RESEARCH PAPER

Eccentricity based Topological Indices of Type II Drugs used for Diabetes and their QSPR Modeling

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Abstract: In Quantitative Structure Property Relationship research, eccentricity-based topological indices are an effective molecular descriptor. The goal of this study is to establish predictive models that correlate the physicochemical properties of critical type II antidiabetic drugs. Linear regression is applied to validate the relation between six physicochemical properties and twelve topological indices. The resulting analysis demonstrated a high degree of correlation between the calculated topological indices and the experimental property values of the drugs.

Keywords: Eccentricity-based topological indices, QSPR analysis, Linear regression, Correlation Analysis.
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1. Introduction

Diabetes is a diverse illness defined by hyperglycemia which is classified as type 1 diabetes, type 2 diabetes, specific types of diabetes and gestational diabetes mellitus [1]. A nonautoimmune, heterogeneously progressive loss of sufficient islet β cells in insulin production, often accompanied by insulin resistance and metabolic syndrome, is the hallmark of type 2 diabetes. 96% of diabetes is caused by type 2 diabetes (T2D), one of the major chronic noncommunicable diseases that pose a major danger to human health without a well understood pathophysiology.

List of few drugs for type II diabetes [4]

1. Insulin and its different types
2. Biguanides: Metformin.1
3. Dipeptidyl Peptidase 4 inhibitors: Linagliptin, Sitagliptin, Saxagliptin
4. Peroxisomal proliferator activating receptor gamma inhibitors: Rosiglitazone, Pioglitazone.
5. Meglitinides: Nateglinide, Repaglinide,
6. Sodium Glucose co-transporter 2 inhibitors: Empagliflozin, Dapagliflozin.

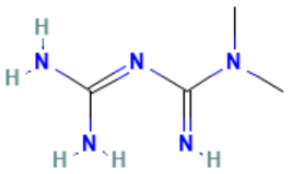
Graph theory is a branch of mathematics that studies network points connected by points connected by lines [3]. Graph theory can be applied to solve a number of practical issues. Graph theory was applied in chemistry during the nineteenth century. After that, a new branch of graph theory called chemical graph theory emerged. In chemical graph theory, chemical structures are represented by chemical graphs [4]. A vertex represents an atom, and an edge represents the connection between atoms.

Most of the compound's chemical information is related to its chemical structure. Topological indices are

numerical invariants that represent a chemical network. In QSAR and QSPR research, the TIs are used to create models that predict the physical, chemical, or biochemical characteristics of specific comp ounds. This idea is widely used as a computational technique for drug design and other structural analysis.

Several studies have predicted particular properties of compounds using various topological indices. Regression models and topological indices were used by Huili Li et al [5] predicted the chemical and physical properties of amino acids by analyzing their structural features.

A molecule's structure can be measured using topological indices. Chemistry and pharmacy have made extensive use of these indices, which are produced using the molecular structure. One of the main uses of the indices is quantitative structure property relationship analysis. These indices can be used to



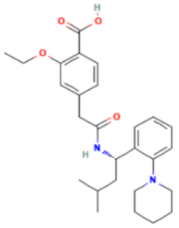
find different information depending on the algorithm chosen. Topological indices serve as a link between molecular structures' actual chemical properties and their abstract mathematical representation. Chemists can develop new medications, materials, and a better understanding of chemical processes by using graph theory to gain insights into molecular behavior.

More than 3000 indices that represent the structural characteristics of graphs have been developed as a result of topological indices research. Suresh et.al [6] used multiple linear regression in QSPR analysis of COVID-19 drugs using various topological indices. Rasheed et.al [7] discussed novel indices and thermodynamics properties of eye infection therapeutics with the help of QSAR modelling.

To ascertain whether a topological index can be used to forecast a chemical compound's behavior, the correlation coefficient between physicochemical properties and topological indices is utilized. In QSPR and QSAR analysis, topological indices with r greater than 0.8 are highly valuable. The goal and purpose of this study encompass the following steps.

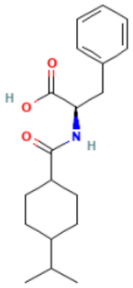
- Molecular graphs of antidiabetic drugs are examined through the computation of various eccentricity based topological indices.
- Linear regression is used to evaluate the relationship between seven topological indices and seven physicochemical properties.
- QSPR models are built using topological indices that exhibit a high correlation coefficient with these characteristics.

