Hindawi
Journal of Chemistry
Volume 2022, Article ID 9749575, 13 pages
https://doi.org/10.1155/2022/9749575

Research Article

Topological Indices of Novel Drugs Used in Cardiovascular Disease Treatment and Its QSPR Modeling

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Received 15 June 2022; Accepted 12 October 2022; Published 4 November 2022

Academic Editor: Patricia E. Allegretti

A topological index is a score function that changes each molecular structure to a unique real number. It aids in determining the physicochemical and biological properties of a wide range of drugs, and it more accurately reflects the theoretical properties of drugs. The task is accomplished through the use of degree-based topological indices (TIs). Heart disease refers to a group of disorders that affect our hearts. Heart diseases include blood vessel disorders such as irregular heartbeat and heart muscle disease. In this article, Eliquis, metoprolol, valsartan, etc., and other drugs employed to treat cardiovascular disease are studied and the QSPR analysis goal will probe the mathematical relationship of properties such as (polarity, boiling point, enthalpy, etc.) and assorted descriptors associated to drug's structure. The present study on TIs imposed on drugs was found to have a good correlation with physical properties.

1. Introduction

The cardiovascular system is made up of the heart and its associated blood vessels. It is a group of illnesses that affect the heart. A buildup of fatty plaques in your arteries can harm your blood vessels and heart. Plaque blocks blood vessels, resulting in a heart attack and chest pain (angina). Cardiovascular disease, also known as heart disease, encompasses four distinct conditions: peripheral artery disease (PAD), coronary heart disease (CHD), coronary artery disease (CAD), and aortic atherosclerosis [1]. CAD is a result of decreased myocardial perfusion that causes angina and results in a heart attack or heart failure. It causes one-third to one-half of cardiovascular disease cases. Cerebrovascular disease is used to designate strokes and transient ischemic attacks (TIAs). Men and women experience shortness of breath, nausea, and extreme fatigue. Your heart beats slowly, too quickly, and irregularly. Heart infection signs are fever, fatigue, changes in your heart rhythm, skin rashes, and so on. Heart attacks, strokes, and other preventable cardiovascular diseases kill or have a significant impact on the population [2]. On a global scale, the disease kills a large number of people. Scientists create and study new drugs and their discovery is an uphill task since it is costly, time-consuming, and becomes incredibly hard in this field. Many drug trials are imposed to treat and halt this deadly disease, and many drug testing is performed to combat lethal disease [3]. It necessitates prompt finding and medication that will devise the disease. Nine drugs Eliquis, vericiguat, Pradaxa, ivabradine, dapagliflozin, empagliflozin, metoprolol, sacubitril, and valsartan are harmless and utmost effective medicines that are obligatory for well-being community. Figure 1 displays the aforementioned drugs.

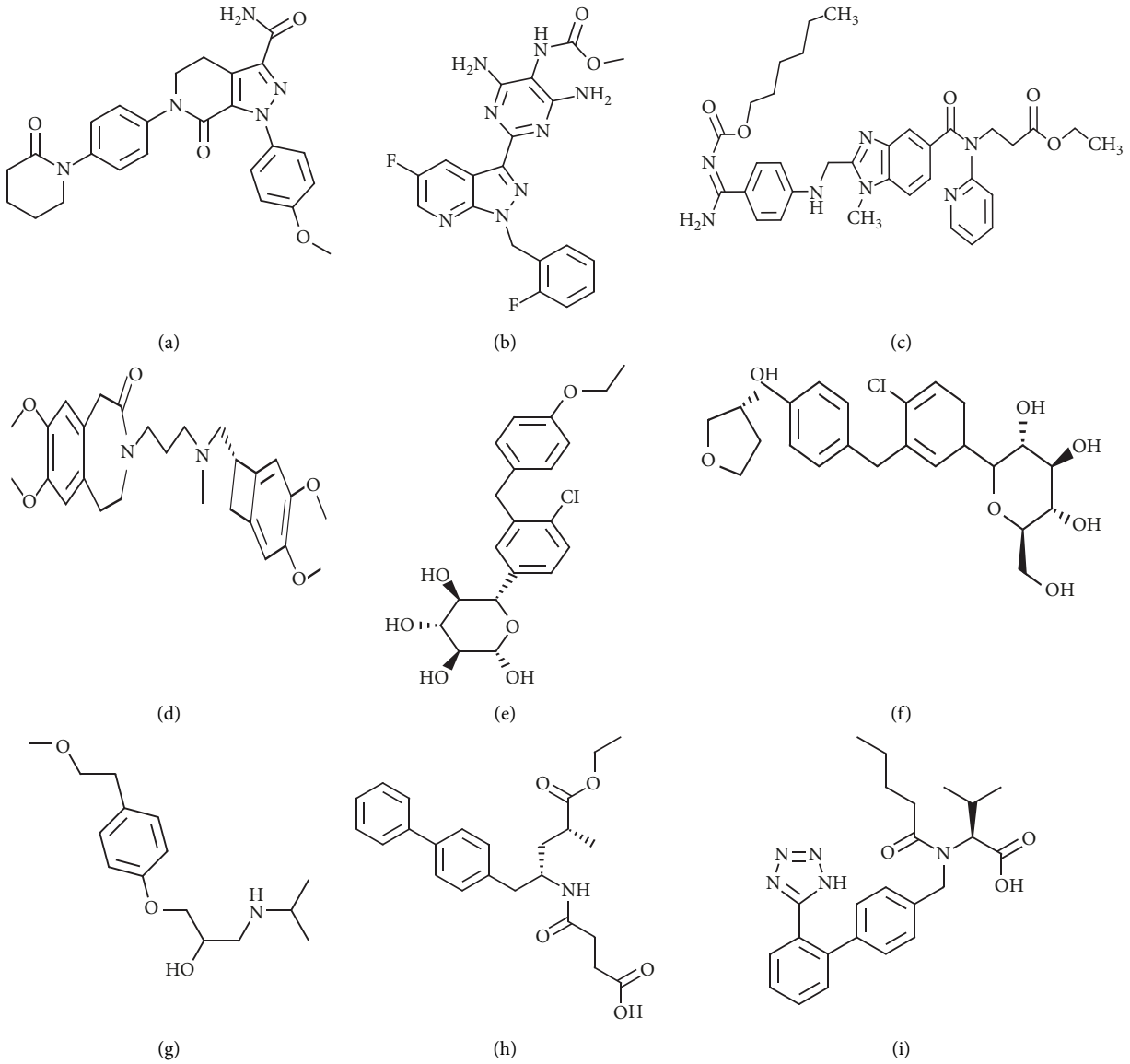


Figure 1: Molecular structure: (a) Eliquis; (b) vericiguat; (c) Pradaxa. (d) ivabradine; (e) dapagliflozin; (f) empagliflozin; (g) metoprolol; (h) sacubitril; (i) valsartan.

