4y^5 + x^7y^8.$$

Now we present the some degree- based and Neighbourhood degree- based topological indices of molecular graph of Zanamivir using M- Polynomial, $\overline{M}$- Polynomial and NM – Polynomial. From Table 1, we obtain the following

$$M(G_2, x, y) = 3xy^2 + 4xy^3 + 11x^2y^3 + x^2y^2 + 3x^3y^3$$

1. $(D_x + D_y)_{x=1,y=1} = 9xy^2 + 16xy^3 + 55x^2y^3 + 4x^2y^2 + 18x^3y^3|_{x=,y=1} = 102.$
2. $(D_xD_y)_{x=1,y=1} = 6xy^2 + 12xy^3 + 66x^2y^3 + 4x^2y^2 + 27x^3y^3|_{x=1,y=1} = 115.$
3. $({D_x}^2 + {D_y}^2)_{x=1,y=1} = 15xy^2 + 40xy^3 + 143x^2y^3 + 8x^2y^2 + 54x^3y^3|_{x=1,y=1} = 260.$
4. $(S_xS_y)_{x=1,y=1} = \frac{3}{2}xy^2 + \frac{4}{3}xy^3 + \frac{11}{6}x^2y^3 + \frac{1}{4}x^2y^2 + \frac{3}{9}x^3y^3|_{x=1,y=1} = 5.25.$
5. $\left(D_xS_y + D_yS_x\right)_{x=1,y=1} = \frac{15}{2}xy^2 + \frac{40}{3}xy^3 + \frac{143}{6}x^2y^3 + 2x^2y^2 + 9x^3y^3|_{x=1,y=1} = 55.6667.$
6. $(2S_xJ)_{x=1,y=1} = 2x^3 + 2x^4 + \frac{25}{5}x^5 + \frac{2}{4}x^4 + x^6|_{x=1,y=1} = 9.9000.$
7. $\left(S_xJD_xD_y\right)_{x=1,y=1} = 2x^3 + 3x^4 + \frac{66}{5}x^5 + x^4 + \frac{27}{6}x^6|_{x=1,y=1} = 23.7.$
8. $\left(S_x^3Q_{-2}JD_x^3D_y^3\right)_{x=1,y=1} = 24x + \frac{108}{8}x^2 + 88x^3 + 8x^2 + \frac{2187}{64}x^4|_{x=1,y=1} = 167.6719.$

Likewise Table 2 we have the following indices,

$$\overline{M}(G_2) = 53xy^2 + 45xy^3 + 45x^2y^3 + 25x^2y^2 + 18x^3y^3$$

1. $\left(D_x + D_y\right)_{x=1,y=1} = 159xy^2 + 180xy^3 + 225x^2y^3 + 108x^2y^2 + 108x^3y^3|_{x=1,y=1}$

$= 780.$

2. $\left(D_xD_y\right)_{x=1,y=1} = 106xy^2 + 135xy^3 + 270x^2y^3 + 108x^2y^2 + 162x^3y^3|_{x=1,y=1}$

$= 781.$

3. $\left({D_x}^2 + {D_y}^2\right)_{x=1,y=1} = 265xy^2 + 450xy^3 + 585x^2y^3 + 216x^2y^2$

$+324x^3y^3|_{x=1,y=1} = 1840.$

4. $\left(S_xS_y\right)_{x=1,y=1} = \frac{53}{2}xy^2 + \frac{45}{3}xy^3 + \frac{45}{6}x^2y^3 + \frac{27}{4}x^2y^2 + \frac{18}{9}x^3y^3|_{x=1,y=1} = 57.75.$

5. $\left(D_xS_y + D_yS_x\right)_{x=1,y=1} = \frac{265}{2}xy^2 + \frac{450}{3}xy^3 + \frac{585}{6}x^2y^3 + \frac{216}{4}x^2y^2$

$+x^3y^3|_{x=1,y=1} = 470.$

6. $(2S_xJ)_{x=1,y=1} = \frac{106}{3}x^3 + \frac{90}{4}x^4 + \frac{90}{5}x^5 + \frac{54}{4}x^4\frac{36}{6}x^6|_{x=1,y=1} = 95.3333.$

