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On The QSPR Analysis of Degree Based Topological Indices of Drugs used in Peripheral Neuropathy

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Abstract:

A numerical invariant that describes the topology of a graph G is known a topological index. The topological indices are ideal tools that can be used for analysing the structure of molecular graphs as it reflects the chemical properties of the molecules. In this article, the drugs used in the treatment of peripheral neuropathy are analysed with the help of topological indices and a QSPR analysis is done. The degree based topological indices are used for this structural analysis of chemical compounds of these drugs. The graph structure of a chemical component is derived from a chemical component by considering the toms as vertices and the bonds connecting two atoms as edges, the edge-partitions are noted and computed the topological indices. The correlation among the chemical properties of the drugs and the topological indices are computed. A detailed diagrammatic illustration of these correlation analyses is done. These comprehensive analyses may help scientists and chemist working in the drug design of peripheral neuropathy.

Keywords: Metal organic frameworks, topological indices, Sombor index, graph invariant, Benzene, Benzoid.

AMS Subject Classification: 05C07, 05C09, 05C92.

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1 Introduction

Peripheral neuropathy, a complex and often debilitating condition affecting the peripheral nervous system, has been a subject of intrigue and investigation throughout the annals of medical history. It is a condition characterized by damage to the peripheral nerves, leading to a range of symptoms such as pain, numbness, tingling, and weakness in the affected areas. The causes of peripheral neuropathy are diverse and can be classified into several categories: (1) Diabetes Mellitus, (2) Trauma or Injury (3) Toxic Substances, (4) Infections, (5) Metabolic disorders (6) Alcohol Abuse (7) Genetic disorders. Over the centuries, the understanding of this condition has evolved from mystical explanations to a more nuanced appreciation of its physiological underpinnings.

The term QSPR stands for Quantitative Structure-Property Relationship. It is a branch of cheminformatics and computational chemistry that involves the development of mathematical models to predict the physical, chemical, or biological properties of molecules based on their chemical structure. QSPR models aim to establish a quantitative relationship between the molecular structure of

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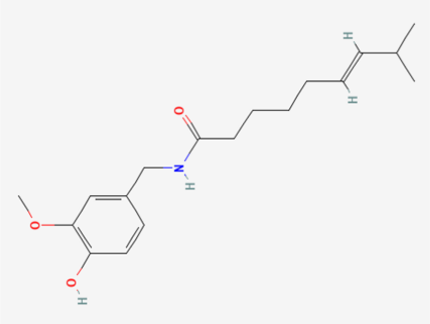
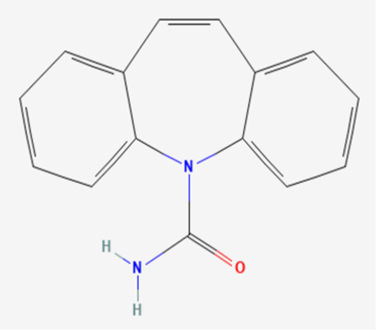
compounds and specific properties of interest. The basic idea behind QSPR is that certain molecular features or descriptors can be correlated with the observed properties of molecules. These descriptors can include various aspects of molecular structure, such as size, shape, electronic distribution, and connectivity. By analysing a set of molecules with known properties, researchers can use statistical techniques to derive mathematical equations or models that relate the molecular descriptors to the properties in question.

QSPR models find applications in several fields, including drug design, environmental chemistry, material science, and toxicology. In drug design, for example, QSPR models can be used to predict the biological activity, solubility, or toxicity of new drug candidates based on their chemical structures. This can be valuable in the early stages of drug development to prioritize compounds for further testing. It's important to note that QSPR models are empirical and rely on the availability of accurate and diverse experimental data for training. The quality and reliability of the predictions depend on the representativeness and completeness of the training dataset, and caution should be exercised when extrapolating predictions to new, untested compounds.