1.1 Molecular Structure of the drugs

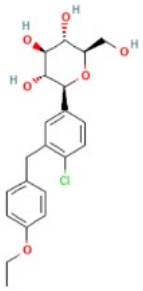


(a) Metformin

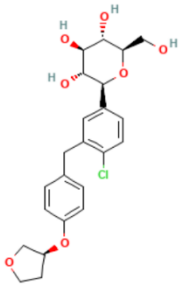
(b) Repaglinide



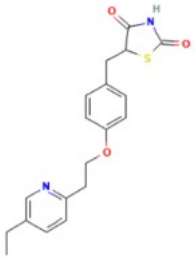
(c) Nateglinide



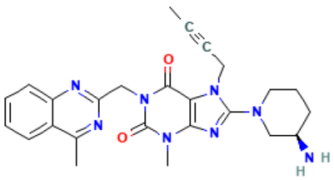
(d) Sitagliptin



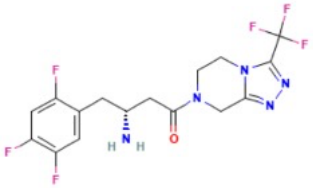
(e) Empagliflozin



(f) Dapagliflozin



(g) Linagliptin



(h) Pioglitazone

Figure 1 2D Structure of Type II Anti-Diabetic Drug

2. Materials and Methods

The data of the physicochemical properties of the compounds are used in QSPR/ QSAR study by chemists and pharmacists to create novel drugs. This study gives a step-by-step approach to comprehend the characteristics of the drugs so as to enhance the ability to target various aspects of the disease.

Topological indices play a major role in QSPR analysis to design a drug. The component of a drug is selected according the accessibility of information related to the compound, along with its properties and structural information to calculate topological indices. The above give eccentricities are used for the computation in QSPR analysis.

The physicochemical properties of the antidiabetic drugs considered for QSPR analysis are taken from the ChemSpider database and are summarized in Table 1.

Table 1 Physicochemical Properties of Drugs

PROPERTIES / DRUGS	BP	Enthalpy	FP	MR	Polarizability	MV
Metformin	224	40.9	58.1	33.4	13.2	100.8
Repalinide	672.9	103.8	360.8	130.1	51.6	397.9
Nateglinide	527.6	84.4	272.9	89.6	35.5	287.3
Sitagliptin	529.9	80.5	274.3	85.2	33.8	252.4
Empaglifliozin	665	102.7	355.7	114.4	45.4	322.4
Dapaglifliozin	609	95.1	322.1	105.6	41.9	303.1
Linagliptin	661.2	97.3	353.7	133.1	52.8	338
Pioglitazone	574.45	86.2	301.8	98.2	38.9	282.8

A molecular structure of chemical compound is represented by simple graph denoted by $G = (V, E)$ where V and E are the set of vertices and edges respectively. In this work, $\zeta(u)$ represents the eccentricity of the vertex $u \in V$.Formally expressed as :

$$\zeta(v) = \max\{d(v,u) | \forall\, u \in V(G)\}$$

For computing the topological indices, we make use of the edge partitioning method. This is an effective method computing topological indices by classifying edges according to the eccentricity of the vertices. Let $E_{u,v}$ represent the set of edges joining the vertices u and v. Here, $\zeta(u)$ and $\zeta(v)$ represents the eccentricity of vertices of u and v respectively.

In this work we analyze the six physicochemical properties of eight selected drugs of type II diabetes using linear regression.