TIs are unique numeric descriptors obtained from the graph and completely describe a chemical structure. These are employed efficiently to describe the physical properties of numerous drugs. Several types of TIs and polynomials are employed for this purpose and exactly depict the hidden information in graph theory [4–7]. All TIs are important and show a noteworthy role in chemical graphs. In the past few years, there has been a big interest in the use of graph invariants (TIs) in quantitative structure-property relationships (QSPR) and quantitative structure-activity relationships (QSAR) studies. For a detailed review of QSPR studies, readers are offered to read [8–13]. Topological indices are widely used in the fields of cheminformatics, bioinformatics, and mathematics but they have the most substantial use in QSPR [14]. The ABC, Wiener, and Randic index can all be used to predict drug bioactivity. QSPR models support to decide the best relationship between TIs and drug properties. In the present paper, we calculated degree-based TIs for cardiovascular drugs. Correspondingly, cardiovascular disease drugs are thoroughly investigated with topological indices and imposed QSPR. It has been calculated with a linear regression model (RM) those TIs and drug properties have a good relation.

2. Material and Methods

Atoms denote vertices in drug structure, and the corresponding bonds are referred to as edges. Graph $G(V, E)$ is thought to be simple and connected. The V and E are referred to as vertex and edge set, respectively. The degree of a vertex is denoted by d_u and is the number of vertices adjacent to it. We used the following TIs:

Definition 1. ABC index [15] G is given under

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

Definition 2. Randic index [16] is given under

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

Definition 3. sum connectivity index [17] is given under

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

Definition 4. GA index [18] is given under:

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

Definition 5. Zagreb indices [19] are given under

$$\begin{aligned} M_1(G) &= \sum_{uv \in E(G)} (d_u + d_v) \\ M_2(G) &= \sum_{uv \in E(G)} (d_u + d_v) \end{aligned} \quad (5)$$

Definition 6. harmonic index [20] of G is given under:

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

Definition 7. hyper-Zagreb index [21] is given under

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

Definition 8. forgotten index [22] is given under

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

The π-electron energy of a molecule was calculated in [23]. ChemSpider is used to calculate the values of physical properties. As an outcome, the RM is preeminent to check and use for the aforementioned examination.

Sacubitril propionate has molecular formula $C_{24}H_{29}$ N O_5. This is a neprilysin inhibitor used in conjunction with valsartan as an adjunct to decrease the risk of cardiovascular death. In Europe and Canada, medication is only sanctioned for adults with symptomatic chronic heart failure irrespective of ejection fraction. Dabigatran etexilate propionate has the molecular formula $C_{34}H_{41}$ N_7O_5. It is an anticoagulant that is used to prevent venous thromboembolic events or strokes in patients who have recently had hip or knee replacement surgery. The molecular formula for ivabradine is $C_{27}H_{36}$ N_2O_5. This medication is used to reduce the risk of hospitalization for exacerbating heart failure in adult patients and to treat stable symptomatic heart failure in pediatric patients due to dilated cardiomyopathy. The molecular formula of dapagliflozin propionate is $C_{21}H_{25}$ Cl O_6. The medication is a sodium-glucose cotransporter inhibitor that is used to treat the disease. $C_{15}H_{25}$ N O_3 is the molecular formula for metoprolol propionate. Valsartan was first approved in Europe in 1996 for the treatment of adult hypertension. This is commonly used to treat hypertension, heart failure, and diabetes.

Previous research on Covid-19, anticancer, blood cancer, and QSPR studies of various topological indices for various chemical structures motivated us to work on the current research problem. The purpose of this study is to look into the use of TIs in determining the physical properties and its QSPR modeling of cardiovascular disease drug regimens used in therapeutic management.

3. Regression Model and Quantitative Structure Analysis

In this section, TIs are discussed as cardiovascular disease treatment drugs. Calculation between QSPR and TIs clearly depicts that these are vastly correlated for the aforementioned drugs of disease [24,25]. Nine medicines Eliquis, vericiguat, Pradaxa, ivabradine, dapagliflozin, empagliflozin, metoprolol, sacubitril, and valsartan are used in a mathematical analysis for cardiovascular disease. The drug structure is shown in Figure 1. The chemical structure of a drug is characterized by a graph and its elements denote vertices and bonds that represent edges. Regression analysis was used to find the best cardiovascular treatment options. In this article, nine TIs for QSPR modeling tenacity are performed and the following properties, molar refractivity (R), polarity (P), complexity (C), molar volume (MV) enthalpy (E) and boiling point (BP), and flash point (FP) for nine remedies used for cardiovascular treatment are listed in Table 1. The regression model (RM) imposed on drugs is tested by applying the following equation:

$$P = A + b(TI) \quad (9)$$

P denotes the property of the given drug. The TI is an independent variable, A stands for constant, and b stands for regression coefficient. Statistix, SageMath, and MATLAB are useful for determining the results. A linear QSPR model is used to analyze nine TIs for cardiovascular drugs and their properties. Equation (9) is pertinent for the aforementioned calculation.

Theorem 1. *Let G_1 be the graph of Eliquis, TIs of G_1 are given as follows:*

(i) $ABC(G_1) = 46.80$

(ii) $RA(G_1) = 26.41$

(iii) $S(G_1) = 27.27$

(iv) $GA(G_1) = 58.10$

Table 1: physical properties of drugs.

Drug	Boiling point (℃)	Enthalpy (℃)	Flash Point (℃)	Molar Refractivity (cm^3)	Polarity (cm^3)	Molar Volume (cm^3)	Complexity	Density (g/cm^3)	Polar surface area (A^2)
Eliquis	770.5	112.2	419.8	125.6	49.8	323.4	777	1.4	111
Vericiguat	535.9	81.2	277.9		41.5	260.8	622	1.6	147
Pradaxa	827.9	120.3	454.5	175.9	69.7	504	991	1.2	154
Ivabradine	626.9	92.8	332.9	132.2	52.4	408.7	663	1.1	60
Dapagliflozin	609	95.1	322.1	105.6	41.9	303.1	472	1.3	99
Empagliflozin	664	102.7	355.7	114.4	45.4	322.4	558	1.4	109
Metoprolol	398.6	68.5	194.9	77.1	30.6	258.7	215	1.0	51
Sacubitril	656.9	101.6	351.1	113.6	45	357.4	550	1.2	93
Valsartan		105.5	368	120.6	47.8	359.1	608	1.2	112

(v) $M1(G_1) = 346$

(vi) $M2(G_1) = 444$

(vii) $F(G_1) = 1086$

(viii) $H(G_1) = 23.84$

(ix) $HM(G_1) = 1974$

Proof. Let G_1 be the graph of Eliquis with edge set E and $E_{m,n}$ are edges in G_1 with, $|E_{1,3}| = 13$, $|E_{1,4}| = 15$, $|E_{2,4}| = 1$, $|E_{3,3}| = 23$, $|E_{3,4}| = 4$, $|E_{4,4}| = 4$, $|E_{2,3}| = 3$. By applying Definitions 1–8 we obtain the following results:

(i) $\mathrm{ABC}(G_1) = 13\sqrt{(1+3-2)/(1\times 3)} + 15\sqrt{(1+4-2)/(1\times 4)} + 3\sqrt{(2+3-2)/(2\times 3)} + 1\sqrt{(2+4-2)/(2\times 4)} + 23\sqrt{(3+3-2)/(3\times 3)} + 4\sqrt{(3+4-2)/(3\times 4)} + 4\sqrt{(4+4-2)/(4\times 4)} = 46.80$

(ii) $RA(GG_1) = 13\sqrt{1/(1\times 3)} + 15\sqrt{1/(1\times 4)} + 3\sqrt{1/(2\times 3)} + 1\sqrt{1/(2\times 4)} + 23\sqrt{1/(3\times 3)} + 4\sqrt{1/(3\times 4)} + 4\sqrt{1/(4\times 4)} = 46.41$

(iii) $S(G_1) = 13\sqrt{1/(1+3)} + 15\sqrt{1/(1+4)} + 3\sqrt{1/(2+3)} + 1\sqrt{1/(2+4)} + 23\sqrt{1/(3+3)} + 4\sqrt{1/(3+4)} + 4\sqrt{1/(4+4)} = 27.27$

(iv) $GA(G_1) = 26\sqrt{1\times 3}/(1+3) + 30\sqrt{1\times 4}/(1+4) + 6\sqrt{2\times 3}/(2+3) + 2\sqrt{2\times 4}/(2+4) + 46\sqrt{3\times 3}/(3+3) + 8\sqrt{3\times 4}/(3+4) + 8\sqrt{4\times 4}/(4+4) = 58.10$

(v) $M1(G_1) = 13(1+3) + 15(1+4) + 3(2+3) + 1(2+4) + 23(3+3) + 4(3+4) + 4(4+4) = 346$

(vi) $M2 = (G_1)13(1\times 3) + 15(1\times 4) + 3(2\times 3) + 1(2\times 4) + 23(3\times 3) + 4(3\times 4) + 4(4\times 4) = 444$

(vii) $H(G_1) = 13(1/(1+3)) + 15(1/(1+4)) + 3(1/(2+3)) + 1(1/(2+4)) + 23(1/(3+3)) + 4(1/(3+4)) + 4(1/(4+4)) = 23.84$

(viii) $HM(G_1) = 13(1+3)^2 + 15(1+4)^2 + 4(2+3)^2 + 5(2+4)^2 + 3(3+3)^2 + 1(3+4)^2 + 4(4+4)^2 = 1974$

(ix) $F(G_1) = 13(1+9) + 15(1+16) + 3(4+9) + 1(4+16) + 23(9+9) + 4(9+16) + 4(16+16) = 1086$ □

Theorem 2. *Let G_2 be the graph of dapagliflozin, TIs in G_2 are given as follows:*

(i) $ABC(G_2) = 40.75$

(ii) $\mathrm{RA}(\mathrm{G}_2) = 23.70$

(iii) $\mathrm{S}(\mathrm{G}_2) = 24.03$

(iv) $\mathrm{GA}(\mathrm{G}_2) = 50.45$

(v) $\mathrm{M1}(\mathrm{G}_2) = 302$

(vi) $\mathrm{M2}(\mathrm{G}_2) = 390$

(vii) $\mathrm{F}(\mathrm{G}_2) = 974$

(viii) $\mathrm{H}(\mathrm{G}_2) = 21.36$

(ix) $HM(G_2) = 1754$

Proof. Let G_2 be the graph of dapagliflozin with edge set E, let $E_{m,n}$ are edges of G_2 with $|E_{1,2}| = 4$, $|E_{2,3}| = 1$, $|E_{2,4}| = 7$, $|E_{3,3}| = 12$, $|E_{3,4}| = 3$, $|E_{1,3}| = 8$, $|E_{1,4}| = 14$. By applying Definitions 1–8 we obtain the following results:

(i) $\mathrm{ABC}(\mathrm{G}_2) = = 4\sqrt{(1+2-2)/(1\times 2)} + 8\sqrt{(1+3-2)/(1\times 3)} + 14\sqrt{(1+4-2)/(1\times 4)} + 1\sqrt{(2+3-2)/(2\times 3)} 7\sqrt{(2+4-2)/(2\times 4)} + 12\sqrt{(3+3-2)/(3\times 3)} + 3\sqrt{(3+4-2)/(3\times 4)} = 22.04.$

(ii) $\mathrm{RA}(\mathrm{G}_2) = 4\sqrt{1/(1\times 2)} + 8\sqrt{1/(1\times 3)} + 14\sqrt{1/(1\times 4)} + 1\sqrt{1/(2\times 3)} + 7\sqrt{1/(2\times 4)} + 12\sqrt{1/(3\times 3)} + 3\sqrt{1/(3\times 4)} = 13.12.$

(iii) $\mathrm{S}(\mathrm{G}_2) = 4\sqrt{1/(1+2)} + 8\sqrt{1/(1+3)} + 14\sqrt{1/(1+4)} + 1\sqrt{1/(2+3)} 7\sqrt{1/(2+4)} + 12\sqrt{1/(3+3)} + 3\sqrt{1/(3+4)} = 13.46.$

(iv) $\mathrm{GA}(\mathrm{G}_2) = 8\sqrt{1\times 2}/(1+2) + 16\sqrt{1\times 3}/(1+3) + 28\sqrt{1\times 4}/(1+4) + 2\sqrt{2\times 3}/(2+3) + 14\sqrt{2\times 4}/(2+4) + 24\sqrt{3\times 3}/(3+3) + 6\sqrt{3\times 4}/(3+4) = 27.72$

(v) $\mathrm{M1}(\mathrm{G}_2) = 4(1+2) + 8(1+3) + 14(1+4) + 1(2+3) + 7(2+4) + 12(3+3) + 3(3+4) = 162.$

(vi) $\mathrm{M2}(G_2) = 4(1\times 2) + 8(1\times 3) + 14(1\times 4) + 1(2\times 3) + 7(2\times 4) + 12(3\times 3) + 3(3\times 4) = 209.$

(vii) $H(G_2) = 4(1/(1+2)) + 8(1/(1+3)) + 14(1/(1+4)) + 1(1/(2+3)) + 7(1/(2+4)) + 12(1/(3+3)) + 3(1/(3+4)) = 11.95$

(viii) $HM(\mathrm{G}_2) = 4(1+2)^2 + 8(1+3)^2 + 14(1+4)^2 + 1(2+3)^2 + 7(2+4)^2 + 12(3+3)^2 + 3(3+4)^2 = 934$

(ix) $\mathrm{F}(\mathrm{G}_2) = 4(1+4) + 8(1+9) + 14(1+16) + 1(4+9) + 7(4+16) + 12(9+9) + 3(9+16) = 516.$

