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# Topological Indices and QSPR/QSAR Analysis of Some Drugs Being Investigated for the Treatment of Alzheimer's Disease Patients

***Mohammed Yasin H*[1], *Suresh M**[*1], *Jalal Hatem Hussein Bayati*[2]

[1]Department of Mathematics, College of Engineering and Technology, SRM Institute of Science and Technology, Kattankulathur-603203, Tamilnadu, India.
[2] Department of Mathematics, College of Science for Women, University of Baghdad, Iraq.
*Corresponding Author.

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## Abstract

The quantitative structure-property/activity relationships (QSAR/QSPR) analysis are important for the several properties of estimating/predicting drug-related activities, particularly in the context of the drugs used for the treatment of Alzheimer's disease. This study uses innovative methods, such as the utilization of $\mathcal{V}_e$ -degree and $\mathcal{E}_v$-degree-based topological indices, to evaluate the physicochemical features and attributes of five medications used for the treat Alzheimer's disease: Tacrine, Donepezil, Rivastigmine, Galantamine and Huperzine A. By reducing the number of descriptors and improving their correlation with a variety of molecular properties, these topological indices provide a unique method for capturing critical molecular structural information. The main objective of this work is to clarify the complex molecular structural characteristics of Alzheimer's disease treatment drugs pharmaceuticals by conducting thorough computations of these indices. Additionally, QSPR and QSAR analyses were performed to establish the relationship between the several physicochemical properties of the drugs and the calculated topological indices. More valuable insightful observations are obtained through the utilization of these methodologies in our investigation. The results not only advance our comprehension of the drug properties of Alzheimer's disease but also have implications for the development and optimization of drugs in the management of the disease. The objective is to enhance understanding of the properties of these compounds to address the multifactorial nature of Alzheimer's disease and to enhance therapeutic interventions.

**Keywords:** Alzheimer, Drugs, $E_v$-degree, Topological Indices, $V_e$-degree.

## Introduction

Alzheimer's disease, a neurodegenerative disorder characterized by cognitive decline and memory loss, presents a significant challenge to global healthcare systems. As researchers strive to find effective treatment drugs, it becomes crucial to explore innovative analytical approaches that can unveil the complex relationships between drug efficacy and various molecular characteristics[1].

Tacrine, once among the first drugs for Alzheimer's disease (AD), operates by inhibiting acetylcholinesterase (AChE), thereby bolstering acetylcholine availability in the brain. Despite its efficacy, Tacrine's usage dwindled due to hepatotoxicity and side effects, prompting discontinuation in many regions. Donepezil, a widely prescribed AD medication, also inhibits

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AChE but boasts a longer half-life, facilitating once-daily dosing. It aids in cognitive enhancement and symptom management, though common side effects include nausea, diarrhea, and insomnia. Rivastigmine, another AChE inhibitor additionally targets butyrylcholinesterase (BuChE), offering dual inhibition, and is available in oral and transdermal formulations. Galantamine stands out for modulating nicotinic acetylcholine receptors alongside AChE inhibition, potentially enhancing cholinergic neurotransmission more effectively. It's utilized for mild to moderate AD in oral form[1,2]. Huperzine A, derived from Huperzia serrata, mirrors synthetic AChE inhibitors' mechanisms, showing promise in cognitive improvement, yet its long-term safety and efficacy necessitate further exploration[3]. these drugs aim to alleviate symptoms of Alzheimer's disease by increasing the availability of acetylcholine in the brain, thereby enhancing cholinergic neurotransmission and improving cognitive function. Each drug has its own unique characteristics and side effect profile, and the choice of medication depends on individual Patient factors and preferences.

Topological indices have become an important tool in theoretical chemistry, particularly in chemical graph theory. These indices, also known as connectivity indices, provide a molecular graph descriptor that is calculated based on the molecular graph of a chemical compound. The indices are defined utilizing the concept of vertex degree and have been utilized to develop the mathematical characteristics of real-world network models[4-6]. Throughout the article atoms and bonds are represented as vertex and edges respectively. Also, all the molecular structures are used as hydrogen-suppressed graphs. To provide a comprehensive overview of current research trends, Ullah et al., conducted a review of recent literature on topological indices, covering studies such as On the construction of some bioconjugate networks and their structural modeling via irregularity topological indices [7], Zaman et al., contributed with works like Structural modeling and topological characterization of three kinds of dendrimer networks [8], On the topological descriptors and structural analysis of cerium oxide nanostructures [9], Ullah et al., conducted a Network-based modeling of the molecular topology of fuchsine acid dye with respect to some irregular molecular descriptors [10]. Hayat et al. introduced Valency-based molecular descriptors for measuring the π-electronic energy of lower polycyclic aromatic hydrocarbons [11]. Ullah et al. studied Zagreb connection topological descriptors and structural property of the triangular chain structures [12]. Zaman et al. studied the Zagreb connection topological descriptors and structural properties of triangular chain structures [13]. Hakeem et al., performed the Computation of some important degree-based topological indices for γ-graphyne and Zigzag graphyne nanoribbon [14]. Zaman et al. also contributed Mathematical analysis and molecular descriptors of two novel metal-organic models with chemical applications [15].

This review aims to identify gaps in existing research and underscores the importance of our study in advancing the field of development, focusing on the $V_e$ and $\mathcal{E}_v$-degree-based indices. They explore various aspects including the $\mathcal{V}_e$-degree ABC, sum connectivity, GA, and harmonic indices of copper oxide[16], along with molecular properties of copper oxides[17]. Siddiqui et al. delve into the topological properties of H-naphthalenic nanotube[18], single-walled titanium dioxide nanotube[19], and silicon carbide Si2C3-II [p, q][20]. They also investigate topological indices for the series of benzenoid graphs[21] using $\mathcal{V}_e$ and $\mathcal{E}_v$ degree-based topological indices, for more recent works regarding $\mathcal{V}_e$ and $\mathcal{E}_v$ degree-based topological indices see details[22-24]. Inspired by these ideas, the investigation aims to focus on $\mathcal{E}_v$ and $\mathcal{V}_e$ degree-based topological indices.

In this study, the relationships between $\mathcal{E}_v$ and $\mathcal{V}_e$ degree-based topological indices and the efficacy of five widely used drugs: Tacrine, Donepezil, Rivastigmine, Galantamine, and Huperzine A were investigated[2,3]. By applying curvilinear regression models, including linear and quadratic forms, both linear and non-linear associations between these indices and the efficacy of Alzheimer's disease treatment drugs can be examined. The selection of these drugs and the calculation process for the $\mathcal{V}_e$ and $\mathcal{E}_v$-degree-based indices are described in the methodology section. In the context of Alzheimer's disease, each index was calculated carefully and formed by considering their importance to the drug performance. Also, linear and quadratic regression

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analyses were performed to frame the model which indicates the relationship between measures and drug performance.

The Correlation values for the $\mathcal{V}_e$ and $\mathcal{E}_v$-degree-based indices, as well as those from the linear and quadratic regression models, are shown in the result section. These values provided important information about the possible impact of the indices on medication efficacy by acting as markers of the direction and strength of the associations Following QSAR analysis for the biological IC50, the data was taken from articles [25-27]. The data for the rivastigmine drug was extracted from the Selleckchem website.

Using $\mathcal{V}_e$ and $\mathcal{E}_v$-degree-based indices, this study concludes by introducing the curvilinear regression analysis as a unique way to investigate the relationship between the effectiveness of Alzheimer's disease therapy medicines and molecular features. This research contributes to the development of Alzheimer's disease treatment drugs to improve the quality of life for every individual affected by this terrible disease.

## Materials and Methods

In this section, some basic concepts are presented. Let $\mathcal{G}$ be a simple connected graph denoted by $\mathcal{G} = (V, E)$ with vertex set $V$ and edge set $E$. The degree of vertex $v$ is denoted by $d(v)$, which is the number of distinct edges that are incident to a vertex. The open neighborhood of $v$, denoted as $N(v)$, refers to the set of all vertices adjacent to $v$. If the vertex $v$ is included in the set $N(v)$, the closed neighborhood $v$ is obtained, denoted as $N[v]$. The $\mathcal{E}_v$-degree of an edge $e = uv \in E$, denoted by $d_{ev}(e)$. The $\mathcal{V}_e$-degree of the vertex $v \in V$, denoted by $d_{ve}(v)$, the number of different edges that are incident to any vertex from the closed neighborhood of $v$. Now some fundamental definitions regarding $\mathcal{V}_e$-degree and $\mathcal{E}_v$-degree topological indices are presented[28-30].

For a connected graph $\mathcal{G}$, the $\mathcal{E}_v$-degree Zagreb, first $\mathcal{V}_e$-degree Zagreb alpha, $\mathcal{V}_e$-degree Zagreb beta, second $\mathcal{V}_e$-degree Zagreb, $\mathcal{V}_e$-degree Randic, $\mathcal{E}_v$-degree Randic, $\mathcal{V}_e$-degree atom-bond connectivity, $\mathcal{V}_e$-degree geometric-arithmetic, $\mathcal{V}_e$-degree harmonic and $\mathcal{V}_e$-degree sum connectivity indices were introduced by Ediz[29-31].

$$M^{ev}(\mathcal{G}) = \sum_{e\in E(\mathcal{G})} d_{ev}(e)^2 \quad (1)$$

$$M_1^{ave}(\mathcal{G}) = \sum_{v\in V(\mathcal{G})} d_{ve}(v)^2 \quad (2)$$

$$M_1^{\beta ve}(\mathcal{G}) = \sum_{uv\in E(\mathcal{G})} d_{ve}(u) + d_{ve}(v) \quad (3)$$

$$M_2^{ve}(\mathcal{G}) = \sum_{uv\in E(\mathcal{G})} d_{ve}(u) \times d_{ve}(v) \quad (4)$$

$$R^{ve}(\mathcal{G}) = \sum_{uv\in E(\mathcal{G})} (d_{ve}(u) \times d_{ve}(v))^{-1/2} \quad (5)$$

$$R^{ev}(\mathcal{G}) = \sum_{e\in E(\mathcal{G})} (`e))^{-1/2} \quad (6)$$

$$ABC^{ve}(\mathcal{G}) = \sum_{uv\in E(\mathcal{G})} \sqrt{\frac{d_{ve}(u)+d_{ve}(v)-2}{d_{ve}(u)\times d_{ve}(v)}} \quad (7)$$

$$GA^{ve}(\mathcal{G}) = \sum_{uv\in E(\mathcal{G})} \frac{2\sqrt{d_{ve}(u)\times d_{ve}(v)}}{d_{ve}(u)+d_{ve}(v)} \quad (8)$$

$$H^{ve}(\mathcal{G}) = \sum_{uv\in E(\mathcal{G})} \frac{2}{d_{ve}(u)+d_{ve}(v)} \quad (9)$$

$$\chi^{ve}(\mathcal{G}) = \sum_{uv\in E(\mathcal{G})} (d_{ve}(u) + d_{ve}(v))^{-1/2} \quad (10)$$

The first and second hyper $\mathcal{V}_e$-degree, $F - \mathcal{V}_e$ degree and $F_1 - \mathcal{V}_e$-degree, arithmetic-geometric $\mathcal{V}_e$-degree indices were introduced by Kulli[32,33].

$$HM_1^{ve}(\mathcal{G}) = \sum_{uv\in E(\mathcal{G})} (d_{ve}(u) + d_{ve}(v))^2 \quad (11)$$

$$HM_2^{ve}(\mathcal{G}) = \sum_{uv\in E(\mathcal{G})} (d_{ve}(u) \times d_{ve}(v))^2 \quad (12)$$

$$F^{ve}(\mathcal{G}) = \sum_{uv\in E(\mathcal{G})} [d_{ve}(u)^2 + d_{ve}(v)^2] \quad (13)$$

$$F_1^{ve}(\mathcal{G}) = \sum_{u\in V(\mathcal{G})} d_{ve}(u)^3 \quad (14)$$

$$AG^{ve}(\mathcal{G}) = \sum_{uv\in E(\mathcal{G})} \frac{d_{ve}(u)+d_{ve}(v)}{2\sqrt{d_{ve}(u).d_{ve}(v)}} \quad (15)$$

Recently, kulli[34], introduce the modified $\mathcal{E}_v$-degree Zagreb, $\mathcal{E}_v$-degree inverse, F-$\mathcal{E}_v$-degree, reciprocal $\mathcal{E}_v$-degree randic indices as follows:

$$mM^{ev}(\mathcal{G}) = \sum_{e\in E(\mathcal{G})} \frac{1}{d_{ev}(e)^2} \quad (16)$$

$$ID^{ev}(\mathcal{G}) = \sum_{e\in E(\mathcal{G})} \frac{1}{d_{ev}(e)} \quad (17)$$

$$F^{ev}(\mathcal{G}) = \sum_{e\in E(\mathcal{G})} d_{ev}(e)^3 \quad (18)$$

$$RR^{ev}(\mathcal{G}) = \sum_{e\in E(\mathcal{G})} d_{ev}(e)^{1/2} \quad (19)$$

The following $\mathcal{V}_e$-degree indices are defined in a manner that parallels their corresponding degree versions[35-37], they are redefine third $\mathcal{V}_e$-degree zagreb, $\mathcal{V}_e$-degree inverse sum indeg, inverse $\mathcal{V}_e$-

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degree, zeroth order $\mathcal{V}_e$-degree, modified first $\mathcal{V}_e$-degree indices are as follows:

$$ReZG_3^{ve}(\mathcal{G}) = \sum_{uv\in E(\mathcal{G})} ((d_{ve}(u) \times d_{ve}(v))(d_{ve}(u) + d_{ve}(v)) \quad 20$$

$$ISI^{ve}(\mathcal{G}) = \sum_{uv\in E(\mathcal{G})} \frac{d_{ve}(u)\times d_{ve}(v)}{d_{ve}(u)+d_{ve}(v)} \quad 21$$

$$ID^{ve}(\mathcal{G}) = \sum_{u\in V(\mathcal{G})} \frac{1}{d_{ve}(u)} \quad 22$$

$$ZD^{ve}(\mathcal{G}) = \sum_{u\in V(\mathcal{G})} \frac{1}{\sqrt{d_{ve}(u)}} \quad 23$$

$$mM_1^{ve}(\mathcal{G}) = \sum_{u\in V(\mathcal{G})} \frac{1}{d_{ve}(u)^2} \quad 24$$

The focus of this article is to estimate the chemical graph of some Alzheimer's disease treatment drugs, including Tacrine, Donepezil, Rivastigmine, Galantamine, and Huperzine A. Specifically, the analysis centers on the $\mathcal{E}_v$-degree Zagreb index, the first $\mathcal{V}_e$-degree Zagreb alpha index, the first $\mathcal{V}_e$-degree Zagreb beta index, the second $\mathcal{V}_e$-degree Zagreb beta index, the $\mathcal{V}_e$-degree Randic index, the $\mathcal{E}_v$-degree Randic index, the $\mathcal{V}_e$-degree atom-bond connectivity ($ABC^{ve}$) index, the $\mathcal{V}_e$-degree geometric-arithmetic ($GA^{ve}$) index, the $\mathcal{V}_e$-degree harmonic ($H^{ve}$) index, and the $\mathcal{V}_e$-degree sum-connectivity ($\chi^{ve}$) index. These topological indices will allow us to estimate the physicochemical properties of these drugs. Please refer to the relevant literature to learn more about these topological indices and their associated formulas[38-40].

The methodology employed in this article is as follows. Firstly, the preliminaries of $\mathcal{E}_v$ and $\mathcal{V}_e$-degree-based topological indices are introduced. Secondly, the structures of Alzheimer's disease treatment drugs are examined. Thirdly, $\mathcal{V}_e$-degree and $\mathcal{E}_v$-degree-based topological indices and their numerical values are calculated. Fourthly, the computed results using curvilinear regression analysis obtained using SPSS statistical software are compared. Afterward, the QSAR analysis using the MLR method is presented along with the significance level of the predicted biological data. Lastly, the conclusion of this article is presented.

The following notation will be used in the discussion hereafter.

$$E_{k,l} = \{uv \in E(G_n) | d_{ve}(u) = k, d_{ve}(v) = l\},$$

$$V_k = \{u \in V(G_n) | d_{ve}(u) = k\},$$

$$E_l = \{e = uv \in E(G_n) | d_{ev}(e) = l, \quad \text{where } n = 1,2,\dots,5$$

Here $G_1, G_2, G_3, G_4, G_5$ represents the molecular structures of Tacrine, Donepezil, Rivastigmine, Galantamine, and Huperzine A respectively.

## Results and Discussion

In this section, degree-based $\mathcal{V}_e$ and $\mathcal{E}_v$ indices are computed for Tacrine, Donepezil, Rivastigmine, Galantamine, and Huperzine A.

From the molecular graph of the above-mentioned drugs, the total number of vertices and edges are tabulated in Table 1.

