Original Research Article

On The QSPR Analysis of Diabetic Nephropathy with the Degree-Based Topological Indices

ABSTRACT

Aims: In this article, the drugs used in the treatment of Diabetic Nephropathy are analysed using the topological indices, and a QSPR analysis of the chemical properties is done.
Study design: The degree based topological indices are used for this structural analysis of chemical compounds of these drugs. The graph structure of a chemical structure is derived from a chemical component by considering the atoms as vertices and the bonds connecting two atoms as edges, the edge-partitions are computed and used to obtain the topological indices.
Results: The topological indices of these drugs are calculated and compared with the theoretical properties of the drugs. The diagrammatic visualization of the data is plotted in Box graph, Line graph and in scatter diagram. 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 is given as regression equations. These equations contain vital information about the structural relationship and the numerical invariants and the properties in terms of numerical values and may be used for drug design.
Conclusion: The computed topological indices are visualized in various aspects and the regression analysis among the chemical properties of the drugs and the topological indices is done. This degree-based QSPR analysis helps to design medicines for the diabetic nephropathy.

Keywords: QSPR Analysis, Drug design, diabetic nephropathy, nephropathy, topological indices.

1. INTRODUCTION

Diabetic nephropathy stands as a formidable complication of diabetes mellitus, constituting a significant burden on global healthcare systems and posing substantial challenges to patient management. Characterized by progressive kidney damage and eventual renal failure, diabetic nephropathy not only diminishes quality of life but also heightens mortality rates among affected individuals. Despite considerable advancements in medical science, the prevalence of this condition continues to rise, underscoring the critical need for comprehensive research to elucidate its pathogenesis, identify effective preventive measures, and devise innovative therapeutic strategies.

Preventing and managing diabetic nephropathy involves controlling blood sugar levels through diet, exercise, and medication as prescribed by a healthcare provider. Managing high blood pressure is also crucial, as it can further damage the kidneys. In advanced stages, treatments may include medications to lower blood pressure, as well as dialysis or kidney transplant for those with kidney failure. Regular monitoring of kidney function through

blood and urine tests is essential for people with diabetes to detect any signs of kidney damage early and take appropriate steps to manage it. Additionally, maintaining a healthy lifestyle and following medical advice can help reduce the risk of developing diabetic nephropathy and slow its progression if already present. The pathophysiology of diabetic nephropathy is multifaceted, involving a complex interplay of metabolic, hemodynamic, and inflammatory factors. Chronic hyperglycemia serves as the primary instigator, triggering a cascade of molecular events that culminate in glomerular injury, tubular dysfunction, and interstitial fibrosis. Furthermore, aberrations in the renin-angiotensin-aldosterone system, oxidative stress, and activation of pro-inflammatory pathways contribute synergistically to the progression of renal damage. Understanding the intricate mechanisms underlying diabetic nephropathy is pivotal in delineating novel targets for intervention and advancing the development of more efficacious treatment modalities.

Numerous risk factors predispose individuals with diabetes to the development and progression of nephropathy. Beyond glycemic control, hypertension emerges as a key determinant, exacerbating renal injury through its hemodynamic effects and amplifying the deleterious impact of hyperglycemia on the kidneys. Genetic susceptibility, obesity, dyslipidemia, and smoking further augment the risk, highlighting the multifactorial nature of diabetic nephropathy. Moreover, emerging evidence suggests that socio-economic disparities, inadequate access to healthcare, and suboptimal adherence to therapeutic regimens contribute significantly to the disproportionate burden of nephropathy among certain demographic groups.

In light of the escalating prevalence of diabetes and its attendant complications, diabetic nephropathy looms large as a global health crisis necessitating urgent attention and concerted research efforts. By unraveling the intricacies of its pathogenesis, delineating modifiable risk factors, and exploring innovative therapeutic avenues, the scientific community endeavors to mitigate the burden of diabetic nephropathy and improve outcomes for affected individuals worldwide.

In the realm of drug discovery and development, The Quantitative Structure-Property Relationship (QSPR) analysis emerges as a powerful computational tool, offering unparalleled insights into the structure-activity relationships governing the pharmacological behavior of small molecules and biomolecules alike. The intricate interplay between molecular structure and physicochemical properties underpins the efficacy, selectivity, and safety of candidate compounds, thereby necessitating sophisticated predictive models to expedite the drug discovery process.

