https://doi.org/10.48047/AFJBS.6.Si4.2024.247-268

African Journal of Biological Sciences

AN ESTIMATION OF CORDIAL LABEL-BASED TOPOLOGICAL INDICES VIA QSPR ANALYSIS FOR HEART ATTACK MEDICATION TREATMENT

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Article info Volume 6, Issue Si4, 2024
Received: 17 Apr 2024
Accepted: 24 May 2024
doi:10.48047/AFJBS.6.Si4.2024.247-268

Abstract. An index of topology is a numerical value. Utilizing a chemical substance's molecular structure, we can theoretically derive the attributes of a graph and determine its topology. Myocardial infarctions, commonly referred to as heart attacks, are exceedingly common worldwide. In this paper, we are going to investigate and analyze the chemical structures of anti-heart attack drugs and compare correlation coefficients derived from a linear regression analysis by using cordial label-based topological indices by QSPR model. In this, the data analysis of several properties such as boiling point, flash point, enthalpy, molar refraction, molar volume, and surface tension indicates a strong correlation with topological indices, indicating the significance of all computations. Additionally, a comparison of topological indices based on cordial labelling with those derived from a degree-based approach is provided. Furthermore, exponential, and logarithmic regression models are presented for reference.

Keywords: Correlation coefficients, QSPR Analysis, Regression model, Topological Indices.

1. Introduction

When a portion of the heart muscle does not receive enough blood, it can result in myocardial infarction, which is another term for a heart attack. Insufficient blood flow of oxygen-rich blood to the affected area of the heart may cause harm. A heart attack is frequently brought on by an obstruction in the arteries that provide blood to the heart. Not getting the blood and oxygen the heart needs to function properly can put it at risk for heart failure and other serious issues. A part of the heart that is unable to pump blood due to a scarcity of blood destroys the heart's entire pumping sequence [1].

A heart attack can cause a number of symptoms which includes feel pain and tightness in the left side of the chest and pain spread beyond the chest to the upper shoulders, arms, pain in the jaw,

neck, back, shortness of breath, nausea, sweating, exhaustion, discomfort, weakness and difficulty in breathing. Depending on gender, these symptoms differ. Heart attacks can be broadly classified into two categories. Type I heart attacks are caused by a rupture of the plaque on the inner wall of the artery, which releases chemicals and bad cholesterol into the bloodstream. Although a type II heart attack does not totally stop blood flow to the heart, it does not get the necessary quantity of oxygen-rich blood. The main factors contributing to heart attacks are physical inactivity, diabetes, stress and illegal drug use, smoking, alcohol consumption, enrich of bad cholesterol, obesity, high blood pressure and sleep Apnea [2]. Bypass surgery, Stent, angioplasties, valve surgeries, heart transplants, and other operations are some ways to avoid and treat a heart attack. The process of producing drugs to treat this condition is costly, time-consuming, and challenging to make sense of these molecular structures, scientists developed a variety of methods [3].

A molecular graph represents the structural formula of a compound graph theoretically, with the atoms of the compound represented by their vertices and the chemical bonds by their edges. To depict a graph, one can use a matrix, polynomial, sequence of integers, or numeric number. Combining math, information science, and chemistry is a new branch of research known as" chem-informatics." To evaluate the biological activities and qualities of different chemical substances, it investigates correlations between quantitative structure-activity relationship (QSAR) and quantitative structure-property relationship (QSPR). An associated numerical value is called a topological index, which describes the topology of a graph and its invariant under graph automorphism. Topological indexes are numerical values associated with graphs that describe their topology and their invariant under graph automorphisms [4].

A topological index is a numerical number that is obtained from each graph of a chemical structure using the function $f : G \rightarrow R$. It can determine a chemical molecule's physical features, which sets it apart from other graph invariant. Its ability to compute a chemical molecule's physio-chemical properties sets it apart from other graph invariant. Indexes can be classified in a variety of ways, including ev-degree based, eccentricity based, distance based, and vertex degree based. Harold Wiener [5] introduced the idea of indices when calculating the boiling point of organic compounds. In 1975, Milan Randic [6] introduced the most widely used degree-based measure, which is referred to as the Randic index.