**Table 1. Total number of vertices and edges of Tacrine, Donepezil, Rivastigmine, Galantamine and Huperzine A**

| S. No. | Drug Name | No. of Vertices | No. of Edges |
|---|---|---|---|
| 1 | Tacrine | 15 | 17 |
| 2 | Donepezil | 28 | 31 |
| 3 | Rivastigmine | 18 | 18 |
| 4 | Galantamine | 19 | 22 |
| 5 | Huperzine A | 18 | 20 |

Based on the $\mathcal{V}_e$-degree of vertices, the edge set of drugs can be partitioned. Molecular structure analysis and observations reveal that the edge set of drugs can be classified according to the $\mathcal{V}_e$-degree of

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their end vertices, as summarized in Table 2 and Table 3. The $\mathcal{V}_e$-degree of vertices is given in Table 4, also the $E_v$-degree of the edges is tabulated in Table 5.

**Table 2. The $V_e$-degree of the end vertices of Tacrine, Donepezil, Rivastigmine, Galantamine, and Huperzine A**

| Drug Name | $E_{2,4}$ | $E_{3,5}$ | $E_{3,6}$ | $E_{3,7}$ | $E_{4,4}$ | $E_{4,5}$ | $E_{4,6}$ | $E_{4,7}$ | $E_{4,9}$ | $E_{5,5}$ | $E_{5,6}$ | $E_{5,7}$ | $E_{5,8}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Tacrine | - | - | - | 1 | 2 | 4 | - | - | - | - | - | 2 | 2 |
| Donepezil | 2 | - | - | 1 | 2 | 5 | - | 2 | - | 2 | 3 | - | - |
| Rivastigmine | 1 | 2 | 2 | 1 | - | 2 | 1 | - | - | - | 1 | 2 | - |
| Galantamine | 1 | 1 | 1 | - | - | - | - | 1 | - | 1 | 2 | 2 | - |
| Huperzine A | 1 | 2 | - | - | - | - | - | - | 2 | 2 | 2 | 1 | - |

**Table 3. The $V_e$-degree of the end vertices of Tacrine, Donepezil, Rivastigmine, Galantamine, and Huperzine A**

| Drug Name | $E_{5,9}$ | $E_{6,6}$ | $E_{6,7}$ | $E_{6,8}$ | $E_{7,7}$ | $E_{7,8}$ | $E_{7,9}$ | $E_{8,8}$ | $E_{8,9}$ | $E_{9,9}$ |
|---|---|---|---|---|---|---|---|---|---|---|
| Tacrine | - | - | 2 | - | - | 4 | - | - | - | - |
| Donepezil | - | 3 | 6 | 1 | 2 | 2 | - | - | - | - |
| Rivastigmine | - | 4 | 1 | - | 1 | - | - | - | - | - |
| Galantamine | - | 1 | 3 | 3 | - | 1 | 2 | - | 2 | 1 |
| Huperzine A | 1 | - | 4 | - | - | - | 3 | - | - | 2 |

**Table 4. The $V_e$-degree of the vertices of Tacrine, Donepezil, Rivastigmine, Galantamine, and Huperzine A**

| $\mathcal{V}_e$-degree $d_{ve}(u)$ | Number of vertices | | | | | Vertex set |
|---|---|---|---|---|---|---|
| | Tacrine | Donepezil | Rivastigmine | Galantamine | Huperzine A | $V_i$ |
| 2 | - | 2 | 1 | 1 | 1 | $V_2$ |
| 3 | 1 | 1 | 5 | 2 | 2 | $V_3$ |
| 4 | 4 | 5 | 2 | 1 | 2 | $V_4$ |
| 5 | 4 | 6 | 3 | 3 | 4 | $V_5$ |
| 6 | 1 | 8 | 5 | 4 | 3 | $V_6$ |
| 7 | 3 | 5 | 2 | 3 | 3 | $V_7$ |
| 8 | 2 | 1 | - | 2 | - | $V_8$ |
| 9 | - | - | - | 2 | 3 | $V_9$ |

**Table 5. The $E_v$-degree of the edges of Tacrine, Donepezil, Rivastigmine, Galantamine , and Huperzine A**

| Degree of end vertices $(d(u), d(v))$ | No. of edges | | | | | $E_v$-degrees |
|---|---|---|---|---|---|---|
| | Tacrine | Donepezil | Rivastigmine | Galantamine | Huperzine A | |
| (1,2) | - | 2 | 1 | 1 | 1 | 3 |
| (1,3),(2,2) | 7 | 7 | 7 | 3 | 3 | 4 |
| (1,4),(2,3) | 6 | 18 | 7 | 11 | 11 | 5 |
| (2,4),(3,3) | 4 | 4 | 3 | 7 | 3 | 6 |
| (3,4) | - | - | - | - | 2 | 7 |

## TACRINE

In this subsection, $\mathcal{V}_e$ and $\mathcal{E}_v$-degree based topological indices are calculated for the structure Tacrine. The molecular structure of Tacrine is shown in Fig. 1.

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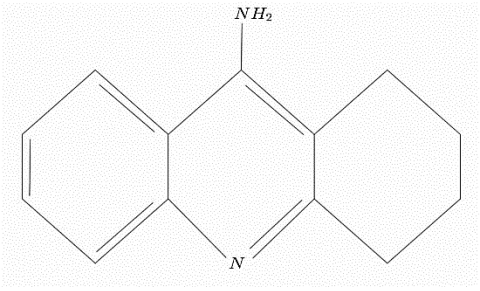


**Figure 1. Molecular structure of Tacrine[2].**

Let $G_1$ be a simple connected graph of Tacrine, the $\mathcal{V}_e$-degree based Topological Indices are,

$M_1^{\beta ve}(\mathcal{G}_1) = \sum_{uv\in E(\mathcal{G}_1)} d_{ve}(u) + d_{ve}(v)$

$= 1(3+7) + 2(4+4) + 4(4+5) + 2(5+7) + 2(5+8) + 2(6+7) + 4(7+8)$

$= 198$

$M_2^{ve}(\mathcal{G}_1) = \sum_{uv\in E(\mathcal{G}_1)} d_{ve}(u) \times d_{ve}(v)$

$= 1(3\times 7) + 2(4\times 4) + 4(4\times 5) + 2(5\times 7) + 2(5\times 8) + 2(6\times 7) + 4(7\times 8)$

$= 591$

$R^{ve}(\mathcal{G}_1) = \sum_{uv\in E(\mathcal{G}_1)} (d_{ve}(u) \times d_{ve}(v))^{-1/2}$

$= 1(21)^{-\frac{1}{2}} + 2(16)^{-\frac{1}{2}} + 4(20)^{-\frac{1}{2}} + 2(35)^{-\frac{1}{2}} + 2(40)^{-\frac{1}{2}} + 2(42)^{-\frac{1}{2}} + 4(56)^{-1/2}$

$= 3.022$

$\chi^{ve}(\mathcal{R}_1) = \sum_{uv\in E(\mathcal{R}_1)} (d_{ve}(u) + d_{ve}(v))^{-1/2}$

$= 1(3+7)^{-\frac{1}{2}} + 2(4+4)^{-\frac{1}{2}} + 4(4+5)^{-\frac{1}{2}} + 2(5+7)^{-\frac{1}{2}} + 2(5+8)^{-\frac{1}{2}} + 2(6+7)^{-\frac{1}{2}} + 4(7+8)^{-1/2}$

$= 5.074$

$H^{ve}(\mathcal{G}_1) = \sum_{uv\in E(\mathcal{G}_1)} \frac{2}{d_{ve}(u)+d_{ve}(v)}$

$= 1\left(\frac{2}{3+7}\right) + 2\left(\frac{2}{4+4}\right) + 4\left(\frac{2}{4+5}\right) + 2\left(\frac{2}{5+7}\right) + 2\left(\frac{2}{5+8}\right) + 2\left(\frac{2}{6+7}\right) + 4\left(\frac{2}{7+8}\right)$

$= 2.671$

$HM_1^{ve}(\mathcal{G}_1) = \sum_{uv\in E(\mathcal{G}_1)} (d_{ve}(u) + d_{ve}(v))^2$

$= 1(3+7)^2 + 2(4+4)^2 + 4(4+5)^2 + 2(5+7)^2 + 2(5+8)^2 + 2(6+7)^2 + 4(7+8)^2$

$= 2416$

$HM_2^{ve}(\mathcal{G}_1) = \sum_{uv\in E(\mathcal{G}_1)} (d_{ve}(u) \times d_{ve}(v))^2$

$= 1(3\times 7)^2 + 2(4\times 4)^2 + 4(4\times 5)^2 + 2(5\times 7)^2 + 2(5\times 8)^2 + 2(6\times 7)^2 + 4(7\times 8)^2$

$= 24275$

$ReZG_3^{ve}(\mathcal{G}_1) = \sum_{uv\in E(\mathcal{G}_1)} ((d_{ve}(u) \times d_{ve}(v))(d_{ve}(u) + d_{ve}(v))$

$= 1(3\times 7)(3+7) + 2(4\times 4)(4+4) + 4(4\times 5)(4+5) + 2(5\times 7)(5+7) + 2(5\times 8)(5+8) + 2(6\times 7)(6+7) + 4(7\times 8)(7+8).$

$= 7518$

$ABC^{ve}(\mathcal{G}_1) = \sum_{uv\in E(\mathcal{G}_1)} \sqrt{\frac{d_{ve}(u)+d_{ve}(v)-2}{d_{ve}(u)\times d_{ve}(v)}}$

$= 1\left(\sqrt{\frac{3+7-2}{3\times 7}}\right) + 2\left(\sqrt{\frac{4+4-2}{4\times 4}}\right) + 4\left(\sqrt{\frac{4+5-2}{4\times 5}}\right) + 2\left(\sqrt{\frac{5+7-2}{5\times 7}}\right) + 2\left(\sqrt{\frac{5+8-2}{5\times 8}}\right) + 2\left(\sqrt{\frac{6+7-2}{6\times 7}}\right) + 4\left(\sqrt{\frac{7+8-2}{7\times 8}}\right)$

$= 9.279$

$GA^{ve}(\mathcal{G}_1) = \sum_{uv\in E(\mathcal{G}_1)} \frac{2\sqrt{d_{ve}(u)\times d_{ve}(v)}}{d_{ve}(u)+d_{ve}(v)}$

$= 1\left(\frac{2\sqrt{3+7}}{3\times 7}\right) + 2\left(\frac{2\sqrt{4+4}}{4\times 4}\right) + 4\left(\frac{2\sqrt{4+5}}{4\times 5}\right) + 2\left(\frac{2\sqrt{5+7}}{5\times 7}\right) + 2\left(\frac{2\sqrt{5+8}}{5\times 8}\right) + 2\left(\frac{2\sqrt{6+7}}{6\times 7}\right) + 4\left(\frac{2\sqrt{7+8}}{7\times 8}\right)$

$= 3.861$

$AG^{ve}(\mathcal{G}_1) = \sum_{uv\in E(\mathcal{G}_1)} \frac{d_{ve}(u)+d_{ve}(v)}{2\sqrt{d_{ve}(u)\times d_{ve}(v)}}$

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$= 1\left(\frac{3+7}{2\sqrt{3\times7}}\right) + 2\left(\frac{4+4}{2\sqrt{4\times4}}\right) + 4\left(\frac{4+5}{2\sqrt{4\times5}}\right) + 2\left(\frac{5+7}{2\sqrt{5\times7}}\right) + 2\left(\frac{5+8}{2\sqrt{5\times8}}\right) + 2\left(\frac{6+7}{2\sqrt{6\times7}}\right) + 4\left(\frac{7+8}{2\sqrt{7\times8}}\right)$

$= 17.214$

$ISI^{ve}(\mathcal{G}_1) = \sum_{uv\in E(\mathcal{G}_1)} \frac{d_{ve}(u)\times d_{ve}(v)}{d_{ve}(u)+d_{ve}(v)}$

$= 1\left(\frac{3\times7}{3+7}\right) + 2\left(\frac{4\times4}{4+4}\right) + 4\left(\frac{4\times5}{4+5}\right) + 2\left(\frac{5\times7}{5+7}\right) + 2\left(\frac{5\times8}{5+8}\right) + 2\left(\frac{6\times7}{6+7}\right) + 4\left(\frac{7\times8}{7+8}\right)$

$= 48.37$

$F^{ve}(\mathcal{G}_1) = \sum_{uv\in E(\mathcal{G}_1)} [d_{ve}(u)^2 + d_{ve}(v)^2]$

$= 1(3^2 + 7^2) + 2(4^2 + 4^2) + 4(4^2 + 5^2) + 2(5^2 + 7^2) + 2(5^2 + 8^2) + 2(6^2 + 7^2) + 4(7^2 + 8^2)$

$= 1234$

$T^{ve}(\mathcal{G}_1) = \sum_{u\in V(\mathcal{G}_1)} d_{ve}(u)$

$= 1(3) + 4(4) + 4(5) + 1(6) + 3(7) + 2(8)$

$= 82$

$M_1^{ave}(\mathcal{G}_1) = \sum_{v\in V(\mathcal{G}_1)} d_{ve}(v)^2$

$= 1(3)^2 + 4(4)^2 + 4(5)^2 + 1(6)^2 + 3(7)^2 + 2(8)^2$

$= 484$

$F_1^{ve}(\mathcal{G}_1) = \sum_{v\in V(\mathcal{G}_1)} d_{ve}(v)^3$

$= 1(3)^3 + 4(4)^3 + 4(5)^3 + 1(6)^3 + 3(7)^3 + 2(8)^3$

$= 3052$

$ID^{ve}(\mathcal{G}_1) = \sum_{v\in V(\mathcal{G}_1)} \frac{1}{d_{ve}(v)}$

$= 1\left(\frac{1}{3}\right) + 4\left(\frac{1}{4}\right) + 4\left(\frac{1}{5}\right) + 1\left(\frac{1}{6}\right) + 3\left(\frac{1}{7}\right) + 2\left(\frac{1}{8}\right)$

$= 2.979$

$ZD^{ve}(\mathcal{G}_1) = \sum_{v\in V(\mathcal{G}_1)} \frac{1}{\sqrt{d_{ve}(v)}}$

$= 1\left(\frac{1}{\sqrt{3}}\right) + 4\left(\frac{1}{\sqrt{4}}\right) + 4\left(\frac{1}{\sqrt{5}}\right) + 1\left(\frac{1}{\sqrt{6}}\right) + 3\left(\frac{1}{\sqrt{7}}\right) + 2\left(\frac{1}{\sqrt{8}}\right)$

$= 6.615$

$mM_1^{ve}(\mathcal{G}_1) = \sum_{v\in V(\mathcal{G}_1)} \frac{1}{d_{ve}(v)^2}$

$= 1\left(\frac{1}{(3)^2}\right) + 4\left(\frac{1}{(4)^2}\right) + 4\left(\frac{1}{(5)^2}\right) + 1\left(\frac{1}{(6)^2}\right) + 3\left(\frac{1}{(7)^2}\right) + 2\left(\frac{1}{(8)^2}\right)$

$= 0.641$

Let $G_1$ be a simple connected graph of Tacrine, the $\mathcal{E}_v$-degree based Topological Indices are,

$T^{ev}(\mathcal{G}_1) = \sum_{e\in E(\mathcal{G}_1)} d_{ev}(e) = 7(4) + 6(5) + 4(6) = 82$

$M^{ev}(\mathcal{G}_1) = \sum_{e\in E(\mathcal{G}_1)} d_{ev}(e)^2 = 7(4)^2 + 6(5)^2 + 4(6)^2 = 406$

$F^{ev}(\mathcal{G}_1) = \sum_{e\in E(\mathcal{G}_1)} d_{ev}(e)^3 = 7(4)^3 + 6(5)^3 + 4(6)^3 = 2062$

$mM^{ev}(\mathcal{G}_1) = \sum_{e\in E(\mathcal{G}_1)} \frac{1}{d_{ev}(e)^2} = 7\left(\frac{1}{(4)^2}\right) + 6\left(\frac{1}{(5)^2}\right) + 4\left(\frac{1}{(6)^2}\right) = 0.786$

$ID^{ev}(\mathcal{G}_1) = \sum_{e\in E(\mathcal{G}_1)} \frac{1}{d_{ev}(e)} = 7\left(\frac{1}{(4)}\right) + 6\left(\frac{1}{(5)}\right) + 4\left(\frac{1}{(6)}\right) = 3.617$

$R^{ev}(\mathcal{G}_1) = \sum_{e\in E(\mathcal{G}_1)} (e)^{-1/2} = 7(4)^{-1/2} + 6(5)^{-1/2} + 4(6)^{-1/2} = 7.816$

$RR^{ev}(\mathcal{G}_1) = \sum_{e\in E(\mathcal{G}_1)} (e)^{1/2} = 7(4)^{1/2} + 6(5)^{1/2} + 4(6)^{1/2} = 37.214$

## DONEPEZIL

In this subsection, $\mathcal{V}_e$ and $\mathcal{E}_v$-degree based topological indices are calculated for the structure Donepezil. The molecular structure of Donepezil is shown in Fig 2.

