TO PREDICT THE ZAGREB ENERGIES ON MOLECULAR STRUCTURE OF ANTI-HIV DRUGS

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Abstract

Molecular topology plays a significant role in establishing quantitative structure-property relationships (QSAR) between chemical structures and their activity. QSAR provides direction to design optimized structures as potential therapeutic agents. In view of the contribution of topological energies (Zagreb energies) in the Human Immunodeficiency Virus-1(HIV-1) drug research, few reverse transcriptase inhibitors were selected and their Zagreb energies were calculated using graph theory derived mathematical models.

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1. INTRODUCTION

Chemical graph theory provides reliable descriptors which define topological information using mathematical modelling. These descriptors are derived mathematically and do not consider physicochemical properties of a chemical structure [1]. In the recent years, topological descriptors are extensively applied in the research areas of drug development by QSAR, nanotechnology, theoretical and mathematical chemistry. Two-dimensional structure is used to derive topological descriptors. The pattern of branching, size and shape characteristics of structure can be calculated. Structural similarity and diversity can be very well analyzed with these types of descriptors. Calculation of topological descriptors does not require any tedious chemical experimentation as required for computing chemical properties and hence are much appreciated [2-4].

Estrada et.al [5, 6] revealed a strong association of topology of molecular structures and their physic-chemical (melting point &boiling point) and bioactivity values. Literature reveals existence of various mathematical ways to derive topological descriptors. Some of the important indices important in drug research include Zagreb index [7], harmonic index[8], connectivity index[9] and Wiener index [10]. In 2016, Gao et al., determined topological indices for smart polymers used in the drug delivery of anticancer drugs [11].

In chemical graph theory chemical structures are represented as molecular graphs in which every vertex denotes an atom of a molecule and every edge corresponds to covalent bounds between two atoms. Let $G = (V(G), E(G))$ be a 2-dimensional molecular graph with vertex set $V(G)$ and edge set $E(G)$.

2. ZAGREB MATRICES AND ZAGREB ENERGIES OF A GRAPH

In 2005, Rodriguez [12] studied that the spectral properties of indices are interrelationship between the weighted adjacency matrix to the topological indices. Since then, major developments of chemical graph theory has occurred [2,3,6,8,10,13]. Recently Banasode et.al., [13] studied various Zagreb indices and energies of few biologically important compounds such as glucose, cholesterol and vitamins.

Antiretroviral drugs are effective as anti-HIV drugs but the unwanted effects include skin rashes, renal abnormalities etc. Hence there is a need for newer drugs that offer both safety and efficacy [14,15].

Definition: For a graph G, the Zagreb matrices are defined as

$$\text{(i)}\quad Z^{(1)} = Z_{ij} = \begin{cases} {d_{ij}}^2 & for\ v_i \in V(G) \\ 0 & otherwise \end{cases}$$

is called a First Zagreb matrix of G,

$$\text{(ii)}\quad Z^{(2)} = Z_{ij} = \begin{cases} d_i d_i & for\ v_i v_j \in E(G) \\ 0 & for\ i = 1 \\ 0 & otherwise \end{cases}$$

is called a Second Zagreb matrix of $G$and

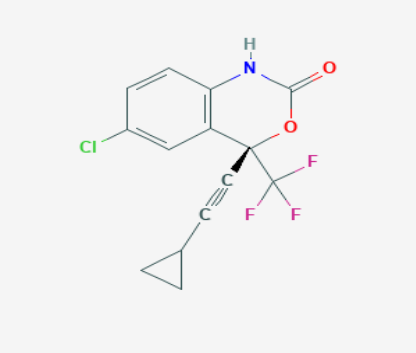
$$\text{(iii)}\quad Z^{(H)} = Z_{ij} = \begin{cases} (d_i + d_i)^2 & for\ v_i v_j \in E(G) \\ 0 & for\ i = 1 \\ 0 & otherwise \end{cases}$$

is called a Hyper Zagreb matrix of G

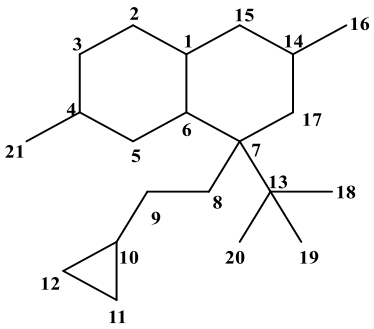
By using these Zagreb matrices we have calculated Zagreb energies for the Anti- HIV drugs.

3.1 EFAVIRENZ

Efavirenz is a non-nucleoside reverse transcriptase (RT) inhibitor.



Molecular structure of Efavirenz



Molecular graph of Efavirenz

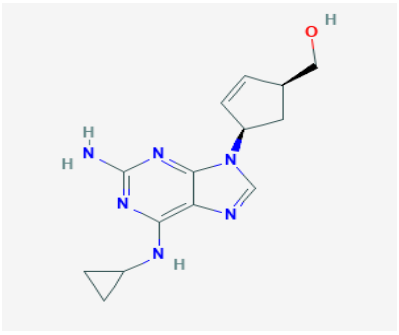
Let $G(V,E)$ be the molecular graph. Then e_{ij} represents the edges joining the vertices v_i, v_j of degrees d_i, d_j respectively.