At its core, QSPR analysis seeks to establish quantitative correlations between the physicochemical properties of chemical entities and their molecular structures, thereby enabling the rational design and optimization of drug candidates with desired attributes. Leveraging principles from computational chemistry, statistical modeling, and machine learning, QSPR methodologies afford researchers the ability to predict a diverse array of molecular properties encompassing solubility, lipophilicity, bioavailability, toxicity, and biological activity. By elucidating the intricate nuances of molecular interactions and structure-activity relationships, QSPR analysis transcends traditional trial-and-error approaches, fostering a paradigm shift towards rational and data-driven drug design strategies.

The foundational principles of QSPR analysis emanate from the rich tapestry of theoretical chemistry, wherein molecular structures are represented as mathematical descriptors encapsulating pertinent physicochemical attributes. Through the judicious selection of molecular descriptors and robust statistical algorithms, QSPR models endeavor to capture

the underlying patterns and correlations intrinsic to structure-property relationships. Notably, the advent of computational chemistry techniques, encompassing molecular docking, quantum mechanics, and molecular dynamics simulations, has further enriched the predictive capabilities of QSPR methodologies, enabling the elucidation of intricate molecular mechanisms underlying drug-receptor interactions and pharmacological responses.

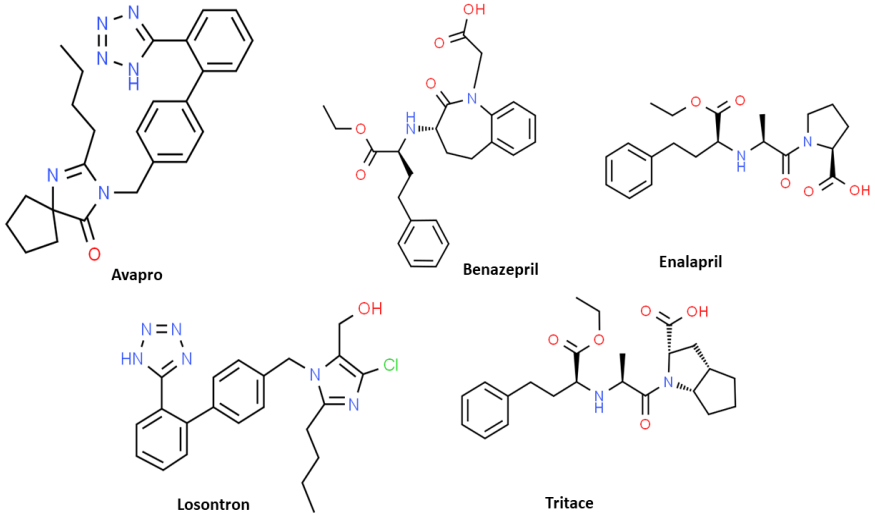
A topological index [9] is a numerical value or set of values derived from the molecular structure of a chemical compound. It encapsulates information about the connectivity of atoms within the molecule but does not consider the spatial arrangement of atoms. Some of the well-known topological indices are Wiener Index [8, 22], Sum Connectivity Index, Randic 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].

In this article, we studied the QSPR analysis of drugs used in the treatment of diabetic nephropathy, namely (i) Avapro, (ii) Benazepril, (iii) Enalapril, (iv) Losontron, and (v) Tritace. The Physio-chemical properties are compared with the theoretical values calculated from the topological indices and the regression lines are plotted.

2. METHODOLOGY

The medicines used in the treatment of diabetic nephropathy are found and their chemical structures and the physio-chemical properties of these chemicals are taken from Chemspider (Table 1). We found various topological indices for these structures and the physical properties are compared with the topological indices. The properties are attained in terms of the topological indices as regression lines. The graphs of the chemical structure are given in the following figure:

Figure 1: Chemical structures of the drugs



The chemical properties such as (a) Density, (b) Index of refractivity, (c) Boiling point, (d) Enthalpy of vaporization, (e) Flash point, (f) Molar refractivity, (g) Polar surface Area, (h) Polarizability, (i) Surface tension, (j) Molar volume of these medicines are extracted from Chemspider and are shown in Table 1:

Table 1: The Physio-chemical properties of the chemicals used in the Diabetic Nephropathy treatment