Table 2 Eccentricity Based Topological Indices used for Computation

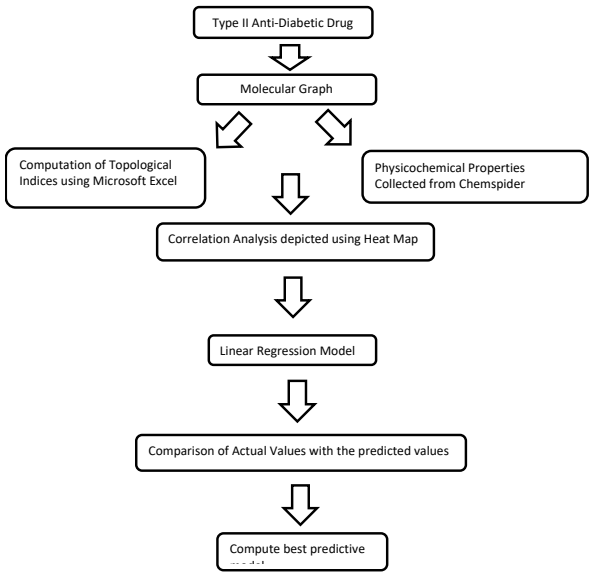
First Zagreb Index [8]	$M_1(G) = \sum_{u,v \in E(G)} \zeta(u) + \zeta(v)$
Second Zagreb Index [8]	$M_2(G) = \sum_{u,v \in E(G)} \zeta(u).\zeta(v)$
Eccentricity Sum-Connectivity Index [9]	$SCI = \sum_{u,v \in E(G)} \sqrt{\frac{1}{\zeta(u)+\zeta(v)}}$
Hyper Zagreb Index [10]	$H = \sum_{u,v \in E(G)} \left(\zeta(u) + \zeta(v)\right)^2$
Atom-Bond Connectivity Index [11]	$ABC(G) = \sum_{u,v \in E(G)} \sqrt{\frac{\zeta(u)+\zeta(v)-2}{\zeta(u).\zeta(v)}}$
Geometric-Arithmetic Index [12]	$GA(G) = \sum_{u,v \in E(G)} \frac{2\sqrt{\zeta(u).\zeta(v)}}{\zeta(u)+\zeta(v)}$
Eccentricity Inverse sum Index [9]	$IS(G) = \sum_{u,v \in G} \frac{\zeta(u).\zeta(v)}{\zeta(u)+\zeta(v)}$
SK index [13]	$SK(G) = \sum_{u,v \in E(G)} \frac{\zeta(u)+\zeta(v)}{2}$

Reciprocal Randic Index [14]	$RR(G) = \sum_{u,v \in E(G)} \sqrt{\zeta(u).\zeta(v)}$
Gourava indices based on eccentricity [16]	$GO_1 = \sum_{u,v \in E(G)} [(\zeta(u) + \zeta(v)) + \zeta(u).\zeta(v)]$ $GO_2 = \sum_{u,v \in E(G)} [(\zeta(u) + \zeta(v)).\zeta(u).\zeta(v)]$

Similar to this eccentricity based topological indices we give a new index product sum eccentricity index

$$PSI(G) = \sum_{u,v \in E(G)} \sqrt{\frac{\zeta(u).\zeta(v)}{\zeta(u)+\zeta(v)}}.$$

2.1 Methodology framework of the study:



3. Results and Discussion

In this section, eccentricity based topological indices are executed on anti-diabetic drugs. The relation between QSPR analysis and topological indices demonstrates that the characteristics are significantly correlated regarding physicochemical properties for drugs. The seven drugs are Metformin, Repaglinide, Nateglinide, Sitagliptin, Empagliflozin, Dapagliflozin, Linagliptin and Pioglitazone are taken for consideration. The drug structures are shown in FIG 1. As a graph, the molecular structure represents drug atoms as vertices and the bonds between them as edges. We employ linear regression analysis for this study.

3.1. Theorem. Let G_1 be the molecular graph of metformin. Various topological indices of G_1 are given as follows:

1. $M_1(G_1) = 63$

2. $M_2(G_1) = 125$

3. $SCI(G_1) = 2.87547$

4. $PS(G_1) = 357.2925$

5. $ABC(G_1) = 507$

6. $GO_1(G_1) = 4.96959$

7. $GO_2(G_1) = 345$

8. $SK(G_1) = 2316$

9. $HM(G_1) = 31.5$

10. $ISI(G_1) = 35$

11. $RR(G_1) = 31.28085$

12. $GA(G_1) = 7.9444$

Proof. Let G_1 be the graph of metformin with edge set E.

Let $E_{m,n}$ represent the class of edges of G_1 joining vertices of eccentricity m and n.