From the molecular graph of Efavirenz, we have

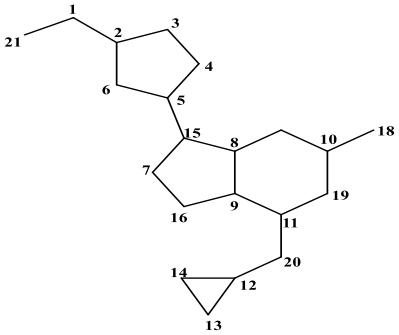
$$|e_{13}| = 2, |e_{14}| = 3, |e_{22}| = 3, |e_{23}| = 10, |e_{24}| = 2, |e_{33}| = 1, |e_{34}| = 1 \text{ and } |e_{44}| = 1.$$

3.2 ABACAVIR

Abacavir is a nucleoside reverse transcriptase inhibitor



Molecular structure of Abacavir



Molecular graph of Abacavir

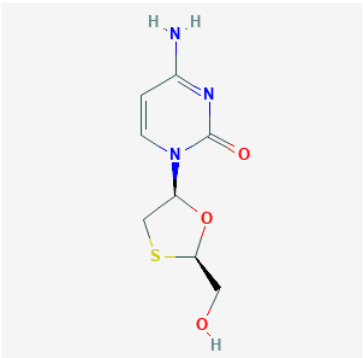
Let $G(V,E)$ be the molecular graph. Then e_{ij} represents the edges joining the vertices v_i, v_j of degrees d_i, d_j respectively.

From the molecular graph of Abacavir, we have

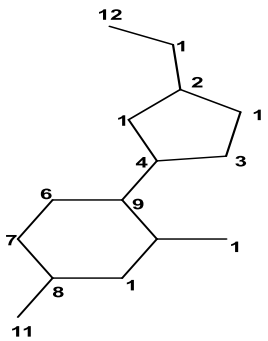
$$|e_{12}| = 1, |e_{13}| = 1, |e_{22}| = 3, |e_{23}| = 15 \text{ and } |e_{33}| = 4.$$

3.3 LAMIVUDINE

Lamivudine is a nucleoside reverse transcriptase inhibitor



Molecular structure of Lamivudine



Molecular graph of Lamivudine

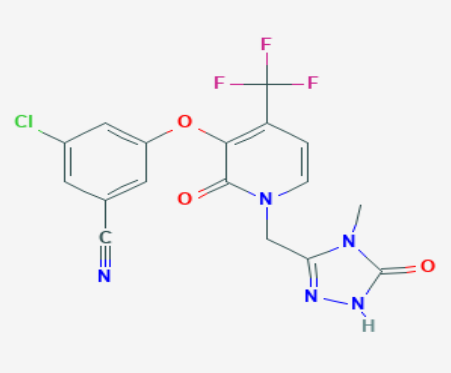
Let $G(V,E)$ be the molecular graph. Then e_{ij} represents the edges joining the vertices v_i, v_j of degrees d_i, d_j respectively.

From the molecular graph of Lamivudine, we have

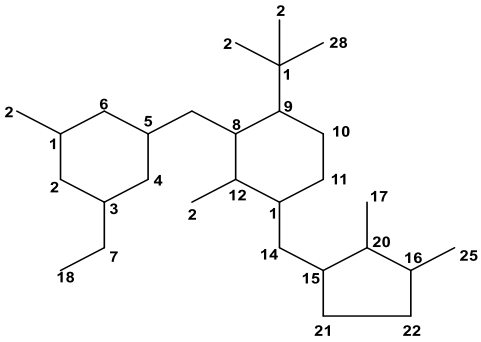
$$|e_{12}| = 1, |e_{13}| = 2, |e_{22}| = 2, |e_{23}| = 9 \text{ and } |e_{33}| = 2.$$

3.4 DORAVIRINE

It is a non-nucleoside reverse transcriptase (RT) inhibitor.



Molecular structure of Doravirine



Molecular graph of Doravirine

Let $G(V,E)$ be the molecular graph. Then e_{ij} represents the edges joining the vertices v_i, v_j of degrees d_i, d_j respectively.

From the molecular graph of Doravirine,

$$|e_{12}| = 1, |e_{13}| = 4, |e_{14}| = 3, |e_{22}| = 2, |e_{23}| = 15, |e_{33}| = 5 \text{ and } |e_{34}| = 1.$$

Based on the biological activity of selected drugs compared with the reported anti-HIV activity, we have evaluated the topological indices for the identification of active ranges.

4 CALCULATIONS OF ZAGREB ENERGIES

In this section, Zagreb matrices to the mentioned drugs are developed and the results on Zagreb energies are presented.

Theorem 4.1: The First Zagreb energy of Efavirenz is $Z^{(1)}\mathcal{E}(C_{14}H_9ClF_3NO_2) = 118$.

Proof: Consider the 2-dimensional molecular structure of $C_{14}H_9ClF_3NO_2$.
The First Zagreb matrix of Efavirenz is
$Z^{(1)}(C_{14}H_9ClF_3NO_2) =$

$$\begin{pmatrix}
9&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&4&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&4&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&9&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&4&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&9&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&16&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&4&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&4&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&9&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&4&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&4&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&16&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&9&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&4&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&4&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1
\end{pmatrix}$$

and the characteristic equation of the above matrix is

$$\lambda^{21} - \lambda^{20} + \lambda^{19} - \lambda^{18} + \lambda^{17} - \lambda^{16} + \lambda^{15} - (0.0001)\lambda^{14} - (0.0008)\lambda^{13} - (0.0053)\lambda^{12}$$
$$+(0.0269)\lambda^{11} - (0.1094)\lambda^{10} + (0.3575)\lambda^{9} - (0.9399)\lambda^{8} + (1.9349)\lambda^{7}$$
$$-(3.1398)\lambda^{6} + (3.9197)\lambda^{5} - (3.6686)\lambda^{4} + (2.4772)\lambda^{3} - (1.1346)\lambda^{2} + (0.3143)\lambda - (0.0396) = 0.$$

