Research Article

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

Fozia Bashir Farooq, 1 Nadeem Ul Hassan Awan, 2 Saima Parveen, 3 Nazeran Idrees, 3 Salma Kanwal, 4 and Tarig A. Abdelhaleem 5

1Department of Mathematics and Statistics, Imam Muhammad Ibn Saud Islamic University, Riyadh, Saudi Arabia
2Department of Mathematics, Faculty of Science, Ghazi University, Dera Ghazi Khan, Pakistan
3Department of Mathematics, Government College University Faisalabad, Faisalabad 38000, Pakistan
4Department of Mathematics, Lahore College for Women University, Lahore, Pakistan
5Department of Mathematics, College of Computer and Mathematical Science, University of Bahri, Khartoum, Sudan

Correspondence should be addressed to Tarig A. Abdelhaleem; tarig.azim@bahri.edu.sd

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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.
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 $d_v$, and is the number of vertices adjacent to it. We used the following TIs:
Definition 1. ABC index [15] \( G \) is given under
\[
ABC(G) = \sum_{u,v \in E(G)} \sqrt{\frac{d_u d_v}{d_u + d_v}} - 2
\]  

Definition 2. Randic index [16] is given under
\[
RA(G) = \sum_{u,v \in E(G)} \frac{1}{\sqrt{d_u d_v}} \tag{2}
\]

Definition 3. sum connectivity index [17] is given under
\[
S(G) = \sum_{u,v \in E(G)} \frac{1}{d_u + d_v} \tag{3}
\]

Definition 4. GA index [18] is given under:
\[
GA(G) = \sum_{u,v \in E(G)} 2\sqrt{\frac{d_u d_v}{d_u + d_v}} \tag{4}
\]

Definition 5. Zagreb indices [19] are given under
\[
M_1(G) = \sum_{u,v \in E(G)} (d_u + d_v) \tag{5}
\]
\[
M_2(G) = \sum_{u,v \in E(G)} (d_u + d_v) \tag{5}
\]

Definition 6. harmonic index [20] of \( G \) is given under:
\[
H(G) = \sum_{u,v \in E(G)} \frac{2}{d_u + d_v} \tag{6}
\]

Definition 7. hyper-Zagreb index [21] is given under
\[
HM(G) = \sum_{u,v \in E(G)} (d_u + d_v)^2 \tag{7}
\]

Definition 8. forgotten index [22] is given under
\[
F(G) = \sum_{u,v \in E(G)} \left[ (d_u)^2 + (d_v)^2 \right] \tag{8}
\]

The \( n \)-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 \( C_{24}H_{29}N\_O_\_ \). This is a nephrisin 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 \( C_{31}H_{41}N_2O_5 \). 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 \( C_{25}H_{25}ClO_6 \). The medication is a sodium-glucose cotransporter inhibitor that is used to treat the disease. \( C_{13}H_{25}N_2O_3 \) is the molecular formula of 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:
\[
P = A + b(TI) \tag{9}
\]

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.