$|V(G_1)| = 9$ and $|E(G_1)| = 8$, edge partition is as follows

$$E_{3,3} = \{\zeta = ab \in E(G_1) | \zeta(u) = 3, \zeta(v) = 3\}$$

$$E_{3,4} = \{\zeta = ab \in E(G_1) | \zeta(u) = 3, \zeta(v) = 4\}$$

$$E_{4,5} = \{\zeta = ab \in E(G_1) | \zeta(u) = 4, \zeta(v) = 5\}$$

Such that $|E_{3,3}| = 1, |E_{3,4}| = 3, |E_{4,5}| = 4$.

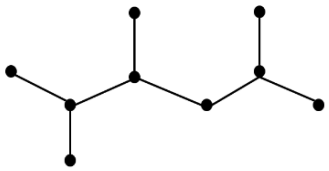


Figure 1. Molecular Graph of Metformin

The results are obtained using the definitions in table 1.

(1) $M_1(G_1) = (3+3) + 3(3+4) + 4(4+5) = 63$

(2) $M_2(G_1) = (3.3) + 3(3.4) + 4(4.5) = 125$

(3) $SCI(G_1) = \sqrt{\frac{1}{3+3}} + 3\sqrt{\frac{1}{3+4}} + 4\sqrt{\frac{1}{4+5}} = 2.87547$

(4) $PS(G_1) = \frac{3.3}{\sqrt{3+3}} + 3\left(\frac{3.4}{\sqrt{3+4}}\right) + 4\left(\frac{4.5}{\sqrt{4+5}}\right) = 357.2925$

(5) $HM(G_1) = (3+3)^2 + 3(3+4)^2 + 4(4+5)^2 = 507$

(6) $ABC(G_1) = \sqrt{\frac{3+3-2}{3.3}} + 3\sqrt{\frac{3+4-2}{3.4}} + 4\sqrt{\frac{4+5-2}{4.5}} = 4.96959$

(7) $GO_1(G_1) = [(3+3) + (3.3)] + 3[(3+4) + (3.4)] + 4[(4+5) + (4.5)] = 345$

(8) $GO_2(G_1) = [(3+3).(3.3)] + 3[(3+4).(3.4)] + 4[(4+5).(4.5)] = 2316$

(9) $SK(G_1) = \frac{3.3}{2} + 3\left(\frac{3+4}{2}\right) + 4\left(\frac{4+5}{2}\right) = 31.5$

(10) $ISI(G_1) = \frac{3.3}{3+3} + 3\left(\frac{3+4}{3+4}\right) + 4\left(\frac{4+5}{4+5}\right) = 35$

(11) $RR(G_1) = \sqrt{(3+3)} + 3\sqrt{(3+4)} + 4\sqrt{(4+5)} = 31.28085$

(12) $GA(G_1) = \frac{2\sqrt{3.3}}{3+3} + 3\left(\frac{\sqrt{3.4}}{3+4}\right) + 4\left(\frac{\sqrt{4.5}}{4+5}\right) = 7.944$

Similarly, the results of other drugs are depicted in table 3.

Table 3 Calculation of Eccentricity Based Topological Indices for antidiabetic drugs

TI / DRUG	M_1	M_2	SCI	PS	HM	ABC	GO_1	GO_2	SK	ISI	RR	GA
Metformin	63	125	2.87547	357.2925	507	4.9695	345	2316	31.5	35	31.28085	7.9444
Repaglinide	818	5230	7.3148	23932.4805	19370	13.9741	11024	250146	409	426	408.63	34.967
Nateglinide	475	2415	5.45749	11018.44395	9683	10.33402	5547	106174	237.5	249	237.2049	23.96889
Sitagliptin	696	4147	6.3012	20461.36492	16616	12.03	9331	211281	348	362	347.69	29.972

Empagliflozin	813	5160	6.7325	26305.08269	20671	12.8882	11525	279808	406.5	422	406.17	32.971
Dapagliflozin	681	3972	6.3692	19401.86355	15916	12.1482	8972	198923	340.5	355	340.1747	29.97
Linagliptin	883	5161	8.3089	25274.25738	20685	15.8409	11650	259809	441.5	460	441.02766	38.955
Pioglitazone	663	4511	4.9088	26766.24228	18067	10.2977	10421	267710	350.5	363	350.2524	26.9798

4. Statistical Computation

4.1 Quantitative Structure analysis and Comparison between Topological indices and Correlation

4.1.1 Coefficient of Physicochemical Properties: Physicochemical properties for eight type II antidiabetic drugs are listed in Table 2. And their TI s computed through the molecular structure are recorded in Table 3. The correlation heat map of TIs and Physicochemical Properties is shown in fig 2.