Then the eigen values of $Z^{(1)}(C_{14}H_9ClF_3NO_2)$ are

$$\lambda_1 = \lambda_2 = 16,$$
$$\lambda_3 = \lambda_4 = \lambda_5 = \lambda_6 = \lambda_7 = 9,$$
$$\lambda_8 = \lambda_9 = \lambda_{10} = \lambda_{11} = \lambda_{12} = \lambda_{13} = \lambda_{14} = \lambda_{15} = \lambda_{16} = 4$$
$$\text{And } \lambda_{17} = \lambda_{18} = \lambda_{19} = \lambda_{20} = \lambda_{21} = 1.$$

Therefore the first Zagreb energy of Efavirenz is

$$Z^{(1)}\mathcal{E}(C_{14}H_9ClF_3NO_2) = \sum_{i=1}^{21}|\lambda_i| = 2(16) + 5(9) + 9(4) + 5(1) = 118.$$

■

Theorem 4.2: The Second Zagreb energy of Efavirenz is

$$Z^{(2)}\mathcal{E}(C_{14}H_9ClF_3NO_2) \approx 156.7834.$$

Proof: Consider the 2-dimensional molecular structure of $C_{14}H_9ClF_3NO_2$.
The Second Zagreb matrix of Efavirenz is $Z^{(2)}(C_{14}H_9ClF_3NO_2) =$

$$\begin{pmatrix}
0 & 6 & 0 & 0 & 0 & 9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0\\
6 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 4 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 6 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3\\
0 & 0 & 0 & 6 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
9 & 0 & 0 & 0 & 6 & 0 & 12 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 12 & 0 & 8 & 0 & 0 & 0 & 0 & 16 & 0 & 0 & 0 & 8 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 6 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 4 & 4 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 3 & 6 & 0 & 0 & 0\\
6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}$$

and the characteristic equation of above matrix is

$$\lambda^{21} - \lambda^{20} - \lambda^{19} - \lambda^{18} - \lambda^{17} + \lambda^{16} - \lambda^{15} - \lambda^{14} + (0.0001)\lambda^{13} + (0.0001)\lambda^{12}$$
$$-(0.0024)\lambda^{11} - (0.0045)\lambda^{10} + (0.0534)\lambda^{9} + (0.1116)\lambda^{8} - (0.5440)\lambda^{7}$$
$$-(1.1468)\lambda^{6} + (1.7700)\lambda^{5} + (3.1838)\lambda^{4} - (0.2510)\lambda^{3} - (0.2378)\lambda^{2} + \lambda = 0.$$

The eigen values of $Z^{(2)}(C_{14}H_9ClF_3NO_2)$ are
$\lambda_1 = -24.4737$, $\lambda_2 = -12.7968$, $\lambda_3 = -9.6712$, $\lambda_4 = -9.4834$
,$\lambda_5 = -7.4036$,$\lambda_6 = -5.2719$, $\lambda_7 = -4$, $\lambda_8 = -3.5399$,
$\lambda_9 = -1.4960$, $\lambda_{10} = -0.2552$, $\lambda_{11} = 0$, $\lambda_{12} = 0$, $\lambda_{13} = 0.2945$, $\lambda_{14} = 2.1808$, $\lambda_{15} = 4.2819$,
$\lambda_{16} = 5.3462$, $\lambda_{17} = 7.4036$, $\lambda_{18} = 9.4917$, $\lambda_{19} = 12.0987$, $\lambda_{20} = 12.8205$, and $\lambda_{21} = 24.4735$.

Therefore the second Zagreb energy of Efavirenz is

$$Z^{(2)}\mathcal{E}(C_{14}H_9ClF_3NO_2) = \sum_{i=1}^{21}|\lambda_i| \approx 156.7834.$$ ■

Theorem 4.3: The Hyper Zagreb energy of Efavirenz is

$$Z^{(H)}\mathcal{E}(C_{14}H_9ClF_3NO_2) \approx 679.7965.$$

Proof: Consider the 2-dimensional molecular structure of $C_{14}H_9ClF_3NO_2$.
The Hyper Zagreb matrix of Efavirenz is

$$Z^{(H)}(C_{14}H_9ClF_3NO_2) =$$

$$\begin{pmatrix}
0 & 25 & 0 & 0 & 0 & 36 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 \\
25 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 16 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 25 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 16 \\
0 & 0 & 0 & 25 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
36 & 0 & 0 & 0 & 25 & 0 & 49 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 49 & 0 & 36 & 0 & 0 & 0 & 0 & 64 & 0 & 0 & 0 & 36 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 36 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 16 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 0 & 25 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 64 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 25 & 25 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 16 & 25 & 0 & 0 & 0 & 0 \\
25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 36 & 0 & 0 & 0 & 0 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}$$

and the characteristic equation is

$$\lambda^{21} - \lambda^{20} - \lambda^{19} - \lambda^{18} + \lambda^{17} + \lambda^{16} - \lambda^{15} - \lambda^{14} + \lambda^{13} + \lambda^{12} - \lambda^{11} - \lambda^{10} + \lambda^{9}$$
$$+(0.0002)\lambda^8 - (0.0055)\lambda^7 - (0.0467)\lambda^6 + (0.3772)\lambda^5 + (2.7154)\lambda^4 - (1.7457)\lambda^3$$
$$-(8.1537)\lambda^2 - \lambda = 0.$$