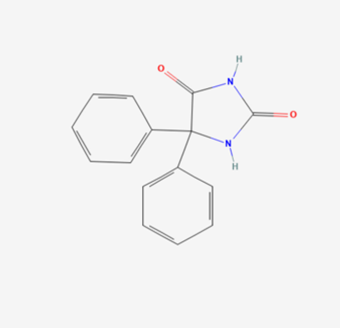
A topological index [9] is a numerical value or set of values derived from the molecular structure of a chemical compound. It encapsulates information about the connectivity of atoms within the molecule but does not consider the spatial arrangement of atoms. Some of the well-known topological indices are Wiener Index [8,22], Sum Connectivity Index, Randić Index [20], Geometric Arithmetic [5,10] Index, Zagreb Indices [1,16]. The molecular descriptors [2,18] are numerical or categorical representations of various aspects of a molecule's structure, composition, or properties. These descriptors are crucial in the field of cheminformatics [3,4,7,12] and computational chemistry, as they serve as the basis for quantitative structure-activity [17] or structure-property relationship models [6,21]. The well-known drugs used for the treatment of the peripheral neuropathy are Gabapentin, duloxetine, Pregabalin, Carbamazepine, Capsaicin and Phenytoin. In this article, we compare the physicochemical properties of these drug components with topological descriptors and find the correlation among of the physiochemical properties of the chemical components with the topological indices.



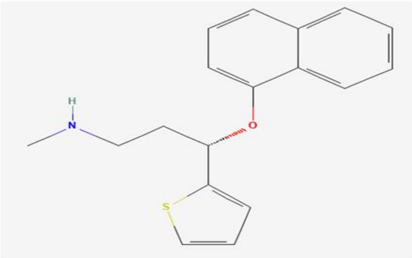
(a) Capsaicin



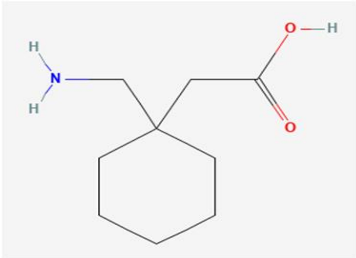
(b) Carbamazepine



(c) Phenytoin



(d) Duloxetine



(e) Gabapentin

Figure 1: Drugs used in the treatment of Peripheral Neuropathy

2 Terminology

Given a graph $G = (V_G, E_G)$, the neighbourhood of a vertex x is a subset of vertices $N_G(x)$ such that every element of $N_G(x)$ is adjacent to x in G and the degree of a vertex $\rho(x)$ is the number of vertices in the neighbourhood of x, that is $|N_G(x)|$. In this article, we compare the theoretical properties of the chemicals with the following topological indices:

Definition 1: The First-Zagreb index [1] is defined as

$$T_1(G) = \sum_{xy \in E(G)} \rho(x) + \rho(y)$$

Definition 2: The Second-Zagreb index [1,19] is defined as

$$T_2(G) = \sum_{xy \in E(G)} \rho(x).\rho(y)$$

Definition 3: The Harmonic index is defined as

$$T_3(G) = \sum_{xy \in E(G)} \frac{1}{\rho(x) + \rho(y)}$$

Definition 4: The Hyper-Zagreb index is defined as

$$T_4(G) = \sum_{xy \in E(G)} \left(\rho(x) + \rho(y)\right)^2$$

Definition 5: The forgotten index [14] is defined as

$$T_5(G) = \sum_{xy \in E(G)} \rho(x)^2 + \rho(y)^2$$

Definition 6: The ABC index is defined as

$$T_6(G) = \sum_{xy \in E(G)} \sqrt{\frac{\rho(x) + \rho(y) - 2}{\rho(x).\rho(y)}}$$

Definition 7: The Randic index [20] is defined as

$$T_7(G) = \sum_{xy \in E(G)} \sqrt{\frac{1}{\rho(x).\rho(y)}}$$

Definition 8: The Sum-connectivity index is defined as

$$T_8(G) = \sum_{xy \in E(G)} \sqrt{\frac{1}{\rho(x)+\rho(y)}}$$

Definition 9: The Sombor index [11] is defined as

$$T_9(G) = \sum_{xy \in E(G)} \sqrt{\rho(x)^2+\rho(y)^2}$$

Definition 10: The Modified Sombor index [23, 24] is defined as

$$T_{10}(G) = \sum_{xy \in E(G)} \frac{1}{\sqrt{\rho(x)^2+\rho(y)^2}}$$

Definition 11: The Reduced Sombor index [13, 15] is defined as

$$T_{11}(G) = \sum_{xy \in E(G)} \sqrt{(\rho(x)-1)^2+(\rho(y)-1)^2}$$

3 Methodology

The theoretical properties of the proposed chemicals are compared with the computed topological indices (Definition 1 to 11) and the correlation coefficients are found. The scatter diagrams are drawn and the Regression lines are plotted. Using the regression equations, the theoretical values are computed and compared. For this purpose, the comparison is done on the (a) Density, (b) Boiling point, (c) Vapour pressure, (d) Enthalpy of vaporization, (e) Flash point, (f) Index of refraction, (g) Molar refractivity, (h) Polarizability, (i) Surface tension, (j) Molar volume of the proposed drugs. These data are extracted from chemspider and is given below:

Name of the drug	Density	Boiling Point	Vapour Pressure	Enthalpy of Vaporization	Flash Point
Gabapentin	1.1	314.4	1.4	61.1	144
Pregabalin	1	274	1.2	56.4	119.5
Duloxetine	1.2	466.2	1.2	72.8	235.7
Carbamazepine	1.3	411	1	66.3	202.4
Capsaicin	1	469.7	1.2	77.1	237.9
Phenytoin	1.3	464	1.2	76.4	305.8

Name of the drug	Index of Refraction	Molar Refractivity	Polarizability	Surface Tension	Molar Volume
Gabapentin	1.489	46.7	18.5	47.1	161.8
Pregabalin	1.465	44.1	17.5	37.9	159.6
Duloxetine	1.628	91.1	36.1	46.1	256.8
Carbamazepine	1.67	69.7	27.6	57.3	186.6
Capsaicin	1.508	88.5	35.1	35	297
Phenytoin	1.652	72.4	28.7	53.3	187.9

Table 1: Theoretical values of the drugs

4 Results

Theorem :

If G is the molecular graph of Gabapentin, then the topological indices are respectively,

$(i) T_1(G) = 56$ $(ii)\ T_2(G) = 62$ $(iii)\ T_3(G) = 2.69$ $(iv)\ T_4(G) = 274$

$(v)\ T_5(G) = 150$ $(vi)\ T_6(G) = 8.7$ $(vii)\ T_7(G) = 25.77$ $(viii)\ T_8(G) = 5.66$

$(ix)\ T_9(G) = 41.37$ $(x)\ T_{10}(G) = 3.67$ $(xi)\ T_{11}(G) = 25.54$

Proof:

From the molecular graph of Gabapentin, we have the following edge-partition:

$E_{1,2} = 1, E_{1,3} = 2, E_{22} = 4, E_{2,3} = 1, E_{2,4} = 4$. Thus,

(i) Consider,

$$T_1(G) = \sum_{xy \,\epsilon\, E(G)} \rho(x) + \rho(y)$$

$$= \sum_{xy\, \in E_{1,2}} \rho(x) + \rho(y) + \sum_{xy\, \in E_{1,3}} \rho(x) + \rho(y) + \sum_{xy\, \in E_{2,2}} \rho(x) + \rho(y)$$

$$+ \sum_{xy\, \in E_{2,3}} \rho(x) + \rho(y) + \sum_{xy\, \in E_{2,4}} \rho(x) + \rho(y)$$

$$= \sum_{\square\square\, \in \square_{1,2}} 3 + \sum_{\square\square\, \in \square_{1,3}} 4 + \sum_{\square\square\, \in \square_{2,2}} 4 + \sum_{\square\square\, \in \square_{2,3}} 5 + \sum_{\square\square\, \in \square_{2,4}} 6$$

$$= |E_{1,2}| \times 3 + |E_{1,3}| \times 4 + |E_{2,2}| \times 4 + |E_{2,3}| \times 5 + |E_{2,4}| \times 6$$

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

$$= 3 + 8 + 16 + 5 + 24$$

$$= 56$$

(ii) Consider,

$$T_2(G) = \sum_{xy \in E(G)} \rho(x).\rho(y)$$

$$= \sum_{xy \in E_{1,2}} \rho(x).\rho(y) + \sum_{xy \in E_{1,3}} \rho(x).\rho(y) + \sum_{xy \in E_{2,2}} \rho(x).\rho(y)$$

$$+ \sum_{xy \in E_{2,3}} \rho(x).\rho(y) + \sum_{xy \in E_{2,4}} \rho(x).\rho(y)$$

$$= \sum_{\square\square \in \square_{1,2}} 2 + \sum_{\square\square \in \square_{1,3}} 3 + \sum_{\square\square \in \square_{2,2}} 4 + \sum_{\square\square \in \square_{2,3}} 6 + \sum_{\square\square \in \square_{2,4}} 8$$

$$= |E_{1,2}| \times 2 + |E_{1,3}| \times 3 + |E_{2,2}| \times 4 + |E_{2,3}| \times 6 + |E_{2,4}| \times 8$$

