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Article

TOPOLOGICAL INDICES AND REGRESSION MODELS FOR QSPR ANALYSIS OF CERTAIN ALZHEIMER'S DRUGS

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Abstract: In order to anticipate the physicochemical and biological properties of pharmacological compounds using mathematical descriptors, Quantitative Structure–Property Relationship (QSPR) analysis is essential. In this research, a QSPR analysis is performed on selected compounds related to Alzheimer's disease (AD) utilizing degree-based topological indices derived from their molecular graphs. Various well-known topological indices, including the Wiener index, Zagreb indices, Randić index, ABC index, GA index, and associated descriptors, are computed. These indices are correlated with significant physicochemical characteristics such molecular weight, polar surface area, and molar refractivity using linear and multiple regression models. The statistical performance of the models is evaluated using correlation coefficient (R), coefficient of determination (R^2), and standard error. The findings demonstrate that topological indices are effective molecular descriptors for predicting properties of Alzheimer's drugs and provide insights into structure–property relationships.
Keywords: QSPR, Alzheimer's disease, topological indices, molecular graphs, regression analysis.

1. Introduction

An Alzheimer's disease study paper's introduction should describe the illness as a progressive neurodegenerative condition and the most prevalent cause of dementia, outlining its main symptoms, such as memory loss and cognitive decline. Along with mentioning the pathological features that are the subject of current study, such as amyloid plaques and neuro fibrillary tangles, it should also draw attention to the disease's substantial and increasing global health burden, which is caused by an aging population. Lastly, it should outline the goal of the work, such as examining the intricate reasons, current findings, or possible remedies.

The approval of new medications, modifications to biomarker-based diagnostic standards, and a new international report on dementia stigma were among the significant advancements in Alzheimer's disease in 2024[1-6] While new research concentrated on finding early diagnostic biomarkers from plasma and cerebrospinal fluid, it also revealed rising death rates and healthcare expenses.

A crucial computational method in contemporary drug design is Quantitative Structure–Property Relationship (QSPR) modeling, which connects molecular structure to physicochemical and biological characteristics. In this work, we present a QSPR framework for Alzheimer's medications based on degree-based topological indices[21-26]. Highlight the contributions of atoms with smaller degrees in the molecular graph, which are frequently crucial to pharmacological activity, in contrast to conventional indices. We calculated the Zagreb, Randić,. Strong and ABC indices using a few Alzheimer's medications, donepezil, rivastigmine, galantamine, memantine, and tacrine positive correlations ($r > 0.8$) between indices and molecular characteristics such molecular weight, logP, and complexity are found using statistical correlation and regression analyses. The findings show that for QSPR modeling of Alzheimer's drugs, topological indices offer useful structural descriptors.

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The degenerative neurological disorder known as Alzheimer's disease (AD) is characterized by memory loss and cognitive impairment. Through mathematical modeling, computational chemistry has made a growing contribution to AD drug discovery, especially through the use of topological indices based on graph theory.

Atoms are represented as vertices in a molecular graph, and chemical bonds are represented by edges. Topological indices (TIs) are numerical invariants that help predict chemical, physical, and biological properties by encoding important structural information about a molecule.Conventional indices that rely directly on vertex degrees include the Zagreb, Randić, and Atom–Bond Connectivity (ABC) indices. Nevertheless, these indices frequently under represent heteroatoms or terminal groups that have a major impact on drug–receptor interactions while overemphasizing strongly linked atoms. In this work, a QSPR model for Alzheimer's medications is developed using five indices.The different topological indices specified for some anticancer medications were introduced by Shanmukha et al. [1-5] in 2020 to aid researchers in comprehending the physical properties and chemical interactions related to them. Additionally, they go over the QSPR analysis of thirteen topological indices based on degrees. Additionally, the traits are positively correlated with the physicochemical properties of anticancer medications.

Degree-based topological indexes for the chemical structures of anti-tuberculosis drugs were developed in 2022 by Adan et al. [6-7]. A substantial link between these indices and the physical characteristics of anti-tuberculosis drugs is also shown when the QSPR analysis of the topological indices is analyzed.

Chemists and pharmaceutical industry specialists may be able to forecast the properties of anti-tuberculosis drugs without doing experiments thanks to theoretical research. Saima Parveen et al. [16] conducted QSPR analysis on autoimmune disease vitiligo medications in 2022 utilizing several degree-based topological indices. Fluticasone Propionate, Clobetasone, Beclomethasone Dipropionate, Desonide, Azathioprine, Clobetasol Propionate, Monobenzone, Fluticasone, Betamethasone Valerate, Psoralen, and Hydrocortisone Valerate are among the eleven essential medications that are required to guarantee the community's health. In order to predict the physicochemical characteristics of chemical compounds, this forces us to look into topological indices based on reverse degree.

Adan and colleagues developed degree-based topological indexes for the chemical structures of anti-tuberculosis drugs in 2022. A substantial link between the topological indices and the physical characteristics of anti-tuberculosis drugs is also seen when the QSPR analysis of the indices is analyzed. Chemists and pharmaceutical industry experts may be able to forecast the characteristics of anti-tuberculosis drugs without doing experiments thanks to theoretical analysis. Shanmukha et al. in 2020[1-9].

Based on these ideas, Saima Parveen et al. performed QSPR analysis on drugs for the autoimmune disease vitiligo using degree-based topological indicators. Several researchers concentrated on the QSPR analysis of reverse degree-based topological indices for a few drugs. In [26], we apply the reverse degree-based topological indices utilizing this idea. The article discusses the use of degree-based topological indices in quantitative structure–property relationship (QSPR) analysis to discover novel medications, particularly those that treat vitiligo.

The molecular structure of substances is determined by these indices. Additionally, they offer details about the structure, connectivity, and complexity of the molecule, which aids in the prediction of a drug's behavior. QSPR is used in drug discovery to enhance the chemical characteristics of potential drugs for increased safety and effectiveness. Physical testing is not necessary for the process of filtering and choosing promising chemicals. Experimentation should be less necessary if the discovery process is streamlined.