7. $\left(S_xJD_xD_y\right)_{x=1,y=1} = \frac{106}{3}x^3 + \frac{135}{4}x^4 + \frac{270}{5}x^5 + \frac{108}{4}x^4 + \frac{162}{6}x^6|_{x=1,y=1}$

$= 177.0833.$

8. $\left(S_x^3Q_{-2}JD_x^3D_y^3\right)_{x=1,y=1} = \frac{424}{1}x + \frac{1215}{8}x^2 + \frac{9720}{27}x^3 + \frac{1728}{8}x^2 + \frac{13122}{64}x^4|_{x=1,y=1}$

$= 1356.9063.$

Finally from Table 3, we obtain the value of following neighbourhood degree- based indices

$$NM(G_1, x, y) = 2x^2y^4 + x^2y^3 + 2x^3y^4 + x^3y^5 + 3x^4y^6 + x^5y^6 + 2x^6y^6 + 5x^6y^7 + x^7y^8 + 2x^3y^6 + 2x^6y^8.$$

1. $\left(D_x + D_y\right)_{x=1,y=1} = 12x^2y^4 + 5x^2y^3 + 14x^3y^4 + 8x^3y^5 + 30x^4y^6 + 11x^5y^6$

$+24x^6y^6 + 65x^6y^7 + 15x^7y^8 + 18x^3y^6 + 26x^6y^8|_{x=1,y=1} = 228.$

2. $\left(D_xD_y\right)_{x=1,y=1} = 16x^2y^4 + 6x^2y^3 + 24x^3y^4 + 15x^3y^5 + 72x^4y^6 + 30x^5y^6 + 72x^6y^6$

$+210x^6y^7 + 56x^7y^8 + 36x^3y^6 + 96x^6y^8|_{x=1,y=1} = 633.$

3. $\left({D_x}^2 + {D_y}^2\right)_{x=1,y=1} = 40x^2y^4 + 13x^2y^3 + 50x^3y^4 + 34x^3y^5 + 156x^4y^6 + 61x^5y^6$

$+144x^6y^6 + 425x^6y^7 + 113x^7y^8 + 90x^3y^6 + 200x^6y^8|_{x=1,y=1}$

$= 1326.$

4. $\left(S_xS_y\right)_{x=1,y=1} = \frac{2}{8}x^2y^4 + \frac{2}{8}x^2y^3 + \frac{2}{12}x^3y^4 + \frac{1}{15}x^3y^5 + \frac{3}{24}x^4y^6 + \frac{1}{30}x^5y^6$

$$+\frac{2}{36}x^6y^6+\frac{5}{42}x^6y^7+\frac{1}{56}x^7y^8+\frac{2}{18}x^3y^6+\frac{2}{48}x^6y^8|_{x=1,y=1}$$

$$=1.1535.$$

5. $\left(D_xS_y+D_yS_x\right)_{x=1,y=1}=5x^2y^4+\frac{13}{6}x^2y^3+\frac{42}{12}x^3y^4+\frac{34}{15}x^3y^5+\frac{156}{24}x^4y^6+\frac{61}{30}x^5y^6+4x^6y^6+\frac{425}{42}x^6y^7+\frac{113}{56}x^7y^8+\frac{90}{18}x^3y^6+\frac{200}{48}x^6y^8|_{x=1,y=1}=47.4910.$

6. $(2S_xJ)_{x=1,y=1}=\frac{4}{6}x^6+\frac{2}{5}x^5+\frac{4}{7}x^7+\frac{2}{8}x^8+\frac{6}{10}x^{10}+\frac{2}{11}x^{11}+x^{12}+\frac{10}{13}x^{13}+\frac{2}{15}x^{15}+\frac{4}{9}x^9+\frac{4}{14}x^{14}|_{x=1,y=1}=4.6358.$