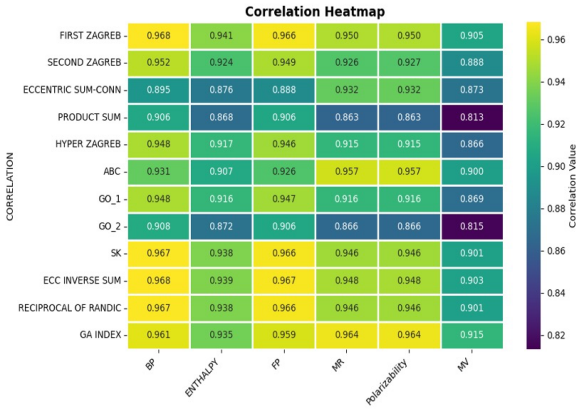


Figure 2 Correlation Heat map of Physicochemical Properties vs Topological Indices

Properties / TI	BP	Enthalpy	FP	MR	Polarizability	MV
$M_1(G)$	0.9681	0.9413	0.9662	0.9496	0.9498	0.9048
$M_2(G)$	0.9521	0.9236	0.9488	0.9264	0.9266	0.8879
$SCI(G)$	0.8947	0.8757	0.888	0.9318	0.9323	0.8731
$PS(G)$	0.9064	0.8683	0.9057	0.8633	0.8634	0.8134
$HM(G)$	0.9484	0.9166	0.9463	0.9151	0.9154	0.8658
$ABC(G)$	0.931	0.9068	0.9256	0.9569	0.9573	0.9
$GO_1(G)$	0.9482	0.9158	0.9465	0.916	0.9161	0.8687
$GO_2(G)$	0.9082	0.8723	0.9058	0.8657	0.8658	0.8148
SK	0.9672	0.938	0.9659	0.946	0.9463	0.9011
$ISI(G)$	0.9678	0.9388	0.9665	0.9476	0.9478	0.9027
$RR(G)$	0.9672	0.938	0.9659	0.946	0.9462	0.901
$GA(G)$	0.9609	0.9351	0.9585	0.964	0.9643	0.9151

Table 4 Correlation Coefficient values for the properties of antidiabetic drugs

4.1.2 Calculation of Statistical Parameters: In this section, we find the relation between eccentricity based topological indices and physicochemical properties of the drugs. This is achieved with the help of QSPR modelling, whereas b and r represent the regression model coefficient and correlation coefficient respectively.

It is noted that the value of $r > 0.7$ and value of $p < 0.5$. Therefore, the computation confirms that all characteristics are highly relevant.