The eigen values of $Z^{(H)}(C_{14}H_9ClF_3NO_2)$ are
$\lambda_1 = -103.4983$, $\lambda_2 = -54.7602$, $\lambda_3 = -40.8901$, $\lambda_4 = -40.5209$,
$\lambda_5 = -31.9921$, $\lambda_6 = -28.1814$, $\lambda_7 = -16.0395$, $\lambda_8 = -16$,
$\lambda_9 = -6.3870$, $\lambda_{10} = -1.6286$, $\lambda_{11} = 0$, $\lambda_{12} = 0$,
$\lambda_{13} = 1.8831$, $\lambda_{14} = 10.0410$, $\lambda_{15} = 17.7782$, $\lambda_{16} = 28.8269$,
$\lambda_{17} = 31.9943$, $\lambda_{18} = 40.8814$, $\lambda_{19} = 50.2220$, $\lambda_{20} = 54.7787$
and $\lambda_{21} = 103.4988$.

Therefore the Hyper Zagreb energy of Efavirenz is

$$Z^{(H)}\mathcal{E}(C_{14}H_9ClF_3NO_2) = \sum_{i=1}^{21} |\lambda_i| \approx 679.7965.$$ ■

Theorem 4.4: The First Zagreb energy of Abacavir is $Z^{(1)}\mathcal{E}(C_{14}H_{18}N_6O) = 118$.
Proof: Consider the 2-dimensional molecular structure of $C_{14}H_{18}N_6O$.
The First Zagreb matrix of Abacavir is $Z^{(1)}(C_{14}H_{18}N_6O) =$

$$\begin{pmatrix}
4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{pmatrix}$$

and the characteristic equation is

$$\lambda^{21}-\lambda^{20}+\lambda^{19}-\lambda^{18}+\lambda^{17}-\lambda^{16}+\lambda^{15}-\lambda^{14}+(0.0001)\lambda^{13}-(0.0010)\lambda^{12}$$
$$+(0.0061)\lambda^{11}-(0.0295)\lambda^{10}+(0.1176)\lambda^{9}-(0.3827)\lambda^{8}+(1.0079)\lambda^{7}$$
$$-(2.1220)\lambda^{6}+(3.5073)\lambda^{5}-(4.4309)\lambda^{4}+(4.1085)\lambda^{3}-(2.6190)\lambda^{2}+(1.0181)\lambda-(0.1806)=0.$$

The eigen values of $Z^{(1)}(C_{14}H_{18}N_6O)$ are

$$\lambda_1=\lambda_2=\lambda_3=\lambda_4=\lambda_5=\lambda_6=\lambda_7=\lambda_8=9,$$
$$\lambda_9=\lambda_{10}=\lambda_{11}=\lambda_{12}=\lambda_{13}=\lambda_{14}=\lambda_{15}=\lambda_{16}=\lambda_{17}=\lambda_{18}=\lambda_{19}=4$$
$$\text{and } \lambda_{20}=\lambda_{21}=1.$$

Therefore the first Zagreb energy of Abacavir is

$$Z^{(1)}\mathcal{E}(C_{14}H_{18}N_6O)=\sum_{i=1}^{21}|\lambda_i|=8(9)+11(4)+2(1)=118.$$

■

Theorem 4.5: The Second Zagreb energy of Abacavir is

$$Z^{(2)}\mathcal{E}(C_{14}H_{18}N_6O)\approx 159.9405.$$

Proof: Consider the 2-dimensional molecular structure of $C_{14}H_{18}N_6O$.
The Second Zagreb matrix of Abacavir is $Z^{(2)}(C_{14}H_{18}N_6O)=$

$$\begin{pmatrix}
0&6&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1\\
6&0&6&0&0&6&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&6&0&4&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&4&0&6&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&6&0&6&0&0&0&0&0&0&0&0&9&0&0&0&0&0&0\\
0&6&0&0&6&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&6&4&0&0&0&0&0\\
0&0&0&0&0&0&0&0&9&0&0&0&0&0&9&0&6&0&0&0&0\\
0&0&0&0&0&0&0&9&0&0&9&0&0&0&0&6&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&6&3&6&0&0\\
0&0&0&0&0&0&0&0&9&0&0&0&0&0&0&0&0&0&6&6&0\\
0&0&0&0&0&0&0&0&0&0&0&0&6&6&0&0&0&0&0&6&0\\
0&0&0&0&0&0&0&0&0&0&0&6&0&4&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&6&4&0&0&0&0&0&0&0&0\\
0&0&0&0&9&0&6&9&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&4&0&6&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&6&0&6&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&3&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&6&6&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&6&6&0&0&0&0&0&0&0&0&0\\
2&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0
\end{pmatrix}$$

and the characteristic equation is

$$\lambda^{21}+\lambda^{20}-\lambda^{19}-\lambda^{18}+\lambda^{17}+\lambda^{16}-\lambda^{15}-\lambda^{14}+\lambda^{13}+\lambda^{12}-(0.0004)\lambda^{11}$$
$$-(0.0003)\lambda^{10}+(0.0117)\lambda^{9}+(0.0078)\lambda^{8}-(0.1909)\lambda^{7}-(0.0427)\lambda^{6}+(1.4052)\lambda^{5}$$
$$-(0.3919)\lambda^{4}-(3.1087)\lambda^{3}+(1.6385)\lambda^{2}+(0.4363)\lambda-(0.1806)=0.$$