7. $\left(S_xJD_xD_y\right)_{x=1,y=1}=\frac{16}{6}x^6+\frac{6}{5}x^5+\frac{24}{7}x^7+\frac{15}{8}x^8+\frac{72}{10}x^{10}+\frac{30}{11}x^{11}\frac{72}{12}x^{12}+\frac{210}{13}x^{13}+\frac{56}{15}x^{15}+\frac{36}{9}x^9+\frac{96}{14}x^{14}=55.8418.$

8. $\left(S_x^3Q_{-2}JD_x^3D_y^3\right)_{x=1,y=1}=\frac{1024}{64}x^4+\frac{216}{27}x^3+\frac{3456}{125}x^5+\frac{3375}{216}x^6+\frac{41472}{512}x^8+\frac{27000}{729}x^9+\frac{93312}{1000}x^{10}\frac{370440}{1331}x^{11}+\frac{175616}{2197}x^{13}+\frac{11664}{343}x^7+\frac{221184}{1728}x^{12}|_{x=1,y=1}=798.9094.$

Graph Descriptors	**Drug 1**			**Drug 2**		
	M	$\bar{M}$	NM	M	$\bar{M}$	NM
First Zagreb index	104	704	217	102	780	228
Second Zagreb index	116	702	555	115	781	633
F-index	272	1726	17.69	260	1840	1326
Second modified Zagreb index	5	166	1.14	5.25	57.75	1.1535
Symmetric Division index	58.667	437.67	46.56	55.67	470	47.49
Harmonic index	9.57	82.97	2.5456	9.9	95.3333	4.6358
Inverse sum index	23.62	155.98	52.74	23.7	177.08	55.84

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Augmented Zagreb index	153.79	1149.61	679.27	167.67	1356.91	798.91

Table 4. Topological descriptors of the Drugs.

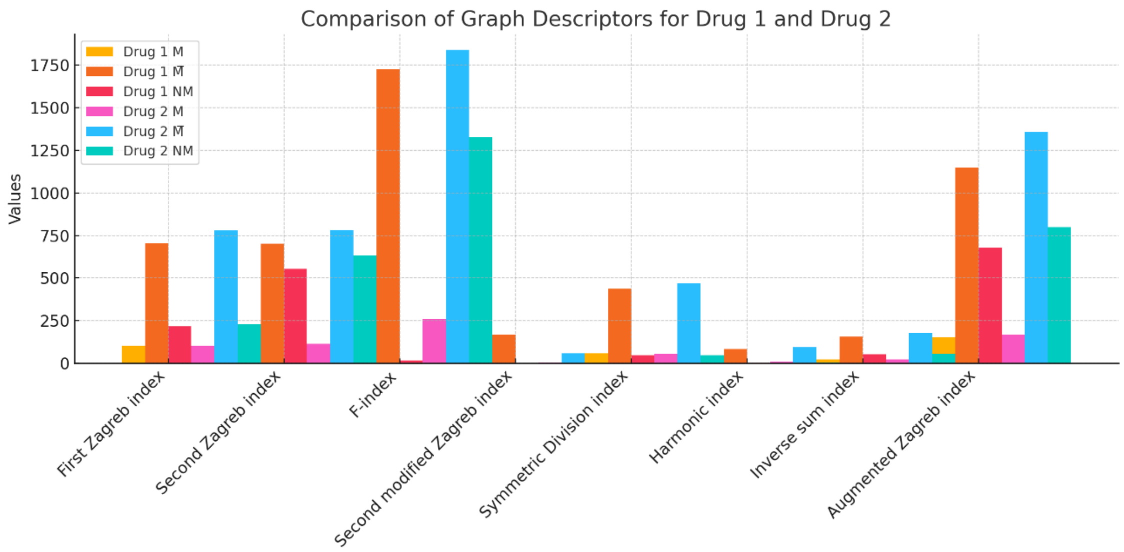

Figure 5. Bar graph comparing the graph descriptors of Drug 1 and Drug 2 across different parameters.

4. Conclusion

This study highlights the significance of topological indices in understanding the structural properties of oseltamivir and zanamivir. The correlations established with physicochemical properties emphasize their potential in drug discovery and molecular characterization, contributing to the development of more effective antiviral agents.

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