<table>
<thead>
<tr>
<th>Drug</th>
<th>Boiling point (°C)</th>
<th>Enthalpy (°C)</th>
<th>Flash point (°C)</th>
<th>Molar Refractivity (cm&lt;sup&gt;3&lt;/sup&gt;)</th>
<th>Polarity (g/cm&lt;sup&gt;3&lt;/sup&gt;)</th>
<th>Molar Volume (cm&lt;sup&gt;3&lt;/sup&gt;)</th>
<th>Complexity</th>
<th>Density (g/cm&lt;sup&gt;3&lt;/sup&gt;)</th>
<th>Polar surface area (Å&lt;sup&gt;2&lt;/sup&gt;)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eliquis</td>
<td>770.5</td>
<td>112.2</td>
<td>419.8</td>
<td>125.6</td>
<td>49.8</td>
<td>323.4</td>
<td>777</td>
<td>1.4</td>
<td>111</td>
</tr>
<tr>
<td>Verciguat</td>
<td>535.9</td>
<td>81.2</td>
<td>277.9</td>
<td>41.5</td>
<td>260.8</td>
<td>622</td>
<td>1.6</td>
<td>147</td>
<td></td>
</tr>
<tr>
<td>Pradaxa</td>
<td>827.9</td>
<td>120.3</td>
<td>454.5</td>
<td>69.7</td>
<td>504</td>
<td>991</td>
<td>1.2</td>
<td>154</td>
<td></td>
</tr>
<tr>
<td>Iprabradine</td>
<td>626.9</td>
<td>92.7</td>
<td>332.9</td>
<td>132.2</td>
<td>408.7</td>
<td>663</td>
<td>1.1</td>
<td>60</td>
<td></td>
</tr>
<tr>
<td>Dipaglifozin</td>
<td>609</td>
<td>95.1</td>
<td>322.1</td>
<td>105.6</td>
<td>303.1</td>
<td>472</td>
<td>1.3</td>
<td>99</td>
<td></td>
</tr>
<tr>
<td>Empaglifozin</td>
<td>664</td>
<td>102.7</td>
<td>357.7</td>
<td>114.4</td>
<td>322.4</td>
<td>558</td>
<td>1.4</td>
<td>109</td>
<td></td>
</tr>
<tr>
<td>Metoprolol</td>
<td>398.6</td>
<td>68.5</td>
<td>194.9</td>
<td>77.1</td>
<td>258.7</td>
<td>215</td>
<td>1.0</td>
<td>51</td>
<td></td>
</tr>
<tr>
<td>Sacubitril</td>
<td>656.9</td>
<td>101.6</td>
<td>351.1</td>
<td>113.6</td>
<td>357.4</td>
<td>550</td>
<td>1.2</td>
<td>93</td>
<td></td>
</tr>
<tr>
<td>Valsartan</td>
<td>105.5</td>
<td>368</td>
<td>120.6</td>
<td>47.8</td>
<td>359.1</td>
<td>608</td>
<td>1.2</td>
<td>112</td>
<td></td>
</tr>
</tbody>
</table>

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

(v) \( M1(G_1) = 346 \)

(vi) \( M2(G_1) = 444 \)

(vii) \( F(G_1) = 1086 \)

(viii) \( H(G_1) = 23.84 \)

(ix) \( HM(G_1) = 1974 \)

Theorem 2. Let \( G_2 \) be the graph of dapaglifozin, TIs in \( G_2 \) are given as follows:

(i) \( ABC(G_2) = 40.75 \)

(ii) \( RA(G_2) = 23.70 \)

(iii) \( S(G_2) = 24.03 \)

(iv) \( GA(G_2) = 50.45 \)

(v) \( M1(G_2) = 302 \)

(vi) \( M2(G_2) = 390 \)

(vii) \( F(G_2) = 974 \)

(viii) \( H(G_2) = 21.36 \)

(ix) \( HM(G_2) = 1754 \)

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

(i) \( ABC(G_2) = 4 \sqrt{(1 + 2 - 2)/(1 × 2)} + 8 \sqrt{(1 + 3 - 2)/(1 × 3)} + 14 \sqrt{(1 + 4 - 2)/(1 × 4)} + 1 \sqrt{(2 + 3 - 2)/(2 × 3)} + 7 \sqrt{(2 + 4 - 2)/(2 × 4)} + 12 \sqrt{(3 + 3 - 2)/(3 × 3)} + 3 \sqrt{(3 + 4 - 2)/(3 × 4)} = 22.04 \)

(ii) \( RA(G_2) = 4 \sqrt{1/(1 × 2)} + 8 \sqrt{1/(1 × 3)} + 14 \sqrt{1/(1 × 4)} + 1 \sqrt{1/(2 × 3)} + 7 \sqrt{1/(2 × 4)} + 12 \sqrt{1/(3 × 3)} + 3 \sqrt{1/(3 × 4)} = 13.12 \)

(iii) \( S(G_2) = 4 \sqrt{1/(1 + 2)} + 8 \sqrt{1/(1 + 3)} + 14 \sqrt{1/(1 + 4)} + 1 \sqrt{1/(2 + 3)} + 7 \sqrt{1/(2 + 4)} + 12 \sqrt{1/(3 + 3)} + 3 \sqrt{1/(3 + 4)} = 13.46 \)

(iv) \( GA(G_2) = 8 \sqrt{1 × 2/(1 + 2)} + 16 \sqrt{1 × 3/(1 + 3)} + 28 \sqrt{1 × 4/(1 + 4)} + 2 \sqrt{2 × 3/(2 + 3)} + 14 \sqrt{2 × 4/(2 + 4)} + 24 \sqrt{3 × 3/(3 + 3)} + 6 \sqrt{3 × 4/(3 + 4)} = 27.72 \)

