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Research Article

Topological Indices of Novel Drugs Used in Diabetes Treatment and Their QSPR Modeling

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A topological index is a real number obtained from the chemical graph structure. It is helpful to calculate the physicochemical and biological properties of numerous drugs. This is done through degree-based topological indices. In this paper, acarbose, tolazamide, miglitol, prandin, metformin, and so on used to treat diabetes are discussed, and the purpose of the QSPR study is to determine the mathematical relation between the properties under investigation (e.g., boiling point and flash point) and different descriptors related to the molecular structure of the drugs. In this study, it is observed that topological indices (TIs) applied to said drugs have a good correlation with physicochemical properties in this course.

1. Introduction

Diabetes is a metabolic disease that develops when the pancreas cannot generate enough insulin, and its effective use is retarded. This chronic disease leads to high blood glucose and is named blood sugar. Glucose is obtained from food and becomes an energy source in our body. Pancreas generates a hormone named insulin. The hormone helps glucose to digest in cells and is used as energy. Glucagon is another hormone that associates with insulin and controls blood sugar. When our immune system is not functioning properly, it fights infections and kills insulin-producing agents. As a result, there is a chance that insulin does not work well and glucose becomes to stay in our blood and will not become part of our cells. With the passage of time, diabetes leads to severe damage to nerves and blood vessels, the amount of glucose becomes very high, and it will generate other health issues. Every year 422 million persons become sick with diabetes, and 1.5 million lead to death because of this disease. The risk of diabetes increases when you are 45 or above, and high blood pressure will also increase the chance of the said disease [1–4]. The disease has no proper treatment, but effective care can help you manage diabetes and live a healthier life. Drugs are used to cure this malignant disease, and many drugs tests are accompanied to fight the fatal disease. This needs timely diagnosis, screening, and medication that benefits patients to control the deadly disease in future. The ten essential drugs acarbose, tolazamide, miglitol, prandin, metformin, glimepiride, linagliptin, pioglitazone, bromocriptine, and alogliptin are safe and the most efficient medicines that are required for well-being community. Figure 1 depicts the chemical structure of the said drugs.

Topological indices (TIs) are termed numeric descriptors that are obtained through a molecular graph in order to completely mention the chemical system and widely used in the investigation of physicochemical properties of many drugs. Since there are several kinds of polynomials and topological indices which are extensively calculated, represent the chemical structure, and have a vital position in

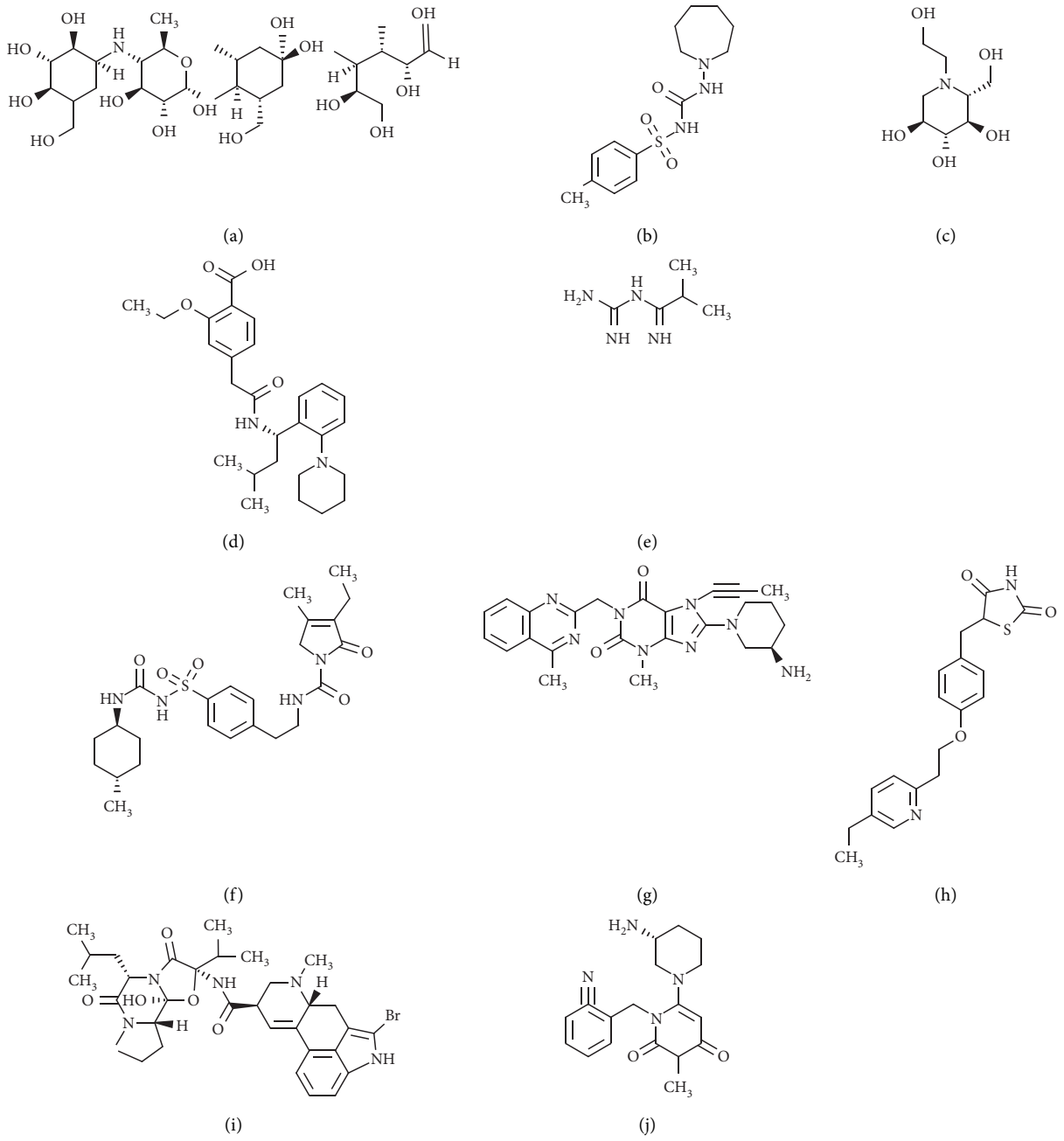

Figure 1: Molecular structure of drugs. (a) Acarbose. (b) Tolazamide. (c) Miglitol. (d) Prandin. (e) Metformin. (f) Glimepiride. (g) Linagliptin. (h) Pioglitazone. (i) Bromocriptine. (j) Alogliptin.