The eigen values of $Z^{(2)}(C_{14}H_{18}N_6O)$ are
$\lambda_1=-18.0683$, $\lambda_2=-14.0381$, $\lambda_3=-10.7771$, $\lambda_4=-9.7456$,
$\lambda_5=-7.2659$, $\lambda_6=-8.6017$, $\lambda_7=-5.2681$, $\lambda_8=-4$,
$\lambda_9=-1.8481$, $\lambda_{10}=-0.3575$, $\lambda_{11}=0.2772$, $\lambda_{12}=0.6806$,
$\lambda_{13}=1.8203$, $\lambda_{14}=3.1537$, $\lambda_{15}=3.8939$, $\lambda_{16}=6.6736$,
$\lambda_{17}=8.5709$, $\lambda_{18}=10.3213$, $\lambda_{19}=12.0787$, $\lambda_{20}=14.0414$
and $\lambda_{21}=18.4587$.

Therefore the second Zagreb energy of Abacavir is

$$Z^{(2)}\mathcal{E}(C_{14}H_{18}N_6O)=\sum_{i=1}^{21}|\lambda_i|\approx 159.9405.$$ ■

Theorem 4.6: The Hype Zagreb energy of Abacavir is

$$Z^{(H)}\mathcal{E}(C_{14}H_{18}N_6O) \approx 665.7209.$$

Proof: Consider the 2-dimensional molecular structure of $C_{14}H_{18}N_6O$.
The Hyper Zagreb matrix of Abacavir is

$$Z^{(H)}\mathcal{E}(C_{14}H_{18}N_6O) =$$

$$\begin{pmatrix}
0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9 \\
25 & 0 & 25 & 0 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 25 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 16 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 25 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 36 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 25 & 0 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 16 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 36 & 0 & 0 & 0 & 0 & 36 & 0 & 25 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 36 & 0 & 0 & 36 & 0 & 0 & 0 & 25 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 16 & 25 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 36 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 25 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 25 & 0 & 0 & 0 & 0 & 25 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 36 & 0 & 25 & 36 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 16 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}$$

and the characteristic equation is

$$\lambda^{21} + \lambda^{20} - \lambda^{19} - \lambda^{18} + \lambda^{17} + \lambda^{16} - \lambda^{15} - \lambda^{14} + \lambda^{13} + \lambda^{12} - (0.0004)\lambda^{11} - (0.0003)\lambda^{10} + (0.0117)\lambda^9 + (0.0078)\lambda^8 - (0.1909)\lambda^7 - (0.0427)\lambda^6 + (1.4052)\lambda^5 - (0.3919)\lambda^4 - (3.1087)\lambda^3 + (1.6385)\lambda^2 + (0.4363)\lambda - (0.1806) = 0.$$

The eigen values of $Z^{(H)}(C_{14}H_{18}N_6O)$ are
$\lambda_1 = -73.1504$, $\lambda_2 = -57.5198$, $\lambda_3 = -44.9520$, $\lambda_4 = -40.7040$,
$\lambda_5 = -36.7040$. $\lambda_6 = -30.1525$, $\lambda_7 = -21.9588$, $\lambda_8 = -16$,
$\lambda_9 = -9.6131$, $\lambda_{10} = -2.1079$, $\lambda_{11} = 1.5774$, $\lambda_{12} = 4.1382$,
$\lambda_{13} = 7.9992$, $\lambda_{14} = 13.1247$, $\lambda_{15} = 16.0844$, $\lambda_{16} = 27.9599$,
$\lambda_{17} = 36.5486, \lambda_{18} = 42.8580, \lambda_{19} = 50.0503, \lambda_{20} = 54.7429$
and $\lambda_{21} = 79.7769$.
Therefore the Hyper Zagreb energy of Abacavir is

$$Z^{(H)}\mathcal{E}(C_{14}H_{18}N_6O) = \sum_{i=1}^{21} |\lambda_i| \approx 665.7209. \qquad \blacksquare$$

Theorem 4.7: The First Zagreb energy of Lamivudine is $Z^{(1)}\mathcal{E}(C_8H_{11}N_3O_3S) = 76$.

Proof: Consider the 2-dimensional molecular structure of $C_8H_{11}N_3O_3S$.
The First Zagreb matrix of Lamivudine is

$$Z^{(1)}(C_8H_{11}N_3O_3S) =$$

$$\begin{pmatrix}
4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4
\end{pmatrix}$$

and the characteristic equation is

$$\lambda^{15} - \lambda^{14} + \lambda^{13} - \lambda^{12} + (0.0001)\lambda^{11} - (0.0008)\lambda^{10} + (0.0056)\lambda^{9} - (0.0307)\lambda^{8} + (0.1256)\lambda^{7} - (0.3847)\lambda^{6} + (0.8698)\lambda^{5} - (1.4197)\lambda^{4} + (1.6105)\lambda^{3} - (1.1924)\lambda^{2} + (0.5133)\lambda - (0.0967) = 0.$$

The eigen values of $Z^{(1)}\mathcal{E}(C_8H_{11}N_3O_3S)$ are

$$\lambda_1 = \lambda_2 = \lambda_3 = \lambda_4 = \lambda_5 = 9.$$
$$\lambda_6 = \lambda_7 = \lambda_8 = \lambda_9 = \lambda_{10} = \lambda_{11} = \lambda_{12} = 9,$$
$$\text{and } \lambda_{13} = \lambda_{14} = \lambda_{15} = 1.$$