(v) \( M1(G_2) = 4/(1 + 2) + 8/(1 + 3) + 14/(1 + 4) + 1/(2 + 3) + 7/(2 + 4) + 12/(3 + 3) + 3/(3 + 4) = 162 \)

(vi) \( M2(G_2) = 4/(1 × 2) + 8/(1 × 3) + 14/(1 × 4) + 1/(2 × 3) + 7/(2 × 4) + 12/(3 × 3) + 3/(3 × 4) = 209 \)

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

(viii) \( HM(G_2) = 4/(1 × 2) + 8/(1 × 3) + 14/(1 × 4) + 1/(2 × 3) + 7/(2 × 4) + 12/(3 × 3) + 3/(3 × 4) = 934 \)

(ix) \( F(G_2) = 4/(1 × 4) + 8/(1 × 9) + 14/(1 × 16) + 1/(4 × 9) + 7/(4 × 16) + 12/(9 × 9) + 3/(9 × 16) = 516 \)

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.
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) $P = -21.820 + 13.843 [ABC (G)]$

(vi) $MV = 212.050 + 9.447 [ABC (G)]$

(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) $MV = -15.044 + 13.343 [S (G)]$

Figure 2: 2D graph of medicines with TIs.

Figure 3: 3D graph of medicines with TI.
Table 2: TIs of drugs.

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

(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) \( FP = 55.837 + 5.409 \) [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) \( E = 41.290 + 0.166 \) [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) \( MV = 0.702 + 0.136 \) [M1 (G)]
(vii) \( C = -199.614 + 15.830 \) [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) \( C = -315.098 + 38.955 \) [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) \( E = 46.714 + 0.047 \) [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).

<table>
<thead>
<tr>
<th>Property</th>
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<th>r</th>
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<td>0.590</td>
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<td>0.642</td>
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</tr>
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<td>0.936</td>
<td>101.578</td>
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### Table 4: RM of RA (G).

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<td>0.637</td>
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<td>0.010</td>
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<td>0.684</td>
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<td>Molar Refractivity</td>
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<td>-15.727</td>
<td>5.040</td>
<td>0.990</td>
<td>0.979</td>
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<tr>
<td>Polarity</td>
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<td>1.896</td>
<td>0.980</td>
<td>0.960</td>
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<th>p</th>
</tr>
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<td>Enthalpy</td>
<td>9</td>
<td>36.901</td>
<td>2.261</td>
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<td>0.647</td>
<td>12.817</td>
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</tr>
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<td>Flash Point</td>
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<td>36.666</td>
<td>11.337</td>
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<td>.005</td>
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<td>-13.430</td>
<td>4.872</td>
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<td>388.144</td>
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<tr>
<td>Polarity</td>
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<td>-2.758</td>
<td>1.853</td>
<td>0.985</td>
<td>0.971</td>
<td>235.553</td>
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<td>Molar Volume</td>
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<td>-15.044</td>
<td>13.343</td>
<td>0.974</td>
<td>0.949</td>
<td>129.876</td>
<td>≤ 0.001</td>
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<tr>
<td>Complexity</td>
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<td>-286.200</td>
<td>33.148</td>
<td>0.877</td>
<td>0.770</td>
<td>23.397</td>
<td>0.002</td>
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<td>Boiling Point</td>
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<td>18.672</td>
<td>0.841</td>
<td>0.707</td>
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### Table 6: RM of GA (G).

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<th>F</th>
<th>p</th>
</tr>
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<tbody>
<tr>
<td>Enthalpy</td>
<td>9</td>
<td>36.896</td>
<td>1.076</td>
<td>0.813</td>
<td>0.661</td>
<td>13.625</td>
<td>0.008</td>
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<td>Flash Point</td>
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<td>35.837</td>
<td>5.409</td>
<td>0.848</td>
<td>0.720</td>
<td>17.980</td>
<td>0.004</td>
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<td>8</td>
<td>-11.636</td>
<td>2.289</td>
<td>0.994</td>
<td>0.988</td>
<td>477.849</td>
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<td>-2.372</td>
<td>0.875</td>
<td>0.988</td>
<td>0.976</td>
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<td>6.227</td>
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<td>26.594</td>
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<td>0.727</td>
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### Table 7: RM of M1 (G).