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

$$= 62$$

(iii) Consider,

$$T_3(G) = \sum_{xy \in E(G)} \frac{1}{\rho(x) + \rho(y)}$$

$$= \sum_{xy \in E_{1,2}} \frac{1}{\rho(x) + \rho(y)} + \sum_{xy \in E_{1,3}} \frac{1}{\rho(x) + \rho(y)} + \sum_{xy \in E_{2,2}} \frac{1}{\rho(x) + \rho(y)}$$

$$+ \sum_{xy \in E_{2,3}} \frac{1}{\rho(x) + \rho(y)} + \sum_{xy \in E_{2,4}} \frac{1}{\rho(x) + \rho(y)}$$

$$= \sum_{\square\square \in \square_{1,2}} \frac{1}{2} + \sum_{\square\square \in \square_{1,3}} \frac{1}{3} + \sum_{\square\square \in \square_{2,2}} \frac{1}{4} + \sum_{\square\square \in \square_{2,3}} \frac{1}{6} + \sum_{\square\square \in \square_{2,4}} \frac{1}{8}$$

$$= |E_{1,2}| \times \frac{1}{2} + |E_{1,3}| \times \frac{1}{3} + |E_{2,2}| \times \frac{1}{4} + |E_{2,3}| \times \frac{1}{6} + |E_{2,4}| \times \frac{1}{8}$$

$$= 2.69$$

(iv) Consider,

$$T_4(G) = \sum_{xy \in E(G)} \left(\rho(x) + \rho(y)\right)^2$$

$$= \sum_{xy \in E_{1,2}} \left(\rho(x) + \rho(y)\right)^2 + \sum_{xy \in E_{1,3}} \left(\rho(x) + \rho(y)\right)^2 + \sum_{xy \in E_{2,2}} \left(\rho(x) + \rho(y)\right)^2$$

$$+ \sum_{xy \in E_{2,3}} \left(\rho(x) + \rho(y)\right)^2 + \sum_{xy \in E_{2,4}} \left(\rho(x) + \rho(y)\right)^2$$

$$= \sum_{\square\square \in \square_{1,2}} 3^2 + \sum_{\square\square \in \square_{1,3}} 4^2 + \sum_{\square\square \in \square_{2,2}} 4^2 + \sum_{\square\square \in \square_{2,3}} 5^2 + \sum_{\square\square \in \square_{2,4}} 6^2$$

$$= \left|E_{1,2}\right| \times 9 + \left|E_{1,3}\right| \times 16 + \left|E_{2,2}\right| \times 16 + \left|E_{2,3}\right| \times 25 + \left|E_{2,4}\right| \times 36$$

$$=274$$

(v) Consider,

$$T_5(G) = \sum_{xy \in E(G)} \rho(x)^2 + \rho(y)^2$$

$$= \sum_{xy \in E_{1,2}} \rho(x)^2 + \rho(y)^2 + \sum_{xy \in E_{1,3}} \rho(x)^2 + \rho(y)^2 + \sum_{xy \in E_{2,2}} \rho(x)^2 + \rho(y)^2$$

$$+ \sum_{xy \in E_{2,3}} \rho(x)^2 + \rho(y)^2 + \sum_{xy \in E_{2,4}} \rho(x)^2 + \rho(y)^2$$

$$= \sum_{\square\square \in \square_{1,2}} 5 + \sum_{\square\square \in \square_{1,3}} 10 + \sum_{\square\square \in \square_{2,2}} 8 + \sum_{\square\square \in \square_{2,3}} 13 + \sum_{\square\square \in \square_{2,4}} 20$$

$$= \left|E_{1,2}\right| \times 5 + \left|E_{1,3}\right| \times 10 + \left|E_{2,2}\right| \times 8 + \left|E_{2,3}\right| \times 13 + \left|E_{2,4}\right| \times 20$$