Table 5 Regression Models for various topological indices

Regression model for $M_1(G)$ index	p	F	r^2	**Indicator**

$BP = 0.5404\ (M_1(G)) + 214$	< 0.0001	89.70	0.9373	$Significant$
$E = 0.0236\ (M_1(G)) + 40.31$	0.0005	46.60	0.8861	$Significant$
$FP = 0.3636\ (M_1(G)) + 56.02$	< 0.0001	84.25	0.9335	$Significant$
$MR = 0.11\ \ (M_1(G)) + 26.21$	0.0003	55.01	0.9017	$Significant$
$P = 0.04525\ (M_1(G)) + 10.33$	0.0003	55.35	0.9022	$Significant$
$MV = 0.02967\ (M_1(G)) + 96.72$	0.002	27.08	0.8186	$Significant$
Regression model for $M_2(G)$ index	p	F	r^2	**Indicator**
$BP = 0.07933\ (M_2(G)) + 253.4$	0.0003	58.22	0.9066	$Significant$
$E = 0.01060(M_2(G)) + 45.66$	0.0011	34.85	0.8531	$Significant$
$FP = 0.05329\ (M_2(G)) + 82.77$	0.0003	54.13	0.9002	$Significant$
$MR = 0.01659\ (M_2(G)) + 35.01$	0.0009	36.30	0.8582	$Significant$
$P = 0.006590(M_2(G)) + 13.83$	0.0009	36.41	0.8585	$Significant$
$MV = 0.04347\ (M_2(G)) + 118.7$	0.0032	22.36	0.7884	$Significant$
Regression model for $SCI(G)$ index	p	F	r^2	**Indicator**
$BP = 79.75\ (SCI(G)) + 76.82$	0.0027	24.09	0.8006	$Significant$
$E = 10.75\ (SCI(G)) + 21.51$	0.0044	19.74	0.7669	$Significant$
$FP = 53.36\ (SCI\ (G)) - 34.50$	0.0032	23.38	0.7886	$Significant$
$MR = 17.85\ (SCI\ (G)) - 8.983$	0.0008	39.55	0.8683	$Significant$
$P = 7.093\ (SCI\ (G)) - 3.658$	0.0007	38.86	0.8692	$Significant$
$MV = 45.72\ (SCI\ (G)) + 9.706$	0.0046	19.24	0.7623	$Significant$
Regression model for $PS(G)$ index	p	F	r^2	**Indicator**
$BP = 0.01451\ (PS(G)) + 279.5$	0.0019	27.62	0.8215	$Significant$
$E = 0.001915\ (PS(G)) + 49.62$	0.0052	18.38	0.7539	$Significant$
$FP = 0.0097\ \ (PS\ (G)) + 99.83$	0.002	27.37	0.8202	$Significant$
$MR = 0.002971\ (PS\ (G) + 41.69$	0.0057	17.56	0.7454	$Significant$
$P = 0.001180\ (PS\ (G)) + 16.49$	0.0057	17.57	0.7454	$Significant$
$MV = 0.007653\ (PS\ (G) + 138.7$	0.0141	11.73	0.6616	$Significant$
Regression model for $HM(G)$ index	p	F	r^2	**Indicator**
$BP = 0.02018\ (HM(G)) + 251.5$	0.0003	53.66	0.8994	$Significant$
$E = 0.002686\ (HM(G)) + 45.56$	0.0014	31.55	0.8402	$Significant$
$FP = 0.01357\ (HM(G)) + 81.24$	0.0004	51.42	0.8955	$Significant$
$MR = 0.004185\ (HM(G)) + 35.14$	0.0014	30.92	0.8375	$Significant$
$P = 0.001663\ (HM(G)) + 13.88$	0.0014	31.02	0.8379	$Significant$
	0.0055	17.96	0.7476	$Significant$