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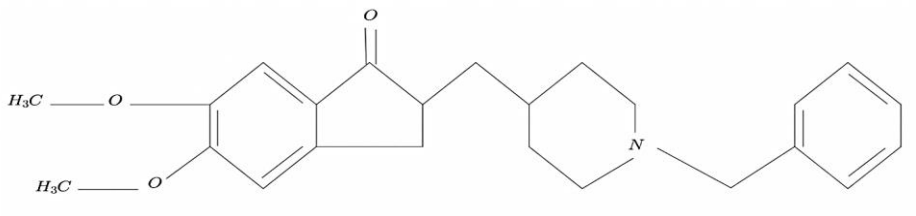


**Figure 2. Molecular structure of Donepezil[2].**

Let $G_2$ be a simple connected graph of Donepezil, the $\mathcal{V}_e$-degree-based Topological Indices are,

$M_1^{\beta ve}(\mathcal{G}_2) = \sum_{uv\in E(\mathcal{G}_2)} d_{ve}(u) + d_{ve}(v)$

$= 2(2+4) + 1(3+7) + 2(4+4) + 5(4+5) + 2(4+7) + 2(5+5) + 2(5+6) + 3(6+6)$

$+6(6+7) + 1(6+8) + 2(7+7) + 2(7+8)$

$= 344$

$M_2^{ve}(\mathcal{G}_2) = \sum_{uv\in E(\mathcal{G}_2)} d_{ve}(u) \times d_{ve}(v)$

$= 2(2\times 4) + 1(3\times 7) + 2(4\times 4) + 5(4\times 5) + 2(4\times 7) + 2(5\times 5) + 2(5\times 6)$

$+3(6\times 6) + 6(6\times 7) + 1(6\times 8) + 2(7\times 7) + 2(7\times 8)$

$= 983$

$R^{ve}(\mathcal{G}_2) = \sum_{uv\in E(\mathcal{G}_2)} (d_{ve}(u)\times d_{ve}(v))^{-1/2}$

$= 2(2\times 4)^{-\frac{1}{2}} + 1(3\times 7)^{-\frac{1}{2}} + 2(4\times 4)^{-\frac{1}{2}} + 2(4\times 5)^{-\frac{1}{2}} + 2(4\times 7)^{-\frac{1}{2}} + 2(5\times 5)^{-\frac{1}{2}}$

$+3(5\times 6)^{-1/2} + 3(6\times 6)^{-1/2} + 6(6\times 7)^{-1/2} + 1(6\times 8)^{-1/2} + 2(7\times 7)^{-1/2} + 2(7\times 8)^{-1/2}$

$= 5.996$

$\chi^{ve}(\mathcal{G}_2) = \sum_{uv\in E(\mathcal{G}_2)} (d_{ve}(u) + d_{ve}(v))^{-1/2}$

$= 2(2+4)^{-\frac{1}{2}} + 1(3+7)^{-\frac{1}{2}} + 2(4+4)^{-\frac{1}{2}} + 2(4+5)^{-\frac{1}{2}} + 2(4+7)^{-\frac{1}{2}} + 2(5+5)^{-\frac{1}{2}}$

$+3(5+6)^{-1/2} + 3(6+6)^{-1/2} + 6(6+7)^{-1/2} + 1(6+8)^{-1/2} + 2(7+7)^{-1/2} + 2(7+8)^{-1/2}$

$= 9.493$

$H^{ve}(\mathcal{G}_2) = \sum_{uv\in E(\mathcal{G}_2)} \frac{2}{d_{ve}(u)+d_{ve}(v)}$

$= 2\left(\frac{2}{2+4}\right) + 1\left(\frac{2}{3+7}\right) + 2\left(\frac{2}{4+4}\right) + 5\left(\frac{2}{4+5}\right) + 2\left(\frac{2}{4+7}\right) + 2\left(\frac{2}{5+5}\right) + 3\left(\frac{2}{5+6}\right) + 3\left(\frac{2}{6+6}\right)$

$+6\left(\frac{2}{6+7}\right) + 1\left(\frac{2}{6+8}\right) + 2\left(\frac{2}{7+7}\right) + 2\left(\frac{2}{7+8}\right)$

$= 5.905$

$HM_1^{ve}(\mathcal{G}_2) = \sum_{uv\in E(\mathcal{G}_2)} (d_{ve}(u) + d_{ve}(v))^2$

$= 2(2+4)^2 + 1(3+7)^2 + 2(4+4)^2 + 2(4+5)^2 + 2(4+7)^2 + 2(5+5)^2 + 3(5+6)^2$

$+3(6+6)^2 + 6(6+7)^2 + 1(6+8)^2 + 2(7+7)^2 + 2(7+8)^2$

$= 3994$

$HM_2^{ve}(\mathcal{G}_2) = \sum_{uv\in E(\mathcal{G}_2)} (d_{ve}(u)\times d_{ve}(v))^2$

$= 2(2\times 4)^2 + 1(3\times 7)^2 + 2(4\times 4)^2 + 2(4\times 5)^2 + 2(4\times 7)^2 + 2(5\times 5)^2 + 3(5\times 6)^2$

$+3(6\times 6)^2 + 6(6\times 7)^2 + 1(6\times 8)^2 + 2(7\times 7)^2 + 2(7\times 8)^2$

$= 36449$

$ReZG_3^{ve}(\mathcal{G}_2) = \sum_{uv\in E(\mathcal{G}_2)} ((d_{ve}(u)\times d_{ve}(v))(d_{ve}(u) + d_{ve}(v))$

$= 2(2\times 4)(2+4) + 1(3\times 7)(3+7) + 2(4\times 4)(4+4) + 5(4\times 5)(4+5) + 2(4\times 7)(4+7)$

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$+2(5\times5)(5+5)+2(5\times6)(5+6)+3(6\times6)(6+6)+6(6\times7)(6+7)+1(6\times8)(6+8)$

$+2(7\times7)(7+7)+2(7\times8)(7+8)$

$=11878$

$ABC^{ve}(\mathcal{G}_2)=\sum_{uv\in E(\mathcal{G}_2)}\sqrt{\frac{d_{ve}(u)+d_{ve}(v)-2}{d_{ve}(u)\times d_{ve}(v)}}$

$=2\left(\sqrt{\frac{2+4-2}{2\times4}}\right)+1\left(\sqrt{\frac{3+7-2}{3\times7}}\right)+2\left(\sqrt{\frac{4+4-2}{4\times4}}\right)+5\left(\sqrt{\frac{4+5-2}{4\times5}}\right)+2\left(\sqrt{\frac{4+7-2}{4\times7}}\right)+2\left(\sqrt{\frac{5+5-2}{5\times5}}\right)$

$+3\left(\sqrt{\frac{5+6-2}{5\times6}}\right)+3\left(\sqrt{\frac{6+6-2}{6\times6}}\right)+6\left(\sqrt{\frac{6+7-2}{6\times7}}\right)+1\left(\sqrt{\frac{6+8-2}{6\times8}}\right)+2\left(\sqrt{\frac{7+7-2}{7\times7}}\right)+2\left(\sqrt{\frac{7+8-2}{7\times8}}\right)$

$=17.223$

$GA^{ve}(\mathcal{G}_2)=\sum_{uv\in E(\mathcal{G}_2)}\frac{2\sqrt{d_{ve}(u)\times d_{ve}(v)}}{d_{ve}(u)+d_{ve}(v)}$

$=2\left(\frac{2\sqrt{2+4}}{2\times4}\right)+1\left(\frac{2\sqrt{3+7}}{3\times7}\right)+2\left(\frac{2\sqrt{4+4}}{4\times4}\right)+5\left(\frac{2\sqrt{4+5}}{4\times5}\right)+2\left(\frac{2\sqrt{4+7}}{4\times7}\right)+2\left(\frac{2\sqrt{5+5}}{5\times5}\right)+3\left(\frac{2\sqrt{5+6}}{5\times6}\right)$

$+3\left(\frac{2\sqrt{6+6}}{6\times6}\right)+6\left(\frac{2\sqrt{6+7}}{6\times7}\right)+1\left(\frac{2\sqrt{6+8}}{6\times8}\right)+2\left(\frac{2\sqrt{7+7}}{7\times7}\right)+2\left(\frac{2\sqrt{7+8}}{7\times8}\right)$

$=7.721$

$AG^{ve}(\mathcal{G}_2)=\sum_{uv\in E(\mathcal{G}_2)}\frac{d_{ve}(u)+d_{ve}(v)}{2\sqrt{d_{ve}(u)\times d_{ve}(v)}}$

$=2\left(\frac{2+4}{2\sqrt{2\times4}}\right)+1\left(\frac{3+7}{2\sqrt{3\times7}}\right)+2\left(\frac{4+4}{2\sqrt{4\times4}}\right)+5\left(\frac{4+5}{2\sqrt{4\times5}}\right)+2\left(\frac{4+7}{2\sqrt{4\times7}}\right)+2\left(\frac{5+5}{2\sqrt{5\times5}}\right)+3\left(\frac{5+6}{2\sqrt{5\times6}}\right)$

$+3\left(\frac{6+6}{2\sqrt{6\times6}}\right)+6\left(\frac{6+7}{2\sqrt{6\times7}}\right)+1\left(\frac{6+8}{2\sqrt{6\times8}}\right)+2\left(\frac{7+7}{2\sqrt{7\times7}}\right)+2\left(\frac{7+8}{2\sqrt{7\times8}}\right)$

$=31.366$

$ISI^{ve}(\mathcal{G}_2)=\sum_{uv\in E(\mathcal{G}_2)}\frac{d_{ve}(u)\times d_{ve}(v)}{d_{ve}(u)+d_{ve}(v)}$

$=2\left(\frac{2\times4}{2+4}\right)+1\left(\frac{3\times7}{3+7}\right)+2\left(\frac{4\times4}{4+4}\right)+5\left(\frac{4\times5}{4+5}\right)+2\left(\frac{4\times7}{4+7}\right)+2\left(\frac{5\times5}{5+5}\right)+3\left(\frac{5\times6}{5+6}\right)+3\left(\frac{6\times6}{6+6}\right)+6\left(\frac{6\times7}{6+7}\right)$

$+1\left(\frac{6\times8}{6+8}\right)+2\left(\frac{7\times7}{7+7}\right)+2\left(\frac{7\times8}{7+8}\right)$

$=84.432$

$F^{ve}(\mathcal{G}_2)=\sum_{uv\in E(\mathcal{G}_2)}[d_{ve}(u)^2+d_{ve}(v)^2]$

$=2(2^2+4^2)+1(3^2+7^2)+2(4^2+4^2)+5(4^2+5^2)+2(4^2+7^2)+2(5^2+5^2)+3(5^2+6^2)$

$+3(6^2+6^2)+6(6^2+7^2)+1(6^2+8^2)+2(7^2+7^2)+2(7^2+8^2)$

$=1234$

$T^{ve}(\mathcal{G}_2)=\sum_{u\in V(\mathcal{G}_2)}d_{ve}(u)$

$=2(2)+1(3)+5(4)+6(5)+8(6)+5(7)+1(8)$

$=148$

$M_1^{ave}(\mathcal{G}_2)=\sum_{v\in V(\mathcal{G}_2)}d_{ve}(v)^2$

$=2(2)^2+1(3)^2+5(4)^2+6(5)^2+8(6)^2+5(7)^2+1(8)^2$

$=844$

$F_1^{ve}(\mathcal{G}_2)=\sum_{v\in V(\mathcal{G}_2)}d_{ve}(v)^3$

$=2(2)^3+1(3)^3+5(4)^3+6(5)^3+8(6)^3+5(7)^3+1(8)^3$

$=5068$

$ID^{ve}(\mathcal{G}_2)=\sum_{v\in V(\mathcal{G}_2)}\frac{1}{d_{ve}(v)}$

$=2\left(\frac{1}{2}\right)+1\left(\frac{1}{3}\right)+5\left(\frac{1}{4}\right)+6\left(\frac{1}{5}\right)+8\left(\frac{1}{6}\right)+5\left(\frac{1}{7}\right)+1\left(\frac{1}{8}\right)$

$=5.956$

$ZD^{ve}(\mathcal{G}_2)=\sum_{v\in V(\mathcal{G}_2)}\frac{1}{\sqrt{d_{ve}(v)}}$

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$$= 2\left(\frac{1}{\sqrt{2}}\right) + 1\left(\frac{1}{\sqrt{3}}\right) + 5\left(\frac{1}{\sqrt{4}}\right) + 6\left(\frac{1}{\sqrt{5}}\right) + 8\left(\frac{1}{\sqrt{6}}\right) + 5\left(\frac{1}{\sqrt{7}}\right) + 1\left(\frac{1}{\sqrt{8}}\right)$$

$$= 12.684$$

$$mM_1^{ve}(\mathcal{G}_2) = \sum_{v\in V(\mathcal{G}_2)} \frac{1}{d_{ve}(v)^2}$$

$$= 2\left(\frac{1}{(2)^2}\right) + 1\left(\frac{1}{(3)^2}\right) + 5\left(\frac{1}{(4)^2}\right) + 6\left(\frac{1}{(5)^2}\right) + 8\left(\frac{1}{(6)^2}\right) + 5\left(\frac{1}{(7)^2}\right) + 1\left(\frac{1}{(8)^2}\right)$$

$$= 1.504$$

Let $G_2$ be a simple connected graph of Donepezil, the $\mathcal{E}_v$-degree-based Topological Indices are,

$$T^{ev}(\mathcal{G}_2) = \sum_{e\in E(\mathcal{G}_2)} d_{ev}(e)$$

$$= 2(3) + 7(4) + 18(5) + 4(6)$$

$$= 148$$

$$M^{ev}(\mathcal{G}_2) = \sum_{e\in E(\mathcal{G}_2)} d_{ev}(e)^2 = 2(3)^2 + 7(4)^2 + 18(5)^2 + 4(6)^2 = 724$$

$$F^{ev}(\mathcal{G}_2) = \sum_{e\in E(\mathcal{G}_2)} d_{ev}(e)^3 = 2(3)^3 + 7(4)^3 + 18(5)^3 + 4(6)^3 = 3616$$

$$mM^{ev}(\mathcal{G}_2) = \sum_{e\in E(\mathcal{G}_2)} \frac{1}{d_{ev}(e)^2} = 2(\frac{1}{(3)^2}) + 7(\frac{1}{(4)^2}) + 18(\frac{1}{(5)^2}) + 4(\frac{1}{(6)^2}) = 1.491$$

$$ID^{ev}(\mathcal{G}_2) = \sum_{e\in E(\mathcal{G}_2)} \frac{1}{d_{ev}(e)} = 2(\frac{1}{(3)}) + 7(\frac{1}{(4)}) + 18(\frac{1}{(5)}) + 4(\frac{1}{(6)}) = 6.683$$

$$R^{ev}(\mathcal{G}_2) = \sum_{e\in E(\mathcal{G}_2)} (e)^{-1/2} = 2(3)^{-1/2} + 7(4)^{-1/2} + 18(5)^{-1/2} + 4(6)^{-1/2} = 14.338$$

$$RR^{ev}(\mathcal{G}_2) = \sum_{e\in E(\mathcal{G}_2)} (e)^{1/2} = 2(3)^{1/2} + 7(4)^{1/2} + 18(5)^{1/2} + 4(6)^{1/2} = 67.511$$

## RIVASTIGMINE

In this subsection, $\mathcal{V}_e$ and $\mathcal{E}_v$-degree based topological indices are calculated for the structure Rivastigmine. The molecular structure of Rivastigmine is shown in Fig 3.