chemical graph theory, among such families, degree-based topological indices are of great significance and play a vital part in chemical graph theory. The use of graph invariants (TIs) in QSPR and QSAR studies has taken key interest in recent years. Topological indices have applications in various areas of mathematics, bioinformatics, mathematics, informatics, biology, and so on, but their utmost significant use to date is in the nonempirical Quantitative Structure-Property Relationships (QSPR) [5, 6].

ABC index, Wiener index, and Randic index are helpful to predict the bioactivity of drugs. The QSPR models assist in determining the optimal relationship between topological indices and psychochemical characteristics. These psychochemical qualities are being studied because they have a big impact on bioactivity and drug transit in the human body. In this paper, we have computed degree-based TIs related to diabetes drugs. Similarly, antidiabetes drugs represent a chemical compound on which the given topological indices are thoroughly defined and deliberate QSPR analysis. The corresponding characteristic estimated through this method is highly correlated with the characteristic of diabetes drugs with the help of linear regression. It is observed that a high correlation exists between the properties of drugs and TIs.

Table 1: The TIs values of candidate drugs.

Name of drug	ABC(G)	RA(G)	S(G)	GA(G)	M1(G)	M2(G)	F(G)	H(G)	HM(G)
Acarbose	65.44	38.18	38.57	81.16	506	682	1730	3094	34.29
Tolazamide	32.73	18.23	18.43	38.61	242	310	806	1426	15.98
Miglitol	23.07	13.67	13.55	27.99	174	230	596	1056	12.16
Prandin/repaglinide	53.61	30.23	30.62	64.24	396	509	1300	2318	26.73
Metformin	14.75	8.75	8.57	17.00	96	104	290	498	7.72
Glimepiride	53.27	29.46	29.86	62.77	398	515	1342	2370	25.75
Linagliptin	50.23	27.92	28.81	60.92	372	472	1196	2140	24.99
Pioglitazone	35.22	20.02	20.52	43.02	256	322	808	1452	17.96
Bromocriptine	66.57	36.33	37.57	80.68	518	699	1762	3160	32.12
Alogliptin	35.88	20.38	20.77	43.86	266	344	858	1546	18.21

2. Material and Method

In drug structures, atoms denote vertices, and the corresponding bonds connecting the atoms are termed edges. Graph G (V, E) is considered as simple, finite, and connected, whereas V and E represented in the chemical graph are termed as vertex and edge set, respectively. The degree of a vertex in a graph G is the number of vertices adjacent to it and is denoted by d_u. Valence of a compound in chemistry and the degree of a vertex in a graph are meticulously related concepts [7–10]. Degree-based topological indices used are given as follows.

Definition 1. The ABC index [10] of a molecular graph G is defined as

$$ABC(G) = \sum_{uv \in E(G)} \sqrt{\frac{d_{u+}d_v - 2}{d_u d_v}}. \tag{1}$$

Definition 2. The first degree-based topological index is the Randic index $RA(G)$ introduced by Milan Randic in 1975 [11]. Randic index is defined as

$$RA(G) = \sum_{uv \in E(G)} \sqrt{\frac{1}{d_u d_v}}. \tag{2}$$

Definition 3. The sum connectivity index [12] of a molecular graph G is defined as

$$S(G) = \sum_{uv \in E(G)} \sqrt{\frac{1}{d_u + d_v}}. \tag{3}$$

Definition 4. The GA index [13] of a molecular graph G is defined as

$$GA(G) = \sum_{uv \in E(G)} \frac{2\sqrt{d_u d_v}}{d_u + d_v}. \tag{4}$$

Definition 5. The first and second Zagreb indices [14] of a molecular graph G are defined as

$$\begin{aligned} M1(G) &= \sum_{uv \in E(G)} (d_u + d_v), \\ M2(G) &= \sum_{uv \in E(G)} (d_u d_v). \end{aligned} \tag{5}$$

Definition 6. The harmonic index [15] of a molecular graph G is defined as

$$H(G) = \sum_{uv \in E(G)} \frac{2}{d_u + d_v}. \tag{6}$$

Definition 7. The hyper-Zagreb index [16] of a molecular graph G is defined as

$$HM(G) = \sum_{uv \in E(G)} (d_u + d_v)^2. \tag{7}$$

Definition 8. The forgotten index [17] of a molecular graph G is defined as

$$F(G) = \sum_{uv \in E(G)} \left[(d_u)^2 + (d_v)^2 \right]. \tag{8}$$

The π – electron energy of molecule was found with the help of the first and second Zagreb indices in [18]. Alkane heat of formation is best predicted by applying the augmented Zagreb index in [19]. The values of physical properties are taken from ChemSpider. It is observed from data in Table 1 and is found that these data values are normally distributed. Therefore, the linear regression model is the most adequate to test and adopt for the said analysis. For more insight on degree-based topological indices, we offer the reader to visit the following articles [5, 7, 20–24].

3. Results and Discussions

In this section, degree-based TIs are executed on diabetes drugs. The relation between QSPR analysis and topological indices portrays that the properties are vastly correlated in terms of physicochemical properties for the said disease. The ten medicines acarbose, tolazamide, miglitol, prandin, metformin, glimepiride, linagliptin, pioglitazone, bromocriptine, and alogliptin are used in the analysis for diabetes. The drug structures are displayed in Figure 1. We consider

Table 2: Correlation coefficients.