$$= 150$$

(vi) Consider,

$$T_6(G) = \sum_{xy \in E(G)} \sqrt{\frac{\rho(x) + \rho(y) - 2}{\rho(x).\rho(y)}}$$

$$= \sum_{xy\in E_{1,2}} \sqrt{\frac{\rho(x)+\rho(y)-2}{\rho(x).\rho(y)}} + \sum_{xy\in E_{1,3}} \sqrt{\frac{\rho(x)+\rho(y)-2}{\rho(x).\rho(y)}} + \sum_{xy\in E_{2,2}} \sqrt{\frac{\rho(x)+\rho(y)-2}{\rho(x).\rho(y)}} + \sum_{xy\in E_{2,3}} \sqrt{\frac{\rho(x)+\rho(y)-2}{\rho(x).\rho(y)}} + \sum_{xy\in E_{2,4}} \sqrt{\frac{\rho(x)+\rho(y)-2}{\rho(x).\rho(y)}}$$

$$= 8.7$$

(vii) Consider,

$$T_7(G) = \sum_{xy\,\epsilon\, E(G)} \sqrt{\frac{1}{\rho(x).\rho(y)}}$$

$$= \sum_{xy\in E_{1,2}} \sqrt{\frac{1}{\rho(x).\rho(y)}} + \sum_{xy\in E_{1,3}} \sqrt{\frac{1}{\rho(x).\rho(y)}} + \sum_{xy\in E_{2,2}} \sqrt{\frac{1}{\rho(x).\rho(y)}} + \sum_{xy\in E_{2,3}} \sqrt{\frac{1}{\rho(x).\rho(y)}} + \sum_{xy\in E_{2,4}} \sqrt{\frac{1}{\rho(x).\rho(y)}}$$

$$= 25.77$$

(viii) Consider,

$$T_8(G) = \sum_{xy\,\epsilon\, E(G)} \sqrt{\frac{1}{\rho(x)+\rho(y)}}$$

$$= \sum_{xy\in E_{1,2}} \sqrt{\frac{1}{\rho(x)+\rho(y)}} + \sum_{xy\in E_{1,3}} \sqrt{\frac{1}{\rho(x)+\rho(y)}} + \sum_{xy\in E_{2,2}} \sqrt{\frac{1}{\rho(x)+\rho(y)}} + \sum_{xy\in E_{2,3}} \sqrt{\frac{1}{\rho(x)+\rho(y)}} + \sum_{xy\in E_{2,4}} \sqrt{\frac{1}{\rho(x)+\rho(y)}}$$

$$= 5.66$$

(ix) Consider,

$$T_9(G) = \sum_{xy\,\epsilon\, E(G)} \sqrt{\rho(x)^2+\rho(y)^2}$$

$$= \sum_{xy \in E_{1,2}} \sqrt{\rho(x)^2 + \rho(y)^2} + \sum_{xy \in E_{1,3}} \sqrt{\rho(x)^2 + \rho(y)^2} + \sum_{xy \in E_{2,2}} \sqrt{\rho(x)^2 + \rho(y)^2}$$

$$+ \sum_{xy \in E_{2,3}} \sqrt{\rho(x)^2 + \rho(y)^2} + \sum_{xy \in E_{2,4}} \sqrt{\rho(x)^2 + \rho(y)^2}$$

$$= \sum_{xy \in E_{1,2}} \sqrt{5} + \sum_{xy \in E_{1,3}} \sqrt{10} + \sum_{xy \in E_{2,2}} \sqrt{8} + \sum_{xy \in E_{2,3}} \sqrt{13} + \sum_{xy \in E_{2,4}} \sqrt{20}$$

$= 41.37$

(ix) Consider,

$$T_{10}(G) = \sum_{xy \in E(G)} \frac{1}{\sqrt{\rho(x)^2 + \rho(y)^2}}$$

$$= \sum_{xy \in E_{1,2}} \frac{1}{\sqrt{\rho(x)^2 + \rho(y)^2}} + \sum_{xy \in E_{1,3}} \frac{1}{\sqrt{\rho(x)^2 + \rho(y)^2}} + \sum_{xy \in E_{2,2}} \frac{1}{\sqrt{\rho(x)^2 + \rho(y)^2}}$$

$$+ \sum_{xy \in E_{2,3}} \frac{1}{\sqrt{\rho(x)^2 + \rho(y)^2}} + \sum_{xy \in E_{2,4}} \frac{1}{\sqrt{\rho(x)^2 + \rho(y)^2}}$$

$$= \sum_{xy \in E_{1,2}} \frac{1}{\sqrt{5}} + \sum_{xy \in E_{1,3}} \frac{1}{\sqrt{10}} + \sum_{xy \in E_{2,2}} \frac{1}{\sqrt{8}} + \sum_{xy \in E_{2,3}} \frac{1}{\sqrt{13}} + \sum_{xy \in E_{2,4}} \frac{1}{\sqrt{20}}$$