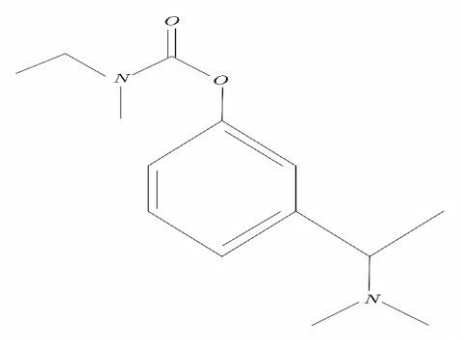


**Figure 3. Molecular structure of Rivastigmine[2].**

Let $G_3$ be a simple connected graph of Rivastigmine, the $\mathcal{V}_e$-degree-based Topological Indices are,

$$M_1^{\beta ve}(\mathcal{G}_3) = \sum_{uv\in E(\mathcal{G}_3)} d_{ve}(u) + d_{ve}(v)$$

$$= 1(2+4) + 2(3+5) + 2(3+6) + 1(3+7) + 2(4+5) + 1(4+6) + 1(5+6) + 2(5+7)$$

$$+4(6+6) + 1(6+7) + 1(7+7)$$

$$= 188$$

$$M_2^{ve}(\mathcal{G}_3) = \sum_{uv\in E(\mathcal{G}_3)} d_{ve}(u) \times d_{ve}(v)$$

$$= 1(2\times 4) + 2(3\times 5) + 2(3\times 6) + 1(3\times 7) + 2(4\times 5) + 1(4\times 6) + 1(5\times 6) + 2(5\times 7)$$

$$+4(6\times 6) + 1(6\times 7) + 1(7\times 7)$$

$$= 494$$

$$R^{ve}(\mathcal{G}_3) = \sum_{uv\in E(\mathcal{G}_3)} (d_{ve}(u) \times d_{ve}(v))^{-1/2}$$

$$= 1(2\times 4)^{-\frac{1}{2}} + 2(3\times 5)^{-\frac{1}{2}} + 2(3\times 6)^{-\frac{1}{2}} + 1(3\times 7)^{-\frac{1}{2}} + 2(4\times 5)^{-\frac{1}{2}} + 1(4\times 6)^{-\frac{1}{2}}$$

$$+1(5\times 6)^{-1/2} + 2(5\times 7)^{-1/2} + 4(6\times 6)^{-1/2} + 1(6\times 7)^{-1/2} + 1(7\times 7)^{-1/2}$$

$$= 3.695$$

$$\chi^{ve}(\mathcal{G}_3) = \sum_{uv\in E(\mathcal{G}_3)} (d_{ve}(u) + d_{ve}(v))^{-1/2}$$

$$= 1(2+4)^{-\frac{1}{2}} + 2(3+5)^{-\frac{1}{2}} + 2(3+6)^{-\frac{1}{2}} + 1(3+7)^{-\frac{1}{2}} + 2(4+5)^{-\frac{1}{2}} + 1(4+6)^{-\frac{1}{2}}$$

$$+1(5+6)^{-1/2} + 2(5+7)^{-1/2} + 4(6+6)^{-1/2} + 1(6+7)^{-1/2} + 1(7+7)^{-1/2}$$

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$= 5.659$

$H^{ve}(\mathcal{G}_3) = \sum_{uv\in E(\mathcal{G}_3)} \frac{2}{d_{ve}(u)+d_{ve}(v)}$.

$= 1\left(\frac{2}{2+4}\right) + 2\left(\frac{2}{3+5}\right) + 2\left(\frac{2}{3+6}\right) + 1\left(\frac{2}{3+7}\right) + 2\left(\frac{2}{4+5}\right) + 1\left(\frac{2}{4+6}\right) + 1\left(\frac{2}{5+6}\right) + 2\left(\frac{2}{5+7}\right) + 4\left(\frac{2}{6+6}\right) + 1\left(\frac{2}{6+7}\right) + 1\left(\frac{2}{7+7}\right)$

$= 3.601$

$HM_1^{ve}(\mathcal{G}_3) = \sum_{uv\in E(\mathcal{G}_3)} (d_{ve}(u) + d_{ve}(v))^2$

$= 1(2+4)^2 + 2(3+5)^2 + 2(3+6)^2 + 1(3+7)^2 + 2(4+5)^2 + 1(4+6)^2 + 1(5+6)^2 + 2(5+7)^2 + 4(6+6)^2 + 1(6+7)^2 + 1(7+7)^2$

$= 2038$

$HM_2^{ve}(\mathcal{G}_3) = \sum_{uv\in E(\mathcal{G}_3)} (d_{ve}(u) \times d_{ve}(v))^2$

$= 1(2\times 4)^2 + 2(3\times 5)^2 + 2(3\times 6)^2 + 1(3\times 7)^2 + 2(4\times 5)^2 + 1(4\times 6)^2 + 1(5\times 6)^2$

$+2(5\times 7)^2 + 4(6\times 6)^2 + 1(6\times 7)^2 + 1(7\times 7)^2$

$= 15678$

$ReZG_3^{ve}(\mathcal{G}_3) = \sum_{uv\in E(\mathcal{G}_3)} ((d_{ve}(u) \times d_{ve}(v))(d_{ve}(u) + d_{ve}(v))$

$= 1(2\times 4)(2+4) + 2(3\times 5)(3+5) + 2(3\times 6)(3+6) + 1(3\times 7)(3+7) + 2(4\times 5)(4+5) + 1(4\times 6)(4+6) + 1(5\times 6)(5+6) + 2(5\times 7)(5+7) + 4(6\times 6)(6+6) + 1(6\times 7)(6+7) + 1(7\times 7)(7+7)$

$= 5552$

$ABC^{ve}(\mathcal{G}_3) = \sum_{uv\in E(\mathcal{G}_3)} \sqrt{\frac{d_{ve}(u)+d_{ve}(v)-2}{d_{ve}(u)\times d_{ve}(v)}}$

$= 1\left(\sqrt{\frac{2+4-2}{2\times 4}}\right) + 2\left(\sqrt{\frac{3+5-2}{3\times 5}}\right) + 2\left(\sqrt{\frac{3+6-2}{3\times 6}}\right) + 1\left(\sqrt{\frac{3+7-2}{3\times 7}}\right) + 2\left(\sqrt{\frac{4+5-2}{4\times 5}}\right) + 1\left(\sqrt{\frac{4+6-2}{4\times 6}}\right)$

$+1\left(\sqrt{\frac{5+6-2}{5\times 6}}\right) + 2\left(\sqrt{\frac{5+7-2}{5\times 7}}\right) + 4\left(\sqrt{\frac{6+6-2}{6\times 6}}\right) + 1\left(\sqrt{\frac{6+7-2}{6\times 7}}\right) + 1\left(\sqrt{\frac{7+7-2}{7\times 7}}\right)$

$= 10.328$

$GA^{ve}(\mathcal{G}_3) = \sum_{uv\in E(\mathcal{G}_3)} \frac{2\sqrt{d_{ve}(u)\times d_{ve}(v)}}{d_{ve}(u)+d_{ve}(v)}$

$= 1\left(\frac{2\sqrt{2+4}}{2\times 4}\right) + 2\left(\frac{2\sqrt{3+5}}{3\times 5}\right) + 2\left(\frac{2\sqrt{3+6}}{3\times 6}\right) + 1\left(\frac{2\sqrt{3+7}}{3\times 7}\right) + 2\left(\frac{2\sqrt{4+5}}{4\times 5}\right) + 1\left(\frac{2\sqrt{4+6}}{4\times 6}\right) + 1\left(\frac{2\sqrt{5+6}}{5\times 6}\right)$

$+2\left(\frac{2\sqrt{5+7}}{5\times 7}\right) + 4\left(\frac{2\sqrt{6+6}}{6\times 6}\right) + 1\left(\frac{2\sqrt{6+7}}{6\times 7}\right) + 1\left(\frac{2\sqrt{7+7}}{7\times 7}\right)$

$= 5.394$

$AG^{ve}(\mathcal{G}_3) = \sum_{uv\in E(\mathcal{G}_3)} \frac{d_{ve}(u)+d_{ve}(v)}{2\sqrt{d_{ve}(u)\times d_{ve}(v)}}$

$= 1\left(\frac{2+4}{2\sqrt{2\times 4}}\right) + 2\left(\frac{3+5}{2\sqrt{3\times 5}}\right) + 2\left(\frac{3+6}{2\sqrt{3\times 6}}\right) + 1\left(\frac{3+7}{2\sqrt{3\times 7}}\right) + 2\left(\frac{4+5}{2\sqrt{4\times 5}}\right) + 1\left(\frac{4+6}{2\sqrt{4\times 6}}\right) + 1\left(\frac{5+6}{2\sqrt{5\times 6}}\right)$

$+2\left(\frac{5+7}{2\sqrt{5\times 7}}\right) + 4\left(\frac{6+6}{2\sqrt{6\times 6}}\right) + 1\left(\frac{6+7}{2\sqrt{6\times 7}}\right) + 1\left(\frac{7+7}{2\sqrt{7\times 7}}\right) = 18.947$

$ISI^{ve}(\mathcal{G}_3) = \sum_{uv\in E(\mathcal{G}_3)} \frac{d_{ve}(u)\times d_{ve}(v)}{d_{ve}(u)+d_{ve}(v)}$

$= 1\left(\frac{2\times 4}{2+4}\right) + 2\left(\frac{3\times 5}{3+5}\right) + 2\left(\frac{3\times 6}{3+6}\right) + 1\left(\frac{3\times 7}{3+7}\right) + 2\left(\frac{4\times 5}{4+5}\right) + 1\left(\frac{4\times 6}{4+6}\right) + 1\left(\frac{5\times 6}{5+6}\right) + 2\left(\frac{5\times 7}{5+7}\right) + 4\left(\frac{6\times 6}{6+6}\right)$

$+1\left(\frac{6\times 7}{6+7}\right) + 1\left(\frac{7\times 7}{7+7}\right)$

$= 45.318$

$F^{ve}(\mathcal{G}_3) = \sum_{uv\in E(\mathcal{G}_3)} [d_{ve}(u)^2 + d_{ve}(v)^2]$

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$= 1(2^2 + 4^2) + 2(3^2 + 5^2) + 2(3^2 + 6^2) + 1(3^2 + 7^2) + 2(4^2 + 5^2) + 1(4^2 + 6^2)$

$+1(5^2 + 6^2) + 2(5^2 + 7^2) + 4(6^2 + 6^2) + 1(6^2 + 7^2) + 1(7^2 + 7^2)$

$= 1050$

$T^{ve}(\mathcal{G}_3) = \sum_{u \in V(\mathcal{G}_3)} d_{ve}(u)$

$= 1(2) + 5(3) + 2(4) + 3(5) + 5(6) + 2(7)$

$= 84$

$M_1^{ave}(\mathcal{G}_3) = \sum_{v \in V(\mathcal{G}_3)} d_{ve}(v)^2$

$= 1(2)^2 + 5(3)^2 + 2(4)^2 + 3(5)^2 + 5(6)^2 + 2(7)^2$

$= 434$

$F_1^{ve}(\mathcal{G}_3) = \sum_{v \in V(\mathcal{G}_3)} d_{ve}(v)^3$

$= 1(2)^3 + 5(3)^3 + 2(4)^3 + 3(5)^3 + 5(6)^3 + 2(7)^3$

$= 2412$

$ID^{ve}(\mathcal{G}_3) = \sum_{v \in V(\mathcal{G}_3)} \frac{1}{d_{ve}(v)}$

$= 1\left(\frac{1}{2}\right) + 5\left(\frac{1}{3}\right) + 2\left(\frac{1}{4}\right) + 3\left(\frac{1}{5}\right) + 5\left(\frac{1}{6}\right) + 2\left(\frac{1}{7}\right)$

$= 4.386$

$ZD^{ve}(\mathcal{G}_3) = \sum_{v \in V(\mathcal{G}_3)} \frac{1}{\sqrt{d_{ve}(v)}}$

$= 1\left(\frac{1}{\sqrt{2}}\right) + 5\left(\frac{1}{\sqrt{3}}\right) + 2\left(\frac{1}{\sqrt{4}}\right) + 3\left(\frac{1}{\sqrt{5}}\right) + 5\left(\frac{1}{\sqrt{6}}\right) + 2\left(\frac{1}{\sqrt{7}}\right)$

$= 8.733$

$mM_1^{ve}(\mathcal{G}_3) = \sum_{v \in V(\mathcal{G}_3)} \frac{1}{d_{ve}(v)^2}$

$= 1\left(\frac{1}{(2)^2}\right) + 5\left(\frac{1}{(3)^2}\right) + 2\left(\frac{1}{(4)^2}\right) + 3\left(\frac{1}{(5)^2}\right) + 5\left(\frac{1}{(6)^2}\right) + 2\left(\frac{1}{(7)^2}\right)$

$= 1.231$

Let $G_3$ be a simple connected graph of Rivastigmine, the $\mathcal{E}_v$-degree-based Topological Indices are,

$T^{ev}(\mathcal{G}_3) = \sum_{e \in E(\mathcal{G}_3)} d_{ev}(e) = 1(3) + 7(4) + 7(5) + 3(6) = 84$

$M^{ev}(\mathcal{G}_3) = \sum_{e \in E(\mathcal{G}_3)} d_{ev}(\mathrm{e})^2 = 1(3)^2 + 7(4)^2 + 7(5)^2 + 3(6)^2 = 404$

$F^{ev}(\mathcal{G}_3) = \sum_{e \in E(\mathcal{G}_3)} d_{ev}(e)^3 = 1(3)^3 + 7(4)^3 + 7(5)^3 + 3(6)^3 = 1998$

$mM^{ev}(\mathcal{G}_3) = \sum_{e \in E(\mathcal{G}_3)} \frac{1}{d_{ev}(e)^2} = 1(\frac{1}{(3)^2}) + 7(\frac{1}{(4)^2}) + 7(\frac{1}{(5)^2}) + 3(\frac{1}{(6)^2}) = 0.912$

$ID^{ev}(\mathcal{G}_3) = \sum_{e \in E(\mathcal{G}_3)} \frac{1}{d_{ev}(e)} = 1(\frac{1}{(3)}) + 7(\frac{1}{(4)}) + 7(\frac{1}{(5)}) + 3(\frac{1}{(6)}) = 3.983$

$R^{ev}(\mathcal{G}_3) = \sum_{e \in E(\mathcal{G}_3)} (e)^{-1/2} = 1(3)^{-1/2} + 7(4)^{-1/2} + 7(5)^{-1/2} + 3(6)^{-1/2} = 8.433$

$RR^{ev}(\mathcal{G}_3) = \sum_{e \in E(\mathcal{G}_3)} (e)^{1/2} = 1(3)^{1/2} + 7(4)^{1/2} + 7(5)^{1/2} + 3(6)^{1/2} = 38.733$

## GALANTAMINE

In this subsection, $\mathcal{V}_e$ and $\mathcal{E}_v$-degree based topological indices are calculated for the structure Galantamine. The molecular structure of Galantamine is shown in Fig 4.

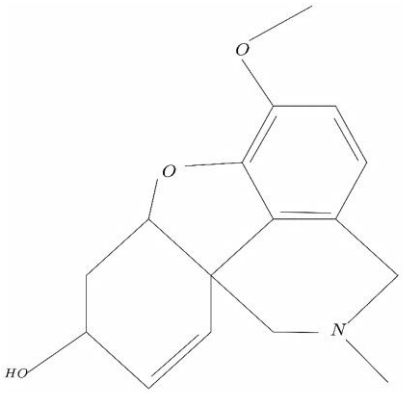


**Figure 4. Molecular structure of Galantamine[2].**

Let $G_4$ be a simple connected graph of Galantamine, the $\mathcal{V}_e$-degree based Topological Indices are,

$M_1^{\beta ve}(\mathcal{G}_4) = \sum_{uv \in E(\mathcal{G}_4)} d_{ve}(u) + d_{ve}(v)$

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$= 1(2+4) + 1(3+5) + 1(3+6) + 1(4+7) + 1(5+5) + 2(5+6) + 2(5+7) + 1(6+6)$

$+3(6+7) + 3(6+8) + 1(7+8) + 2(7+9) + 2(8+9) + 1(9+9)$

$= 282$

$M_2^{ve}(\mathcal{G}_4) = \sum_{uv \in E(\mathcal{G}_4)} d_{ve}(u) \times d_{ve}(v)$

$= 1(2\times4) + 1(3\times5) + 1(3\times6) + 1(4\times7) + 1(5\times5) + 2(5\times6) + 2(5\times7) + 1(6\times6) + 3(6\times7) + 3(6\times8) + 1(7\times8) + 2(7\times9) + 2(8\times9) + 1(9\times9)$

$= 937$

$R^{ve}(\mathcal{G}_4) = \sum_{uv \in E(\mathcal{G}_4)} (d_{ve}(u) \times d_{ve}(v))^{-1/2}$

$= 1(2\times4)^{-1/2} + 1(3\times5)^{-1/2} + 1(3\times6)^{-1/2} + 1(4\times7)^{-1/2} + 1(5\times5)^{-1/2} + 2(5\times6)^{-1/2} + 2(5\times7)^{-1/2} + 1(6\times6)^{-1/2} + 3(6\times7)^{-1/2} + 3(6\times8)^{-1/2} + 1(7\times8)^{-1/2} + 2(7\times9)^{-1/2} + 2(8\times9)^{-1/2} + 1(9\times9)^{-1/2}$

$= 3.736$

$\chi^{ve}(\mathcal{G}_4) = \sum_{uv \in E(\mathcal{G}_4)} (d_{ve}(u) + d_{ve}(v))^{-1/2}$

$= 1(2+4)^{-1/2} + 1(3+5)^{-1/2} + 1(3+6)^{-1/2} + 1(4+7)^{-1/2} + 1(5+5)^{-1/2} + 2(5+6)^{-1/2} + 2(5+7)^{-1/2} + 1(6+6)^{-1/2} + 3(6+7)^{-1/2} + 3(6+8)^{-1/2} + 1(7+8)^{-1/2} + 2(7+9)^{-1/2} + 2(8+9)^{-1/2} + 1(9+9)^{-1/2}$

$= 6.295$

$H^{ve}(\mathcal{G}_4) = \sum_{uv \in E(\mathcal{G}_4)} \frac{2}{d_{ve}(u)+d_{ve}(v)}$