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<td>Enthalpy</td>
<td>9</td>
<td>41.290</td>
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<td>0.778</td>
<td>0.606</td>
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<td>Flash Point</td>
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<td>59.202</td>
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<td>0.809</td>
<td>0.654</td>
<td>13.254</td>
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<td>-11.830</td>
<td>0.378</td>
<td>0.978</td>
<td>0.957</td>
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<td>0.702</td>
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<tr>
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### Table 8: RM of M2 (G).

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### Table 9: RM of HM (G).

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<td>0.626</td>
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<td>0.931</td>
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### Table 10: RM of H (G).

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### Table 11: RM of F (G).

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### Table 12: Correlation coefficients.

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<th>Fp</th>
<th>refractivity</th>
<th>Polarity</th>
<th>Molar volume</th>
<th>C</th>
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<tr>
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<td>0.801</td>
<td>0.98</td>
<td>0.967</td>
<td>0.984</td>
<td>0.841</td>
</tr>
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<td>0.798</td>
<td>0.827</td>
<td>0.99</td>
<td>0.98</td>
<td>0.982</td>
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<td>0.837</td>
<td>0.992</td>
<td>0.985</td>
<td>0.974</td>
<td>0.877</td>
</tr>
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<td>GA(G)</td>
<td>0.852</td>
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<td>0.988</td>
<td>0.965</td>
<td>0.89</td>
</tr>
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<td>0.814</td>
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<td>0.826</td>
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<td>0.959</td>
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</tr>
<tr>
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<td>0.951</td>
<td>0.903</td>
<td>0.964</td>
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<tr>
<td>H(G)</td>
<td>0.852</td>
<td>0.818</td>
<td>0.849</td>
<td>0.995</td>
<td>0.990</td>
<td>0.969</td>
<td>0.887</td>
</tr>
</tbody>
</table>
Figure 4: Continued.
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.

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

Table 14: Standard error of the estimate.

See
### Table 15: Comparison.

<table>
<thead>
<tr>
<th>Drug</th>
<th>Polarity</th>
<th>Polarity computed from RM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eliquis</td>
<td>49.8 ± 0.5 cm³</td>
<td>42.2134 ± 120.6</td>
</tr>
<tr>
<td>Vercigatu</td>
<td>41.5 ± 0.5 cm³</td>
<td>36.7798 ± 357.4</td>
</tr>
<tr>
<td>Pradaxa</td>
<td>69.7 ± 0.5 cm³</td>
<td>46.1755 ± 77.1</td>
</tr>
<tr>
<td>Iveradine</td>
<td>52.4 ± 0.5 cm³</td>
<td>40.4107 ± 113.6</td>
</tr>
<tr>
<td>Dapagliflozin</td>
<td>41.9 ± 0.5 cm³</td>
<td>41.7420 ± 322.4</td>
</tr>
<tr>
<td>Empagliflozin</td>
<td>45.4 ± 0.5 cm³</td>
<td>22.5683 ± 114.4</td>
</tr>
<tr>
<td>Metoprolol</td>
<td>30.6 ± 0.5 cm³</td>
<td>22.9150 ± 258.7</td>
</tr>
<tr>
<td>Sacubitril</td>
<td>45.00 ± 0.5 cm³</td>
<td>44.5321 ± 22.5</td>
</tr>
<tr>
<td>Valsartan</td>
<td>47.8 ± 0.5 cm³</td>
<td>19.5935 ± 105.5</td>
</tr>
</tbody>
</table>