Topological indices for other drugs can be premeditated via the equivalent procedure as in Theorems 1 and 2 and Definitions 1–8. Table 2 includes estimates for drugs' TIs. Figures 2 and 3 depict a 2D and 3D graphical representation of calculated TIs for various medicines. Using (1), we calculated the following models of TIs and are given under: □

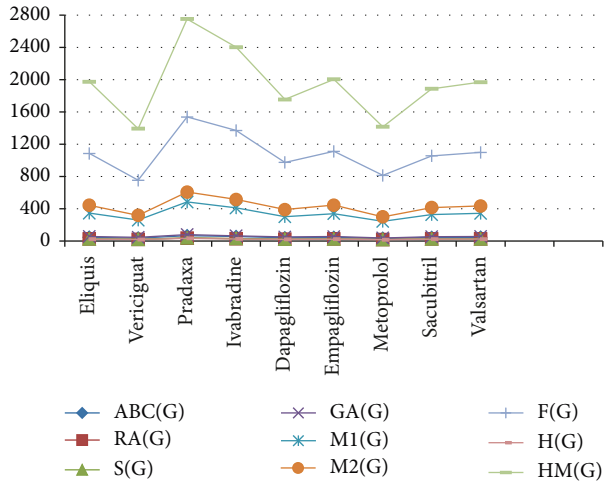


Figure 2: 2D graph of medicines with TIs.

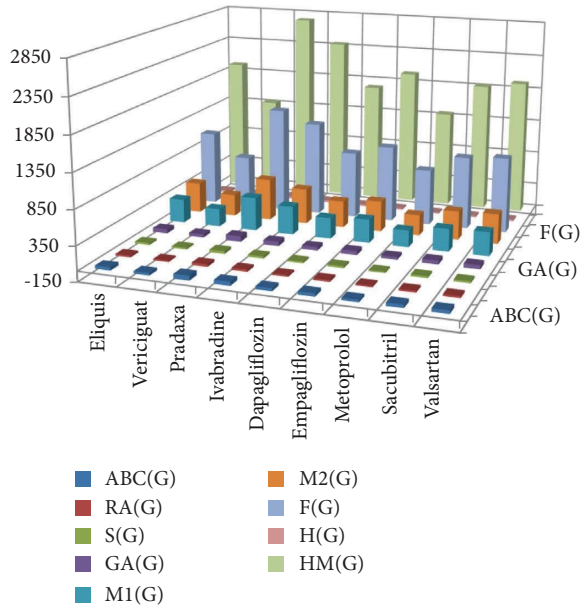


Figure 3: 3D graph of medicines with TI.

3.1. Regression Models for ABC (G)

(i) BP = 171.475 + 10.018 [ABC (G)]
(ii) EP = 41.507 + 1.210 [ABC (G)]
(iii) FP = 59.120 + 6.082 [ABC (G)]
(iv) $M = -10.427 + 2.747$ [ABC (G)]
(v) $P = -0.273 + 1.019$ [ABC (G)]
(vi) MV = −7.037 + 7.554 [ABC (G)]
(vii) $C = -221.857 + 17.811$ [ABC (G)]

3.2. RM for RA (G)]

(i) BP = 136.030 + 18.971 [RA (G)]
(ii) $E = 36.702 + 2.310$ [RA (G)]
(iii) FP = 37.149 + 11.525 [RA (G)]
(iv) $R = -3.007 + 1.896$ [RA (G)]
(v) $P = -21.820 + 13.843$ [RA (G)]
(vi) MV = 212.050 + 9.447 [RA (G)]
(vii) $C = -227.825 + 33.436$ [RA (G)]

3.3. RM for S (G)

(i) BP = 134.715 + 18.672 [S (G)]
(ii) $E = 36.901 + 2.261$ [S (G)]
(iii) FP = 36.666 + 11.337 [S (G)]
(iv) $R = -13.430 + 4.872$ [S (G)]
(v) $P = -2.758 + 1.853$ [S (G)]
(vi) MV = −15.044 + 13.343 [S (G)]

Table 2: TIs of drugs.

Drug	S (G)	ABC (G)	RA (G)	HM (G)	GA (G)	F (G)	M2 (G)	H (G)	M1 (G)
Eliquis	27.27	46.80	26.41	1974	58.10	1086	444	23.84	346
Vericiguat	22.18	36.79	21.52	1392	46.86	754	319	19.84	260
Pradaxa	38.68	66.98	37.98	2751	81.20	1537	607	33.95	485
Ivabradine	31.09	55.64	30.40	2402	65.52	1370	516	26.67	412
Dapagliflozin	24.03	40.75	23.70	1754	50.45	974	390	21.36	302
Empagliflozin	26.45	45.12	25.90	2004	55.93	1112	446	23.32	340
Metoprolol	19.01	33.78	19.03	1416	39.19	814	301	16.61	244
Sacubitril	26.16	45.26	25.99	1886	54.45	1056	415	23.10	328
Valsartan	27.43	47.31	27.03	1968	57.49	1098	435	24.17	344

(vii) $C = -286.200 + 33.148$ [S (G)]

3.4. RM for GA (G)

(i) BP = 132.919 + 8.914 [GA (G)]
(ii) $E = 36.896 + 1.076$ [GA (G)]
(iii) FP = 35.837 + 5.409 [GA (G)]
(iv) R = -11.830 + 2.289 [GA (G)]
(v) $P = -2.372 + 0.875$ [GA (G)]
(vi) MV = −8.142 + 6.227 [GA (G)]
(vii) $C = -289.368 + 15.830$ [GA (G)]

3.5. RM for M1 (G)

(i) BP = 170.708 + 1.371 [M1 (G)]
(ii) EP = 41.290 + 0.166 [M1 (G)]
(iii) FP = 59.202 + 0.831 [M1 (G)]
(iv) $R = -11.830 + 0.378$ [M1 (G)]
(v) $P = 0.702 + 0.136$ [M1 (G)]
(vi) MV = −0.381 + 1.013 [M1 (G)]
(vii) $C = -199.614 + 2.369$ [M1 (G)]

3.6. RM for HM (G)

(i) BP = 90.149 + 0.229 [HM (G)]
(ii) $E = 43.148 + 0.028$ [HM (G)]
(iii) FP = 71.169 + 0.039 [HM (G)]
(iv) $R = -14.022 + 0.067$ [HM (G)]
(v) $P = 3.155 + 0.023$ [HM (G)]
(vi) MV = 10.033 + 0.171 [HM (G)]
(vii) $C = -134.240 + 0.380$ [HM (G)]

3.7. RM for M2 (G)

(i) BP = 156.992 + 1.115 [M2 (G)]
(ii) $E = 39.081 + 0.361$ [M2 (G)]
(iii) FP = 50.928 + 0.676 [M2 (G)]
(iv) $R = -14.688 + 0.305$ [M2 (G)]
(v) $P = 1.255 + 0.107$ [M2 (G)]
(vi) MV = 6.006 + 0.786 [M2 (G)]
(vii) $C = -190.310 + 1.851$ [M2 (G)]

3.8. RM for F (G)

(i) BP = 219.223 + 0.383 [F (G)]
(ii) EP = 46.714 + 0.047 [F (G)]
(iii) FP = 88.903 + 0.232 [F (G)]
(iv) $R = -12.042 + 0.117$ [F (G)]
(v) $P = 5.016 + 0.039$ [F (G)]
(vi) MV = 16.534 + 0.301 [F (G)]
(vii) $C = -85.217 + 0.635$ [F (G)]

3.9. RM for H (G)

(i) BP = 117.355 + 21.998 [H (G)]
(ii) $E = 34.520 + 2.674$ [H (G)]
(iii) FP = 243.838 + 13.363 [H (G)]
(iv) R = -15.356 + 5.636 [H (G)]
(v) P = -4.046 + 2.163 [H (G)]
(vi) MV = -20.739 + 15.429 [H (G)]
(vii) C = -315.098 + 38.955 [H (G)]

Tables 3–11 are statistical parameters in QSPR models of TIs.