Topological index	Correlation coefficient of boiling point	Correlation coefficient of refractive index	Correlation coefficient of flash point	Correlation coefficient of polarity	Correlation coefficient of molar volume	Correlation coefficient of complexity
ABC(G)	0.910	**0.961**	0.929	**0.993**	**0.960**	0.946
RA(G)	0.898	0.947	0.939	0.985	0.947	0.931
S(G)	0.904	0.953	0.938	0.989	0.951	0.938
GA(G)	0.909	0.956	0.938	0.991	0.952	0.943
M1(G)	**0.912**	0.953	0.940	0.990	0.949	**0.947**
M2(G)	**0.912**	0.940	**0.950**	0.983	0.935	0.943
HM(G)	0.896	0.944	0.942	0.983	0.942	0.928
F(G)	0.907	0.937	0.947	0.982	0.935	0.941
H(G)	0.909	0.939	0.949	0.983	0.935	0.942

the molecular structure as a graph, the drug elements denote vertices, and bonds among atoms are their edges. We use regression analysis calculation for drugs study.

3.1. Regression Model. In this paper, drug computable structure analysis about ten topological indices is done for QSPR modeling tenacity. The six physical properties, flash point (FP), polarity, boiling point (BP), molar volume (MV), and refractivity (R) for ten medicine arranged in Table 2 are used in diabetes treatment. We execute the regression analysis for the drugs, and the linear regression model is tested with the help of equation

$$P = A + b(TI). \tag{9}$$

Here, P represents the physicochemical property of given drugs. TI is the topological index, A is constant, and b represents the regression coefficient. The IBM SPSS Statistics version-24 software is helpful to find out the results. Nine TIs of diabetes drugs and physiochemical properties are analyzed with a linear QSPR model. Equation (9) is suitable for the said calculation purpose.

Theorem 1. *Let G_1 be the graph metformin. Various topological indices of G_1 are given as follows:*

(i) $ABC(G_1) = 14.75$.
(ii) $RA(G_1) = 8.75$.
(iii) $S(G_1) = 8.57$.
(iv) $GA(G_1) = 17.00$.
(v) $M1(G_1) = 96$.
(vi) $M2(G_1) = 104$.
(vii) $F(G_1) = 290$.
(viii) $H(G_1) = 498$.
(ix) $HM(G_1) = 7.72$.

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 degrees m and n. With $|E_{1,3}| = 5$, $|E_{1,4}| = 6$, $|E_{2,3}| = 3$, $|E_{2,4}| = 1$, $|E_{3,3}| = 3$, and $|E_{3,4}| = 1$, one has the following:

(i) By using Definition 1 and the above given edge partitions $E_{m,n}$, we get

$$AB(G_1) = 5\sqrt{\frac{1+3-2}{1\times 3}} + 6\sqrt{\frac{1+4-2}{1\times 4}} + 3\sqrt{\frac{2+3-2}{2\times 3}} + 1\sqrt{\frac{2+4-2}{2\times 4}} + 3\sqrt{\frac{3+3-2}{3\times 3}} + 1\sqrt{\frac{3+4-2}{3\times 4}} = 14.75. \tag{10}$$

(ii) By using Definition 2 and the above given edge partitions $E_{m,n}$, we get

$$RA(GG_1) = 5\sqrt{\frac{1}{1\times 3}} + 6\sqrt{\frac{1}{1\times 4}} + 3\sqrt{\frac{1}{2\times 3}} + 1\sqrt{\frac{1}{2\times 4}} + 3\sqrt{\frac{1}{3\times 3}} + 1\sqrt{\frac{1}{3\times 4}} = 8.75. \tag{11}$$

(iii) By using Definition 3 and the above given edge partitions $E_{m,n}$, we get

$$S(G_1) = 5\sqrt{\frac{1}{1+3}} + 6\sqrt{\frac{1}{1+4}} + 3\sqrt{\frac{1}{2+3}} + 1\sqrt{\frac{1}{2+4}} + 3\sqrt{\frac{1}{3+3}} + 1\sqrt{\frac{1}{3+4}} = 8.57. \tag{12}$$

(iv) By using Definition 4 and the above given edge partitions $E_{m,n}$, we get

$$GA(G_1) = \frac{5\sqrt{1\times 3}}{1+3} + \frac{6\sqrt{1\times 4}}{1+4} + \frac{3\sqrt{2\times 3}}{2+3} + \frac{1\sqrt{2\times 4}}{2+4} + \frac{3\sqrt{3\times 3}}{3+3} + \frac{1\sqrt{3\times 4}}{3+4} = 17.00. \tag{13}$$

(v) By using Definition 5 and the above given edge partitions $E_{m,n}$, we get

$$M1(G_1) = 5(1+3) + 6(1+4) + 3(2+3) + 1(2+4) + 3(3+3) + 1(3+4) = 96. \tag{14}$$

(vi) By using Definition 5 and the above given edge partitions $E_{m,n}$, we get

$$M2(G_1) = 5(1\times 3) + 6(1\times 4) + 3(2\times 3) + 1(2\times 4) + 3(3\times 3) + 1(3\times 4) = 104. \tag{15}$$

(vii) By using Definition 6 and the above given edge partitions $E_{m,n}$, we get

$$H(G_1) = 5\left(\frac{1}{1+3}\right) + 6\left(\frac{1}{1+4}\right) + 3\left(\frac{1}{2+3}\right) + 1\left(\frac{1}{2+4}\right) + 3\left(\frac{1}{3+3}\right) + 1\left(\frac{1}{3+4}\right) = 498. \tag{16}$$

(viii) By using Definition 7 and the above given edge partitions $E_{m,n}$, we get

$$HM(G_1) = 5(1+3)^2 + 6(1+4)^2 + 3(2+3)^2 + 1(2+4)^2 + 3(3+3)^2 + 1(3+4)^2 = 7.72. \tag{17}$$

(ix) By using Definition 8 and the above given edge partitions $E_{m,n}$, we get

$$F(G_1) = 5(1+9) + 6(1+16) + 3(4+9) + 1(4+16) + 3(9+9) + 1(9+16) = 290. \tag{18}$$

□

Theorem 2. *Let G_2 be the graph of tolazamide. Various topological indices of G_2 are given as follows:*

(i) $ABC(G_2) = 32.73$.
(ii) $RA(G_2) = 18.23$.
(iii) $S(G_2) = 18.43$.
(iv) $GA(G_2) = 38.61$.
(v) $M1(G_2) = 242$.
(vi) $M2(G_2) = 310$.
(vii) $F(G_2) = 806$.
(viii) $H(G_2) = 1426$.
(ix) $HM(G_2) = 15.98$.