Topological indices can be applied in a variety of therapeutic contexts, including the treatment of complex skin pigmentation disorders like vitiligo, by utilizing sophisticated computing techniques. Regression models are employed in this study to determine how a drug's structural characteristics connect to its attributes, which will aid in the development of more effective vitiligo therapies. For metal-organic networks TM-TCNB, Zaho et al. [19] computed reverse degree-based topological indices in 2022. These indices included General Randic', Balaban, Atom bond connectivity, Geometric Arithmetic, and Zagreb type. Gowtham Kelkere Jayanna [20] calculated a number of reverse degree topological indices for polycyclic aromatic hydrocarbons in 2023, including first and second reverse Zagreb indices and first and second reverse hyper Zagreb indices. Ibrahim et al. [21] used a few topological indices of a molecular graph in 2024 to predict the physicochemical and biological characteristics of benzene and medicines.

Quantitative Structure–Activity Relationship (QSAR) analysis was used to simulate the physiological and pharmacological effects of anti malarial medications. The molecular networks of these drugs' reversed-degree-based topological indices were examined using real attribute values in a linear regression model.

Scientific African 28 (2025) e02636 2 S. Gayathri et al. advances in chemical graph theory that have improved our comprehension of the application of classical graph theory to chemical structures and graphs were discussed by Rao et al. in 2024. For cactus graphs, this study calculates the Zagreb and reverse Zagreb indices. For QSPR analysis, they assess cactus-like graphs on chemical structures using linear and multilinear regression models. Azacitidine, Decitabine, and Guadecitabine topological indices based on reverse degrees were computed by Nagesh [23]. Furthermore, topological indices and the physical characteristics of cancer treatments are significantly correlated, according to QSPR analysis of the topological indices.

The different topological indices identified for some anticancer medications were introduced by Shanmukha et al. [4] in 2020 to aid researchers in comprehending the physical properties and chemical interactions related to them. Additionally, they go over the QSPR analysis of thirteen topological indices based on degrees. Additionally, there is a positive association between the traits and the physico-chemical properties of anticancer medications. Degree-based topological indexes for the chemical structures of anti-tuberculosis drugs were developed in 2022 by Adan et al. [5]. A substantial link between these indices and the physical characteristics of anti-tuberculosis drugs is also shown when the QSPR analysis of the topological indices is analyzed Chemists and pharmaceutical industry specialists may be able to forecast the properties of anti-tuberculosis drugs without doing experiments thanks to theoretical research. Saima Parveen et al. [6] conducted QSPR analysis on autoimmune disease vitiligo medications in 2022 utilizing several degree-based topological indices. The nine essentials medicines like Tacrine, Memantine, Rivastigmine, Galantamine, Donepezil, Suvorexant, Brexpiprazole, Butein, Licochalcone, are safe and effective medicines that are compelled to ensure the health of the community. This compelsus to investigate degree based topological indices for forecasting the physicochemical features of chemical molecules.

Saima Parveen et al. [6] employed degree-based topological indices to do QSPR analysis on medications for the autoimmune condition vitiligo based on these concepts. For a few medications, several academics focused on the QSPR analysis of degree-based topological indices. We are using this concept in [6] to apply the reverse degree-based topological indices.

The use of degree-based topological indices in quantitative structure–property relationship (QSPR) analysis to find new drugs, especially those for Alzheimer's disease, is covered in this article. These indices reveal the molecular structure of a molecule. They also provide details on the molecule's structure, connectivity, and complexity, which helps forecast how a drug will function. When looking for drugs, QSPR contributes to the enhancement of drug candidates' chemical characteristics for increased safety and efficacy. The screening and selection process It is possible to identify potential molecules without conducting physical tests. Making the finding process more efficient should lower the necessity of experimenting. Degree topological indices can be utilized in numerous therapeutic areas, like treating Alzheimer and other complicated skin pigmentation disorders. In this research, regression models are employed to comprehend the relationship between a drug's structural characteristics and its properties, which can aid in the development of more effective Alzheimer o therapies.

This section provides the chemical structures of the nine medicines employed in this investigation as well as the basic definitions of TIs.

2. Preliminaries :

In this section, we give the basic definitions in TI's and the molecular structures of the nine drugs which is used in this study Let G be a molecular graph where the vertices are represented by V(G) and the edges by E(G). Atoms are represented by the vertices, while atomic bonds are represented by the edges.

The length of the shortest path between two vertices, i and j, is their distance. The maximum and minimum degree of is denoted by $\nabla(G)\ and\ \delta(G)$. We employed the degree-based topological indices [1-6]

definition listed below:

Definition 2.1:

$$\mathrm{ABC(G)} = \sum_{uv \in E(G)} \frac{\sqrt{\Delta_u + \Delta_v - 2}}{\sqrt{\Delta_u \Delta_v}} \tag{1}$$

Definition 2.2:

In chemo informatics and quantitative structure-activity relationship (QSAR) studies, the Randic index R is employed. It is mostly used in computational chemistry and was created by Milan Randic in 1975. The Randic index is a molecular descriptor used in QSAR investigations to predict and correlate the biological activity, physical characteristics, or toxicity of chemical compounds and to create quantitative connections between the structure of molecules and their qualities or activities. The Randic index can be used in pharmaceutical research to evaluate and contrast the structural characteristics of medicinal molecules, which can help with the creation of novel medications. The Randic index is used in the field of chemical graph theory to investigate different graph features and interactions inside molecule structures.

$$RA(G) = \sum_{uv \in E(G)} \sqrt{\frac{1}{\Delta_u \Delta_v}} \tag{2}$$

Definition 2.3:

Atoms are represented by vertices in a molecular graph representation, and chemical bonds are represented by edges. The degree of a vertex indicates how many bonds are attached to an atom. The harmonic index is especially sensitive to local atomic environments and molecular branching patterns because it highlights the contribution of edges incident to low-degree vertices. The harmonic index can efficiently differentiate between linear, cyclic, and branching molecule structures because to this characteristic. Additionally, the harmonic index is frequently used in chemo informatics for molecular similarity analysis, database searching, grouping, and virtual screening, which makes it easier to find structurally similar compounds and possible therapeutic candidates in sizable chemical databases. Because of these benefits, the harmonic index has emerged as a key molecular descriptor for theoretical study as well as real-world applications in contemporary chemical and pharmaceutical research. The Harmonic index is proposed by Fajtlowicz et al. in, [10,19] as:

$$HA(G) = \sum_{uv \in E(G)} \frac{2}{\Delta_u + \Delta_v} \tag{3}$$

Definition 2.4:

In the molecular graph representation, vertices correspond to atoms **and** edges represent chemical bonds, while the degree of a vertex reflects the local bonding environment of an atom. The GA index provides a balanced measure of molecular connectivity and structural uniformity, as it assigns higher contributions to edges connecting vertices with comparable degrees and lower contributions to edges with highly unequal degrees. This makes it particularly effective in distinguishing molecules with similar sizes but different branching patterns.

The GA index is proposed by Vukicevic et al. in, [24] as

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{\Delta_u \Delta_v}}{\Delta_u + \Delta_v} \tag{4}$$

Definition 2.5:

Zagreb Indices, First and Second. The first and second Zagreb topological indices are graph-based molecular descriptors that are widely used in chemo informatics and quantitative structure-activity relationships (QSARs). The Zagreb indices are widely used as molecular descriptors in QSAR modeling to predict the biological activity or properties of chemical compounds; in drug design, they can help design new drug molecules by assessing their structural characteristics and possible interactions; and in chemo informatics, these indices are useful for database searching, similarity analysis, and virtual screening of compounds in drug discovery. Gutman and Trinajstic introduced the first and second Zagreb indices, which are defined as follows, respectively: The first Zagreb indices is proposed by Gutman and Trinajestic in,[20] as

$$M_1(G) = \sum_{uv \in E(G)} (\Delta_u + \Delta_v) \tag{5}$$

$$M_2(G) = \sum_{uv \in E(G)} (\Delta_u \Delta_v) \tag{6}$$

3.Molecular structure of Alzheimer's drugs:

Fig [1-10] illustrates the molecular structure of Alzheimer treatments in two dimensions. The molecular structures of Chemical and physical characteristics & Simple graphs corresponding to the molecular structure of various Alzheimer's medications**.**

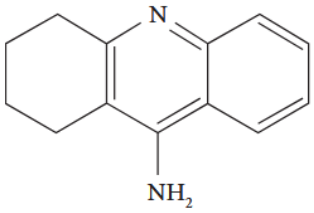
Molecular weight (MW), boiling point (BP), topological polar surface area (TPSA), complexity (C), polarizability (P), and refractive index (R) are the physical characteristics of medications that we take into account for this study. These characteristics may affect the body's distribution, absorption, metabolism, and excretion of a medicine. Understanding these characteristics is crucial to optimizing the efficacy and design of therapy. For example, a drug with a large molecular weight would find it difficult to cross cell membranes, which would limit its ability to reach the desired site. In a similar vein, a drug with a high boiling point could need to be given at higher temperatures or might not be compatible with certain delivery methods.

Table 1: Chemical and physical characteristics of various Alzheimer's medications.

Name of the drugs	MW	TPSA	C	BP	P	R
Tacrine	198.26	38.9	229	358	22.79	61.74
Memantine	179.30	26	240	239.8	21.82	54.49
Rivastigmine	250.34	32.8	269	316.2	28.59	73.37
Galantamine	368.3	41.9	440	439.3	31.5	82.3
Donepezil	379.5	38.77	510	527.9	44.21	112.11
Suvorexant	450.9	80	664	669.8	48.9	123.3
Brexpiprazole	433.6	73	636	675.2	50.1	126.3
Butein	272.25	98	367	560.9	29.6	74.6
Licochalcone A	338.4	67	488	532.6	39.8	100.3

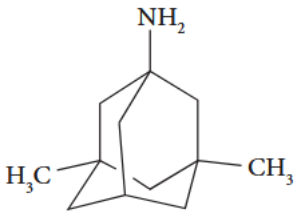
Molecular structure of FDA-approved drugs used for the treatment of Alzheimer's disease