$= 1\left(\frac{2}{2+4}\right) + 1\left(\frac{2}{3+5}\right) + 1\left(\frac{2}{3+6}\right) + 1\left(\frac{2}{4+7}\right) + 1\left(\frac{2}{5+5}\right) + 2\left(\frac{2}{5+6}\right) + 2\left(\frac{2}{5+7}\right) + 1\left(\frac{2}{6+6}\right) + 3\left(\frac{2}{6+7}\right) + 3\left(\frac{2}{6+8}\right) + 1\left(\frac{2}{7+8}\right) + 2\left(\frac{2}{7+9}\right) + 2\left(\frac{2}{8+9}\right) + 1\left(\frac{2}{9+9}\right)$

$= 3.664$

$HM_1^{ve}(\mathcal{G}_4) = \sum_{uv \in E(\mathcal{G}_4)} (d_{ve}(u) + d_{ve}(v))^2$

$= 1(2+4)^2 + 1(3+5)^2 + 1(3+6)^2 + 1(4+7)^2 + 1(5+5)^2 + 2(5+6)^2 + 2(5+7)^2 + 1(6+6)^2 + 3(6+7)^2 + 3(6+8)^2 + 1(7+8)^2 + 2(7+9)^2 + 2(8+9)^2 + 1(9+9)^2$

$= 3810$

$HM_2^{ve}(\mathcal{G}_4) = \sum_{uv \in E(\mathcal{G}_4)} (d_{ve}(u) \times d_{ve}(v))^2$

$= 1(2\times4)^2 + 1(3\times5)^2 + 1(3\times6)^2 + 1(4\times7)^2 + 1(5\times5)^2 + 2(5\times6)^2 + 2(5\times7)^2 + 1(6\times6)^2 + 3(6\times7)^2 + 3(6\times8)^2 + 1(7\times8)^2 + 2(7\times9)^2 + 2(8\times9)^2 + 1(9\times9)^2$

$= 47775$

$ReZG_3^{ve}(\mathcal{G}_4) = \sum_{uv \in E(\mathcal{G}_4)} ((d_{ve}(u) \times d_{ve}(v))(d_{ve}(u) + d_{ve}(v))$

$= 1(2\times4)(2+4) + 1(3\times5)(3+5) + 1(3\times6)(3+6) + 1(4\times7)(4+7) + 1(5\times5)(5+5) + 2(5\times6)(5+6) + 2(5\times7)(5+7) + 1(6\times6)(6+6) + 3(6\times7)(6+7) + 3(6\times8)(6+8) + 1(7\times8)(7+8) + 2(7\times9)(7+9) + 2(8\times9)(8+9) + 1(9\times9)(9+9)$

$= 13236$

$ABC^{ve}(\mathcal{G}_4) = \sum_{uv \in E(\mathcal{G}_4)} \sqrt{\frac{d_{ve}(u)+d_{ve}(v)-2}{d_{ve}(u)\times d_{ve}(v)}}$

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$$= 1\left(\sqrt{\frac{2+4-2}{2\times4}}\right) + 1\left(\sqrt{\frac{3+5-2}{3\times5}}\right) + 1\left(\sqrt{\frac{3+6-2}{3\times6}}\right) + 1\left(\sqrt{\frac{4+7-2}{4\times7}}\right) + 1\left(\sqrt{\frac{5+5-2}{5\times5}}\right) + 2\left(\sqrt{\frac{5+6-2}{5\times6}}\right)$$

$$+2\left(\sqrt{\frac{5+7-2}{5\times7}}\right) + 1\left(\sqrt{\frac{6+6-2}{6\times6}}\right) + 3\left(\sqrt{\frac{6+7-2}{6\times7}}\right) + 3\left(\sqrt{\frac{6+8-2}{6\times8}}\right) + 1\left(\sqrt{\frac{7+8-2}{7\times8}}\right) + 2\left(\sqrt{\frac{7+9-2}{7\times9}}\right)$$

$$+2\left(\sqrt{\frac{8+9-2}{8\times9}}\right) + 1\left(\sqrt{\frac{9+9-2}{9\times9}}\right)$$

$$= 11.604$$

$$GA^{ve}(\mathcal{G}_4) = \sum_{uv\in E(\mathcal{G}_4)} \frac{2\sqrt{d_{ve}(u)\times d_{ve}(v)}}{d_{ve}(u)+d_{ve}(v)}$$

$$= 1\left(\frac{2\sqrt{2+4}}{2\times4}\right) + 1\left(\frac{2\sqrt{3+5}}{3\times5}\right) + 1\left(\frac{2\sqrt{3+6}}{3\times6}\right) + 1\left(\frac{2\sqrt{4+7}}{4\times7}\right) + 1\left(\frac{2\sqrt{5+5}}{5\times5}\right) + 2\left(\frac{2\sqrt{5+6}}{5\times6}\right) + 2\left(\frac{2\sqrt{5+7}}{5\times7}\right)$$

$$+1\left(\frac{2\sqrt{6+6}}{6\times6}\right) + 3\left(\frac{2\sqrt{6+7}}{6\times7}\right) + 3\left(\frac{2\sqrt{6+8}}{6\times8}\right) + 1\left(\frac{2\sqrt{7+8}}{7\times8}\right) + 2\left(\frac{2\sqrt{7+9}}{7\times9}\right) + 2\left(\frac{2\sqrt{8+9}}{8\times9}\right) + 1\left(\frac{2\sqrt{9+9}}{9\times9}\right)$$

$$= 4.551$$

$$AG^{ve}(\mathcal{G}_4) = \sum_{uv\in E(\mathcal{G}_4)} \frac{d_{ve}(u)+d_{ve}(v)}{2\sqrt{d_{ve}(u)\times d_{ve}(v)}}$$

$$= 1\left(\frac{2+4}{2\sqrt{2\times4}}\right) + 1\left(\frac{3+5}{2\sqrt{3\times5}}\right) + 1\left(\frac{3+6}{2\sqrt{3\times6}}\right) + 1\left(\frac{4+7}{2\sqrt{4\times7}}\right) + 1\left(\frac{5+5}{2\sqrt{5\times5}}\right) + 2\left(\frac{5+6}{2\sqrt{5\times6}}\right) + 2\left(\frac{5+7}{2\sqrt{5\times7}}\right)$$

$$+1\left(\frac{6+6}{2\sqrt{6\times6}}\right) + 3\left(\frac{6+7}{2\sqrt{6\times7}}\right) + 3\left(\frac{6+8}{2\sqrt{6\times8}}\right) + 1\left(\frac{7+8}{2\sqrt{7\times8}}\right) + 2\left(\frac{7+9}{2\sqrt{7\times9}}\right) + 2\left(\frac{8+9}{2\sqrt{8\times9}}\right) + 1\left(\frac{9+9}{2\sqrt{9\times9}}\right)$$

$$= 22.291$$

$$ISI^{ve}(\mathcal{G}_4) = \sum_{uv\in E(\mathcal{G}_4)} \frac{d_{ve}(u)\times d_{ve}(v)}{d_{ve}(u)+d_{ve}(v)}$$

$$= 1\left(\frac{2\times4}{2+4}\right) + 1\left(\frac{3\times5}{3+5}\right) + 1\left(\frac{3\times6}{3+6}\right) + 1\left(\frac{4\times7}{4+7}\right) + 1\left(\frac{5\times5}{5+5}\right) + 2\left(\frac{5\times6}{5+6}\right) + 2\left(\frac{5\times7}{5+7}\right) + 1\left(\frac{6\times6}{6+6}\right)$$

$$+3\left(\frac{6\times7}{6+7}\right) + 3\left(\frac{6\times8}{6+8}\right) + 1\left(\frac{7\times8}{7+8}\right) + 2\left(\frac{7\times9}{7+9}\right) + 2\left(\frac{8\times9}{8+9}\right) + 1\left(\frac{9\times9}{9+9}\right)$$

$$= 69.098$$

$$F^{ve}(\mathcal{G}_4) = \sum_{uv\in E(\mathcal{G}_4)} [d_{ve}(u)^2 + d_{ve}(v)^2]$$

$$\begin{aligned} &= 1(2^2+4^2) + 1(3^2+5^2) + \\ &\quad 1(3^2+6^2) + 1(4^2+7^2) + \\ &\quad 1(5^2+5^2) + 2(5^2+6^2) + \\ &\quad 2(5^2+7^2) + 1(6^2+6^2) + \\ &\quad 3(6^2+7^2) + 3(6^2+8^2) + \\ &\quad 1(7^2+8^2) + 2(7^2+9^2) + \\ &\quad 2(8^2+9^2) + 1(9^2+9^2) \end{aligned}$$

$$= 1936$$

$$T^{ve}(\mathcal{G}_4) = \sum_{u\in V(\mathcal{G}_4)} d_{ve}(u)$$

$$= 1(2) + 2(3) + 1(4) + 3(5) + 4(6) + 3(7) + 2(8) + 2(9)$$

$$= 106$$

$$M_1^{ave}(\mathcal{G}_4) = \sum_{v\in V(\mathcal{G}_4)} d_{ve}(v)^2$$

$$= 1(2)^2 + 2(3)^2 + 1(4)^2 + 3(5)^2 + 4(6)^2 + 3(7)^2 + 2(8)^2 + 2(9)^2$$

$$= 694$$

$$F_1^{ve}(\mathcal{G}_4) = \sum_{v\in V(\mathcal{G}_4)} d_{ve}(v)^3$$

$$= 1(2)^3 + 2(3)^3 + 1(4)^3 + 3(5)^3 + 4(6)^3 + 3(7)^3 + 2(8)^3 + 2(9)^3$$

$$= 4876$$

$$ID^{ve}(\mathcal{G}_4) = \sum_{v\in V(\mathcal{G}_4)} \frac{1}{d_{ve}(v)}$$

$$= 1\left(\frac{1}{2}\right) + 2\left(\frac{1}{3}\right) + 1\left(\frac{1}{4}\right) + 3\left(\frac{1}{5}\right) + 4\left(\frac{1}{6}\right) + 3\left(\frac{1}{7}\right) + 2\left(\frac{1}{8}\right) + 2\left(\frac{1}{9}\right)$$

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$= 3.584$

$ZD^{ve}(\mathcal{G}_4) = \sum_{v\in V(\mathcal{G}_4)} \frac{1}{\sqrt{d_{ve}(v)}}$

$= 1\left(\frac{1}{\sqrt{2}}\right) + 2\left(\frac{1}{\sqrt{3}}\right) + 1\left(\frac{1}{\sqrt{4}}\right) + 3\left(\frac{1}{\sqrt{5}}\right) + 4\left(\frac{1}{\sqrt{6}}\right) + 3\left(\frac{1}{\sqrt{7}}\right) + 2\left(\frac{1}{\sqrt{8}}\right) + 2\left(\frac{1}{\sqrt{9}}\right)$

$= 7.844$

$mM_1^{ve}(\mathcal{G}_4) = \sum_{v\in V(\mathcal{G}_4)} \frac{1}{d_{ve}(v)^2}$

$= 1\left(\frac{1}{(2)^2}\right) + 2\left(\frac{1}{(3)^2}\right) + 1\left(\frac{1}{(4)^2}\right) + 3\left(\frac{1}{(5)^2}\right) + 4\left(\frac{1}{(6)^2}\right) + 3\left(\frac{1}{(7)^2}\right) + 2\left(\frac{1}{(8)^2}\right) + 2\left(\frac{1}{(9)^2}\right)$

$= 0.833$

Let $G_4$ be a simple connected graph of Galantamine, the $\mathcal{E}_v$-degree based Topological Indices are,

$T^{ev}(\mathcal{G}_4) = \sum_{e\in E(\mathcal{G}_4)} d_{ev}(e) = 1(3) + 3(4) + 11(5) + 7(6) = 112$

$M^{ev}(\mathcal{G}_4) = \sum_{e\in E(\mathcal{G}_4)} d_{ev}(e)^2 = 1(3)^2 + 3(4)^2 + 11(5)^2 + 7(6)^2 = 584$

$F^{ev}(\mathcal{G}_4) = \sum_{e\in E(\mathcal{G}_4)} d_{ev}(e)^3 = 1(3)^3 + 3(4)^3 + 11(5)^3 + 7(6)^3 = 3106$

$mM^{ev}(\mathcal{G}_4) = \sum_{e\in E(\mathcal{G}_4)} \frac{1}{d_{ev}(e)^2} = 1(\frac{1}{(3)^2}) + 3(\frac{1}{(4)^2}) + 11(\frac{1}{(5)^2}) + 7(\frac{1}{(6)^2}) = 0.933$

$ID^{ev}(\mathcal{G}_4) = \sum_{e\in E(\mathcal{G}_4)} \frac{1}{d_{ev}(e)} = 1(\frac{1}{(3)}) + 3(\frac{1}{(4)}) + 11(\frac{1}{(5)}) + 7(\frac{1}{(6)}) = 4.450$

$R^{ev}(\mathcal{G}_4) = \sum_{e\in E(\mathcal{G}_4)} (e)^{-1/2} = 1(3)^{-1/2} + 3(4)^{-1/2} + 11(5)^{-1/2} + 7(6)^{-1/2} = 9.854$

$RR^{ev}(\mathcal{G}_4) = \sum_{e\in E(\mathcal{G}_4)} (e)^{1/2} = 1(3)^{1/2} + 3(4)^{1/2} + 11(5)^{1/2} + 7(6)^{1/2} = 49.475$

## HUPERZINE A

In this subsection, $\mathcal{V}_e$ and $\mathcal{E}_v$-degree based topological indices are calculated for the structure Huperzine A. The molecular structure of Huperzine A is shown in Fig 5.

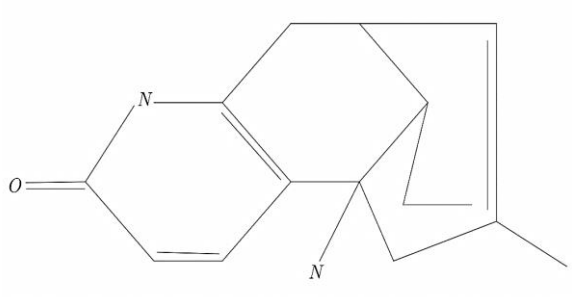


**Figure 5. Molecular structure of Huperzine A[3].**

Let $G_5$ be a simple connected graph of Huperzine A, the $\mathcal{V}_e$-degree-based Topological Indices are,

$M_1^{\beta ve}(\mathcal{G}_5) = \sum_{uv\in E(\mathcal{G}_5)} d_{ve}(u) + d_{ve}(v)$

$= 1(2+4) + 2(3+5) + 2(4+9) + 2(5+5) + 2(5+6) + 1(5+7) + 1(5+9) + 4(6+7) + 3(7+9) + 2(9+9)$

$= 252$

$M_2^{ve}(\mathcal{G}_5) = \sum_{uv\in E(\mathcal{G}_5)} d_{ve}(u) \times d_{ve}(v)$

$= 1(2\times 4) + 2(3\times 5) + 2(4\times 9) + 2(5\times 5) + 2(5\times 6) + 1(5\times 7) + 1(5\times 9) + 4(6\times 7) + 3(7\times 9) + 2(9\times 9)$

$= 819$

$R^{ve}(\mathcal{G}_5) = \sum_{uv\in E(\mathcal{G}_5)} (d_{ve}(u) \times d_{ve}(v))^{-1/2}$

$= 1(2\times 4)^{-1/2} + 2(3\times 5)^{-1/2} + 2(4\times 9)^{-1/2} + 2(5\times 5)^{-1/2} + 2(5\times 6)^{-1/2}$

$+1(5\times 7)^{-1/2} + 1(5\times 9)^{-1/2} + 4(6\times 7)^{-1/2} + 3(7\times 9)^{-1/2} + 2(9\times 9)^{-1/2}$

$= 3.504$

$\chi^{ve}(\mathcal{G}_5) = \sum_{uv\in E(\mathcal{G}_5)} (d_{ve}(u) + d_{ve}(v))^{-1/2}$

$= 1(2+4)^{-1/2} + 2(3+5)^{-1/2} + 2(4+9)^{-1/2} + 2(5+5)^{-1/2} + 2(5+6)^{-1/2}$