Proof. Let G_2 be the graph of tolazamide with edge set $E'E'$. Let $E_{(m,n)}'$ represent the class of edges of G_2 joining vertices of degrees m and n. With $|E_{(1,3)}'| = 7$, $|E_{(1,4)}'| = 17$, $|E_{(3,3)}'| = 9$, $|E_{(3,4)}'| = 5$, and $|E_{(4,4)}'| = 5$, one has the following:

(i) By using Definition 1 and edge partitions $E_{(m,n)}'$, we get

$$ABC(G_2) = 7\sqrt{\frac{1+3-2}{1\times 3}} + 17\sqrt{\frac{1+4-2}{1\times 4}}9\sqrt{\frac{3+3-2}{3\times 3}} + 5\sqrt{\frac{3+4-2}{3\times 4}} + 5\sqrt{\frac{4+4-2}{4\times 4}} = 32.73. \tag{19}$$

(ii) By using Definition 2 and edge partition $E_{(m,n)}'$, we get

$$RA(G_2) = 7\sqrt{\frac{1}{1\times 3}} + 17\sqrt{\frac{1}{1\times 4}} + 9\sqrt{\frac{1}{3\times 3}} + 5\sqrt{\frac{1}{3\times 4}} + 5\sqrt{\frac{1}{4\times 4}} = 18.23. \tag{20}$$

(iii) Definition 3 and edge partition $E_{(m,n)}'$ give

$$S(G_2) = 7\sqrt{\frac{1}{1+3}} + 17\sqrt{\frac{1}{1+4}} + 9\sqrt{\frac{1}{3+3}} + 5\sqrt{\frac{1}{3+4}} + 5\sqrt{\frac{1}{4+4}} = 18.43. \tag{21}$$

(iv) By using Definition 4 and edge partition $E_{(m,n)}'$, we get

$$GA(G_2) = \frac{7\sqrt{1\times 3}}{1+3} + \frac{17\sqrt{1\times 4}}{1+4} + \frac{9\sqrt{3\times 3}}{3+3} + \frac{5\sqrt{3\times 4}}{3+4}\,\frac{5\sqrt{4\times 4}}{4+4} = 38.61. \tag{22}$$

(v) By using Definition 5 and edge partition $E_{(m,n)}'$, we get

$$M1(G_2) = 9(3+3) + 5(3+4) + 5(4+4) = 242. \tag{23}$$

(vi) By using Definition 5 and edge partition $E_{(m,n)}'$, we get

$$M2(G_2) = 9(3\times 3) + 5(3\times 4) + 5(4\times 4) = 310. \tag{24}$$

(vii) By using Definition 6 and edge partition $E_{(m,n)}'$, we get

$$H(G_2) = 14\left(\frac{1}{1+3}\right) + 34\left(\frac{1}{1+4}\right) + 18\left(\frac{1}{3+3}\right) + 10\left(\frac{1}{3+4}\right) + 10\left(\frac{1}{4+4}\right) = 15.98. \tag{25}$$

(viii) By using Definition 7 and edge partition $E_{(m,n)}'$, we get

$$HM(G) = 7(1+3)^2 + 17(1+4)^2 + 9(3+3)^2 + 5(3+4)^2 + 5(4+4)^2 = 1426. \tag{26}$$

(ix) By using Definition 8 and edge partition $E_{(m,n)}'$, we get

Table 3: Statistical parameters used in the QSPR model of ABC(G).

Physiochemical property	N	A	b	r	r^2	F	p	Indicator
Boiling point	8	103.153	10.44	0.910	0.828	28.947	0.002	Significant
Refractivity	10	18.569	2.093	0.961	0.923	96.186	0.000	Significant
Flash point	10	20.160	7.125	0.929	0.863	50.209	0.000	Significant
Polarity	10	0.172	0.980	0.993	0.987	601.829	0.000	Significant
Molar volume	10	31.785	6.065	0.960	0.922	94.658	0.000	Significant
Complexity	10	−182.330	19.139	0.946	0.895	68.075	0.000	Significant

Table 4: Statistical parameters used in the QSPR model of R(G).

Physiochemical property	N	A	b	r	r^2	F	p	Indicator
Boiling point	8	100.512	18.552	0.898	0.806	24.869	0.002	Significant
Refractivity	10	18.020	3.731	0.947	0.896	68.952	0.000	Significant
Flash point	10	10.148	13.033	0.939	0.882	59.738	0.000	Significant
Polarity	10	−0.380	1.759	0.985	0.971	269.242	0.000	Significant
Molar volume	10	29.935	10.820	0.947	0.897	69.435	0.000	Significant
Complexity	10	−186.139	34.060	0.931	0.866	51.682	0.000	Significant

Table 5: Statistical parameters used in the QSPR model of S(G).

Physiochemical property	N	A	b	r	r^2	F	p	Indicator
Boiling point	8	105.293	18.056	0.904	0.818	26.895	0.002	Significant
Refractivity	10	18.772	3.638	0.953	0.909	79.844	0.000	Significant
Flash point	10	15.429	12.603	0.938	0.880	58.418	0.000	Significant
Polarity	10	0.122	1.710	0.989	0.978	361.056	0.000	Significant
Molar volume	10	32.905	10.520	0.951	0.904	75.428	0.000	Significant
Complexity	10	−180.010	33.247	0.938	0.880	58.669	0.000	Significant

Table 6: Statistical parameters used in the QSPR model of GA(G).