### Table 16: Comparison.

<table>
<thead>
<tr>
<th>Drug</th>
<th>Molar volume</th>
<th>Molar volume computed from RM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eliquis</td>
<td>323.4 ± 7.0 cm³</td>
<td>344.058 ± 152.6</td>
</tr>
<tr>
<td>Vercigatu</td>
<td>260.8 ± 7.0 cm³</td>
<td>294.874 ± 303.1</td>
</tr>
<tr>
<td>Pradaxa</td>
<td>504 ± 7.0 cm³</td>
<td>379.923 ± 77.1</td>
</tr>
<tr>
<td>Iveradine</td>
<td>408.7 ± 3.0 cm³</td>
<td>327.741 ± 45.4</td>
</tr>
<tr>
<td>Dapagliflozin</td>
<td>303.1 ± 3.0 cm³</td>
<td>339.791 ± 102.7</td>
</tr>
<tr>
<td>Empagliflozin</td>
<td>322.4 ± 3.0 cm³</td>
<td>166.235 ± 113.6</td>
</tr>
<tr>
<td>Metoprolol</td>
<td>258.7 ± 3.0 cm³</td>
<td>166.235 ± 258.7</td>
</tr>
<tr>
<td>Sacubitril</td>
<td>357.4 ± 3.0 cm³</td>
<td>365.047 ± 303.1</td>
</tr>
<tr>
<td>Valsartan</td>
<td>359.1 ± 3.0 cm³</td>
<td>139.308 ± 258.7</td>
</tr>
</tbody>
</table>

### Table 17: Comparison.

<table>
<thead>
<tr>
<th>Drug</th>
<th>Enthalpy</th>
<th>Enthalpy computed from RM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eliquis</td>
<td>112.2 ± 3.0 °C</td>
<td>99.7525 ± 99.6680</td>
</tr>
<tr>
<td>Vercigatu</td>
<td>81.2 ± 3.0 °C</td>
<td>92.8517 ± 92.4671</td>
</tr>
<tr>
<td>Pradaxa</td>
<td>120.3 ± 3.0 °C</td>
<td>104.784 ± 104.966</td>
</tr>
<tr>
<td>Iveradine</td>
<td>92.8 ± 3.0 °C</td>
<td>97.4630 ± 97.2102</td>
</tr>
<tr>
<td>Dapagliflozin</td>
<td>95.1 ± 3.0 °C</td>
<td>99.1358 ± 98.8878</td>
</tr>
<tr>
<td>Empagliflozin</td>
<td>102.7 ± 3.0 °C</td>
<td>74.8029 ± 74.885</td>
</tr>
<tr>
<td>Metoprolol</td>
<td>68.5 ± 3.0 °C</td>
<td>74.8029 ± 75.4412</td>
</tr>
<tr>
<td>Sacubitril</td>
<td>101.6 ± 3.0 °C</td>
<td>102.697 ± 102.942</td>
</tr>
<tr>
<td>Valsartan</td>
<td>105.5 ± 3.0 °C</td>
<td>71.0249 ± 137.285</td>
</tr>
</tbody>
</table>

### Table 18: Comparison.

<table>
<thead>
<tr>
<th>Drug</th>
<th>Molar refractivity</th>
<th>Molar refractivity computed from RM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Eliquis</td>
<td>125.6 ± 5.0 cm³</td>
<td>119.352 ± 119.326</td>
</tr>
<tr>
<td>Vercigatu</td>
<td>175.9 ± 5.0 cm³</td>
<td>130.423 ± 131.125</td>
</tr>
<tr>
<td>Pradaxa</td>
<td>132.2 ± 3.0 cm³</td>
<td>114.314 ± 113.857</td>
</tr>
<tr>
<td>Iveradine</td>
<td>105.6 ± 3.0 cm³</td>
<td>118.035 ± 117.813</td>
</tr>
<tr>
<td>Dapagliflozin</td>
<td>110.4 ± 3.0 cm³</td>
<td>64.457 ± 64.149</td>
</tr>
<tr>
<td>Empagliflozin</td>
<td>110.4 ± 3.0 cm³</td>
<td>64.457 ± 64.149</td>
</tr>
<tr>
<td>Metoprolol</td>
<td>77.1 ± 3.0 cm³</td>
<td>64.457 ± 65.3874</td>
</tr>
<tr>
<td>Sacubitril</td>
<td>113.6 ± 3.0 cm³</td>
<td>125.831 ± 126.619</td>
</tr>
<tr>
<td>Valsartan</td>
<td>120.6 ± 3.0 cm³</td>
<td>56.1444 ± 54.9986</td>
</tr>
</tbody>
</table>
In this section, we find the relation of TIs with the properties of aforementioned drugs of said disease, such as Eliquis, vericiguat, Pradaxa, ivabradine, dapaglifozin, empaglifozin, metoprolol, sacubitril, and valsartan, and it will best be calculated with the aid of QSAR modeling, whereas TIs, $h$, $r$, 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 statistical 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 QSAR 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.

**References**