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$$+1(5+7)^{-1/2}+1(5+9)^{-1/2}+4(6+7)^{-1/2}+3(7+9)^{-1/2}+2(9+9)^{-1/2}$$

$$=5.792$$

$$H^{ve}(\mathcal{G}_5)=\sum_{uv\in E(\mathcal{G}_5)}\frac{2}{d_{ve}(u)+d_{ve}(v)}$$

$$=1\left(\frac{2}{2+4}\right)+2\left(\frac{2}{3+5}\right)+2\left(\frac{2}{4+9}\right)+2\left(\frac{2}{5+5}\right)+2\left(\frac{2}{5+6}\right)+1\left(\frac{2}{5+7}\right)+1\left(\frac{2}{5+9}\right)$$

$$+4\left(\frac{2}{6+7}\right)+3\left(\frac{2}{7+9}\right)+2\left(\frac{2}{9+9}\right)$$

$$=3.427$$

$$HM_1^{ve}(\mathcal{G}_5)=\sum_{uv\in E(\mathcal{G}_5)}(d_{ve}(u)+d_{ve}(v))^2$$

$$=1(2+4)^2+2(3+5)^2+2(4+9)^2+2(5+5)^2+2(5+6)^2+1(5+7)^2+1(5+9)^2$$

$$+4(6+7)^2+3(7+9)^2+2(9+9)^2$$

$$=3376$$

$$HM_2^{ve}(\mathcal{G}_5)=\sum_{uv\in E(\mathcal{G}_5)}(d_{ve}(u)\times d_{ve}(v))^2$$

$$=1(2\times4)^2+2(3\times5)^2+2(4\times9)^2+2(5\times5)^2+2(5\times6)^2+1(5\times7)^2+1(5\times9)^2$$

$$+4(6\times7)^2+3(7\times9)^2+2(9\times9)^2$$

$$=41491$$

$$ReZG_3^{ve}(\mathcal{G}_5)=\sum_{uv\in E(\mathcal{G}_5)}((d_{ve}(u)\times d_{ve}(v))(d_{ve}(u)+d_{ve}(v))$$

$$=1(2\times4)(2+4)+2(3\times5)(3+5)+2(4\times9)(4+9)+2(5\times5)(5+5)+2(5\times6)(5+6)+1(5\times7)(5+7)+1(5\times9)(5+9)+4(6\times7)(6+7)+3(7\times9)(7+9)+2(9\times9)(9+9)$$

$$=11558$$

$$ABC^{ve}(\mathcal{G}_5)=\sum_{uv\in E(\mathcal{G}_5)}\sqrt{\frac{d_{ve}(u)+d_{ve}(v)-2}{d_{ve}(u)\times d_{ve}(v)}}$$

$$=1\left(\sqrt{\frac{2+4-2}{2\times4}}\right)+2\left(\sqrt{\frac{3+5-2}{3\times5}}\right)+2\left(\sqrt{\frac{4+9-2}{4\times9}}\right)+2\left(\sqrt{\frac{5+5-2}{5\times5}}\right)+2\left(\sqrt{\frac{5+6-2}{5\times6}}\right)$$

$$+1\left(\sqrt{\frac{5+7-2}{5\times7}}\right)+1\left(\sqrt{\frac{5+9-2}{5\times9}}\right)+4\left(\sqrt{\frac{6+7-2}{6\times7}}\right)+3\left(\sqrt{\frac{7+9-2}{7\times9}}\right)+2\left(\sqrt{\frac{9+9-2}{9\times9}}\right)$$

$$=10.706$$

$$GA^{ve}(\mathcal{G}_5)=\sum_{uv\in E(\mathcal{G}_5)}\frac{2\sqrt{d_{ve}(u)\times d_{ve}(v)}}{d_{ve}(u)+d_{ve}(v)}$$

$$=1\left(\frac{2\sqrt{2+4}}{2\times4}\right)+2\left(\frac{2\sqrt{3+5}}{3\times5}\right)+2\left(\frac{2\sqrt{4+9}}{4\times9}\right)+2\left(\frac{2\sqrt{5+5}}{5\times5}\right)+2\left(\frac{2\sqrt{5+6}}{5\times6}\right)+1\left(\frac{2\sqrt{5+7}}{5\times7}\right)$$

$$+1\left(\frac{2\sqrt{5+9}}{5\times9}\right)+4\left(\frac{2\sqrt{6+7}}{6\times7}\right)+3\left(\frac{2\sqrt{7+9}}{7\times9}\right)+2\left(\frac{2\sqrt{9+9}}{9\times9}\right)$$

$$=4.356$$

$$AG^{ve}(\mathcal{G}_5)=\sum_{uv\in E(\mathcal{G}_5)}\frac{d_{ve}(u)+d_{ve}(v)}{2\sqrt{d_{ve}(u)\times d_{ve}(v)}}$$

$$=1\left(\frac{2+4}{2\sqrt{2\times4}}\right)+2\left(\frac{3+5}{2\sqrt{3\times5}}\right)+2\left(\frac{4+9}{2\sqrt{4\times9}}\right)+2\left(\frac{5+5}{2\sqrt{5\times5}}\right)+2\left(\frac{5+6}{2\sqrt{5\times6}}\right)+1\left(\frac{5+7}{2\sqrt{5\times7}}\right)$$

$$+1\left(\frac{5+9}{2\sqrt{5\times9}}\right)+4\left(\frac{6+7}{2\sqrt{6\times7}}\right)+3\left(\frac{7+9}{2\sqrt{7\times9}}\right)+2\left(\frac{9+9}{2\sqrt{9\times9}}\right)$$

$$=20.394$$

$$ISI^{ve}(\mathcal{G}_5)=\sum_{uv\in E(\mathcal{G}_5)}\frac{d_{ve}(u)\times d_{ve}(v)}{d_{ve}(u)+d_{ve}(v)}$$

$$=1\left(\frac{2\times4}{2+4}\right)+2\left(\frac{3\times5}{3+5}\right)+2\left(\frac{4\times9}{4+9}\right)+2\left(\frac{5\times5}{5+5}\right)+2\left(\frac{5\times6}{5+6}\right)+1\left(\frac{5\times7}{5+7}\right)+1\left(\frac{5\times9}{5+9}\right)+4\left(\frac{6\times7}{6+7}\right)$$

$$+3\left(\frac{7\times9}{7+9}\right)+2\left(\frac{9\times9}{9+9}\right)$$

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$= 60.943$

$F^{ve}(\mathcal{G}_5) = \sum_{uv \in E(\mathcal{G}_5)} [d_{ve}(u)^2 + d_{ve}(v)^2]$

$= 1(2^2 + 4^2) + 2(3^2 + 5^2) + 2(4^2 + 9^2) + 2(5^2 + 5^2) + 2(5^2 + 6^2) + 1(5^2 + 7^2) + 1(5^2 + 9^2) + 4(6^2 + 7^2) + 3(7^2 + 9^2) + 2(9^2 + 9^2)$

$= 1738$

$T^{ve}(\mathcal{G}_5) = \sum_{u \in V(\mathcal{G}_5)} d_{ve}(u)$

$= 1(2) + 2(3) + 2(4) + 4(5) + 3(6) + 3(7) + 3(9)$

$= 102$

$M_1^{ave}(\mathcal{G}_5) = \sum_{v \in V(\mathcal{G}_5)} d_{ve}(v)^2$

$= 1(2)^2 + 2(3)^2 + 2(4)^2 + 4(5)^2 + 3(6)^2 + 3(7)^2 + 3(9)^2$

$= 652$

$F_1^{ve}(\mathcal{G}_5) = \sum_{v \in V(\mathcal{G}_5)} d_{ve}(v)^3$

$= 1(2)^3 + 2(3)^3 + 2(4)^3 + 4(5)^3 + 3(6)^3 + 3(7)^3 + 3(9)^3$

$= 4554$

$ID^{ve}(\mathcal{G}_5) = \sum_{v \in V(\mathcal{G}_5)} \frac{1}{d_{ve}(v)}$

$= 1\left(\frac{1}{2}\right) + 2\left(\frac{1}{3}\right) + 2\left(\frac{1}{4}\right) + 4\left(\frac{1}{5}\right) + 3\left(\frac{1}{6}\right) + 3\left(\frac{1}{7}\right) + 3\left(\frac{1}{9}\right)$

$= 3.729$

$ZD^{ve}(\mathcal{G}_5) = \sum_{v \in V(\mathcal{G}_5)} \frac{1}{\sqrt{d_{ve}(v)}}$

$= 1\left(\frac{1}{\sqrt{2}}\right) + 2\left(\frac{1}{\sqrt{3}}\right) + 2\left(\frac{1}{\sqrt{4}}\right) + 4\left(\frac{1}{\sqrt{5}}\right) + 3\left(\frac{1}{\sqrt{6}}\right) + 3\left(\frac{1}{\sqrt{7}}\right) + 3\left(\frac{1}{\sqrt{9}}\right)$

$= 8.009$

$mM_1^{ve}(\mathcal{G}_5) = \sum_{v \in V(\mathcal{G}_5)} \frac{1}{d_{ve}(v)^2}$

$= 1\left(\frac{1}{(2)^2}\right) + 2\left(\frac{1}{(3)^2}\right) + 2\left(\frac{1}{(4)^2}\right) + 4\left(\frac{1}{(5)^2}\right) + 3\left(\frac{1}{(6)^2}\right) + 3\left(\frac{1}{(7)^2}\right) + 3\left(\frac{1}{(9)^2}\right)$

$= 0.939$

Let $G_5$ be a simple connected graph of Huperzine A, the $\mathcal{E}_v$-degree based Topological Indices are,

$T^{ev}(\mathcal{G}_5) = \sum_{e \in E(\mathcal{G}_5)} d_{ev}(e) = 1(3) + 3(4) + 11(5) + 3(6) + 2(7) = 102$

$M^{ev}(\mathcal{G}_5) = \sum_{e \in E(\mathcal{G}_5)} d_{ev}(e)^2 = 1(3)^2 + 3(4)^2 + 11(5)^2 + 3(6)^2 + 2(7)^2 = 538$

$F^{ev}(\mathcal{G}_5) = \sum_{e \in E(\mathcal{G}_5)} d_{ev}(e)^3 = 1(3)^3 + 3(4)^3 + 11(5)^3 + 3(6)^3 + 2(7)^3 = 2928$

$mM^{ev}(\mathcal{G}_5) = \sum_{e \in E(\mathcal{G}_5)} \frac{1}{d_{ev}(e)^2} = 1\left(\frac{1}{(3)^2}\right) + 3\left(\frac{1}{(4)^2}\right) + 11\left(\frac{1}{(5)^2}\right) + 3\left(\frac{1}{(6)^2}\right) + 2\left(\frac{1}{(7)^2}\right) = 0.862$

$ID^{ev}(\mathcal{G}_5) = \sum_{e \in E(\mathcal{G}_5)} \frac{1}{d_{ev}(e)} = 1\left(\frac{1}{(3)}\right) + 3\left(\frac{1}{(4)}\right) + 11\left(\frac{1}{(5)}\right) + 3\left(\frac{1}{(6)}\right) + 2\left(\frac{1}{(7)}\right) = 4.069$

$R^{ev}(\mathcal{G}_5) = \sum_{e \in E(\mathcal{G}_5)} (e)^{-1/2} = 1(3)^{-1/2} + 3(4)^{-1/2} + 11(5)^{-1/2} + 3(6)^{-1/2} + 2(7)^{-1/2} = 8.977$

$RR^{ev}(\mathcal{G}_5) = \sum_{e \in E(\mathcal{G}_5)} (`e)^{1/2}.= 1(3)^{1/2} + 3(4)^{1/2} + 11(5)^{1/2} + 3(6)^{1/2} + 2(7)^{1/2} = 44.968.$

## Quantitative Structure Analysis of Chemical Graphs of Tacrine, Donepezil, Rivestigmine, Galantamine, Huperzine A.

In this section, QSPR modeling using specific physicochemical properties of five drugs: Tacrine, Donepezil, Rivastigmine, Galantamine, and Huperzine A was conducted. Additionally, nineteen $\mathcal{V}_e$-degree-based topological indices and seven $\mathcal{E}_v$-degree-based topological indices were utilized for the models. Furthermore, ten physicochemical

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properties, namely Density ($D$), Enthalpy ($E$), Boiling Point ($BP$), Flash point ($FP$), Log P, Molar refraction ($MR$), Polar surface area ($PSA$), Surface tension ($ST$), Molar volume ($MV$), Polarizability ($P$) of the mentioned drugs were considered and tabulated in Table 6. Curvilinear regression analysis using the SPSS statistical software was employed, with the values of the aforementioned topological indices as the independent variables in the models. The objective of this study was to explore and test the following regression models for drugs used in Alzheimer's treatment.

$$Y = a + b_1X_1;$$

(Linear Equation).

$$Y = a + b_1X_2 + b_2X_2^2;$$

(Quadratic Equation).

In the regression equation, $Y$ represents the dependent variable, while "$a$" is the regression model constant. "$b_i$" (where i=1,2,3) represents the coefficients for individual descriptors, and "$X_i$" (where i=1,2) is the independent variable. The regression equation is built using the "n" number of samples. The correlation coefficient, denoted by "R," measures the degree of correlation between the experimental and theoretical results. When the experimental and theoretical results are in close agreement, the correlation coefficient tends to be close to 1, indicating a strong correlation.

Additionally, the standard error of the estimates, denoted as "SE," measures the accuracy of the regression model's predictions. Fisher's statistic[41], represented by "F" is used to assess the overall significance of the regression model.

To evaluate the predictive quality of the model, it is essential to compare the observed values with the model predictions. By assessing the agreement between these values, researchers can determine how well the model performs in predicting the dependent variable based on the independent variables and their corresponding coefficients. For more recent works regarding QSPR analysis using topological indices, see details[42-44].

**Table 6. The physico-chemical properties of drugs used in the Alzheimer's treatment**

| Drugs | $D$ | $BP$ | $E$ | $FP$ | $MR$ | $LogP$ | $PSA$ | $P$ | $ST$ | $MV$ | $IC50$ ($\mu M$) | $PIC50$ ($\mu M$) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| *Tacrine* | 1.3 | 353.8 | 59.9 | 167.8 | 59.8 | 1.78 | 36 | 23.7 | 49.6 | 157.8 | 0.10 | 7.00 |
| *Donepezil* | 1.1 | 527.9 | 80.3 | 273.1 | 110.4 | 4.71 | 39 | 43.8 | 45.2 | 332.5 | 0.021 | 7.678 |
| *Rivastigmine* | 1.0 | 316.2 | 55.8 | 145.0 | 73.1 | 2.14 | 33 | 29.0 | 36.9 | 241.2 | 4.15 | 5.382 |
| *Galantamine* | 1.3 | 439.3 | 73.4 | 219.5 | 80.3 | 1.75 | 42 | 31.8 | 56.6 | 223.9 | 0.35 | 6.456 |
| *HuperzineA* | 1.2 | 505.0 | 77.5 | 259.2 | 71.5 | 0.71 | 55 | 28.3 | 49.5 | 201.8 | 0.6 | 6.222 |

**Linear Regression:** Linear regression is a statistical method used to model the relationship between a dependent variable and one or more independent variables. In this case, linear regression was employed to explore how the calculated indices relate to the efficacy of the drugs. Linear regression assumes a linear relationship between the indices and the drug efficacy, allowing you to estimate the effect of each index on the outcome.

From the Table 7, $mM_1^{ve}$ for density, $M_1\alpha^{ve}$ for boiling point and Flash point, $F_1^{ve}$ for enthalpy, $H^{ve}$ for molar refraction and polarizability, $mM^{ev}$ for Log P, $ReZG_3^{ve}$ for polar surface area, $HM_2^{ve}$ for surface tension and $ID^{ve}$ for molar volume are the best estimator indices in linear regression models.