3.10. Comparison between TIs and Correlation Coefficient of Properties. Table 1 shows the properties of nine cardiovascular disease drugs, and Table 2 shows their TIs computed using molecules. Table 12 lists correlation coefficients between seven physical properties and TIs. Figure 4 depicts the graph between TIs and physical properties.

3.11. Standard Error of Estimate (SEE) and Statistical Parameters. A measure of variation for an observation calculated around the computed regression line is said to be the standard error estimate. This will be helpful in calculating the range of accuracy to predict around the regression line in Table 13. In Table 14 correlation determination describes the percentage of relationship that provides additional info about the association between variables. It is calculated by squaring the value of r. Tables 15–21 associate properties, theoretical, and experimental estimated values that are found with the models.

Table 3: RM of ABC (G).

Property	N	A	b	r	r^2	F	p
Enthalpy	9	41.507	1.210	0.768	0.590	10.056	0.016
Flash Point	9	59.120	6.082	0.801	0.642	12.551	0.009
Molar Refractivity	8	−10.427	2.747	0.980	0.961	147.449	≤ 0.001
Polarity	9	−0.273	1.019	0.967	0.936	101.578	≤ 0.001
Molar Volume	9	−7.037	7.554	0.984	0.968	210.248	≤ 0.001
Complexity	9	−221.857	17.811	0.841	0.707	16.900	0.005
Boiling Point	8	171.475	10.018	0.805	0.647	11.017	0.016

Table 4: RM of RA (G).

Property	N	A	b	r	r^2	F	p
Enthalpy	9	36.702	2.310	0.798	0.637	12.304	0.010
Flash Point	9	37.149	11.525	0.827	0.684	15.164	0.006
Molar Refractivity	8	−15.727	5.040	0.990	0.979	285.580	≤ 0.001
Polarity	9	−3.007	1.896	0.980	0.960	169.494	≤ 0.001
Molar Volume	9	−21.820	13.843	0.982	0.964	189.488	≤ 0.001
Complexity	9	−227.825	33.436	0.860	0.740	19.874	0.003
Boiling Point	8	136.030	18.971	0.830	0.688	13.259	0.011

Table 5: RM of S (G).

Property	N	A	b	r	r^2	F	p
Enthalpy	9	36.901	2.261	0.804	0.647	12.817	.009
Flash Point	9	36.666	11.337	0.827	0.701	16.413	.005
Molar Refractivity	8	−13.430	4.872	0.992	0.985	388.144	≤ 0.001
Polarity	9	−2.758	1.853	0.985	0.971	235.553	≤ 0.001
Molar Volume	9	−15.044	13.343	0.974	0.949	129.876	≤ 0.001
Complexity	9	−286.200	33.148	0.877	0.770	23.397	0.002
Boiling Point	8	134.715	18.672	0.841	0.707	14.452	0.009

Table 6: RM of GA (G).

Property	N	A	b	r	r^2	F	p
Enthalpy	9	36.896	1.076	0.813	0.661	13.625	0.008
Flash Point	9	35.837	5.409	0.848	0.720	17.980	0.004
Molar Refractivity	8	−11.636	2.289	0.994	0.988	477.849	≤0.001
Polarity	9	−2.372	0.875	0.988	0.976	290.534	≤0.001
Molar Volume	9	−8.142	6.227	0.965	0.932	96.106	≤0.001
Complexity	9	−289.368	15.830	0.890	0.792	26.594	0.001
Boiling Point	8	132.919	8.914	0.852	0.727	15.941	0.007

Table 7: RM of M1 (G).

Property	N	A	b	r	r^2	F	p
Enthalpy	9	41.290	0.166	0.778	0.606	10.767	0.013
Flash Point	9	59.202	0.831	0.809	0.654	13.254	0.008
Molar Refractivity	8	−11.830	0.378	0.978	0.957	132.373	≤ 0.001
Polarity	9	0.702	0.136	0.957	0.915	75.687	≤ 0.001
Molar Volume	9	−0.381	1.013	0.975	0.950	133.079	≤ 0.001
Complexity	9	−199.614	2.369	0.826	0.683	15.082	0.006
Boiling Point	8	170.708	1.371	0.814	0.662	11.744	0.014

Table 8: RM of M2 (G).

Property	N	A	b	r	r^2	F	p
Enthalpy	9	39.081	0.136	0.811	0.658	13.476	0.008
Flash Point	9	50.928	0.676	0.835	0.697	16.124	0.005
Molar Refractivity	8	−14.688	0.305	0.979	0.959	139.905	≤ 0.001
Polarity	9	1.255	0.107	0.948	0.899	62.189	≤ 0.001
Molar Volume	9	6.006	0.786	0.959	0.920	80.997	≤ 0.001
Complexity	9	−190.310	1.851	0.819	0.671	14.289	0.007
Boiling Point	8	156.992	1.115	0.840	0.705	14.369	0.009

Table 9: RM of HM (G).

Property	N	A	b	r	r^2	F	p
Enthalpy	9	43.148	0.028	0.769	0.591	10.106	0.016
Flash Point	9	71.169	0.139	0.791	0.626	11.695	0.011
Molar Refractivity	8	−14.022	0.067	0.966	0.934	84.254	≤ 0.001
Polarity	9	3.155	0.023	0.925	0.856	41.582	≤ 0.001
Molar Volume	9	10.033	0.171	0.965	0.931	94.877	≤ 0.001
Complexity	9	−134.240	0.380	0.775	0.601	10.547	0.014
Boiling Point	8	190.149	0.229	0.796	0.633	10.358	0.018

Table 10: RM of H (G).

Property	N	A	b	r	r^2	F	p
Enthalpy	9	34.520	2.674	0.818	0.670	14.202	0.007
Flash Point	9	25.838	13.363	0.849	0.721	18.085	0.004
Molar Refractivity	8	−15.356	5.636	0.995	0.989	563.243	≤ 0.001
Polarity	9	−4.046	2.163	0.990	0.980	346.941	≤ 0.001
Molar Volume	9	−20.739	15.429	0.969	0.939	108.128	≤ 0.001
Complexity	9	−315.098	38.955	0.887	0.787	25.844	0.001
Boiling Point	8	117.355	21.998	0.852	0.726	15.875	0.007

Table 11: RM of F (G).