Therefore, first Zagreb energy of Lamivudine is

$$Z^{(1)}\mathcal{E}(C_8H_{11}N_3O_3S) = \sum_{i=1}^{15}|\lambda_i| = 76.$$

■

Theorem 4.8: The Second Zagreb energy of Lamivudine is

$$Z^{(2)}\mathcal{E}(C_8H_{11}N_3O_3S) \approx 102.3364.$$

Proof: Consider the 2-dimensional molecular structure of $C_8H_{11}N_3O_3S$.
The Second Zagreb matrix of Lamivudine is

$$Z^{(2)}(C_8H_{11}N_3O_3S) =$$

$$\begin{pmatrix}
0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\
6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 6 \\
0 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 \\
0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 9 & 0 & 0 & 0 & 6 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9 & 6 & 0 & 0 & 0 & 3 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 4 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 6 & 0 & 0 & 6 & 3 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 9 & 9 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 6 & 0 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 6 & 0 & 6 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 6 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}$$

and the characteristic equation is

$$\lambda^{15} - \lambda^{14} - \lambda^{13} + \lambda^{12} + \lambda^{11} - \lambda^{10} - (0.0008)\lambda^{9} + (0.0021)\lambda^{8} + (0.0247)\lambda^{7} - (0.055\,4)\lambda^{6} - (0.3057)\lambda^{5} + (0.5564)\lambda^{4} + (0.9762)\lambda^{3} - (1.4572)\lambda^{2} + (1.2177)\lambda = 0.$$

The eigen values of $Z^{(2)}(C_8H_{11}N_3O_3S)$ are
$\lambda_1 = -13.6974$, $\lambda_2 = -10.9375$, $\lambda_3 = -9.6333$, $\lambda_4 = -6.1385$,
$\lambda_5 = -4.1010$, $\lambda_6 = -2.1605$, $\lambda_7 = 0$, $\lambda_8 = 0.1706$,
$\lambda_9 = 1.0492$, $\lambda_{10} = 2.5821$, $\lambda_{11} = 4.6400$, $\lambda_{12} = 5.7648$
$\lambda_{13} = 9.4459$, $\lambda_{14} = 11.6775$, and $\lambda_{15} = 20.8831$.

Therefore second Zagreb energy of Lamivudine is

$$Z^{(2)}\mathcal{E}(C_8H_{11}N_3O_3S) = \sum_{i=1}^{15} |\lambda_i| \approx 102.3364. \quad \blacksquare$$

Theorem 4.9: The Hyper Zagreb energy of Lamivudine is

$$Z^{(H)}\mathcal{E}(C_8H_{11}N_3O_3S) \approx 421.7836.$$

Proof: Consider the 2-dimensional molecular structure of $C_8H_{11}N_3O_3S$.
The Hyper Zagreb matrix of Lamivudine is

$$Z^{(H)}(C_8H_{11}N_3O_3S) =$$

$$\begin{pmatrix}
0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 9 & 0 & 0 & 0 \\
25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 25 & 0 & 25 \\
0 & 0 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 16 \\
0 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 36 & 0 & 0 & 0 & 25 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 36 & 25 & 0 & 0 & 0 & 16 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 16 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 16 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 25 & 0 & 0 & 25 & 16 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 36 & 36 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 25 & 0 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
9 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 25 & 0 & 25 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 25 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{pmatrix}$$

and the characteristic equation is

$$\lambda^{15} - \lambda^{14} - \lambda^{13} - \lambda^{12} + \lambda^{11} - \lambda^{10} - \lambda^9 + \lambda^8 + \lambda^7 - (0.0001)\lambda^6 - (0.0061)\lambda^5 + (0.0231)\lambda^4 + (0.3948)\lambda^3 - (1.4439)\lambda^2 - (1.6577)\lambda = 0.$$

The eigen values of $Z^{(H)}(C_8H_{11}N_3O_3S)$ are
$\lambda_1 = -65.7674$, $\lambda_2 = -45.9120$, $\lambda_3 = -41.1120$, $\lambda_4 = -28.2749$,
$\lambda_5 = -19.4646$, $\lambda_6 = -9.4326$, $\lambda_7 = -0.9283$, $\lambda_8 = 0$,
$\lambda_9 = 4.8207$, $\lambda_{10} = 10.5214$, $\lambda_{11} = 17.9408$ $\lambda_{12} = 25.0199$,
$\lambda_{13} = 38.1106$, $\lambda_{14} = 48.1427$ and $\lambda_{15} = 66.3357$.

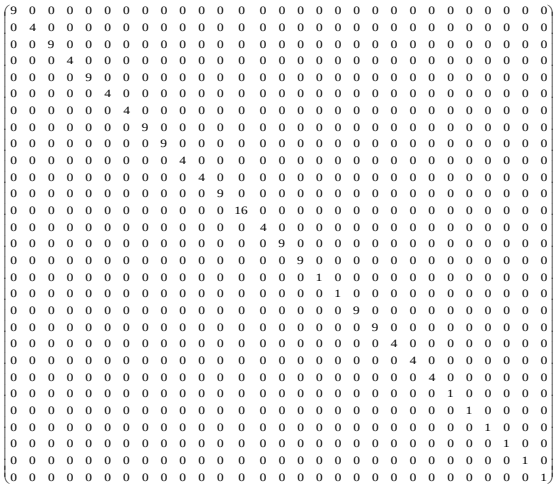
Therefore Hyper Zagreb energy of Lamivudine is

$$Z^{(H)}\mathcal{E}(C_8H_{11}N_3O_3S) = \sum_{i=1}^{15} |\lambda_i| \approx 421.7836. \quad \blacksquare$$