Name of the chemical	Density	Index of refraction	Boiling point	Enthalpy of vapourization	Flash Point	Molar Refractivity	Polar Surface Area	Polarizability	Surface tension	Molar Volume
Avapro	1.3	1.690	648.6	95.6	346	125.4	87	49.7	54.4	328.2
benazepril	1.3	1.608	691.2	106.4	371.8	116.1	96	46	58.9	335.8
enalapril	1.2	1.550	582.3	91.6	306	99.5	96	39.5	51.3	312.6
losartan	1.4	1.681	682	105.1	366.3	118.2	93	46.9	53.3	312.5
Tritace	1.2	1.556	616.2	96.1	326.4	111.4	96	44.2	50.2	346.8

3. TERMINOLOGIES

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 $\rho_G(x)$ 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 3.1: The First-Zagreb index [1] is defined as

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

Definition 3.2: The Second-Zagreb index [1,19] is defined as

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

Definition 3.3: The Harmonic index is defined as

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

Definition 3.4: The Hyper-Zagreb index is defined as

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

Definition 3.5: The forgotten index [14] is defined as

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

Definition 3.6: 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 3.7: The Randic index [20] is defined as

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

Definition 3.8: The Sum-connectivity index is defined as

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

Definition 3.9: The Sombor index [11] is defined as

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

Definition 3.10: The Reduced Sombor index [13, 15] is defined as

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

4. RESULTS AND DISCUSSION

The topological indices are calculated for the drugs in this section. The topological indices we consider for this work are listed in the terminologies section. The computed topological indices are plotted in Heatmap diagram, Box graph, Line graph, and Scatter diagram. The result starts from the following Theorem:

Theorem 4.1 :

If G is the molecular graph of Benazepril, then the topological indices are respectively, $t_1(G) = 153, t_2(G) = 176, t_3(G) = 7.33, t_4(G) = 731, t_5(G) = 379, t_6(G) = 23.52,$ $t_7(G) = 70.79, t_8(G) = 15.50, t_9(G) = 110.34, t_{10}(G) = 65.30.$

Proof:

From the molecular graph of Gabapentin, we have the following edge-partition: $E_{1,2} = 1, E_{1,3} = 4, E_{22} = 12, E_{2,3} = 10, E_{(3,3)} = 6.$ Now,

(i) Consider,

$$\begin{aligned} T_1(G) &= \sum_{xy \in E(G)} \rho(x) + \rho(y) \\ &= \sum_{xy \in E_{1,2}} \rho(x) + \rho(y) + \sum_{xy \in E_{1,3}} \rho(x) + \rho(y) + \sum_{xy \in E_{2,2}} \rho(x) + \rho(y) \\ &\quad + \sum_{xy \in E_{2,3}} \rho(x) + \rho(y) + \sum_{xy \in E_{2,4}} \rho(x) + \rho(y) \\ &= \sum_{xy \in E_{1,2}} 3 + \sum_{xy \in E_{1,3}} 4 + \sum_{xy \in E_{2,2}} 4 + \sum_{xy \in E_{2,3}} 5 + \sum_{xy \in E_{3,3}} 6 \\ &= |E_{1,2}| \times 3 + |E_{1,3}| \times 4 + |E_{2,2}| \times 4 + |E_{2,3}| \times 5 + |E_{3,3}| \times 6 \\ &= (1 \times 3) + (4 \times 4) + (12 \times 4) + (10 \times 5) + (6 \times 6) \\ &= 3 + 16 + 48 + 50 + 36 \\ &= 153 \end{aligned}$$

(ii) Consider,

$$\begin{aligned} T_2(G) &= \textstyle\sum_{xy \in E(G)} \rho(x).\rho(y) \\ &= \sum_{xy \in E_{1,2}} \rho(x).\rho(y) + \sum_{xy \in E_{1,3}} \rho(x).\rho(y) + \sum_{xy \in E_{2,2}} \rho(x).\rho(y) + \sum_{xy \in E_{2,3}} \rho(x).\rho(y) \\ &\quad + \sum_{xy \in E_{2,4}} \rho(x).\rho(y) \\ &= \sum_{xy \in E_{1,2}} 2 + \sum_{xy \in E_{1,3}} 3 + \sum_{xy \in E_{2,2}} 4 + \sum_{xy \in E_{2,3}} 6 + \sum_{xy \in E_{3,3}} 9 \\ &= |E_{1,2}| \times 2 + |E_{1,3}| \times 3 + |E_{2,2}| \times 4 + |E_{2,3}| \times 6 + |E_{3,3}| \times 9 \\ &= (1 \times 2) + (4 \times 3) + (12 \times 4) + (10 \times 6) + (6 \times 8) \\ &= 176 \end{aligned}$$