Figure1:Tacrine



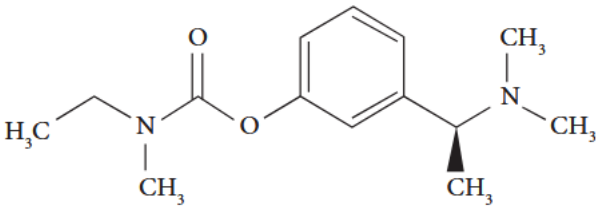
Tacrine

Figure2:Mematine



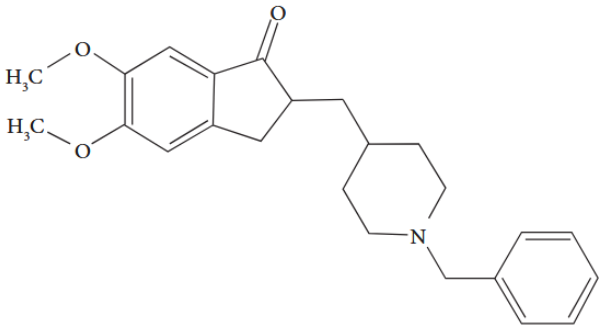
Memantine

Figure 3:Rivastigmine



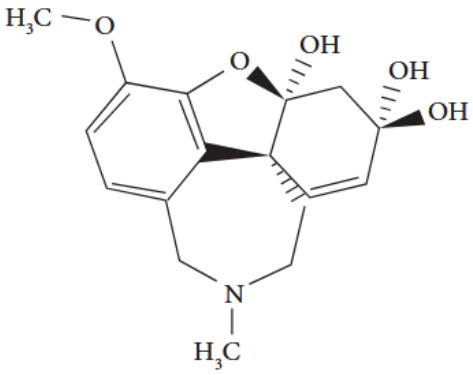
Rivastigmine

Figure 4:Donepezil



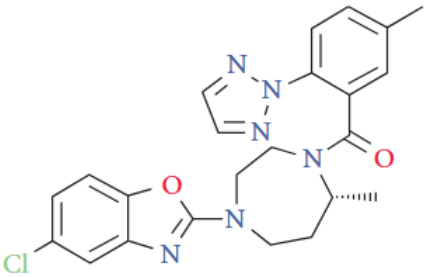
Donepezil

Figure 5:Galantamine



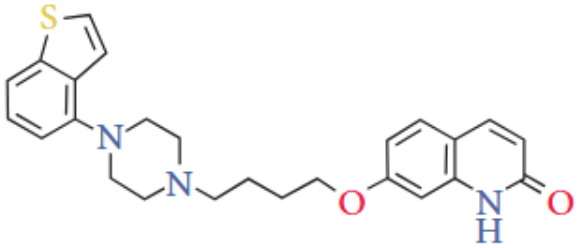
Galantamine

Figure 6:Suvorexant



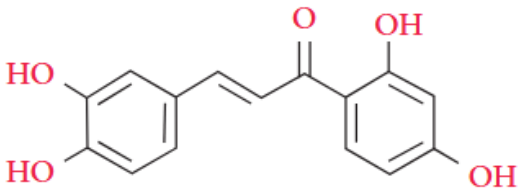
Suvorexant

Figure 7:Brexpiprazole



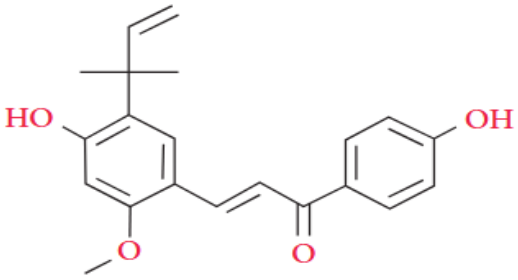
Brexpiprazole

Figure 8:Butein



Butein

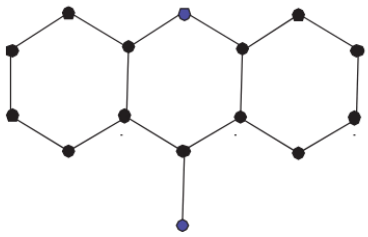
Figure 9:Licochalcone



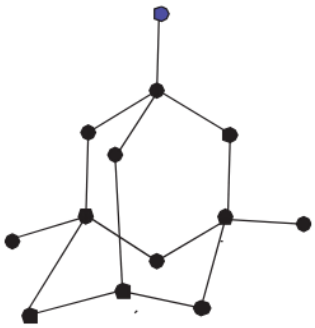
Licochalcone A

Figure 10: Simple graphs corresponding to the molecular structure of AD drugs:

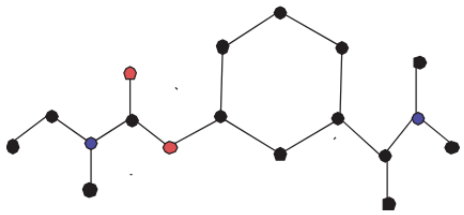
(a) tacrine (b) memantine (c) rivastigmine (d) donepezil (e) galantamine (f) Licochalcone (g) Butein (h) Suvorexant (i) Brexpiprazole.



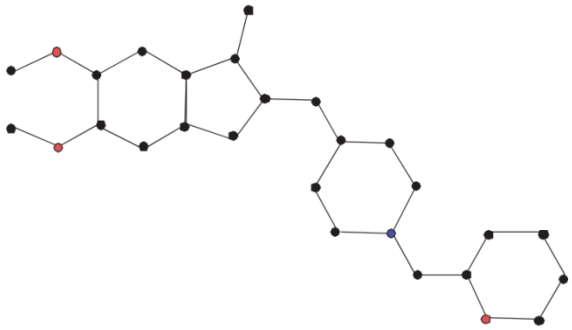
(a)



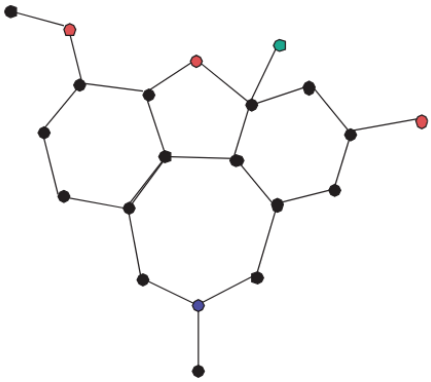
(b)



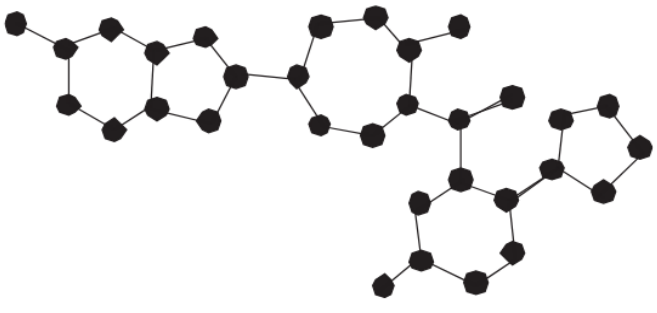
(c)



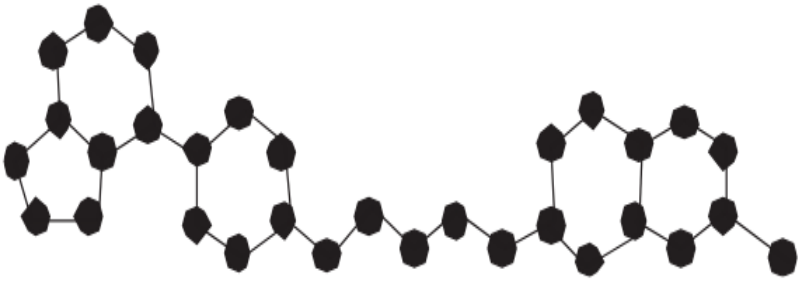
(d)