Physiochemical property	N	A	b	r	r^2	F	p	Indicator
Boiling point	8	113.440	8.420	0.909	0.827	28.661	0.002	Significant
Refractivity	10	20.596	1.694	0.956	0.915	85.807	0.000	Significant
Flash point	10	22.547	5.853	0.938	0.881	58.950	0.000	Significant
Polarity	10	1.044	0.795	0.991	0.981	422.813	0.000	Significant
Molar volume	10	38.721	4.888	0.952	0.906	77.089	0.000	Significant
Complexity	10	−465.288	15.519	0.943	0.890	64.644	0.000	Significant

Table 7: Statistical parameters used in the QSPR model of M1(G).

Physiochemical property	N	A	b	r	r^2	F	p	Indicator
Boiling point	8	126.868	1.316	0.912	0.833	29.851	0.002	Significant
Refractivity	10	24.500	0.261	0.953	0.907	78.261	0.000	Significant
Flash point	10	34.273	0.908	0.940	0.884	60.928	0.000	Significant
Polarity	10	2.745	0.123	0.990	0.980	389.993	0.000	Significant
Molar volume	10	49.701	0.755	0.949	0.901	72.565	0.000	Significant
Complexity	10	−135.869	2.413	0.947	0.897	69.814	0.000	Significant

$$F(G_2) = 7(1+9) + 17(1+16) + 9(9+9) + 5(9+16) + 5(16+16) = 806. \quad (27)$$

One can calculate topological indices of the remaining drugs by adopting a similar procedure applied in Theorem 1 and Theorem 2 and using Definitions 1 to 8. Moreover, the calculated values of all drugs are listed in Table 1.

Using (1), we have calculated the following diverse linear models for all degree-based topological indices, which are given as follows:

Table 8: Statistical parameters used in the QSPR model of M2(G).

Physiochemical property	N	A	b	r	r^2	F	p	Indicator
Boiling point	8	151.218	0.952	0.912	0.831	29.594	0.002	Significant
Refractivity	10	30.535	0.187	0.940	0.884	61.765	0.000	Significant
Flash point	10	48.647	0.665	0.950	0.903	74.726	0.000	Significant
Polarity	10	5.362	0.088	0.983	0.966	227.719	0.000	Significant
Molar volume	10	67.501	0.539	0.935	0.874	55.716	0.000	Significant
Complexity	10	−86.694	1.741	0.943	0.890	64.605	0.000	Significant

Table 9: Statistical parameters used in the QSPR model of HM(G).

Physiochemical property	N	A	b	r	r^2	F	p	Indicator
Boiling point	8	104.181	20.696	0.896	0.802	24.371	0.003	Significant
Refractivity	10	18.567	4.176	0.944	0.891	65.590	0.000	Significant
Flash point	10	10.181	14.677	0.942	0.888	63.253	0.000	Significant
Polarity	10	−0.136	1.970	0.983	0.967	232.095	0.000	Significant
Molar volume	10	32.218	12.080	0.942	0.887	62.921	0.000	Significant
Complexity	10	−181.037	38.124	0.928	0.861	49.617	0.000	Significant

Table 10: Statistical parameters used in the QSPR model of F(G).

Physiochemical property	N	A	b	r	r^2	F	p	Indicator
Boiling point	8	144.280	0.380	0.907	0.823	27.860	0.002	Significant
Refractivity	10	29.397	0.074	0.937	0.878	57.742	0.000	Significant
Flash point	10	44.851	0.264	0.947	0.896	69.058	0.000	Significant
Polarity	10	4.737	0.035	0.982	0.965	217.832	0.000	Significant
Molar volume	10	63.476	0.215	0.935	0.875	55.888	0.000	Significant
Complexity	10	−97.844	0.692	0.941	0.886	61.999	0.000	Significant

Table 11: Statistical parameters used in the QSPR model of H(G).

Physiochemical property	N	A	b	r	r^2	F	p	Indicator
Boiling point	8	147.316	0.211	0.909	0.827	28.627	0.002	Significant
Refractivity	10	29.878	0.041	0.939	0.881	59.168	0.000	Significant
Flash point	10	46.427	0.147	0.949	0.900	71.756	0.000	Significant
Polarity	10	5.004	0.020	0.983	0.965	223.451	0.000	Significant
Molar volume	10	65.210	0.120	0.935	0.875	55.864	0.000	Significant
Complexity	10	−93.085	0.386	0.942	0.888	63.218	0.000	Significant

Table 12: Physical properties of drugs.

Name of drug	Refractive index (m^3mol^{-1})	Flash point (℃)	Molar volume (cm^3)	Polarity (cm^3)	Boiling point (℃)	Complexity (bit)
Acarbose	139.02	541.40	369.80	60.87	675.05	962
Tolazamide	81.34	246.80	237.90	32.82	300	431
Miglitol	48.16	284.30	142.10	20.81	453.7	179
Prandin/ repaglinide	131.83	360.80	397.90	51.49	672.9	619
Metformin	56.64	58.10	100.80	13.43	224	132
Glimepiride	129.80	363.20	378.80	53.49		895
Linagliptin	133.43	353.70	338.00	51.24	661.2	885
Pioglitazone	97.39	301.80	282.80	37.91		466
Bromocriptine	165.51	492.80	429.40	66.44	891.3	1230
Alogliptin	104.26	267.80	252.90	35.44	519.2	622

Figure 2: Physicochemical properties and TIs.

(1) Regression models for atom bond connectivity index ABC(G):

$$\text{Boiling point} = 103.153 + 10.44\ [\text{ABC(G)}].$$
$$\text{Refractivity} = 18.569 + 2.093\ [\text{ABC(G)}].$$
$$\text{Flash point} = 20.160 + 7.125\ [\text{ABC(G)}].$$
$$\text{Polarity} = 0.172 + 0.980\ [\text{ABC(G)}].$$
$$\text{Molar volume} = 31.785 + 6.065\ [\text{ABC(G)}].$$
$$\text{Complexity} = -182.330 + 19.139\ [\text{ABC(G)}].$$

Table 13: Standard error of estimate.