$= 3.67$

(xi) Consider,

$$T_9(G) = \sum_{xy \in E(G)} \sqrt{(\rho(x) - 1)^2 + (\rho(y) - 1)^2}$$

$$= \sum_{xy \in E_{1,2}} \sqrt{(\rho(x) - 1)^2 + (\rho(y) - 1)^2} + \sum_{xy \in E_{1,3}} \sqrt{(\rho(x) - 1)^2 + (\rho(y) - 1)^2}$$

$$+ \sum_{xy \in E_{2,2}} \sqrt{(\rho(x) - 1)^2 + (\rho(y) - 1)^2} + \sum_{xy \in E_{2,3}} \sqrt{(\rho(x) - 1)^2 + (\rho(y) - 1)^2}$$

$$+ \sum_{xy \in E_{2,4}} \sqrt{(\rho(x) - 1)^2 + (\rho(y) - 1)^2}$$

$$= \sum_{\square\square \in \square_{1,2}} 1 + \sum_{\square\square \in \square_{1,3}} 2 + \sum_{\square\square \in \square_{2,2}} \sqrt{2} + \sum_{\square\square \in \square_{2,3}} \sqrt{5} + \sum_{\square\square \in \square_{2,4}} \sqrt{10}$$

$= 25.54$

Similarly, the topological indices of the other Drugs are calculated and listed below:

Name of the drug	T_1	T_2	T_3	T_4	T_5	T_6	T_7	T_8	T_9	T_{10}	T_{11}
Gabapentin	98	105	5.05	446	236	15.95	46.31	10.51	71.38	6.92	41.85
Pregabalin	96	115	4.28	474	244	14.16	43.66	9.22	68.97	5.95	41.46
Duloxetine	102	124	4.49	518	270	14.88	46.04	9.67	73.66	6.23	44.95
Carbamazepine	106	123	5.13	502	256	16.14	49.21	10.83	75.7	7.19	43.75
Capsaicin	56	62	2.69	274	150	8.7	25.77	5.66	41.37	3.67	25.54
Phenytoin	44	44	2.33	198	110	7.51	20.91	4.81	32.91	3.099	20.18

Table 2: Computed topological indices of drugs

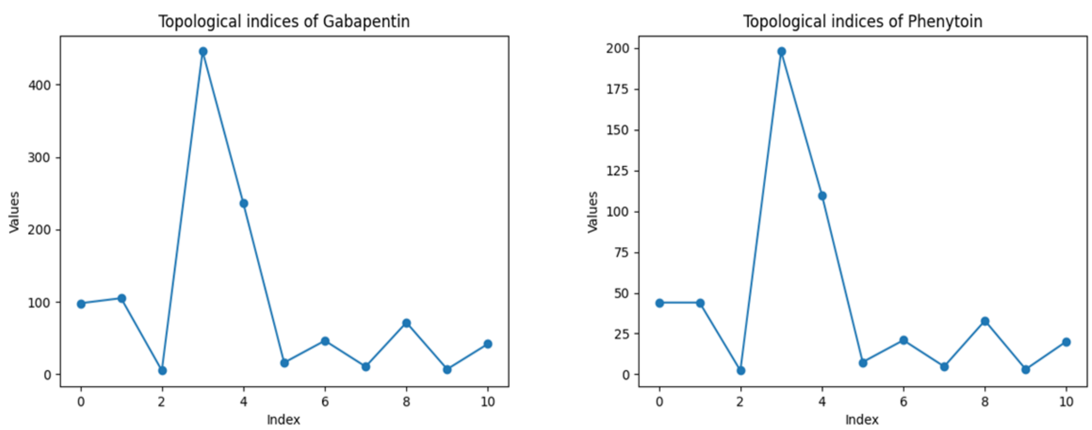


Figure 2 : Graphical representation of Topological Indices

The scatter diagram of the computed values is shown below:

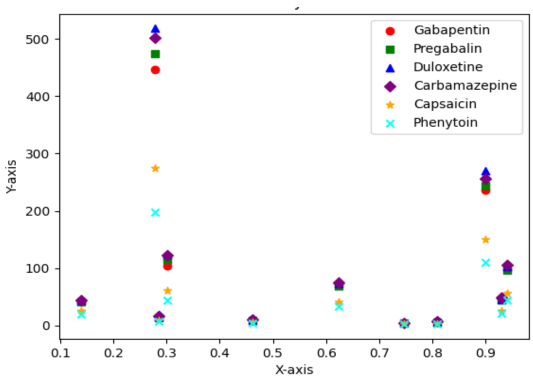


Figure 3: Scatter Plot of Computed Topological Indices

The computed topological indices are plotted and compared in the following diagram:

Advances in Nonlinear Variational Inequalities
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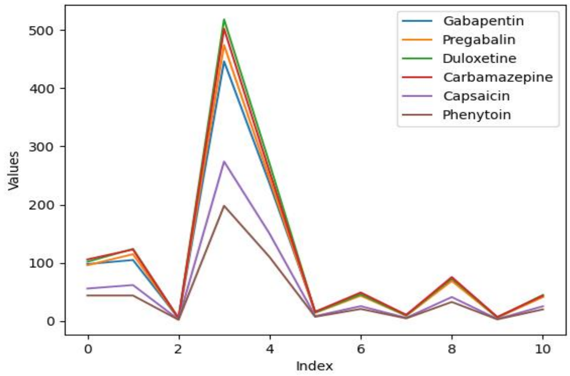


Figure 4: Comparison of Computed Topological Indices

5 Regression Analysis

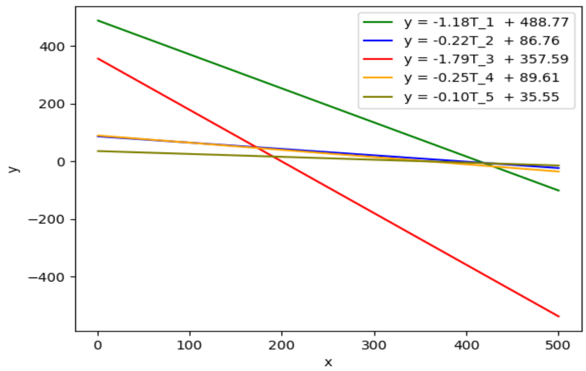
In this section, the computed topological values are statistically analysed. We found the mean, median and standard deviation and the values are listed in Table 5. Then, we compare each property with the topological indices calculated and find the regression lines for the properties, for example boiling point, flash point, etc., Then, the relation between the computed values and theoretical values are found in terms of the regression equations and we plotted the regression lines.

Name of the drug	Mean	Median	Standard Deviation
Capsaicin	98.45	46.31	127.22
Pregabalin	101.52	43.66	135.51
Duloxetine	110.35	46.04	148.63
Carbamazepine	108.63	49.21	49.21
Gabapentin	59.58	25.77	25.77
Phenytoin	44.34	20.91	20.91

Table 5: Mean, Median, Mode of the topological indices

The Regression equations of T_1:

$y = -1.18T_1 + 488.77$, $y = -0.22T_1 + 86.76$, $y = -1.79T_1 + 357.59$,
$y = -0.25T_1 + 89.61$, $y = -0.10T_1 + 35.55$, $y = 0.05T_1 + 41.74$,
$y = -0.71T_1 + 267.69$, $y = -0.00T_1 + 1.59$, $y = -0.25T_1 + 89.61$
$y = -0.10T_1 + 35.55$,