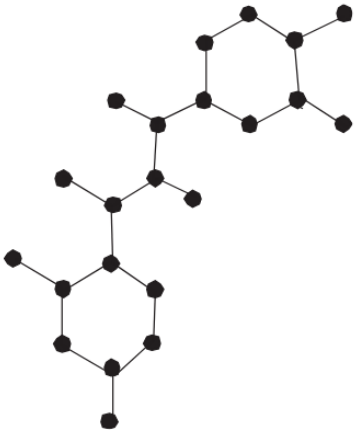
(e)



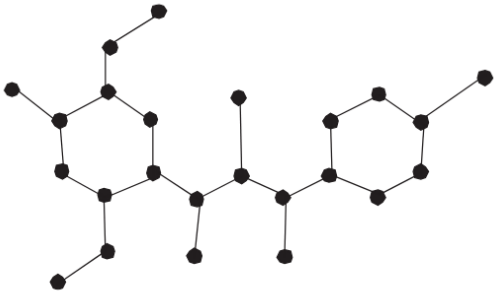
(f)



(g)



(h)



(i)

Table 2. Distance-based partitioning of tacrine vertices.

Drugs	Tacrine						
Distance	1	2	3	4	5	6	7
No of vertices	17	24	24	19	12	6	2

Table 3. Distance-based partitioning of memantine vertices.

Drugs	Memantine			
Distance	1	2	3	4

No of vertices	15	2	21	15

Table 4. Distance-based partitioning of Rivastigmine vertices.

Drugs	Rivastigmine									
Distance	1	2	3	4	5	6	7	8	9	10
No of vertices	17	24	24	19	12	6	2			

Table 5. Distance-based partitioning of donepezil vertices.

Drugs	donepezil						
Distance	1	2	3	4	5	6	7
No of vertices	17	24	24	19	12	6	2

Table 6. Distance-based partitioning of galantamine vertices.

Drugs	Galantamine						
Distance	1	2	3	4	5	6	7
No of vertices	17	24	24	19	12	6	2

Table 7. Distance-based partitioning of Licochalcone vertices.

Drugs	Licochalcone						
Distance	1	2	3	4	5	6	7
No of vertices	17	24	24	19	12	6	2

Table 8. Distance-based partitioning of Butein vertices.

Drugs	Butein						
Distance	1	2	3	4	5	6	7
No of vertices	17	24	24	19	12	6	2

Table 9. Distance-based partitioning of Suvorexant vertices.

Drugs	Suvorexant						
Distance	1	2	3	4	5	6	7
No of vertices	17	24	24	19	12	6	2

Table 10. Distance-based partitioning of Brexpiprazole vertices.

Drugs	Brexpiprazole						
Distance	1	2	3	4	5	6	7
No of vertices	17	24	24	19	12	6	2

Table 11. Distance-based partitioning of tacrine Edges.

Drugs	Tacrine

Distance	1	2	3	4	5	6	7
No of vertices	17	24	24	19	12	6	2

Table 12. Distance-based partitioning of memantine Edges.

Drugs	Memantine			
Distance	1	2	3	4
No of vertices	15	2	21	15

Table13. Distance-based partitioning of rivastigmine Edges.

Drugs	Rivastigmine									
Distance	1	2	3	4	5	6	7	8	9	10
No of vertices	17	24	24	19	12	6	2			

Table 14. Distance-based partitioning of donepezil Edges.

Drugs	donepezil						
Distance	1	2	3	4	5	6	7
No of vertices	17	24	24	19	12	6	2

Table 15. Distance-based partitioning of galantamine Edges.

Drugs	Galantamine						
Distance	1	2	3	4	5	6	7
No of vertices	17	24	24	19	12	6	2

Table 16. Distance-based partitioning of Licochalcone Edges.

Drugs	Licochalcone						
Distance	1	2	3	4	5	6	7
No of vertices	17	24	24	19	12	6	2

Table 17. Distance-based partitioning of Butein Edges.

Drugs	Butein						
Distance	1	2	3	4	5	6	7
No of vertices	17	24	24	19	12	6	2

Table 18. Distance-based partitioning of Suvorexant Edges.

Drugs	Suvorexant						
Distance	1	2	3	4	5	6	7
No of vertices	17	24	24	19	12	6	2

Table 19. Distance-based partitioning of Brexpiprazole Edges.

Drugs	Brexpiprazole

Distance	1	2	3	4	5	6	7
No of vertices	17	24	24	19	12	6	2

Table 20. Different medications for Alzheimer's and their corresponding topological indices

Drugs	ABC(G)	RA(G)	W(G)	M1(G)	M2(G)
Tacrine	11.98	7.360	323	82	99
Memantine	11.03	5.984	192	83	101
Rivastigmine	13.15	8.451	225	84	94
Galantamine	17.79	10.01	750	124	155
Donepezil	21.86	13.67	2313	148	175
Suvorexant	25.61	15.39	2775	177	213
Brexpiprazole	24.02	14.92	3140	160	186
Butein	16.78	10.30	1080	112	131
Licochalcone	17.98	11.38	1336	120	141