Topological index	Std. error of the estimate for boiling point	Std. error of the estimate for r efractive index	Std. error of the estimate for flash point	Std. error of the estimate for polarity	Std. error of the estimate for molar volume	Std. error of the estimate for complexity
ABC(G)	98.43048	11.17466	52.64505	2.09188	32.63778	121.449
RA(G)	104.73051	13.00251	48.80174	3.10250	37.57911	137.117
S(G)	101.45526	12.16978	49.28409	2.68903	36.20431	129.734
GA(G)	98.83581	11.77664	49.08803	2.48884	35.84931	124.284
M1(G)	97.18220	13.28092	48.37844	2.58942	36.84197	120.084
M2(G)	97.53269	13.75484	44.16003	3.36468	41.42791	124.317
HM(G)	105.58577	13.29629	47.58271	3.33388	39.26701	139.553
F(G)	99.99823	14.06750	45.75529	3.43754	41.37206	126.610
H(G)	98.88522	13.91734	44.97484	3.39556	41.37987	125.522

(2) Regression models for atom bond connectivity index RA(G):

Boiling point = 100.512 + 18.552 [RA(G)].
Refractivity = 18.020 + 3.731 [RA(G)].
Flash point = 10.148 + 13.033 [RA(G)].
Polarity = −0.380 + 1.759 [RA(G)].
Molar volume = 29.935 + 10.820 [RA(G)].
Complexity = −186.139 + 34.060 [RA(G)].

(3) Regression models for atom bond connectivity index S(G):

Boiling point = 105.293 + 18.056 [S(G)].
Refractive index = 18.429 + 3.638 [S(G)].
Flash point = 15.429 + 12.603 [S(G)].
Polarity = 0.122 + 1.710 [S(G)].
Molar volume = 32.905 + 10.520 [S(G)].
Complexity = −180.010 + 33.247 [S(G)].

(4) Regression models for atom bond connectivity index GA(G):

Boiling point = 113.440 + 8.420 [GA(G)].
Refractivity = 20.596 + 1.694 [GA(G)].
Flash point = 22.547 + 5.853 [GA(G)].
Polarity = 1.044 + 0.795 [GA(G)].
Molar volume = 38.721 + 4.888 [GA(G)].
Complexity = −465.288 + 15.519 [GA(G)].

(5) Regression models for atom bond connectivity index M1(G):

Boiling point = 126.868 + 1.316 [M1(G)].
Refractivity = 24.500 + 0.261 [M1(G)].
Flash point = 34.273 + .908 [M1(G)].
Polarity = 2.745 + 0.123 [M1(G)].
Molar volume = 49.701 + 0.755 [M1(G)].
Complexity = −135.869 + 2.413 [M1(G)].

(6) Regression models for atom bond connectivity index HM(G):

Boiling point = 104.181 + 20.696 [HM(G)].
Refractivity = 18.567 + 4.176 [HM(G)].
Flash point = 10.181 + 14.677 [HM(G)].
Polarity = −0.136 + 1.970 [HM(G)].
Molar volume = 32.218 + 12.080 [HM(G)].
Complexity = −181.037 + 38.124 [HM(G)].

(7) Regression models for atom bond connectivity index M2(G):

Boiling point = 151.218 + .952 [M2(G)].
Refractivity = 30.535 + 0.187 [M2(G)].
Flash point = 48.647 + 0.665 [M2(G)].
Polarity = 5.362 + 0.088 [M2(G)].
Molar volume = 67.501 + 0.539 [M2(G)].
Complexity = −86.964 + 1.741 [M2(G)].

(8) Regression models for atom bond connectivity index F(G):

Boiling point = 144.280 + 0.380 [F(G)].
Refractivity = 29.397 + 0.074 [F(G)].
Flash point = 44.851 + 0.264 [F(G)].
Polarity = 4.737 + 0.035 [F(G)].
Molar volume = 63.476 + 0.215 [F(G)].
Complexity = −97.844 + 0.692 [F(G)].

(9) Regression models for atom bond connectivity index H(G):

Boiling point = 147.316 + 0.211 [H(G)].
Refractivity = 29.878 + 0.041 [H(G)].
Flash point = 46.427 + 0.147 [H(G)].
Polarity = 5.004 + 0.020 [H(G)].
Molar volume = 65.21.0 + 0.120 [H(G)].
Complexity = −93.085 + 0.386 [H(G)].

Tables 3–11 represent the statistical parameters used in the QSPR models of TIs. □

3.2. Quantitative Structure Analysis and Comparison between Topological Indices and Correlation

3.2.1. Coefficient of Physicochemical Properties. Physical properties for ten diabetes drugs are listed in Table 12, and their TIs computed through the molecular structure are recorded in Table 1. The correlation coefficient between six physical properties and TIs is itemized in Table 2. The graph of TIs and physical properties is shown in Figure 2.

3.3. Calculation of Statistical Parameters. In this section, we find the relation between degree base TIs and physical

Table 14: Comparison of actual and computed values for polarity from regression models.

Name of drug	Polarity of drug	Polarity computed from regression model for ABC(G) index	Polarity computed from regression model for R(G) index	Polarity computed from regression model for S(G) index	Polarity computed from regression model for GA(G) index	Polarity computed from regression model for M1(G) index	Polarity computed from regression model for M2(G) index	Polarity computed from regression model for F(G) index	Polarity computed from regression model for H(G) index	Polarity computed from regression model for HM(G) index
Acarbose	60.87 cm^3	64.3032	66.7786	66.0767	65.5662	64.983	65.378	65.287	66.884	67.4153
Tolazamide	32.82 cm^3	32.2474	31.6865	31.6373	31.7389	32.511	32.642	32.947	33.524	31.3446
Miglitol	20.81 cm^3	22.7806	23.6655	23.2925	23.2960	24.147	25.602	25.597	26.124	23.8192
Prandin	51.49 cm^3	52.7098	52.7945	52.4822	52.1148	51.453	50.154	50.237	51.364	52.5221
Metformin	13.43 cm^3	14.627	15.0112	14.7767	14.559	14.553	14.514	14.887	14.964	15.0724
Glimepiride	53.49 cm^3	52.3766	51.4401	51.1826	50.9461	51.699	50.682	51.707	52.404	50.5915
Linagliptin	51.24 cm^3	49.3974	48.7312	49.3871	49.4754	48.501	46.898	46.597	47.804	49.0943
Pioglitazone	37.91 cm^3	34.6876	34.8351	35.2112	35.2449	34.233	33.698	33.017	34.044	35.2452
Bromocriptine	66.44 cm^3	65.4106	63.5244	64.3667	65.1846	66.459	66.874	66.407	68.204	63.1404
Alogliptin	35.44 cm^3	35.3344	35.4684	35.6387	35.9127	35.463	35.634	34.767	35.924	35.7377

Table 15: Comparison of actual and computed values for molar volume from regression models.