The linear models obtained with these topological indices are as follows:

$$D = 1.319 - 0.002(mM_1^{ve}) \quad F = 5.596 \quad SE = 0.089 \quad P = 0.001 \quad R^2 = 0.649$$

$$B.P = 108.838 + 0.514(M_1\alpha^{ve}) \quad F = 17.334 \quad SE = 40.905 \quad P = 0.030 \quad R^2 = 0.864$$

$$E = 33.861 + 0.009(F_1^{ve}) \quad F = 40.352 \quad SE = 3.312 \quad P = 0.070 \quad R^2 = 0.941$$

$$F.P = 108.838 + 0.514(M_1\alpha^{ve}) \quad F = 17.334 \quad SE = 40.905 \quad P = 0.072 \quad R^2 = 0.856$$

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$M.R = 19.147 + 15.543(H^{ve})$ $F = 182.494$ $SE = 2.793$ P $= 0.022$ $R^2 = 0.983$

$P = 7.521 + 6.178(H^{ve})$ $F = 189.827$ $SE = 1.089$ P $= 0.025$ $R^2 = 0.984$

$LogP = -2.680 + 4.918(mM^{ev})$ $F = 19.588$ $SE = 0.628$ P $= 0.103$ $R^2 = 0.863$

$S.T = 32.142 + 0.000(HM_2^{ve})$ $F = 6.601$ $SE = 4.664$ P $= 0.015$ $R^2 = 0.772$

$PSA = 21.894 + 0.002(ReZG_3^{ve})$ $F = 4.436$ $SE = 6.245$ P $= 0.136$ $R^2 = 0.701$

$M.V = 1.539 + 55.612(ID^{ve})$ $F = 63.330$ $SE = 15.815$ $P = 0.003$ $R^2 = 0.003$

**Table 7. The Correlation coefficient ® obtained by linear regression model between topological indices and physico-chemical properties of drugs.**

| Indices | *D* | *BP* | *E* | *FP* | *MR* | *LogP* | *PSA* | *P* | *ST* | *MV* |
|---|---|---|---|---|---|---|---|---|---|---|
| $M1\beta^{ve}$ | 0.038 | 0.873 | 0.895 | 0.873 | 0.893 | 0.643 | 0.282 | 0.892 | 0.338 | 0.754 |
| $M2^{ve}$ | 0.287 | 0.893 | 0.941 | 0.893 | 0.717 | 0.385 | 0.469 | 0.714 | 0.593 | 0.535 |
| $R^{ve}$ | 0.437 | 0.618 | 0.595 | 0.618 | 0.985 | 0.914 | 0.102 | 0.985 | 0.204 | 0.963 |
| $\chi^{ve}$ | 0.327 | 0.685 | 0.669 | 0.685 | 0.987 | 0.893 | 0.038 | 0.987 | 0.084 | 0.934 |
| $H^{ve}$ | 0.461 | 0.637 | 0.619 | 0.637 | **0.992** | 0.883 | 0.059 | **0.992** | 0.203 | 0.977 |
| $HM^{ve}$ | 0.284 | 0.896 | 0.944 | 0.897 | 0.715 | 0.379 | 0.477 | 0.713 | 0.591 | 0.534 |
| $HM^{ve}$ | 0.557 | 0.764 | 0.841 | 0.764 | 0.362 | 0.035 | 0.644 | 0.358 | **0.829** | 0.159 |
| $ReZG^{ve}$ | 0.436 | 0.885 | 0.932 | 0.885 | 0.418 | 0.015 | **0.772** | 0.414 | 0.718 | 0.227 |
| $ABC^{ve}$ | 0.317 | 0.697 | 0.683 | 0.697 | 0.988 | 0.884 | 0.021 | 0.989 | 0.068 | 0.933 |
| $GA^{ve}$ | 0.617 | 0.452 | 0.418 | 0.452 | 0.940 | 0.928 | 0.245 | 0.941 | 0.414 | 0.977 |
| $AG^{ve}$ | 0.267 | 0.738 | 0.732 | 0.738 | 0.989 | 0.848 | 0.036 | 0.988 | 0.0006 | 0.92 |
| $ISI^{ve}$ | 0.048 | 0.870 | 0.893 | 0.870 | 0.891 | 0.644 | 0.276 | 0.889 | 0.346 | 0.749 |
| $F^{ve}$ | 0.281 | 0.900 | 0.946 | 0.900 | 0.714 | 0.374 | 0.486 | 0.711 | 0.590 | 0.533 |
| $T^{ve}$ | 0.17 | 0.829 | 0.821 | 0.829 | 30.959 | 0.775 | 0.172 | 0.958 | 0.102 | 0.862 |
| $F^{ve}$ | 0.327 | 0.922 | **0.965** | 0.922 | 0.655 | 0.296 | 0.568 | 0.653 | 0.626 | 0.466 |
| $ID^{ve}$ | 0.68 | 0.489 | 0.449 | 0.489 | 0.926 | 0.862 | 0.145 | 0.927 | 0.458 | **0.978** |
| $ZD^{ve}$ | 0.579 | 0.567 | 0.53 | 0.567 | 0.959 | 0.888 | 0.106 | 0.959 | 0.351 | 0.977 |
| $mM^{ve}$ | **0.807** | 0.387 | 0.349 | 0.387 | 0.849 | 0.755 | 0.141 | 0.85 | 0.574 | 0.95 |
| $M_1\alpha^{ve}$ | 0.100 | **0.923** | 0.942 | **0.923** | 0.843 | 0.559 | 0.393 | 0.841 | 0.398 | 0.688 |
| $T^{ev}$ | 0.117 | 0.829 | 0.835 | 0.829 | **0.955** | 0.751 | 0.177 | 0.954 | 0.172 | 0.848 |
| $M^{ev}$ | 0.016 | 0.884 | 0.902 | 0.885 | 0.906 | 0.642 | 0.302 | 0.905 | 0.292 | 0.778 |
| $F^{ev}$ | 0.080 | 0.922 | 0.949 | 0.922 | 0.836 | 0.515 | 0.425 | 0.834 | 0.401 | 0.69 |
| $mM^{ev}$ | 0.407 | 0.605 | 0.581 | 0.605 | 0.978 | **0.931** | 0.131 | 0.979 | 0.188 | 0.949 |
| $ID^{ev}$ | 0.317 | 0.679 | 0.664 | 0.679 | 0.986 | 0.897 | 0.049 | 0.986 | 0.077 | 0.93 |
| $R^{ev}$ | 0.269 | 0.719 | 0.709 | 0.719 | 0.985 | 0.870 | 0.002 | 0.985 | 0.017 | 0.916 |
| $RR^{ev}$ | 0.169 | 0.795 | 0.796 | 0.795 | 0.970 | 0.797 | 0.116 | 0.969 | 0.109 | 0.876 |

**Quadratic Regression:** Quadratic regression extends the linear regression model by including squared terms of the independent variables. By introducing quadratic terms, potential curvilinear relationships between the indices and the drug efficacy can be captured. Quadratic regression allows for non-linear patterns in the data, enabling a more comprehensive analysis of the relationship.

From the Table 8, $GA^{ve}$ for density, $M_1\alpha^{ve}$ for boiling point, Flash point, enthalpy, and surface tension, $\chi^{ve}$ for molar refraction and polarizability, $F^{ev}$ for Log P, $F^{ve}$ for polar surface area and $R^{ve}$ for molar volume are the best estimator indices in quadratic regression models.

The quadratic models obtained with these topological indices are as follows:

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$$D = 3.084 + 0.648(GA^{ve}) + 0.050(GA^{ve})^2 \quad F = 2.490 \ SE = 0.099 \ \text{P} = 0.10 \ R^2 = 0.717$$

$$LogP = 28.950 - 0.022(F^{ev}) + 0.000(F^{ev})^2 \quad F = 138.285 \ SE = 0.179 \ \text{P} = 0.007 \ R^2 = 0.989$$

$$B.P = -234.647 + 1.665(M_1\alpha^{ve}) - 0.000(M_1\alpha^{ve})^2 \ F = 8.264 \ SE = 42.862 \ \text{P} = 0.60 \ R^2 = 0.89894$$

$$PSA = -124.176 + 0.218(F^{ve}) - 0.000(F^{ve})^2 \quad F = 3.534 \ SE = 5.655 \ \text{P} = 0.234 \ R^2 = 0.767$$

$$E = -22.318 + 0.240(M_1\alpha^{ve}) - 0.000(M_1\alpha^{ve})^2 \quad F = 21.261 \ SE = 3.268 \ \text{P} = 0.05 \ R^2 = 0.956$$

$$P = 30.231 + 13.981(\chi^{ve}) + 0.651(\chi^{ve})^2 \quad F = 166.802 \ SE = 0.825 \ \text{P} = 0.015 \ R^2 = 0.993$$

$$F.P = -188.11 + 1.007(M_1\alpha^{ve}) - 0.001(M_1\alpha^{ve})^2 \quad F = 8.279 \ SE = 25.906 \ \text{P} = 0.05 \ R^2 = 0.894$$

$$S.T = -66.287 + 0.363(M_1\alpha^{ve}) - 0.000(M_1\alpha^{ve})^2 \ F = 2.819 \ SE = 5.229 \ \text{P} = 0.316 \ R^2 = 0.737$$

$$M.V = -393.979 + 243.626(R^{ve}) - 20.451(R^{ve})^2 \ F = 58.308 \ SE = 11.85 \ \text{P} = 0.011 \ R^2 = 0.982$$

$$M.R = -77.395 + 35.620(\chi^{ve}) - 1.669(\chi^{ve})^2 \quad F = 179.985 \ SE = 2.000 \ \text{P} = 0.05 \ R^2 = 0.994$$

**Table 8. The Correlation coefficient ® obtained by quadratic regression model between topological indices and physico-chemical properties of drugs**

| *Indices* | *D* | *BP* | *E* | *FP* | *MR* | *LogP* | *PSA* | *P* | *ST* | *MV* |
|---|---|---|---|---|---|---|---|---|---|---|
| $M1\beta^{ve}$ | 0.636 | 0.915 | 0.959 | 0.915 | 0.972 | 0.993 | 0.814 | 0.972 | 0.816 | 0.907 |
| $M2^{ve}$ | 0.716 | 0.914 | 0.957 | 0.914 | 0.934 | 0.846 | 0.875 | 0.934 | 0.804 | 0.905 |
| $R^{ve}$ | 0.554 | 0.618 | 0.602 | 0.618 | 0.993 | 0.939 | 0.208 | 0.993 | 0.215 | **0.992** |
| $\chi^{ve}$ | 0.327 | 0.728 | 0.754 | 0.728 | **0.997** | 0.938 | 0.408 | **0.997** | 0.335 | 0.945 |
| $H^{ve}$ | 0.549 | 0.638 | 0.627 | 0.638 | 0.993 | 0.940 | 0.288 | 0.993 | 0.207 | 0.988 |
| $HM^{ve}$ | 0.713 | 0.916 | 0.959 | 0.916 | 0.936 | 0.848 | 0.879 | 0.936 | 0.802 | 0.908 |
| $HM^{ve}$ | 0.568 | 0.904 | 0.912 | 0.904 | 0.411 | 0.287 | 0.701 | 0.408 | 0.829 | 0.181 |
| $ReZG^{ve}$ | 0.551 | 0.909 | 0.945 | 0.909 | 0.478 | 0.518 | 0.806 | 0.476 | 0.741 | 0.244 |
| $ABC^{ve}$ | 0.320 | 0.745 | 0.774 | 0.745 | 0.996 | 0.939 | 0.445 | 0.996 | 0.356 | 0.940 |
| $GA^{ve}$ | **0.845** | 0.585 | 0.530 | 0.585 | 0.943 | 0.954 | 0.279 | 0.944 | 0.603 | 0.986 |
| $AG^{ve}$ | 0.310 | 0.792 | 0.828 | 0.792 | 0.989 | 0.945 | 0.537 | 0.989 | 0.441 | 0.920 |
| $ISI^{ve}$ | 0.663 | 0.912 | 0.957 | 0.913 | 0.972 | 0.993 | 0.811 | 0.972 | 0.836 | 0.911 |
| $F^{ve}$ | 0.710 | 0.918 | 0.961 | 0.918 | 0.938 | 0.850 | **0.883** | 0.938 | 0.799 | 0.910 |
| $T^{ve}$ | 0.462 | 0.924 | 0.957 | 0.924 | 0.965 | 0.963 | 0.774 | 0.965 | 0.664 | 0.886 |
| $F^{ve}$ | 0.802 | 0.924 | 0.966 | 0.924 | 0.930 | 0.745 | 0.791 | 0.929 | 0.827 | 0.927 |
| $ID^{ve}$ | 0.843 | 0.521 | 0.473 | 0.521 | 0.936 | 0.955 | 0.250 | 0.937 | 0.569 | 0.979 |
| $ZD^{ve}$ | 0.780 | 0.575 | 0.534 | 0.575 | 0.959 | 0.944 | 0.233 | 0.960 | 0.478 | 0.987 |
| $mM^{ve}$ | 0.835 | 0.393 | 0.350 | 0.393 | 0.885 | 0.966 | 0.448 | 0.886 | 0.575 | 0.961 |
| $M_1\alpha^{ve}$ | 0.726 | **0.944** | **0.977** | **0.945** | 0.979 | 0.984 | 0.833 | 0.979 | **0.859** | 0.934 |
| $T^{ev}$ | 0.469 | 0.894 | 0.936 | 0.894 | 0.970 | 0.969 | 0.736 | 0.969 | 0.684 | 0.888 |
| $M^{ev}$ | 0.521 | 0.922 | 0.962 | 0.922 | 0.968 | 0.985 | 0.813 | 0.968 | 0.724 | 0.891 |
| $F^{ev}$ | 0.565 | 0.936 | 0.974 | 0.936 | 0.975 | **0.996** | 0.867 | 0.975 | 0.746 | 0.907 |
| $mM^{ev}$ | 0.509 | 0.606 | 0.585 | 0.606 | 0.994 | 0.939 | 0.142 | 0.995 | 0.191 | 0.989 |
| $ID^{ev}$ | 0.322 | 0.721 | 0.750 | 0.721 | 0.997 | 0.938 | 0.384 | 0.996 | 0.372 | 0.941 |
| $R^{ev}$ | 0.340 | 0.786 | 0.826 | 0.786 | 0.989 | 0.944 | 0.512 | 0.988 | 0.500 | 0.917 |
| $RR^{ev}$ | 0.433 | 0.870 | 0.914 | 0.870 | 0.974 | 0.961 | 0.682 | 0.973 | 0.647 | 0.892 |

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QSPR modeling for linear and quadratic models shows that the best estimating indices are:

1. Modified first $\mathcal{V}_e - degree\ index$ in the linear models, $geometric\ arithmetic\ \mathcal{V}_e - degree\ index$ in the quadratic regression models for density.
2. $First\ \mathcal{V}_e - degree\ zagreb\ alpha\ index$ in the linear and quadratic models for boiling point.
3. $f_1 - \mathcal{V}_e - degree\ index$ in linear, $first\ \mathcal{V}_e - degree\ zagreb\ alpha\ index$ in the quadratic regression model for enthalpy.
4. $First\ \mathcal{V}_e - degree\ zagreb\ alpha\ index$ in the linear and quadratic models for flash point.
5. $\mathcal{V}_e - degree\ harmonic\ index$ in linear, $\mathcal{V}_e - degree\ sum\ connectivity\ index$ in quadratic for molar refraction.
6. $modified\ \mathcal{E}_v - degree\ zagreb\ index$ in linear, $F - \mathcal{E}_v - degree\ index$ in quadratic for logP.
7. $\mathcal{V}_e - degree\ redefined\ zagreb\ index$ in linear, $F - \mathcal{V}_e - degree\ index$ in the quadratic model for polar surface tension.
8. $\mathcal{V}_e - degree\ harmonic\ index$ in linear, $\mathcal{V}_e - degree\ sum\ connectivity\ index$ in quadratic model for polarizability.
9. $second\ hyper\ \mathcal{V}_e - degree\ Zagreb\ index$ in linear, $first\ \mathcal{V}_e - degree\ zagreb\ alpha\ index$ in quadratic for surface tension.
10. $Inverse\ \mathcal{V}_e - degree\ index$ in linear, $\mathcal{V}_e - degree\ randic\ index$ in quadratic for molar volume.

In our comprehensive analysis, the $First\ \mathcal{V}_e - degree\ zagreb\ alpha\ index$ and its neighborhood emerged as robust indicators, exhibiting a strong correlation with crucial properties such as boiling point, enthalpy, flash point, and surface tension. This noteworthy correlation underscores the potential of these topological indices as valuable tools for the quantitative structure-property relationship (QSPR) analysis of drugs designed for Alzheimer's treatment.

Moving forward, our focus shifted to the development of quantitative structure-activity relationship (QSAR) models aimed at estimating the biological activity (pIC50) of the aforementioned drugs. Employing multiple linear regression (MLR), the QSAR model was constrained to a maximum of four topological indices. To ensure the robustness of our models, an intercorrelation matrix analysis of the topological indices was conducted, as detailed in Table 8. Notably, combinations of highly inter-correlated topological indices with $|r| \geq 0.8$, where 'r' represents the simple linear coefficient were excluded.

Our initial step involved constructing simple linear regression models with topological indices that exhibited the least inter-correlation. Notably, a minimal correlation of -0.0807 was observed between $mM_1^{ve}$ and $HM_2^{ve}$, resulting in the formulation of two mono-parameter models. Despite their weak correlation with pIC50, subsequent analysis revealed that the most promising statistical results were obtained from the following model.

Table 9 elucidates that the least inter-correlated values are confined to a single index, specifically the $HM_2^{ve}$ index, which notably avoids multicollinearity issues. The refined model is expressed as follows:

$$pIC50 = 5.765 + 2.362E - 5(\pm 1.250)HM_2^{ve} \quad \text{(Model1)}$$

This model not only demonstrates superior statistical performance but also reinforces the significance of $HM_2^{ve}$ as a singularly influential topological index in predicting the biological activity of Alzheimer's treatment drugs.

The observed activity together with model 1 for the tested drugs calculated using the MLR model are given below. $n = 5, r = 0.358, R^2 = 0.128, R_A^2 = -0.163, S_e = 0.927, F = 0.441, PE = 0.260,$

In order to judge the quality of these models some statistical parameters such as $PE = \frac{2(1-r^2)}{3\sqrt{n}}$, $R_A^2$, $F$, are given.

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**Algorithm 1** Linear Regression Model for Alzheimer's Treatment Drug Evaluation

**Require:** Index
**Require:** predicted data
**Ensure:** Regression model summary
1: Import required libraries:
2: **import** statsmodels.api as sm
3: **import** pandas as pd
4: Prepare the actual data: Create a dictionary with 'Index' and 'predicted data' as keys and corresponding lists of values as values.
5: Create a DataFrame: Convert the dictionary into a pandas DataFrame.
6: Add a constant term for the intercept: Use the stats models to add a constant function to add a column of ones to the DataFrame.
7: Fit the linear regression model: Use the Ordinary Least Squares (OLS) method from stats models to fit the model. Use the fit() method to obtain the model.
8: Print the model summary: Use the summary() method on the model to print detailed regression results.
Display information such as R-squared, coefficients, p-values, etc.