$MV = 0.01082\ (HM\ (G)) + 121.2$				
Regression model for ABC(G) index	p	F	r^2	**Indicator**
$BP = 42.40\ (ABC(G)) + 67.86$	0.0008	39.02	0.8667	$Significant$
$E = 5.687\ (ABC(G)) + 20.62$	0.0019	27.75	0.8222	$Significant$
$FP = 28.44\ (ABC\ (G)) - 41.38$	0.0009	36.35	0.8583	$Significant$
$MR = 9.365\ (ABC(G)) - 9.560$	0.0002	65.19	0.9157	$Significant$
$P = 3.721\ (ABC\ (G)) - 3.881$	0.0002	65.74	0.9164	$Significant$
$MV = 24.08\ (ABC\ (G)) + 7.193$	0.0023	25.57	0.8099	$Significant$
Regression model for $GO_1(G)$ index	p	F	r^2	**Indicator**
$BP = 0.036\ (GO_1(G)) + 248.5$	0.0003	53.49	0.8991	$Significant$
$E = 0.004785\ (GO_1(G)) + 45.20$	0.0014	31.20	0.8387	$Significant$
$FP = 0.02421\ (GO_1\ (G)) + 79.17$	0.0004	51.62	0.8959	$Significant$
$MR = 0.007468(GO_1(G)) + 34.46$	0.0014	31.27	0.8390	$Significant$
$P = 0.002967\ (GO_1\ (G)) + 13.61$	0.0014	31.34	0.8393	$Significant$
$MV = 0.01937\ (GO_1(G)) + 119$	0.0051	18.45	0.7546	$Significant$
Regression model for $GO_2(G)$ index	p	F	r^2	**Indicator**
$BP = 0.001386\ (GO_2(G)) + 284.9$	0.0018	28.24	0.8248	$Significant$
$E = 0.00018\ (GO_2(G)) + 50.23$	0.0047	19.10	0.7609	$Significant$
$FP = 0.009322\ (GO_2(G)) + 103.8$	0.0019	27.43	0.8205	$Significant$
$MR = 0.0002840(GO_2(G)) + 42.75$	0.0055	17.94	0.7494	$Significant$
$P = 0.0001128\ (GO_2\ (G)) + 16.91$	0.0055	17.96	0.7496	$Significant$
$MV = 0.0007308\ (GO_2(G)) + 141.6$	0.0138	11.85	0.6638	$Significant$
Regression model for $SK(G)$ index	p	F	r^2	**Indicator**
$BP = 1.076\ (SK(G)) + 213$	< 0.0001	86.97	0.9355	$Significant$
$E = 0.1437\ (SK(G)) + 40.28$	0.0006	43.92	0.8798	$Significant$
$FP = 0.7245\ (SK\ (G)) + 55.14$	< 0.0001	83.56	0.9330	$Significant$
$MR = 0.2262\ (SK\ (G)) + 26.18$	0.0004	51.14	0.8950	$Significant$
$P = 0.08987\ (SK(G)) + 10.32$	00004	51.38	0.8954	$Significant$
$MV = 0.5891\ (SK\ (G)) + 96.72$	0.0022	25.90	0.8119	$Significant$
Regression model for $ISI(G)$ index	p	F	r^2	**Indicator**
$BP = 1.041\ (ISI(G)) + 210$	< 0.0001	88.74	0.9367	$Significant$

$E = 0.1391\ (ISI(G)) + 39.89$	0.0005	44.59	0.8814	$Significant$
$FP = 0.7011\ (ISI\ (G)) + 53.25$	< 0.0001	85.09	0.9341	$Significant$
$MR = 0.2191\ (ISI(G)) + 25.51$	0.0003	52.77	0.8979	$Significant$
$P = 0.08706\ (ISI(G)) + 10.06$	0.0003	53.02	0.8983	$Significant$
$MV = 0.5707\ \ (ISI\ (G)) + 94.96$	0.0021	26.40	0.8148	$Significant$
Regression model for $RR(G)$ index	p	F	r^2	**Indicator**
$BP = 1.077\ (RR(G)) + 213.2$	< 0.0001	86.98	0.9355	$Significant$
$E = 0.1438\ (RR(G)) + 213.2$	0.0006	43.93	0.8798	$Significant$
$FP = 0.7248\ (RR\ (G)) + 55.27$	< 0.0001	83.59	0.9330	$Significant$
$MR = 0.2263\ (RR(G)) + 26.23$	0.0004	51.07	0.8949	$Significant$
$P = 0.0899\ (RR\ (G)) + 10.34$	0.0004	51.30	0.8953	$Significant$
$MV = 0.5893\ \ (RR\ (G)) + 96.83$	0.0022	25.90	0.8119	$Significant$
Regression model for $GA(G)$ index	p	F	r^2	**Indicator**
$BP = 15.02\ (GA(G)) + 134.3$	0.0001	72.25	0.9233	$Significant$
$E = 2.012\ (GA(G)) + 29.58$	0.0006	41.80	0.8745	$Significant$
$FP = 10.10\ \ (GA\ (G)) + 2.515$	0.0002	67.90	0.9188	$Significant$
$MR = 3.237\ \ (GA(G)) + 7.367$	0.0001	78.78	0.9292	$Significant$
$P = 1.286\ (GA\ (G)) + 2.847$	0.0001	79.46	0.9298	$Significant$
$MV = 8.402\ (GA\ (G)) + 48.52$	0.00014	30.90	0.8374	$Significant$

Python programming is used to create all of the regression models. Here we take into account the following metrics for the assessment

1. The regression coefficient (r), indicates how strongly the actual value and the value computed through the model are related. The values for r falls between -1 to 1. A strong positive correlation and a significant impact of the predictor variable on the dependent parameter are indicated when the r-value is greater than 0.9.
2. r^2 (coefficient of determination): Shows how much of the depend variable's variation the model can account for. A higher r^2 value indicates a better fit.
3. $F-$ statistic: It assesses the model's overall relevance. The variation in the dependent variable is mostly explained by the independent factors when the p value is low and the F-statistic is high.
4. $p-$ value: The statistical significance of the model is assessed. If the p value is less than 0.05, it is considered that the predictor is statistically significant.