Name of drug	Molar volume of drug	Molar volume from regression model for ABC(G) index	Molar volume from regression model for R(G) index	Molar volume from regression model for S(G) index	Molar volume from regression model for GA(G) index	Molar volume from regression model for M1(G) index	Molar volume from regression model for M2(G)index	Molar volume from regression model for F(G) index	Molar volume from regression model for H(G) index	Molar volume from regression model for HM(G) index
Acarbose	369.8 ±5.0 cm^3	428.678	443.042	438.661	435.431	431.731	435.099	435.426	436.49	446.441
Tolazamide	237.9 ±7.0 cm^3	230.292	227.183	226.788	227.446	232.411	234.591	236.766	236.33	225.256
Miglitol	142.1 ±3.0 cm^3	171.704	177.844	175.451	175.536	181.071	191.471	191.616	191.93	179.110
Prandin	397.9 ±3.0 cm^3	356.929	357.023	355.027	352.726	348.681	341.852	342.976	343.37	355.116
Metformin	100.8 ±7.0 cm^3	121.243	124.61	123.061	121.817	122.181	123.557	125.826	124.97	125.475
Glimepiride	378.8 ±5.0 cm^3	354.867	348.692	347.032	345.540	350.191	345.086	352.006	349.61	343.278
Linagliptin	338 ±7.0 cm^3	336.43	332.029	335.986	336.498	330.561	321.909	320.616	322.01	334.097
Pioglitazone	282.8 ±3.0 cm^3	245.394	246.551	248.775	249.002	242.981	241.059	237.196	239.45	249.174
Bromocriptine	429.4 ±5.0 cm^3	435.532	423.025	428.141	433.084	440.791	444.262	442.306	444.41	420.227
Alogliptin	252.9 ±5.0 cm^3	249.397	250.446	251.405	253.108	250.531	252.917	247.946	250.73	252.194

Table 16: Comparison of actual and computed values for flash point from regression models.

Name of drug	Flash point of drug	Flash point computed from regression model for ABC(G) index	Flash point computed from regression model for R(G) index	Flash point computed from regression model for S(G) index	Flash point computed from regression model for GA(G) index	Flash point computed from regression model for M1(G) index	Flash point computed from regression model for M2(G) index	Flash point computed from regression model for F(G) index	Flash point computed from regression model for H(G) index	Flash point computed from regression model for HM(G) index
Acarbose	541.4 ±34.3°C	486.42	507.747	501.526	497.576	493.721	502.177	501.571	501.245	513.455
Tolazamide	246.8 ±26.8°C	253.361	247.739	247.702	248.531	254.009	254.797	257.635	256.049	244.719
Miglitol	284.3 ±27.4°C	184.533	188.309	186.199	186.372	192.265	201.597	202.195	201.659	188.653
Prandin	360.8 ±0.0°C	402.131	404.135	401.332	398.543	393.841	387.132	388.051	387.173	402.497
Metformin	58.1 ±22.6°C	125.253	124.186	123.436	122.048	121.441	117.807	121.411	119.633	123.487
Glimepiride	363.2 ±34.3°C	399.708	394.100	391.754	389.939	395.657	391.122	399.139	394.817	388.113
Linagliptin	353.7 ±34.3°C	378.048	374.029	378.521	379.111	372.049	362.527	360.595	361.007	376.959
Pioglitazone	301.8 ±28.7°C	271.102	271.068	274.042	274.343	266.721	262.777	258.163	259.871	273.779
Bromocriptine	492.8 ±34.3°C	494.471	483.636	488.923	494.767	504.617	513.482	510.019	510.947	481.606
Alogliptin	267.8 ±32.9°C	275.805	275.760	277.193	279.259	275.801	277.407	271.363	273.689	277.449

Table 17: Comparison of actual and computed values for refractive index from regression models.

Name of drug	Refractivity of drug	Refractivity computed from regression model for ABC(G) index	Refractivity computed from regression model for R(G) index	Refractivity computed from regression model for S(G) index	Refractivity computed from regression model for GA(G) index	Refractivity computed from regression model for M1(G) index	Refractivity computed from regression model for M2(G) index	Refractivity computed from regression model for F(G) index	Refractivity computed from regression model for H(G) index	Refractivity computed from regression model for HM(G) index
Acarbose	139.02 $m^3 \cdot mol^{-1}$	155.534	160.469	159.089	158.081	156.566	158.069	157.417	156.732	161.762
Tolazamide	81.34 $m^3 \cdot mol^{-1}$	87.0728	86.0361	85.8203	86.0013	87.662	88.505	89.041	88.344	85.2994
Miglitol	48.16 $m^3 \cdot mol^{-1}$	66.8545	69.0227	68.0669	68.0110	69.914	73.545	73.501	73.174	69.3471
Prandin	131.83 $m^3 \cdot mol^{-1}$	130.774	130.808	130.167	129.418	127.856	125.718	125.597	124.916	130.191
Metformin	56.64 $m^3 \cdot mol^{-1}$	49.4407	50.6662	49.9496	49.394	49.556	49.983	50.857	50.296	50.8057
Glimepiride	129.8 $m^3 \cdot mol^{-1}$	130.063	127.935	127.402	126.928	128.378	126.84	128.705	127.048	126.099
Linagliptin	133.43 $m^3 \cdot mol^{-1}$	123.700	122.189	123.582	123.794	121.592	118.799	117.901	117.618	122.925
Pioglitazone	97.39 $m^3 \cdot mol^{-1}$	92.2844	92.7146	93.4237	93.4718	91.316	90.749	89.189	89.41	93.5679
Bromocriptine	165.51 $m^3 \cdot mol^{-1}$	157.9	153.567	155.451	157.267	159.698	161.248	159.785	159.438	152.700
Alogliptin	104.26 $m^3 \cdot mol^{-1}$	93.6658	94.0577	94.3332	94.8948	93.926	94.863	92.889	93.264	94.6119

Table 18: Comparison of actual and computed values for complexity from regression models.