**Table 9. Intercorrelation matrix of the Topological Indices.**

| | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $RR^{ev}$ | 7 | 0.8362 | 0.9481 | 0.9781 | 0.9496 | 0.8318 | 0.5016 | 0.6596 | 0.9822 | 0.8525 | 0.9938 | 0.9677 | 0.8271 | 0.9967 | 0.7847 | 0.8308 | 0.8924 | 0.7169 | 0.9388 | 0.9971 | 0.9722 | 0.9196 | 0.9474 | 0.9780 | 0.9896 | 1.0000 |
| $R^{ev}$ | 0.9218 | 0.7491 | 0.9822 | 0.9977 | 0.9780 | 0.7436 | 0.3721 | 0.5449 | 0.9987 | 0.9136 | 0.9984 | 0.9224 | 0.7378 | 0.9846 | 0.6880 | 0.8887 | 0.9396 | 0.7807 | 0.8809 | 0.9757 | 0.9286 | 0.8543 | 0.9834 | 0.9978 | 1.0000 | |
| $ID^{ev\,v}$ | 0.8942 | 0.7037 | 0.9914 | 0.9999 | 0.9850 | 0.6978 | 0.3100 | 0.4883 | 0.9995 | 0.9361 | 0.9938 | 0.8949 | 0.6916 | 0.9724 | 0.6388 | 0.9107 | 0.9559 | 0.8070 | 0.8481 | 0.9592 | 0.9023 | 0.8189 | 0.9932 | 1.0000 | | |
| $mM^{ev}$ | 0.8364 | 0.6169 | 0.9983 | 0.9933 | 0.9894 | 0.6105 | 0.1991 | 0.3847 | 0.9906 | 0.9682 | 0.9759 | 0.8370 | 0.6039 | 0.9410 | 0.5465 | 0.9440 | 0.9774 | 0.8520 | 0.7819 | 0.9205 | 0.8478 | 0.7498 | 1.0000 | | | |
| $F^{ev}$ | 0.9839 | 0.9750 | 0.7586 | 0.8206 | 0.7787 | 0.9755 | 0.7923 | 0.8926 | 0.8331 | 0.6049 | 0.8750 | 0.9809 | 0.9756 | 0.9253 | 0.9605 | 0.6028 | 0.6825 | 0.4925 | 0.9941 | 0.9468 | 0.9859 | 1.0000 | | | | |
| $M^{ev}$ | 0.9977 | 0.9376 | 0.8529 | 0.9032 | 0.8652 | 0.9358 | 0.6873 | 0.8139 | 0.9124 | 0.7199 | 0.9426 | 0.9962 | 0.9337 | 0.9733 | 0.9061 | 0.7079 | 0.7822 | 0.5930 | 0.9909 | 0.9872 | 1.0000 | | | | | |
| $T^{ev}$ | 0.9837 | 0.8749 | 0.9225 | 0.9595 | 0.9274 | 0.8713 | 0.5659 | 0.7146 | 0.9653 | 0.8137 | 0.9830 | 0.9833 | 0.8673 | 0.9950 | 0.8294 | 0.7946 | 0.8610 | 0.6794 | 0.9617 | 1.0000 | | | | | | |
| $M_1^{ave}$ | 0.9924 | 0.9673 | 0.7851 | 0.8485 | 0.7957 | 0.9665 | 0.7585 | 0.8697 | 0.8594 | 0.6288 | 0.8959 | 0.9910 | 0.9653 | 0.9451 | 0.9488 | 0.6161 | 0.7023 | 0.4875 | 1.0000 | | | | | | | |
| $mM_1^{ve}$ | 0.5536 | 0.3017 | 0.8740 | 0.8138 | 0.8939 | 0.3003 | -0.0807 | 0.0798 | 0.8095 | 0.9461 | 0.7830 | 0.5469 | 0.2987 | 0.7116 | 0.2378 | 0.9746 | 0.9385 | 1.0000 | | | | | | | | |
| $ZD^{ve}$ | 0.7576 | 0.5180 | 0.9853 | 0.9589 | 0.9868 | 0.5142 | 0.1004 | 0.2826 | 0.9557 | 0.9914 | 0.9354 | 0.7546 | 0.5103 | 0.8912 | 0.4541 | 0.9912 | 1.0000 | | | | | | | | | |
| $ID^{ve}$ | 0.6776 | 0.4236 | 0.9563 | 0.9150 | 0.9624 | 0.4204 | 0.0074 | 0.1859 | 0.9106 | 0.9910 | 0.8852 | 0.6734 | 0.4171 | 0.8282 | 0.3579 | 1.0000 | | | | | | | | | | |
| $F_1^{ve}$ | 0.9132 | 0.9913 | 0.5531 | 0.6396 | 0.5747 | 0.9935 | 0.9238 | 0.9785 | 0.6558 | 0.3611 | 0.7135 | 0.9108 | 0.9953 | 0.7944 | 1.0000 | | | | | | | | | | | |

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| | $M_1^{\beta ve}$ | $M_2^{ve}$ | $R^{ve}$ | $\chi^{ve}$ | $H^{ve}$ | $HM_1^{ve}$ | $HM_2^{ve}$ | $ReZG$ | $^{ve}ABC_3^{v}$ | $^{e}GA^{ve}$ | $AG^{ve}$ | $ISI^{ve}$ | $F^{ve}$ | $T^{ve}$ | $F_1^{ve}$ | $ID^{ve}$ | $ZD^{ve}$ | $mM_1^{ve}$ | $M_1^{\alpha ve}$ | $T^{ev}$ | $M^{ev}$ | $F^{ev}$ | $mM^{ev}$ | $ID^{ev}$ | $R^{ev}$ | $RR^{ev}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $M_1^{\beta ve}$ | 1.0000 | | | | | | | | | | | | | | | | | | | | | | | | | |
| $M_2^{ve}$ | 0.9473 | 1.0000 | | | | | | | | | | | | | | | | | | | | | | | | |
| $R^{ve}$ | 0.8383 | 0.6211 | 1.0000 | | | | | | | | | | | | | | | | | | | | | | | |
| $\chi^{ve}$ | 0.8941 | 0.7036 | 0.9925 | 1.0000 | | | | | | | | | | | | | | | | | | | | | | |
| $H^{ve}$ | 0.8472 | 0.6401 | 0.9960 | 0.9872 | 1.0000 | | | | | | | | | | | | | | | | | | | | | |
| $HM_1^{ve}$ | 0.9445 | 0.9998 | 0.6156 | 0.6979 | 0.6356 | 1.0000 | | | | | | | | | | | | | | | | | | | | |
| $HM_2^{ve}$ | 0.7021 | 0.8925 | 0.2091 | 0.3108 | 0.2428 | 0.8968 | 1.0000 | | | | | | | | | | | | | | | | | | | |
| $ReZG$ | 0.8271 | 0.9633 | 0.3922 | 0.4887 | 0.4200 | 0.9657 | 0.9808 | 1.0000 | | | | | | | | | | | | | | | | | | |
| $^{ve}ABC_3^{v}$ | 0.9032 | 0.7184 | 0.9904 | 0.9997 | 0.9866 | 0.7129 | 0.3313 | 0.5072 | 1.0000 | | | | | | | | | | | | | | | | | |
| $^{e}GA^{ve}$ | 0.6976 | 0.4378 | 0.9733 | 0.9383 | 0.9706 | 0.4320 | 0.0035 | 0.1900 | 0.9327 | 1.0000 | | | | | | | | | | | | | | | | |
| $AG^{ve}$ | 0.9345 | 0.7722 | 0.9773 | 0.9943 | 0.9779 | 0.7674 | 0.4077 | 0.5759 | 0.9964 | 0.9054 | 1.0000 | | | | | | | | | | | | | | | |
| $ISI^{ve}$ | 0.9998 | 0.9465 | 0.8378 | 0.8945 | 0.8454 | 0.9434 | 0.6996 | 0.8253 | 0.9034 | 0.6962 | 0.9343 | 1.0000 | | | | | | | | | | | | | | |
| $F^{ve}$ | 0.9414 | 0.9991 | 0.6098 | 0.6920 | 0.6309 | 0.9998 | 0.9006 | 0.9678 | 0.7072 | 0.4261 | 0.7622 | 0.9399 | 1.0000 | | | | | | | | | | | | | |
| $T^{ve}$ | 0.9663 | 0.8370 | 0.9427 | 0.9730 | 0.9440 | 0.8339 | 0.5072 | 0.6636 | 0.9775 | 0.8438 | 0.9888 | 0.9652 | 0.8306 | 1.0000 | | | | | | | | | | | | |
| $F_1^{ve}$ | | | | | | | | | | | | | | | | | | | | | | | | | | |
| $ID^{ve}$ | | | | | | | | | | | | | | | | | | | | | | | | | | |
| $ZD^{ve}$ | | | | | | | | | | | | | | | | | | | | | | | | | | |
| $mM_1^{ve}$ | | | | | | | | | | | | | | | | | | | | | | | | | | |
| $M_1^{\alpha ve}$ | | | | | | | | | | | | | | | | | | | | | | | | | | |
| $T^{ev}$ | | | | | | | | | | | | | | | | | | | | | | | | | | |
| $M^{ev}$ | | | | | | | | | | | | | | | | | | | | | | | | | | |
| $F^{ev}$ | | | | | | | | | | | | | | | | | | | | | | | | | | |
| $mM^{ev}$ | | | | | | | | | | | | | | | | | | | | | | | | | | |
| $ID^{ev}$ | | | | | | | | | | | | | | | | | | | | | | | | | | |
| $R^{ev}$ | | | | | | | | | | | | | | | | | | | | | | | | | | |
| $RR^{ev}$ | | | | | | | | | | | | | | | | | | | | | | | | | | |

Through the application of the developed algorithm, our analysis reveals compelling statistical metrics affirming the robustness of the linear regression model. The predicted data seamlessly aligns with the model, as evidenced by the high correlation coefficient ($R$=0.999546) and an exceptional coefficient of determination ($R^2$=0.999092). The adjusted $R_A^2$ value further strengthens our model's explanatory power, registering at 0.998789. The F-statistic, calculated at 3300.102, attests to the overall significance of the model. Additionally, the significance error, with a remarkably low value of $1.16 \times 10^{-5}$, is reflected in the corresponding p-value of 0.000. The plot of predicted PIC50 value with $HM_2^{ve}$ index is shown in Fig 6. This culmination of statistical indicators unequivocally underscores the model's significance at the 5% significance level, affirming its efficacy in capturing and explaining the variation in the predicted data.

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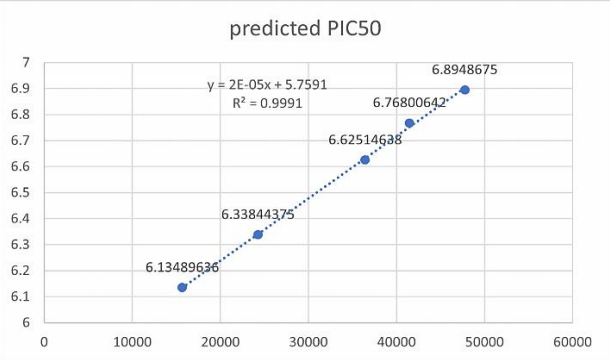


**Figure 6. Correlation of $HM_2$ with Predicted PIC50 value.**

The QSAR studies performed on five Alzheimer's disease treatment drugs produced a model using MLR. The studied model shows that there is sufficient evidence to indicate that these drug's activity ($pIC50$) is well correlated with the topological indices being used at a 5% significance level.

Although the studies have provided valuable insights into the predictive power of topological indices for anti-Alzheimer's drugs, the limitation of the study's focus on a specific set of compounds is acknowledged. The restricted dataset may limit the generalizability of our model to novel drug candidates beyond those initially considered. Future studies will try to enlarge the dataset to encompass a wider variety of chemicals with various structural traits in order to overcome this constraint. We hope to further strengthen the model's resilience by employing external validation methods including clinical results and experimental data, as well as cross-validation approaches. Working together with subject matter specialists will be essential to verifying the model's forecast and guaranteeing its application to actual situations. To understand the structure-activity relationship in Alzheimer's drug development and improve the predictions about the capacity of the computational models.

In future research, studying the relationship between topological measures and drug activity in other disease treatments which help us provide valuable results in their wide application. Discussing the impact of different types of topological measures on drug activity could provide the most relevant structural characteristics that influence therapeutic effectiveness. These efforts help us to a deeper understanding of structure-activity relationships and to inform the development of more effective treatments across various disease domains.

## Conclusion

This article evaluates the use of topological measures to understand the molecular structures of drugs designed for Alzheimer's treatment. Well-known pharmaceuticals like Tacrine, Donepezil, Galantamine, Rivastigmine, and Huperzine A were analyzed by using advanced techniques such as edge partitioning. This research also involves QSPR studies by showing strong correlations between topological measures and the physicochemical properties of the drugs. In particular, $\chi^{ve}$ index performs a compelling positive correlation ($r = 0.997$) with molar refraction and polarizability while the $F^{ev}$ index shows a strong connection ($r = 0.996$) with log P values. Additionally, the $M1$ $\alpha ve$ index illustrates positive correlations with boiling point, enthalpy, and flash point, offering insights through quadratic regression models. Notably, First $HM_2^{ve}$ emerges as a standout predictor for estimating biological activity, supported by a remarkably low p-value (0.000) and an exceptional R-squared value of 0.999. However, caution is advised due to potential numerical challenges in the models. The study underscores the importance of topological indices in drug development while acknowledging the need for further exploration of molecular descriptors. Future research should consider incorporating a broader array of descriptors to advance understanding and improve drug design for Alzheimer's treatment.

## Authors' Declaration

- Conflicts of Interest: None.
- We hereby confirm that all the Figures and Tables in the manuscript are ours. Furthermore, any Figures and images, that are not ours, have been included with the necessary permission for re-publication, which is attached to the manuscript.

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- No animal studies are present in the manuscript.
- No human studies are present in the manuscript.
- Ethical Clearance: The project was approved by the local ethical committee at SRM Institute of Science and Technology, Kattankulathur-603203, Tamilnadu, India.

## Authors' Contribution Statement

This work was carried out in collaboration between all authors. M. Y. H and S. M analyzed the antiviral compounds and numerical values were calculated, J. H. H. B Writing Arabic draft preparation, proofreading, and supervision. All authors read and approved the final manuscript.

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# المؤشرات التبولوجية وتحليل QSPR/QSAR لبعض الادوية التي يتم دراستها لعلاج مرضى الزهايمر

**محمد ياسين[1]، سورش[1]*، جلال حاتم حسين[2]**

[1] قسم الرياضيات كلية الهندسة والتكنولوجيا معهد SRM للعلوم والتكنولوجيا كاتانكولاتور-603203، تاميل نادو، الهند.
[2] قسم الرياضيات، كلية العلوم للبنات، جامعة بغداد، بغداد، العراق.

## الخلاصة

يعد تحليل العلاقات الكمية بين البنية والممتلكات/النشاط (QSPR/QSAR) أمرًا بالغ الأهمية لفهم خصائص المركبات المرتبطة بالمخدرات، خاصة في علاج مرض الزهايمر. في هذه الدراسة، هدفنا هو استخدام أساليب مبتكرة بما في ذلك استخدام المؤشرات الطوبولوجية $\mathcal{V}_e$-درجة و-$E_v$ درجة ، المستمدة من نظرية الرسم البياني، لتقييم الخصائص والخصائص الفيزيائية والكيميائية لخمسة أدوية لمرض الزهايمر: تاكرين، دونيبيزيل، ريفيستيجمين، جالانتامين و والهوبرزين أ . تقدم هذه المؤشرات الطوبولوجية طريقة جديدة لالتقاط المعلومات الهيكلية الجزيئية الأساسية، مما يقلل من عدد الواصفات مع تعزيز ارتباطها بالخصائص الجزيئية المتنوعة. ومن خلال الحسابات الشاملة لهذه المؤشرات، هدفنا هو توضيح الخصائص الجزيئية المعقدة لأدوية مرض الزهايمر. علاوة على ذلك، أجرينا تحليلات QSPR وQSAR لربط المؤشرات الطوبولوجية المحسوبة بالخصائص الفيزيائية والكيميائية المختلفة للأدوية. في حين أن الأساليب المبتكرة المستخدمة في دراستنا توفر رؤى قيمة. لا تساهم النتائج التي توصلنا إليها في تعزيز فهمنا لخصائص أدوية مرض الزهايمر فحسب، بل تحمل أيضًا آثارًا على تطوير الأدوية وتحسينها في إدارة مرض الزهايمر. ومن خلال تعزيز معرفتنا بخصائص هذه المركبات، فإن هدفنا هو معالجة الطبيعة المتعددة العوامل لمرض الزهايمر وتحسين التدخلات العلاجية.

**الكلمات المفتاحية** : مرض الزهايمر، الادوية، الدرجة من النوع $\mathcal{V}_e$ ، المؤشرات التبولوجية، الدرجة من النوع $\mathcal{E}_v$.