In linear regression analysis, most of the indices calculated shows positive correlation with the physicochemical properties of the drugs. Table 6. shows the best predictive model.

Table 6 Best Predictive Model

Equation	p	F	r^2	Indicator
$BP = 0.036\,(GO_1) + 248.5$	0.000	53.4	0.824	$Signific$
$E = 0.00018\,(G + 50.23$	0.004	19.1	0.760	$Signific$
$FP = 0.0097\ (PS + 99.83$	0.002	27.3	0.820	$Signific$
$MR = 0.11\ (M_1(G + 26.21$	0.000	55.0	0.901	$Signific$
$P = 1.286\,(GA + 2.847$	0.000	79.4	0.929	$Signific$
$MV = 8.402\,(GA + 48.52$	0.000	30.9	0.837	$Signific$

We take into account the drug Rosiglitazone in order to validate the predictive model. We compute the eccentricity based topological indices and the results are given in Table7. By substituting the index values in the best predictive model, the physicochemical properties of Rosiglitazone are estimated.

The experimental values of physicochemical properties are gathered from ChemSpider and compared with the predicted values. These findings demonstrate how well the model predicts the properties of new antidiabetic medications. This method may be used to screen a huge number of compounds and find those with a high potential for use as type II antidiabetic drugs.

Table 7 *Computation of various topological indices for the drug Rosiglitazone*

Topological Indices	Computed Value of Rosiglitazone
First Zagreb Index	668
Second Zagreb Index	4271
Eccentricity Sum-Connectivity Index	5.324629
Product- Sum Eccentricity Index	21864.23114
Hyper Zagreb Index	17110
Atom-Bond Connectivity Index	10.54054
Gourava indices based on eccentricity	$GO_1 = 9542$ $GO_2 = 233784$
***SK* index**	334
Eccentricity Inverse sum Index	454
Reciprocal Randic Index	333.72448
Geometric-Arithmetic Index	26.97567

Table 8 Experimental value vs Predicted value

Physicochemical Property	Experimental Value	Predicted Value
Boiling Point	585	591.82
Enthalpy	87.4	92.30
Flash Point	307.6	311.91
Molar Refractivity	98.1	99.69
Polarizability	38.9	37.53
Molar Volume	271.6	275.17

4. Conclusions

In this study, topological indices are effectively utilized to create prediction models for evaluating the physicochemical characteristics of type II antidiabetic drugs. This study effectively demonstrates the potential of topological indices in constructing predictive models for evaluating the physicochemical characteristics of type II antidiabetic drugs. The proposed computational framework offers a rapid, cost-efficient, and reliable first-level screening method, significantly reducing the time, resources, and labour required compared to traditional experimental approaches. While this model provides valuable preliminary insights for drug discovery, it cannot be directly used to determine human applicability without further pharmacological validation and clinical testing. Overall, the integration of graph-theoretical methods with computational chemistry presents a promising direction for accelerating and optimizing the early stages of drug design.

Data Availability Statement

The data used to support the findings of this study are from Pubchem: https://pubchem.ncbi.nlm.nih.gov/ and Chemspider: https://www.chemspider.com/.

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Conflicts of Interest

The authors declare no conflict of interest.

Abbreviations

The following abbreviations are used in this manuscript:

Abbreviation	Definition
TI	Topological Indices
ABC	Atom Bond Connectivity
GA	Geometric-Arithmetic
RR	Reciprocal Randic
SCI	Sum Connectivity Index
ISI	Inverse Sum Index
PSI	Product Sum Index
QSPR	Quantitative Structure-Property Relationship
BP	Boiling Point
FP	Flash Point
MR	Molar Refractivity
MV	Molar Volume

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