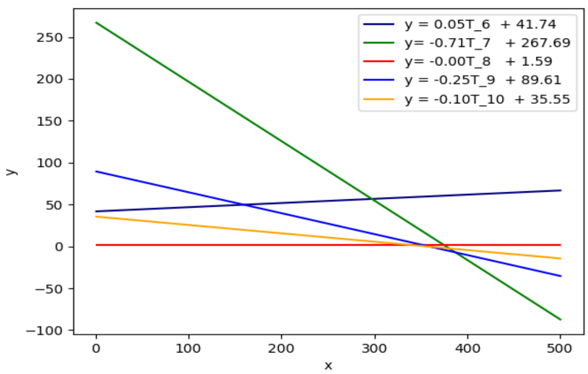


Figure 5: Comparison of Boiling Point of various topological indices

Regression equations of T_2:

y = -0.82x + 468.06, y = -0.16x + 83.78, y = -1.33x + 334.64,

y = -0.15x + 83.15, y = -0.06x + 32.98, y = 0.03x + 43.51,

y = -0.43x + 249.79, y = -0.00x + 1.58, y = -0.15x + 83.15,

y = -0.06x + 32.98,

Regression equations of T_3:

y = -28.03x + 502.07, y = -5.00x + 88.32, y = -39.88x + 366.87,

y = -6.94x + 96.48, y = -2.76x + 38.28, y = 1.93x + 38.39,

y = -20.18x + 288.90, y = -0.00x + 1.58, y = -6.94x + 96.48,

y = -2.76x + 38.28,

Regression equations of T_4:

y = -0.21x + 474.17, y = -0.04x + 84.83, y = -0.34x + 345.13,

y = -0.04x + 83.86, y = -0.01x + 33.27, y = 0.01x + 43.73,

y = -0.10x + 250.44, y = -0.00x + 1.58, y = -0.04x + 83.86,

y = -0.01x + 33.27

Regression equations of T_5:

y = -0.43x + 480.24, y = -0.08x + 85.84, y = -0.70x + 355.65,

y = -0.07x + 84.49, y = -0.03x + 33.52, y = 0.01x + 44.04,

y = -0.20x + 250.55, y = -0.00x + 1.59, y = -0.07x + 84.49,

y = -0.03x + 33.52

Regression equations of T_6:

y = -8.96x + 505.55, y = -1.60x + 88.96, y = -12.82x + 372.75,

y = -2.13x + 96.25, y = -0.85x + 38.19, y = 0.51x + 39.53,

y = -6.11x + 287.06, y = -0.00x + 1.59, y = -2.13x + 96.25,

y = -0.85x + 38.19

Regression equations of T_7:

y = -2.68x + 493.73, y = -0.49x + 87.38, y = -3.98x + 361.42,

y = -0.60x + 91.84, y = -0.24x + 36.44, y = 0.14x + 40.82,

y = -1.71x + 274.50, y = -0.00x + 1.59, y = -0.60x + 91.84,

y = -0.24x + 36.44,

Regression equations of T_8:

y = -13.02x + 500.15, y = -2.34x + 88.13, y = -18.74x + 365.92,

y = -3.13x + 95.17, y = -1.24x + 37.76, y = 0.82x + 39.17,

y = -9.05x + 284.79, y = -0.00x + 1.59, y = -3.13x + 95.17,

y = -1.24x + 37.76,

Regression equations of T_9:

y = -1.70x + 493.24, y = -0.31x + 87.46, y = -2.58x + 363.90,

y = -0.36x + 90.55, y = -0.14x + 35.93, y = 0.07x + 41.70,

y = -1.01x + 269.75, y = -0.00x + 1.59, y = -0.36x + 90.55,

y = -0.14x + 35.93,

Regression equations of T_{10}:

y = -19.33x + 496.60, y = -3.48x + 87.52, y = -27.81x + 360.80,

y = -4.71x + 94.72, y = -1.88x + 37.58, y = 1.34x + 38.75,

y = -13.76x + 284.10, y = -0.00x + 1.58, y = -4.71x + 94.72,

y = -1.88x + 37.58

Regression equations of T_{11}:

y = -2.88x + 494.54, y = -0.54x + 87.84, y = -4.46x + 369.37,

y = -0.57x + 89.39, y = -0.23x + 35.47, y = 0.09x + 42.89,

y = -1.56x + 264.78, y = -0.00x + 1.59, y = -0.57x + 89.39,

y = -0.23x + 35.47

6 Conclusion

In this article, the topological indices of the molecular graphs of the drugs used in the treatment of peripheral neuropathy are computed. The scatter diagram of these values is plotted. The theoretical values are compared with these topological indices and the regression equations are found. The relation between the properties of chemicals in terms of topological indices are given in as equations. These equations contain vital information about the structural relationship and the numerical invariants and the properties in terms of a numerical values and may be used for drug design.

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