Name of drug	Complexity	Complexity computed from regression model for ABC(G) index	Complexity computed from regression model for R(G) index	Complexity computed from regression model for S(G) index	Complexity computed from regression model for GA(G) index	Complexity computed from regression model for M1(G) index	Complexity computed from regression model for M2(G) index	Complexity computed from regression model for F(G) index	Complexity computed from regression model for H(G) index	Complexity computed from regression model for HM(G) index
Acarbose	962	1070.12	1114.27	1102.32	794.234	1085.10	1100.66	1099.31	1101.19	1126.23
Tolazamide	431	444.089	434.774	432.732	133.900	448.077	453.016	459.908	457.351	428.184
Miglitol	179	259.206	279.461	270.486	-30.9112	283.993	313.736	314.588	314.531	282.550
Prandin	619	843.711	843.494	838.013	531.652	819.679	799.475	801.756	801.663	838.017
Metformin	132	99.9702	111.886	104.916	-201.465	95.779	94.37	102.836	99.143	113.280
Glimepiride	895	837.204	817.268	812.745	508.839	824.505	809.921	830.82	821.735	800.656
Linagliptin	885	779.022	764.816	777.836	480.129	761.767	735.058	729.788	732.955	771.681
Pioglitazone	466	491.745	495.742	502.218	202.339	481.859	473.908	461.292	467.387	503.67
Bromocriptine	1230	1091.75	1051.26	1069.08	786.784	1114.06	1130.26	1121.46	1126.67	1043.50
Alogliptin	622	504.377	508.003	510.530	215.375	505.989	512.21	495.892	503.671	513.201

Table 19: Comparison of actual and computed values for boiling point from regression models.

Name of drug	Boiling point of drug	Boiling point computed from regression model for ABC(G) index	Boiling point computed from regression model for R(G) index	Boiling point computed from regression model for S(G) index	Boiling point computed from regression model for GA(G) index	Boiling point computed from regression model for M1(G) index	Boiling point computed from regression model for M2(G) index	Boiling point computed from regression model for F(G) index	Boiling point computed from regression model for H(G) index	Boiling point computed from regression model for HM(G) index
Acarbose	675.05 °C at 760 mmHg	786.34	808.827	801.712	796.80	792.764	800.482	801.68	800.15	813.8468
Tolazamide	300 °C at 760 mmHg	444.85	438.715	438.065	438.53	445.34	446.338	450.56	448.20	434.9031
Miglitol	453.7 °C at 760 mmHg	344.00	354.117	349.951	349.11	355.852	370.178	370.76	370.13	355.8444
Prandin	672.9 °C at 760 mmHg	662.84	661.339	658.167	654.34	648.004	635.786	638.28	636.41	657.3851
Metformin	224 °C at 760 mmHg	257.14	262.842	260.032	256.58	253.204	250.226	254.48	252.39	263.9541
Glimepiride		659.29	647.053	644.445	641.96	650.636	641.498	654.24	647.38	637.103
Linagliptin	661.2 °C at 760 mmHg	627.55	618.483	625.486	626.38	616.42	600.562	598.76	598.85	621.374
Pioglitazone		470.84	471.923	475.802	475.66	463.764	457.762	451.32	453.68	475.8812
Bromocriptine	891.3 °C at 760 mmHg	798.14	774.506	783.656	792.76	808.556	816.666	813.84	814.07	768.9365
Alogliptin	519.2 °C at 760 mmHg	477.74	478.601	480.316	482.74	476.924	478.706	470.32	473.52	481.0552

properties of diabetes drugs such as medicines acarbose, tolazamide, miglitol, prandin, metformin, glimepiride, linagliptin, pioglitazone, bromocriptine, and alogliptin, and this is done with the help of QSPR modeling, whereas TIs, N, b, and r represent regression model constant, correlation coefficient, and sample size, respectively. This will be helpful to compare and improve the model. It is noted that the value of r is greater than 0.6, and p value is less than 0.05. Hence, the calculation verifies that all properties are significant.

3.4. Standard Error (SE) of Estimate and Comparison. Measure of variation for an observation calculated around the computed regression line is said to be the standard error estimate. It measures the amount of accuracy of predictions done around the computed regression line in Table 13. We also compare the physicochemical properties of the experimental and theoretical calculated values of the models as presented in Tables 14–19.

4. Conclusions

It is obvious from statistical parameters used in linear QSPR models and topological indices that ABC(G) index provides a maximum high correlated value for polarity $r = 0.993$, refractive index $r = 0.961$, and molar volume $r = 0.960$. M1 index provides a high correlated value of boiling point; that is, $r = 0.912$ and complexity $r = 0.947$. M2 index depicts the utmost correlation coefficient of flash point $r = 0.950$ and boiling point $r = 0.912$.

In this paper, we have computed topological indices and related them to the linear QSPR model for the drugs used to cure diabetes. The results gained in the following means will be supportive for designing various new drugs to attain defensive measures for the said disease in the pharmaceutical industry. The correlation coefficient plays a substantial impact on the range of topological indices of the drugs and may be considered for the combination to designing novel drugs. The outcomes are helpful to research workers on drugs science in the pharmaceutical industry and offer a pathway to approximate physical properties for novice discoveries of diabetes medicines to cure other specific diseases [25].

Data Availability

The data used to support the findings of this study are included within the paper.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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