Theorem 4.10: The First Zagreb energy of Doravirine is

$$Z^{(1)}\mathcal{E}(C_{17}H_{11}ClF_3N_5O_3) = 154.$$

Proof: Consider the 2-dimensional molecular structure of $C_{17}H_{11}ClF_3N_5O_3$.
The First Zagreb matrix of Doravirine is $Z^{(1)}(C_{17}H_{11}ClF_3N_5O_3) =$



and the characteristic equation is

$$\lambda^{29}-\lambda^{28}+\lambda^{27}-\lambda^{26}+\lambda^{25}-\lambda^{24}+\lambda^{23}-\lambda^{22}+\lambda^{21}-\lambda^{20}+\lambda^{19}-(0.0001)\lambda^{18}$$
$$+(0.0007)\lambda^{17}-(0.0038)\lambda^{16}+(0.0172)\lambda^{15}-(0.0669)\lambda^{14}+(0.2218)\lambda^{13}$$
$$-(0.6240)\lambda^{12}+(1.4848)\lambda^{11}-(2.9738)\lambda^{10}+(4.9809)\lambda^{9}-(6.6190)\lambda^{8}$$
$$+(7.8859)\lambda^{7}-(7.2712)\lambda^{6}+(5.3223)\lambda^{5}-(3.0124)\lambda^{4}+(1.2681)\lambda^{3}-(0.3730)\lambda^{2}+(0.0683)\lambda-$$
$$(0.0058)=0.$$

The eigen values of $Z^{(1)}(C_{17}H_{11}ClF_3N_5O_3)$ are

$$\lambda_1=16,$$
$$\lambda_2=\lambda_3=\lambda_4=\lambda_5=\lambda_6=\lambda_7=\lambda_8=\lambda_9=\lambda_{10}=\lambda_{11}=9,$$
$$\lambda_{12}=\lambda_{13}=\lambda_{14}=\lambda_{15}=\lambda_{16}=\lambda_{17}=\lambda_{18}=\lambda_{19}=\lambda_{20}=\lambda_{21}=4$$
$$\text{And } \lambda_{22}=\lambda_{23}=\lambda_{24}=\lambda_{25}=\lambda_{26}=\lambda_{27}=\lambda_{28}=\lambda_{29}=1.$$

Therefore the first Zagreb energy of Doravirine is

$$Z^{(1)}\mathcal{E}(C_{17}H_{11}ClF_3N_5O_3)=\sum_{i=1}^{29}|\lambda_i|=1(16)+10(9)+10(4)+8(1)=154.$$

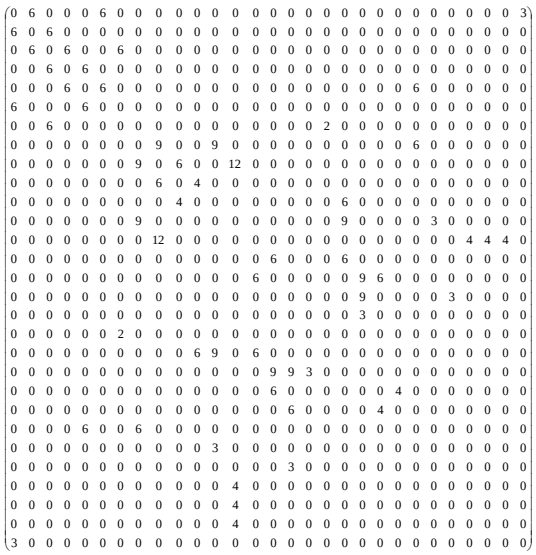
■

Theorem 4.11: The Second Zagreb energy of Doravirine is

$$Z^{(2)}\mathcal{E}(C_{17}H_{11}ClF_3N_5O_3)\approx 198.0378.$$

Proof: Consider the 2-dimensional molecular structure of $C_{17}H_{11}ClF_3N_5O_3$.
The Second Zagreb matrix of Doravirine is

$$Z^{(2)}(C_{17}H_{11}ClF_3N_5O_3)=$$



and the characteristic equation is

$$\lambda^{29} - \lambda^{28} - \lambda^{27} + \lambda^{26} + \lambda^{25} - \lambda^{24} - \lambda^{23} + \lambda^{22} + \lambda^{21} - \lambda^{20} - \lambda^{19} + \lambda^{18}$$
$$+(0.0001)\lambda^{17} - (0.0001)\lambda^{16} - (0.0040)\lambda^{15} + (0.0026)\lambda^{14} + (0.0795)\lambda^{13}$$
$$-(0.0611)\lambda^{12} - (0.8442)\lambda^{11} + (0.6130)\lambda^{10} + (4.1249)\lambda^{9} - (1.6184)\lambda^{8}$$
$$-(8.1189)\lambda^{7} + (1.1493)\lambda^{6} + (5.5105)\lambda^{5} - \lambda^{4} - (0.83361)\lambda^{3} = 0.$$

The eigen values of $Z^{(2)}(C_{17}H_{11}ClF_3N_5O_3)$ are
$\lambda_1 = -18.9015$, $\lambda_2 = -14.9539$, $\lambda_3 = -13.2499$, $\lambda_4 = -12.7862$
$\lambda_5 = -9.1436$, $\lambda_6 = -7.6593$, $\lambda_7 = -7.2424$, $\lambda_8 = -6.1008$,
$\lambda_9 = -4.2429$, $\lambda_{10} = -1.8243$, $\lambda_{11} = -1.5045$, $\lambda_{12} = -0.9037$,
$\lambda_{13} = -0.5$, $\lambda_{14} = 0$, $\lambda_{15} = 0$, $\lambda_{16} = 0$,
$\lambda_{17} = 0.4293$, $\lambda_{18} = 0.9999$, $\lambda_{19} = 1.5167$, $\lambda_{20} = 3.9626$,
$\lambda_{21} = 3.9626$, $\lambda_{22} = 4.7532$, $\lambda_{23} = 6.4841$, $\lambda_{24} = 7.5649$,
$\lambda_{25} = 9.1340$, $\lambda_{26} = 12.8475$, $\lambda_{27} = 13.2603$, $\lambda_{28} = 15.2016$
and $\lambda_{29} = 18.9021$.