(iii) Consider,

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

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

$$= \sum_{xy \in E_{1,2}} \frac{1}{2} + \sum_{xy \in E_{1,3}} \frac{1}{3} + \sum_{xy \in E_{2,2}} \frac{1}{4} + \sum_{xy \in E_{2,3}} \frac{1}{6} + \sum_{xy \in E_{3,3}} \frac{1}{6}$$

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

$$= 7.33$$

(iv) Consider,

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

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

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

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

$$= 731$$

(v) Consider,

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

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

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

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

$$= 379$$

(vi) Consider,

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

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

$= 23.52$

(vii) Consider,

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

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

$= 70.79$

(viii) Consider,

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

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

$= 15.50$

(ix) Consider,

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

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

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

$= 110.34$

(x) Consider,

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

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

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

$= 65.30$

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

Table 2: Computed topological indices of drugs

Name of the drug	T_1	T_2	T_3	T_4	T_5	T_6	T_7	T_8	T_9	T_{10}
Avapro	174	210	7.71	870	450	25.30	78.81	16.59	125.06	75.45
Benazepril	153	176	7.33	731	379	23.52	70.79	15.50	110.34	65.30
Enalapril	130	148	6.22	622	326	20.14	60.10	13.14	94.34	56.58
Losontron	163	188	7.75	781	405	24.87	75.25	16.40	117.54	69.83
Tritace	151	176	7	735	383	22.89	69.24	14.91	109.26	65.89

The computed topological indices and the theoretical properties are undergone a diagrammatical illustration below. The heat map is plotted in Figures 2 and 3. The Box plot is plotted in Figures 4 and 5. The line graphs are plotted in Figures 6 and 7. The scatterplot of the data are plotted in Figures 8 and 9. The different plotting of the data helps us to visualize the variations and similarities in the data and also helps us to understand the behavior of the chemical structures and their properties.