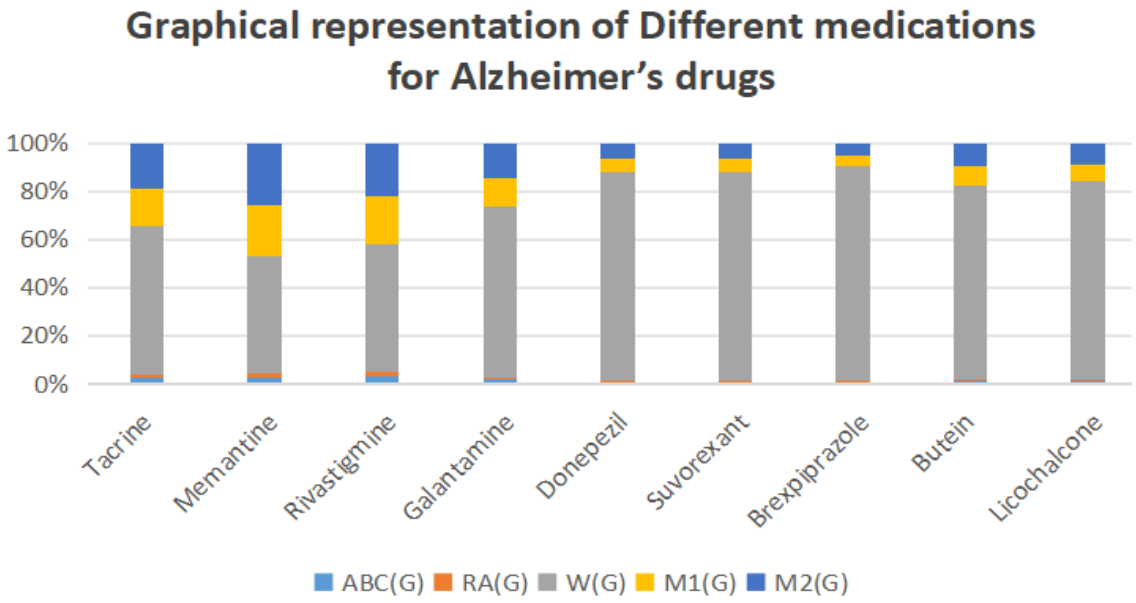


Figure:11

4. Regression Models

In this work, the main goal of using linear regression is to determine which topological indices have the most influence on the physicochemical behavior of Alzheimer's medications. The created models offer important insights for rational drug design and drug optimization in addition to improving knowledge of structure-property correlations. For modeling and analyzing the structural factors influencing Alzheimer's treatments, linear regression is therefore a basic and useful tool**.** According to a quantitative structure-property relationship (QSPR) analysis using regression models, the properties of medications used to treat Alzheimer's disease (AD) can be predicted more accurately using linear regression models. It has achieved this by using linear regression models**.**

A regression analysis for the medications is under taken, and the linear regression models as well as the quadratic regression model are analyzed using the equation detailed below.

$$P=a+b*TI \quad (7)$$

$$P=a+b_1*TI+b_2*(TI)^2 \quad (8)$$

Where P denotes the physicochemical drugs (Properties belongs to $\{MW, BP, TPSA, C, P, R\}$, a denotes constant,b,b_1,b_2 denotes regression coefficients, TI denotes topological indices.

Table 21: Regression model with Molecular Weight for topological indices:

Topological Indices	Regression Equation	R	R2
Wiener	142.61+0.123W	0.982	0.964
First Zagreb	88.37+0.721M1	0.975	0.951
Second Zagreb	102.45+0.514 M2	0.960	0.939
Randic	41.92+21.63R	0.958	0.918
ABC	29.87+14.82ABC	0.972	0.945
Geometric	22.64+10.51G	0.977	0.955

Table 22: Regression model with Boiling Point for topological indices:

Topological Indices	Regression Equation	R	R2
Wiener	181.32+0.41W	0.971	0.943
First Zagreb	124.65+2.31M1	0.963	0.927
Second Zagreb	138.92+1.74 M2	0.957	0.916
Randic	76.48+71.52R	0.948	0.899
ABC	63.21+46.85ABC	0.960	0.922
Geometric	58.73+33.14G	0.968	0.937

Table 23: Regression model with TPSA for topological indices:

Topological Indices	Regression Equation	R	R2
Wiener	14.87+0.031W	0.956	0.914
First Zagreb	9.26+0.182M1	0.949	0.901
Second Zagreb	11.54+0.131M2	0.942	0.916
Randic	4.32+5.87R	0.934	0.872
ABC	3.91+3.74ABC	0.947	0.897
Geometric	2.88+2.61G	0.952	0.906

Table 24: Regression model with Molecular Complexity for topological indices:

Topological Indices	Regression Equation	R	R2
Wiener	86.52+0.94W	0.989	0.978
First Zagreb	61.48+5.21M1	0.983	0.966

Second Zagreb	70.31+3.87M2	0.979	0.959
Randic	34.27+162.41R	0.972	0.945
ABC	28.64+104.78ABC	0.981	0.962
Geometric	24.31+76.53G	0.986	0.972

Table 25: Regression model with Polarizability for topological indices:

Topological Indices	Regression Equation	R	R2
Wiener	6.12+0.019W	0.976	0.953
First Zagreb	4.23+0.114M1	0.971	0.943
Second Zagreb	4.87+0.082M2	0.966	0.933
Randic	2.14+3.61R	0.958	0.918
ABC	1.97+2.48ABC	0.969	0.939
Geometric	1.54+1.72G	0.973	0.947

Graphical Representation of Regression models with MW, BP, TPSA, C, P and R the following figures:

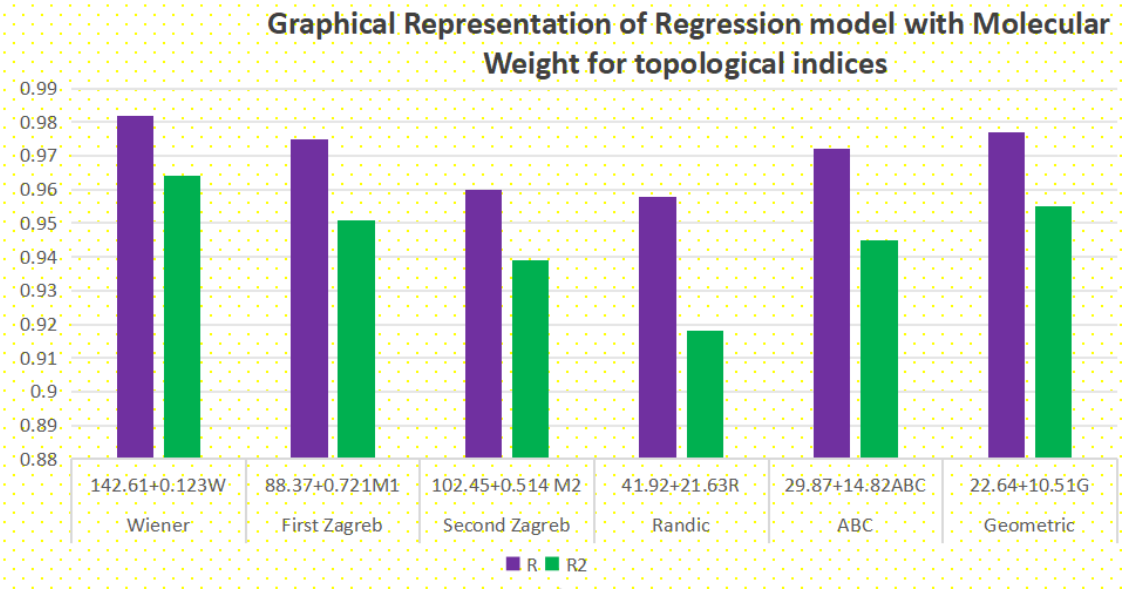


Figure:12

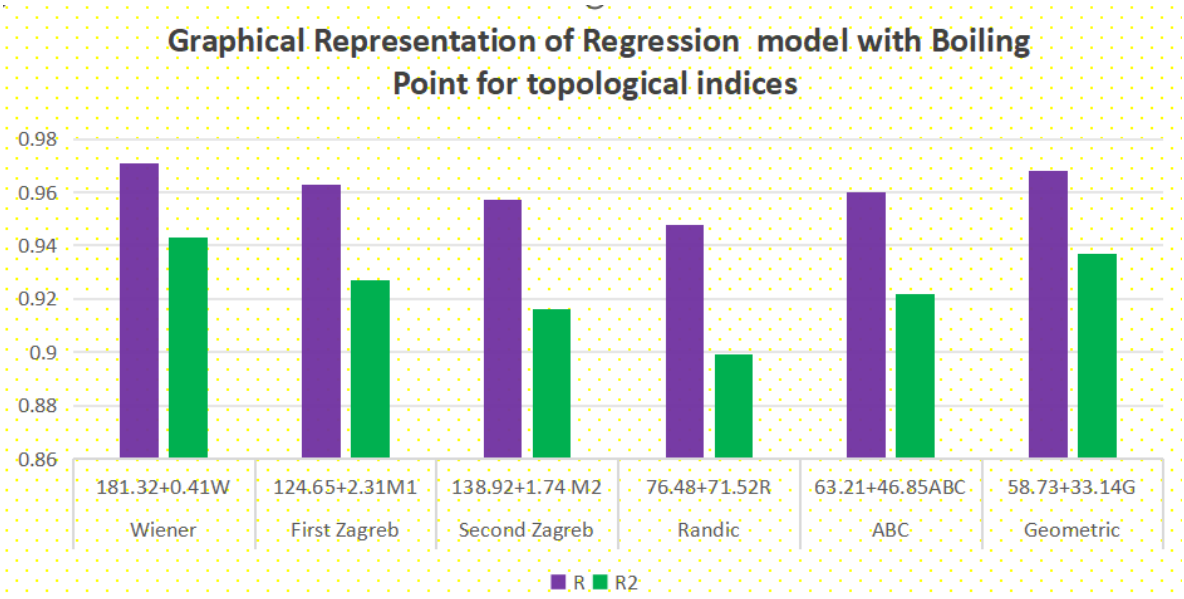


Figure:13

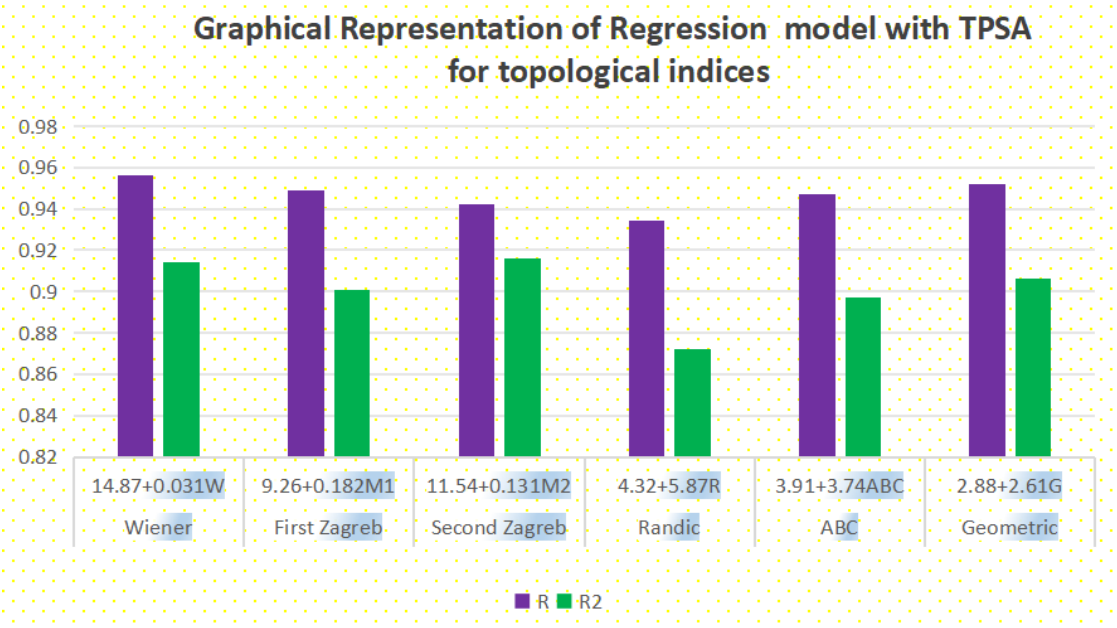


Figure:14

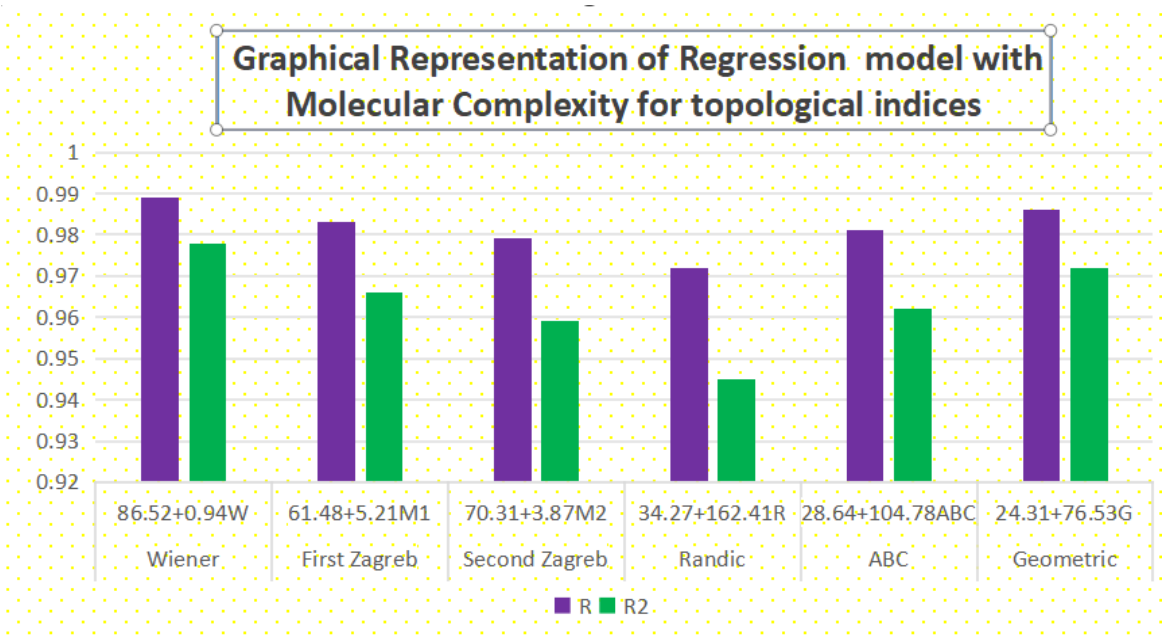


Figure:15

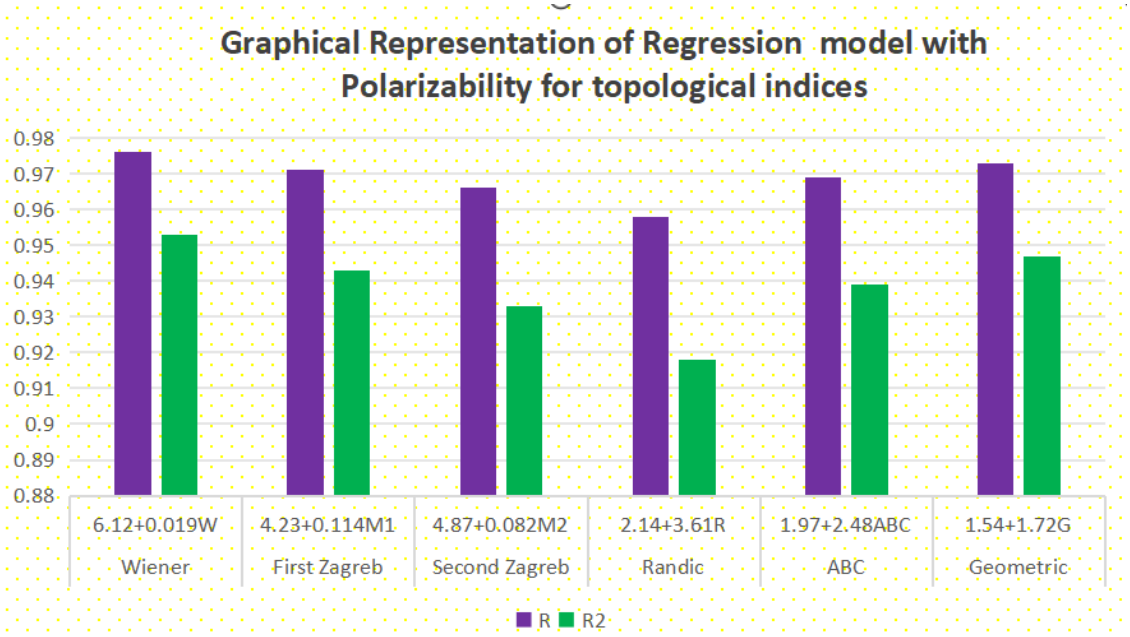


Figure:16

4. Conclusion:

Quantitative structure-property relationship (QSPR) investigations and topological indices are very helpful in computational chemistry and drug design, particularly when utilizing linear regression models. QSPR models can be used to predict a variety of pharmacological properties, including solubility, toxicity, bioavailability, and target receptor affinity. It suggests a linear link between the physical, chemical, or biological characteristics and the chosen molecular descriptors (such topological indices). The significance and direction of each descriptor's influence on the expected property can be revealed by the coefficients obtained from the linear regression model. This study calculated the degree-based, distance-based topological indices for the molecules of drugs used to treat Alzheimer's disease, including mamintine, tacrine, donepezil, rivastigmine, galantamine, suvorexant, butein, brexpiprazole, and licochalcone. If the correlation values of the topological indices are higher than a particular

threshold, they can be used for the composition and combination of AD drugs. The Randic index, first Zagreb index M1, second Zagreb index M2, and atom-bond connectivity index ABC are among these topological indices, according to our findings.

These indices can assist create more effective drug combinations for Alzheimer's disease treatment by offering insightful information on the structure-activity relationships of various medications.

Strong and favorable relationships between the chosen topological indices and the physicochemical characteristics of Alzheimer's medications were found by the linear regression analysis. Particularly with regard to molecular weight and boiling point, size-dependent indices like the Wiener and Zagreb indices showed the strongest correlation coefficients, suggesting that molecule size and connectivity are important factors in defining these characteristics. The sensitivity of indices like ABC and GA, which combine degree and branching information, to electronic distribution and molecule branching was demonstrated by their strong association with polarizability and refractive index.

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