Therefore the second Zagreb energy of Doravirine is

$$Z^{(2)}\mathcal{E}(C_{17}H_{11}ClF_3N_5O_3) = \sum_{i=1}^{29} |\lambda_i| \approx 198.0378. \qquad \blacksquare$$

.

Theorem 4.12: The Hyper Zagreb energy of Doravirine is

$$Z^{(H)}\mathcal{E}(C_{17}H_{11}ClF_3N_5O_3) \approx 864.1557.$$

Proof: Consider the 2-dimensional molecular structure of $C_{17}H_{11}ClF_3N_5O_3$.
The Hyper Zagreb matrix of Doravirine is

$$Z^{(H)}\mathcal{E}(C_{17}H_{11}ClF_3N_5O_3) =$$

$$\begin{pmatrix}
0&25&0&0&0&25&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&16\\
25&0&25&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&25&0&25&0&0&25&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&25&0&25&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&25&0&25&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&25&0&0&0&0&0&0&0\\
25&0&0&0&25&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&25&0&0&0&0&0&0&0&0&0&0&0&0&0&9&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&36&0&0&36&0&0&0&0&0&0&0&0&0&25&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&36&0&25&0&0&49&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&25&0&16&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&16&0&0&0&0&0&0&0&0&25&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&36&0&0&0&0&0&0&0&0&0&36&0&0&0&0&16&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&49&0&0&0&0&0&0&0&0&0&0&0&0&0&0&25&25&25&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&25&0&0&0&25&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&25&0&0&0&0&0&36&25&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&36&0&0&0&0&16&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&16&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&9&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&25&36&0&25&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&36&36&16&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&25&0&0&0&0&0&0&16&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&25&0&0&0&0&16&0&0&0&0&0&0&0&0\\
0&0&0&0&25&0&0&25&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&16&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&16&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&25&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&0&25&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
0&0&0&0&0&0&0&0&0&0&0&0&25&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0\\
16&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0
\end{pmatrix}$$

and the characteristic equation is

$$\lambda^{29} - \lambda^{28} - \lambda^{27} + \lambda^{26} + \lambda^{25} - \lambda^{24} - \lambda^{23} + \lambda^{22} + \lambda^{21} - \lambda^{20} - \lambda^{19} + \lambda^{18} + \lambda^{17} - \lambda^{16}$$
$$-\lambda^{15} + \lambda^{14} + \lambda^{13} - \lambda^{12} - \lambda^{11} + \lambda^{10} + (0.0004)\lambda^{9} - (0.0005)\lambda^{8} - (0.0176)\lambda^{7}$$
$$+(0.0094)\lambda^{6} + (0.3493)\lambda^{5} + \lambda^{4} - (1.8297)\lambda^{3} = 0.$$

The eigen values of $Z^{(H)}(C_{17}H_{11}ClF_3N_5O_3)$ are
$\lambda_1 = -80.4873,$ $\lambda_2 = -62.1918,$ $\lambda_3 = -58.0080,$ $\lambda_4 = -54.2720,$
$\lambda_5 = -41.3011,$ $\lambda_6 = -32.9933,$ $\lambda_7 = -31.2688,$ $\lambda_8 = -26.2732,$
$\lambda_9 = -21.1162,$ $\lambda_{10} = -8.2913,$ $\lambda_{11} = -6.7192,$ $\lambda_{12} = -6.1303,$
$\lambda_{13} = -3.0254,$ $\lambda_{14} = 0,$ $\lambda_{15} = 0,$ $\lambda_{16} = 0,$
$\lambda_{17} = 2.6644,$ $\lambda_{18} = 5.9780,$ $\lambda_{19} = 6.9327,$ $\lambda_{20} = 16,$
$\lambda_{21} = 20.0006, \lambda_{22} = 21.5396, \lambda_{23} = 28.6890, \lambda_{24} = 32.7615,$
$\lambda_{25} = 41.2882, \lambda_{26} = 54.4985, \lambda_{27} = 58.2631, \lambda_{28} = 62.9740$
and $\lambda_{29} = 80.4882.$

Therefore the hyper Zagreb energy of Doravirine is

$$Z^{(H)}\mathcal{E}(C_{17}H_{11}ClF_3N_5O_3) = \sum_{i=1}^{29} |\lambda_i| \approx 864.1557.$$

■

5 CONCLUSION

Zagreb indices and Zagreb energies for efavirenz, abacavir, lamivudine, and doravirine are calculated. The anti-HIV drugs play an important role in antiretroviral therapy. Among the anti-HIV drugs, doravirine has the highest Zagreb energy value. By the clinical information, resistance against doravirine based antiretroviral therapies is expected to be rare. Doravirine is potent than other drugs selected for our analysis. Our results are in accordance with the actual clinical observations suggesting the high activity of the drug might be due to its highest Zagreb energy.

6. REFERENCES

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