Property	N	A	b	r	r^2	F	p
Enthalpy	9	46.714	0.047	0.732	0.536	8.091	0.025
Flash Point	9	88.903	0.232	0.753	0.567	9.182	0.019
Molar Refractivity	8	−12.042	0.117	0.951	0.904	56.541	≤ 0.001
Polarity	9	5.016	0.039	0.903	0.815	30.915	0.001
Molar Volume	9	16.534	0.301	0.964	0.930	93.089	≤ 0.001
Complexity	9	−85.217	0.635	0.738	0.544	8.365	0.023
Boiling Point	8	219.223	0.383	0.758	0.575	8.106	0.029

Table 12: Correlation coefficients.

	Correlation coefficient						
Topological Index	Boiling point	Enthalpy	FP	refractivity	Polarity	Molar volume	C
ABC(G)	0.805	0.768	0.801	0.98	0.967	0.984	0.841
RA(G)	0.830	0.798	0.827	0.99	0.98	0.982	0.86
S(G)	0.841	0.804	0.837	0.992	0.985	0.974	0.877
GA(G)	0.852	0.813	0.848	0.994	0.988	0.965	0.89
M1(G)	0.814	0.778	0.809	0.978	0.957	0.975	0.826
M2(G)	0.84	0.811	0.835	0.979	0.948	0.959	0.819
HM(G)	0.796	0.769	0.791	0.966	0.925	0.965	0.775
F(G)	0.758	0.732	0.753	0.951	0.903	0.964	0.738
H(G)	0.852	0.818	0.849	0.995	0.990	0.969	0.887

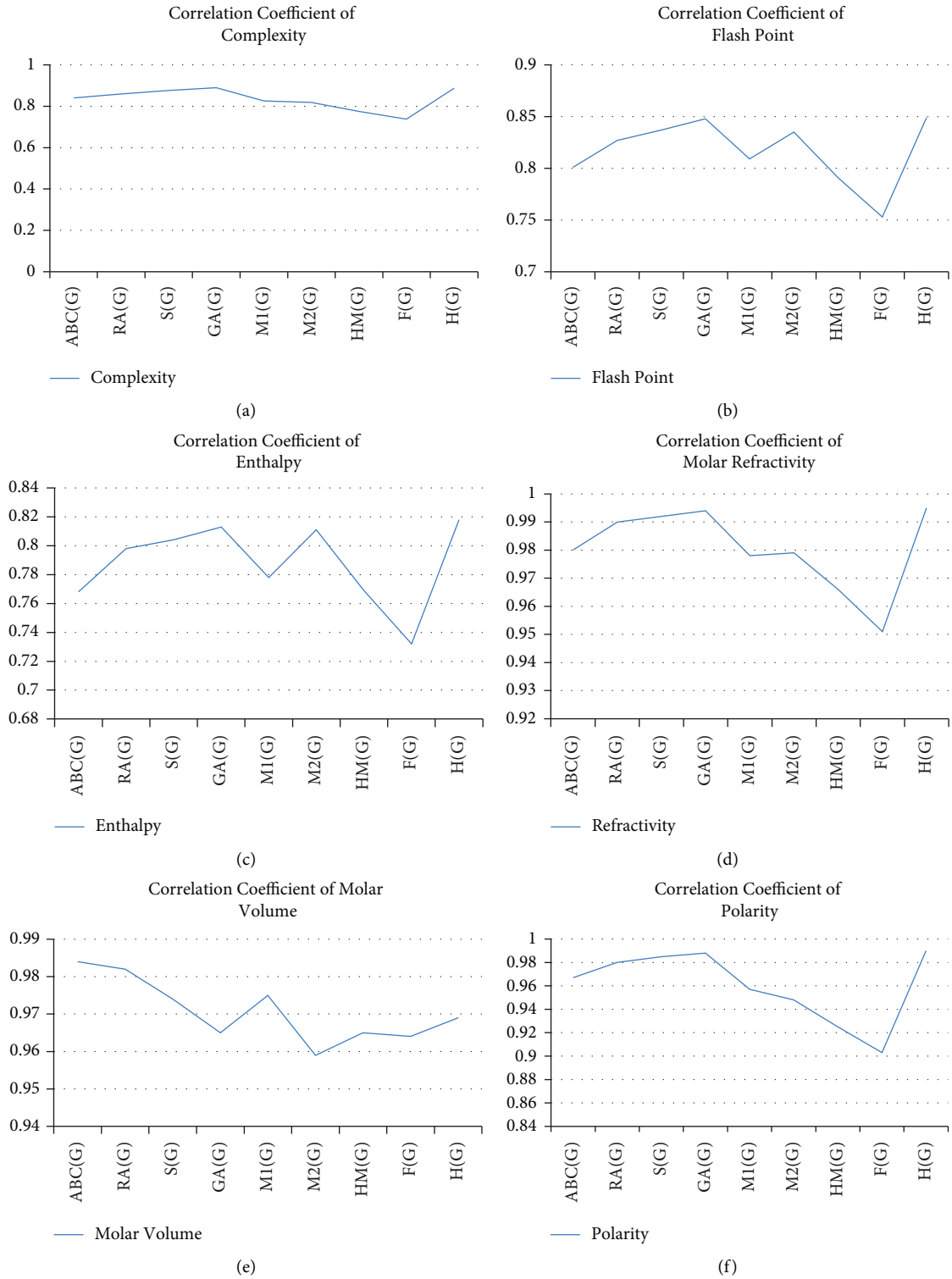
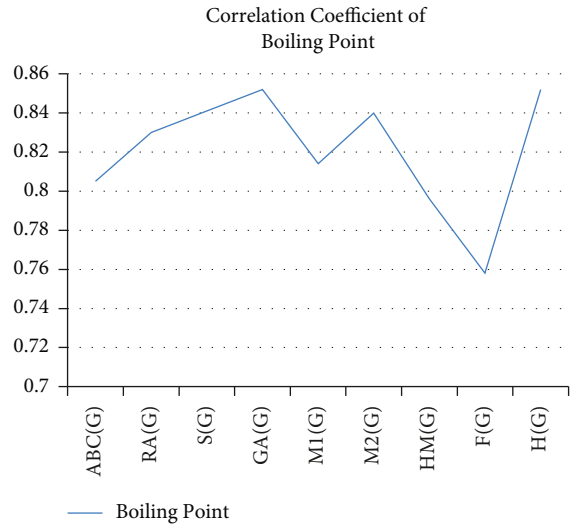


Figure 4: Continued.



(g)

Figure 4: Properties and Tis: (a) complexity on TI; (b) enthalpy on TI; (c) enthalpy on TI; (d) molar refractivity on TI; (e) MV on TI; (f) polarity on TI; (g) boiling point on TI.