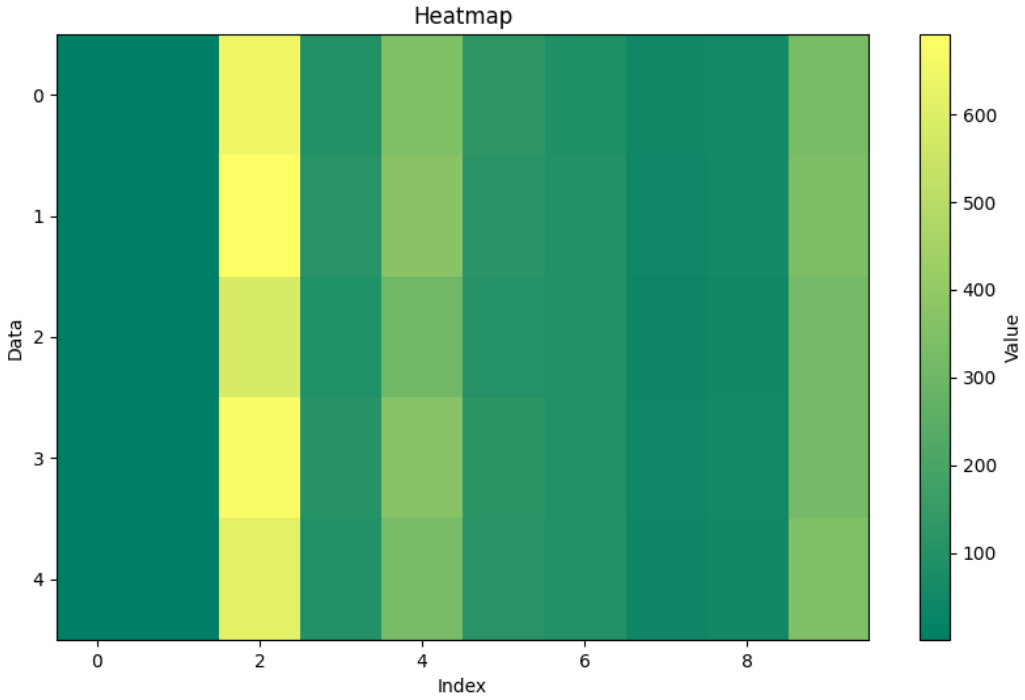


Figure 2: The heat map of topological indices

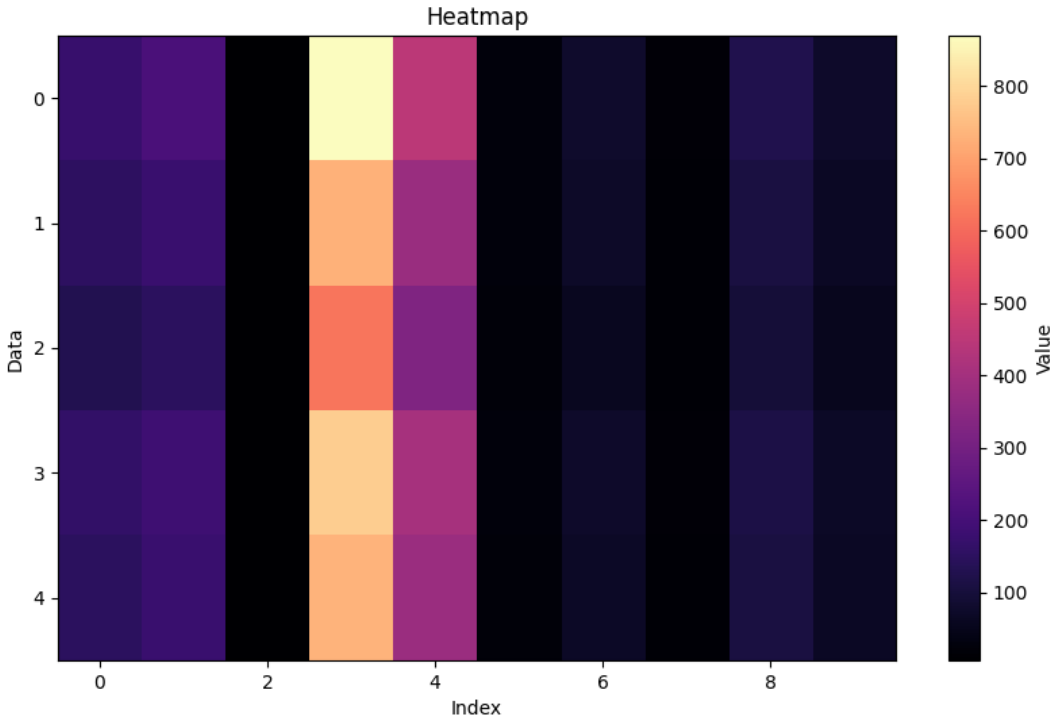


Figure 3: The heat map of chemical properties

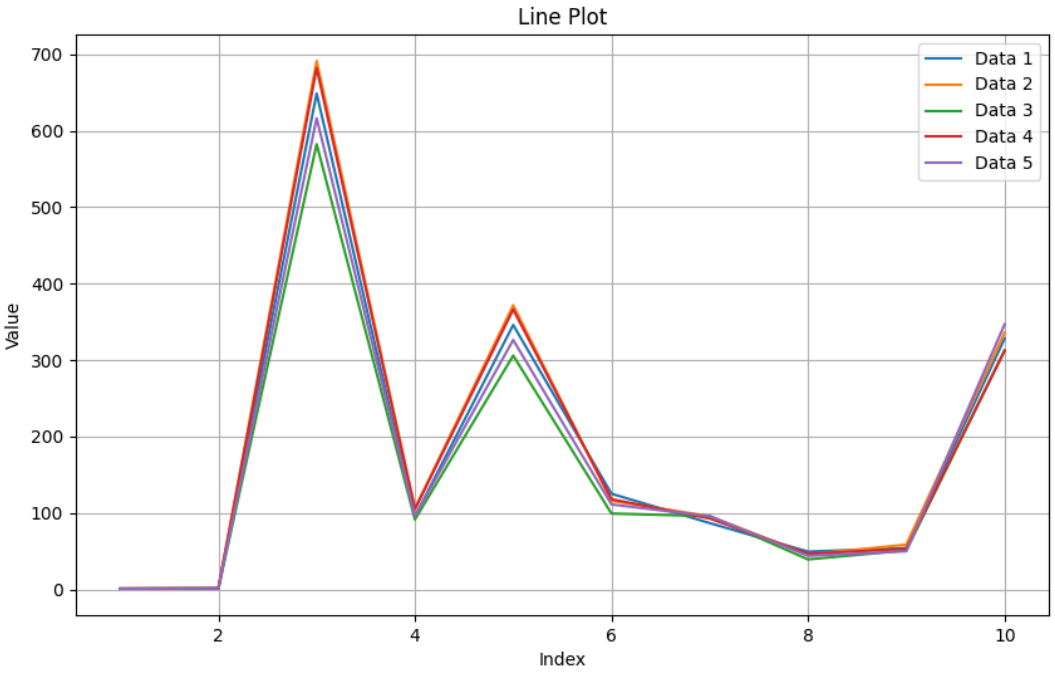


Figure 4: The Line graph of topological indices

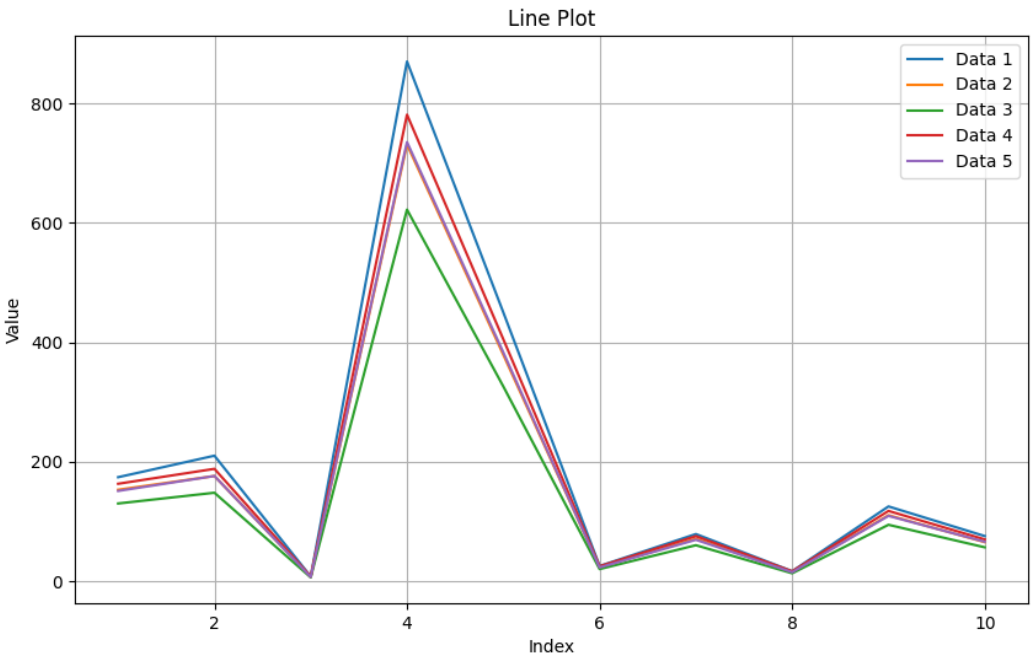


Figure 5: The Line graph of chemical properties

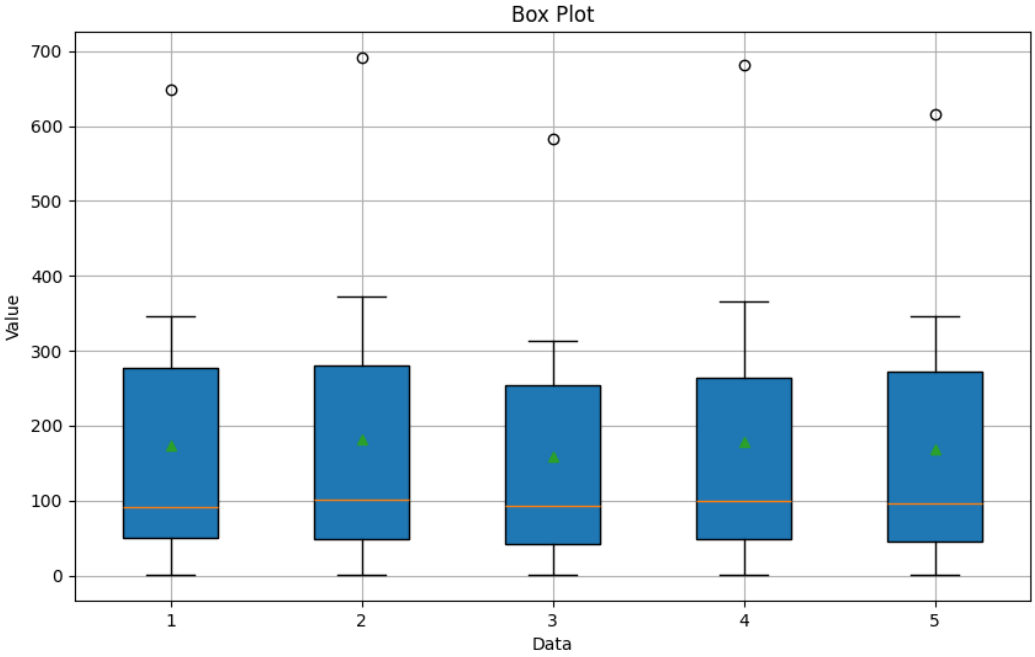


Figure 6: The Box graph of topological indices

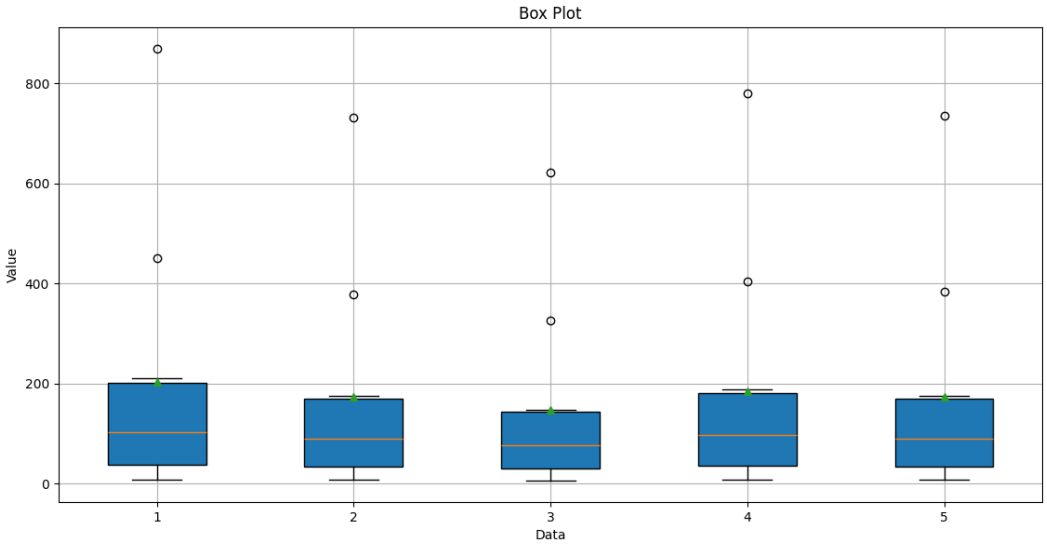


Figure 7: The Box graph of chemical properties

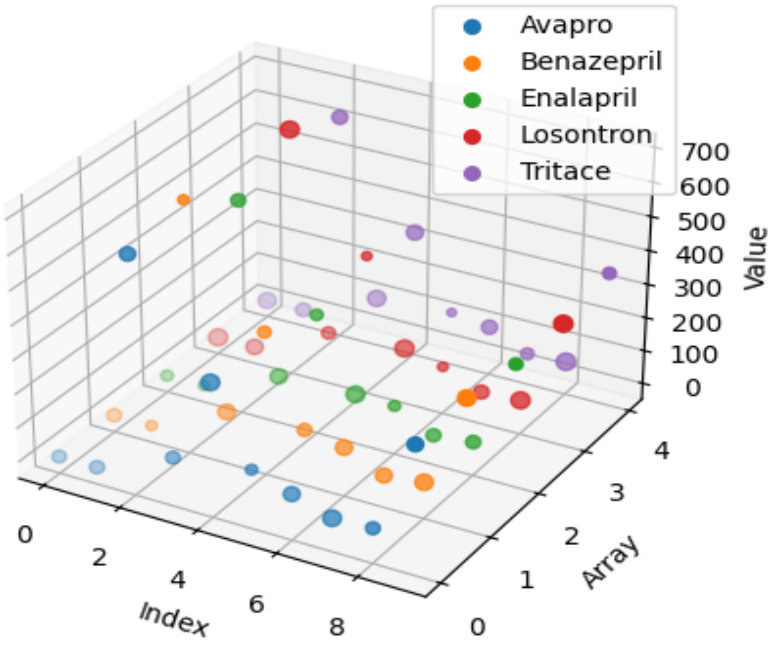


Figure 8: Scatter plot of topological indices of drugs

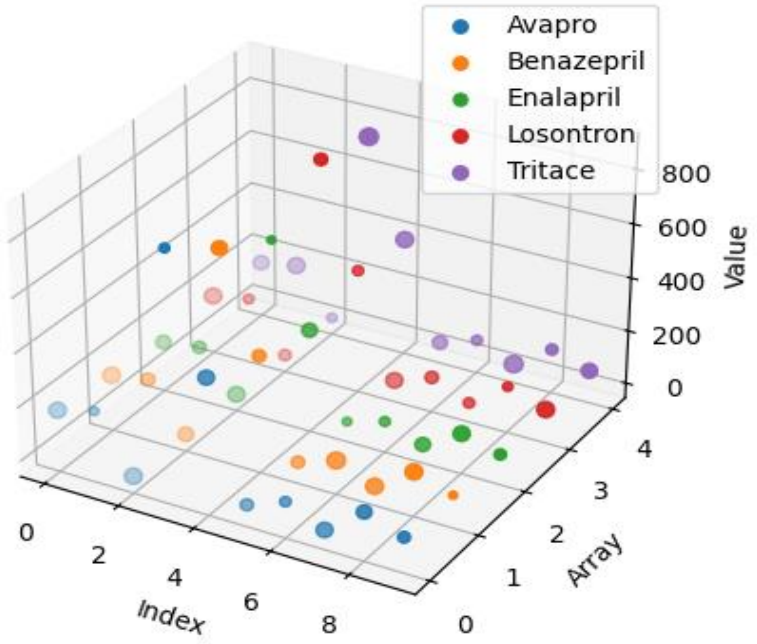


Figure 9: Scatter plot of chemical properties

5. STATISTICAL ANALYSIS

The mean, median and standard deviation of the computed topological indices are found and listed in Table 3 and Table 4:

Table 3: Mean, Median and Standard deviation of the chemical properties

Mean:	**Median:**	**Standard Deviation:**
Avapro: 173.79	Avapro: 91.3	Avapro: 195.95
Benazepril: 182.51	Benazepril: 101.2	Benazepril: 208.63
Enalapril: 158.16	Enalapril: 93.8	Enalapril: 176.64
Losontron: 178.04	Losontron: 99.05	Losontron: 99.05
Tritace: 169.01	Tritace: 96.05	Tritace: 96.05

Table 4: Mean, Median and Standard deviation of the topological indices

Mean:	**Median:**	**Standard Deviation:**
Avapro: 203.292	Avapro: 101.935	Avapro: 254.7583
Benazepril: 173.178	Benazepril: 90.565	Benazepril: 213.255
Enalapril: 147.652	Enalapril: 77.22	Enalapril: 181.737
Losontron: 184.864	Losontron: 96.395	Losontron: 96.395
Tritace: 173.419	Tritace: 89.25	Tritace: 89.25

The computed topological indices are undergone regression analysis and the results are listed below:

Regression equation of Avapro:

$y = -0.17x + 233.36$

$y = -0.15x + 199.15$

y = -0.12x + 169.28
y = -0.16x + 212.53
y = -0.15x + 198.93

Regression equation of Benazepril:

y = -0.14x + 228.99
y = -0.12x + 195.47
y = -0.10x + 166.15
y = -0.13x + 208.60
y = -0.12x + 195.24

Regression equation of Enalapril:

y = -0.19x + 232.88
y = -0.16x + 198.73
y = -0.13x + 168.92
y = -0.17x + 212.08
y = -0.16x + 198.51

Regression equation of Losontron:

y = -0.14x + 228.15
y = -0.12x + 194.77
y = -0.10x + 165.56
y = -0.13x + 207.86
y = -0.12x + 194.54

Regression equation of Tritace:

y = -0.18x + 233.77
y = -0.16x + 199.49
y = -0.13x + 169.57
y = -0.17x + 212.90
y = -0.15x + 199.27

5. CONCLUSION

In this article, the QSPR study of the drugs used in the treatment of diabetic nephropathy are studied. The topological indices of these drugs are calculated and compared with the theoretical properties of the drugs. The diagrammatic visualization of the data are plotted in Box graph, Line graph and in scatter diagram. The theoretical values are compared with these topological indices and the regression equations are found. The relations between the properties of chemicals in terms of topological indices are given as regression equations. These equations contain vital information about the structural relationship and the numerical invariants and the properties in terms of numerical values and may be used for drug design.

Disclaimer (Artificial intelligence)

Option 1:

Author(s) hereby declare that NO generative AI technologies such as Large Language Models (ChatGPT, COPILOT, etc.) and text-to-image generators have been used during the writing or editing of this manuscript.

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