Table 13: coefficient of determination.

	Coefficient of determination						
Topological Index	BP	Enthalpy	FP	refractivity	Polarity	Molar volume	Complexity
ABC (G)	0.647	0.59	0.642	0.961	0.936	0.968	0.707
RA (G)	0.688	0.637	0.684	0.979	0.960	0.964	0.74
S (G)	0.707	0.647	0.701	0.985	0.971	0.949	0.77
GA (G)	0.727	0.661	0.720	0.988	0.976	0.932	0.792
M1 (G)	0.662	0.606	0.654	0.957	0.915	0.950	0.683
M2 (G)	0.705	0.658	0.697	0.959	0.899	0.920	0.671
HM (G)	0.633	0.591	0.626	0.934	0.856	0.931	0.601
F (G)	0.575	0.536	0.567	0.904	0.815	0.930	0.544
H (G)	0.726	0.670	0.721	0.989	0.980	0.939	0.787

Table 14: Standard error of the estimate.

	See						
Topological Index	BP	Enthalpy	FP	Refractivity	Polarity	Molar volume	Complexity
ABC (G)	85.1316	10.7681	48.44341	5.94445	2.85428	14.7016	122.262
RA (G)	80.022	10.1218	45.49855	4.31235	2.23873	15.4588	115.298
S (G)	77.6543	9.98981	44.26847	3.70908	1.90970	18.5216	108.411
GA (G)	74.9728	9.79228	42.85683	3.34764	1.72425	21.3403	103.123
M1 (G)	83.3696	10.5504	47.59531	6.25990	3.27076	18.3087	127.196
M2 (G)	77.8124	9.82774	44.54343	6.09618	3.57560	23.0998	129.542
HM (G)	86.8284	10.7525	19.54067	7.75106	4.26707	21.4687	142.686
F (G)	93.5034	11.4478	53.24734	9.31133	4.83016	21.6596	152.484
H (G)	75.0847	9.65811	42.76757	3.08634	1.58089	20.1954	104.295

Table 15: Comparision.

Drug	Polarity	Polarity computed from RM								
		ABC	R	S	GA	M1	M2	F	H	HM
Eliquis	49.8 ± 0.5 cm^3	42.2134	42.1701	42.1776	42.1525	42.209	41.996	42.303	42.1853	41.18
Vericiguat	41.5 ± 0.5 cm^3	36.7798	36.4476	36.4961	36.6542	37.358	37.756	37.883	36.2585	36.98
Pradaxa	69.7 ± 0.5 cm^3	46.1755	46.3821	46.3295	46.1455	45.674	44.911	45.363	46.5602	44.07
Ivabradine	52.4 ± 0.5 cm^3	40.4107	40.2176	40.5266	40.8631	41.131	41.519	41.383	40.4265	40.47
Dapagliflozin	41.9 ± 0.5 cm^3	41.7420	41.6298	41.6192	41.6129	41.824	41.678	42.003	41.5793	40.88
Empagliflozin	45.4 ± 0.5 cm^3	22.5683	22.473	22.5473	22.5508	22.42	22.174	22.323	22.5427	21.96
Metoprolol	30.6 ± 0.5 cm^3	22.5683	22.9150	22.6687	22.4656	22.42	22.333	22.443	22.8974	22.09
Sacubitril	45.00 ± 0.5 cm^3	44.5321	44.7734	44.9091	44.7312	44.519	44.328	44.463	44.9787	43.33
Valsartan	47.8 ± 0.0 cm^3	19.5935	19.2065	19.3059	19.4836	20.11	20.584	20.523	19.0250	20.31

Table 16: Comparison.

Drug	Molar volume	Molar volume computed from RM								
		AB	R	S	GA	M1	M2	F	H	HM
Eliquis	323.4 ± 7.0 cm^3	344.058	343.528	343.406	343.508	343.293	343.034	343.097	343.143	341.924
Vericiguat	260.8 75.0 cm^3	294.874	292.133	292.413	293.917	298.941	303.514	302.433	290.324	301.919
Pradaxa	504 ± 7.0 cm^3	379.923	381.357	380.670	379.523	374.973	370.204	371.249	382.132	369.539
Ivabradine	408.7 ± 3.0 cm^3	327.741	325.992	328.588	331.879	333.437	338.588	334.633	327.469	335.204
Dapagliflozin	303.1 ± 3.0 cm^3	339.791	338.675	338.394	338.641	339.773	340.07	340.337	337.743	339.089
Empagliflozin	322.4 ± 3.0 cm^3	166.235	166.623	167.218	166.713	162.365	158.278	159.281	168.087	158.489
Metoprolol	258.7 ± 3.0 cm^3	166.235	170.593	168.307	165.945	162.365	159.76	160.385	171.249	159.749
Sacubitril	357.4 ± 3.0 cm^3	365.047	366.909	367.922	366.766	364.413	364.77	362.969	368.038	362.504
Valsartan	359.1 ± 3.0 cm^3	139.308	137.285	138.125	139.049	141.245	143.458	142.721	136.738	142.739

Table 17: Comparison.

Drug	Enthalpy	Enthalpy computed from RM								
		ABC	R	S	GA	M1	M2	F	H	HM
Eliquis	112.2 ± 3.0 ℃	99.7525	99.6668	99.6808	99.6986	99.58	99.441	98.934	99.6577	100.626
Vericiguat	81.2 ± 3.0℃	92.8517	92.4671	92.5110	92.7194	93.406	94.001	93.409	92.2232	94.911
Pradaxa	120.3 ± 3.0 ℃	104.784	104.966	104.920	104.767	103.99	103.181	102.759	105.145	104.571
Ivabradine	92.8 ± 3.0 ℃	97.4630	97.2102	97.5973	98.0620	98.208	98.829	97.784	97.4515	99.666
Dapagliflozin	95.1 ± 3.0℃	99.1538	98.987	98.9761	99.0137	99.09	99.033	98.559	98.8976	100.221
Empagliflozin	102.7 ± 3.0 ℃	74.8029	74.885	74.9084	74.8169	74.394	74.009	73.959	75.0181	74.421
Metoprolol	68.5 ± 3.0 ℃	74.8029	75.4412	75.0616	74.7088	74.394	74.213	74.109	75.4630	74.601
Sacubitril	101.6 ± 3.0 ℃	102.697	102.942	103.127	102.972	102.52	102.433	101.634	103.161	103.566
Valsartan	105.5 ± 3.0 ℃	71.0249	70.7753	70.8179	70.9235	71.454	71.969	71.709	70.6055	72.171

Table 18: Comparison.

Drug	Molar refractivity	Molar refractivity computed from RM								
		ABC	R	S	GA	M1	M2	F	H	HM
Eliquis	125.6 ± 5.0cm^3	119.352	119.326	119.342	119.277	119.06	118.509	118.659	119.309	117.44
Vericiguat		104.168	103.296	103.444	103.905	105.578	106.749	106.504	102.719	105.63
Pradaxa	175.9 ± 5.0 cm^3	130.423	131.125	130.96	130.441	128.69	126.594	127.074	131.554	125.59
Ivabradine	132.2 ± 3.0cm^3	114.314	113.857	114.722	115.672	116.064	117.186	116.129	114.386	115.45
Dapagliflozin	105.6 ± 3.0cm^3	118.035	117.813	117.78	117.768	117.99	117.627	117.834	117.613	116.6
Empagliflozin	114.4 ± 3.0cm^3	64.457	64.149	64.4127	64.4754	64.062	63.531	63.714	64.3285	63.28
Metoprolol	77.1 ± 3.0 cm^3	64.457	65.3874	64.7524	64.2372	64.062	63.972	64.044	65.3214	63.652
Sacubitril	113.6 ± 3.0 cm^3	125.831	126.619	126.985	126.486	125.48	124.977	124.599	127.128	123.51
Valsartan	120.6 ± 3.0cm^3	56.1444	54.9986	55.3427	55.9002	57.642	59.121	58.764	54.4824	58.63

Table 19: Comparison.

Drug	Complexity	Complexity computed from RM								
		ABC	R	S	GA	M1	M2	F	H	HM
Eliquis	777	918.993	916.572	916.631	917.327	916.775	914.103	915.126	915.531	916.04
Vericiguat	622	754.040	744.744	745.703	750.715	768.032	782.023	779.211	738.678	781.54
Pradaxa	991	1039.27	1043.04	1041.54	1038.32	1023.02	1004.90	1009.22	1046.07	1008.9
Ivabradine	663	864.267	857.944	866.96	878.256	883.721	899.244	886.836	863.048	893.44
Dapagliflozin	472	904.683	900.348	899.830	900.976	904.97	904.197	905.901	897.449	906.5
Empagliflozin	558	322.609	325.13	326.054	323.341	309.998	296.629	300.741	329.402	299.34
Metoprolol	215	322.609	338.404	329.706	320.759	309.998	301.582	304.431	339.987	303.58
Sacubitril	550	989.384	994.743	998.808	995.470	987.605	986.747	981.546	998.886	985.22
Valsartan	608	232.301	227.047	228.537	230.396	239.168	247.099	245.391	224.437	246.39

Table 20: Comparison.

Drug	Boiling point of the drug	Boiling point computed from RM								
		ABC	R	S	GA	M1	M2	F	H	HM
Eliquis	770.5 ± 6.0℃	640.3174	637.0541	643.9	677.9733	645.074	652.052	635.161	641.7873	642.2
Vericiguat	535.9 ± 5.0℃	540.0372	544.2859	548.86	621.6272	527.168	512.677	508.005	553.7953	508.92
Pradaxa	827.9 ± 75℃	842.4806	856.5486	856.948	793.7736	835.643	833.797	807.894	864.1871	820.13
Ivabradine	626.9 ± 55℃	728.8765	712.7484	715.227	715.1698	735.56	732.332	743.933	704.0417	740.21
Dapagliflozin	609 ± 55℃	579.7085	585.6427	583.403	639.6239	584.75	591.842	592.265	587.2323	591.82
Empagliflozin	664.5 ± 55℃	623.4872	627.3789	628.589	667.0951	636.848	654.282	645.119	630.3484	649.07
Metoprolol	398.6 ± 37℃	509.883	497.0481	489.67	583.1775	505.232	492.607	530.985	482.7418	514.41
Sacubitril	656.9 ± 55℃	624.8897	629.0863	623.175	659.6759	620.396	619.717	623.671	625.5088	622.04
Valsartan		645.4266	648.8161	646.888	674.9154	642.332	642.017	639.757	649.0467	640.82

Table 21: Comparison.

Drug	Flash point	Flash point computed from RM								
		ABC	R	S	GA	M1	M2	F	H	HM
Eliquis	419 ± 32℃	343.7576	341.5243	345.826	350.0999	346.728	351.072	340.855	344.4119	148.155
Vericiguat	277.9 ± 30℃	282.8768	285.167	288.1207	289.3027	275.262	266.572	263.831	290.9599	125.457
Pradaxa	454.5 ± 3℃	466.4924	474.8685	475.1812	475.0478	462.237	461.26	445.487	479.5119	178.458
Ivabradine	332.9 ± 31.5℃	397.5225	387.509	389.1333	390.2347	401.574	399.744	406.743	382.2292	164.847
Dapagliflozin	322. ± 31.5℃	306.9615	310.2915	309.0941	308.7211	310.164	314.568	314.871	311.2717	139.575
Empagliflozin	355.7 ± 31.5℃	333.5398	335.6465	336.5297	338.3624	341.742	352.424	346.887	337.4632	149.325
Metoprolol	194.9 ± 26.5℃	264.57	256.4698	252.1824	247.8157	261.966	254.404	277.751	247.7974	126.393
Sacubitril	351.1 ± 31.5℃	334.3913	336.6838	333.2419	330.3571	331.77	331.468	333.895	334.5233	144.723
Valsartan	368 ± 34.3℃	346.8594	348.6698	347.6399	346.8004	345.066	344.988	343.639	348.8217	147.921

In this section, we find the relation of TIs with the properties of aforementioned drugs of said disease, such as Eliquis, vericiguat, Pradaxa, ivabradine, dapagliflozin, empagliflozin, metoprolol, sacubitril, and valsartan, and it will best be calculated with the aid of QSPR modeling, whereas TIs, b, r, and N are independent variables, RM constant, correlation coefficient, and sample size, respectively. This test can associate and decide the enhancement of the model. The observations evaluate that p should be less than 0.05 and r is greater than 0.6. Therefore, based on the calculating procedure used above, it is clearly shown that the features listed in Tables 3–11 are important.

4. Conclusions

The statistical parameters applied to the models and TIs that: H(G) delivers maximum correlation of molar polarity $r = 0.990$. ABC(G) delivers highly correlated worth for molar volume $r = 0.984$. H(G) index offers a maximum correlated value of flash point i.e., $r = 0.849$. GA (G) and H (G) index describe the extreme correlation coefficient of BP $r = 0.852$. H(G) delivers the ultimate correlated value of molar refractivity $r = 0.995$. Tables 3–11 display various statical parameters of correlation between seven physical properties of medicine and the values of nine degree-based topological indices. There was no correlation between TIs and density and between polar surface area and surface tension.

In this paper, we calculated TIs and compared them to the QSPR model for drugs employed in cardiovascular disease. In the pharmaceutical industry, the calculated value gained through this will be useful in designing novel drugs that will obviously be helpful in obtaining preventive measures for the aforementioned disease. The correlation coefficient subsidizes meaningfully with many TIs for the drugs. Drugs calculated values are eye-opening to chemists

deployed on drug discovering phenomenon in the pharmaceutical industry. They deliver methods for the estimation of properties for new exposures to other specific diseases.

Data Availability

All the data used in the manuscript are within the manuscript.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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