The investigation of benzene derivatives, ev-and ve-degrees approaches to understanding breast cancer drugs, and entropy-based indices to compute benzene derivative attributes [7]. According to Gnanaraj et al. [8], degree-based indices were employed for the purpose of computing, analyzing, and investigating the two-dimensional structures of non-steroidal anti-inflammatory drugs (NSAIDs). Azeem et al. [9] examined the characteristics of anxiety drugs using a topological indicator and a linear regression model. Adnan et al. [10] study on anti-tuberculosis drugs employed a linear regression model in combination with eleven degree-based topological indices. They noted that a number of indices, such as the Randic index ($r = 0.984$), the geometric arithmetic index ($r = 0.917$), the harmonic index ($r = 0.891$), the sum connectivity index ($r = 0.919$), and polarization ability, are helpful in determining molar refraction measurement. The strongest correlation ($r = 0.980$) is seen by the ABC-index. The Zagreb index has a 0.963 association with enthalpy, which is one of the distinctive features of anti-malarial medications that Zhang [11] explained through the analysis of degree-based-indices. The polarizability and the Sum Connectivity index have a strong correlation ($r = 0.969$); the redefined Zagreb indices with enthalpy have 0.947, 0.958, and 0.962, respectively; the forgotten index with enthalpy has $r = 0.969$; and the Sum connectivity index has the strongest correlation with the boiling point and flash point (0.948). Muhammad Waheed Rasheed et al. [12] used a linear regression model and topological indicators to investigate and highlight a number of

useful indices, such as the RR index (r =0.9664), the sum connectivity index, which has a very high correlation with Enthalpy (0.9677), flash point (0.9297), molar refractivity (0.9898), and molar volume (0.9273). The Zagreb indices for heart attack medications range from 0.8035 to 0.968. In this article, we examine the idea of cordial label-based topological indices for a linear regression model, since there are many studies with applications for degree-based indices.

The following points outline how our work contributed to this paper:

• To investigate heart attack drugs, the eight topological indices on cordial label-based topological indices are used to calculate the results.

• We use the linear, quadratic, cubic, logarithmic and exponential curves to find the regression model to find a relationship between topological indices and experimental graph data. It is quite easy to use basic linear regression to look at the relationship between two variables. Calculating the value of an output variable in order to ascertain the value of an input variable.

• Although the physicochemical property values have already been determined by laboratory testing, we estimate the heart attack's properties using statistical methods. All the statistical parameters and regression equations are obtained by using SPSS software.

• In the computations, the correlation coefficient is very important because its values show how well the theoretical experiments were conducted. When developing drugs for heart attack conditions, pharmacists and chemists can benefit from these characteristics. The P-test shows how significant the correlation coefficients are. Significant results require both high correlation coefficients and a low P-value.

• Every line in the graphs is created using Microsoft Excel to make it simple to analyze the graphical data that is shown.

The paper is organized as follows:

In Section 2, fundamental definitions, all topological indices are defined, and an overview of their literature is provided. Section 3 provides an explanation of every method utilized to calculate findings linked to the topological index. Tables containing topological indices and experimental values for anti-heart attack drugs are provided in Section 4. Section 5 contains all statistical computations, including a comparison of topological indices based on cordial labelling and those derived from a degree-based approach for reference. A graphical comparison of each correlation coefficient may be seen in Section 6. Section 7 discusses applications of the topological indices used in the article. Section 8 presents the findings, conversation, and concluding remarks. Reference is listed at the conclusion of the work.

2. Fundamental definitions and an overview of the literature

If a connection exists between any two nodes in a basic graph G (V, E), which consists of nodes V(G) and edges E(G), then the graph is said to be connected. Every graph in this article is two-dimensional, planar (no crossings), undirected (unordered), and simple (no multiple edges or loops). The total number of edges that occur on a vertex is its degree. One is the least vertex degree, and three is the maximum. The joining of two vertices forms an edge, or a bridge, and is represented as e = rs = (r, s). In chemistry, the concept of valence is connected to the idea of degree. See Sonawane et al. [13] for additional details regarding the fundamentals of graph theory.

1. Cordial Labelling

Cordial labelling was initially introduced and defined by Cahit [14] in 1987 as a function $f: V(G) \rightarrow \{1, 0\}$ and for each $\alpha\,\beta$ assign the label $|f(\varphi) - f(\omega)|$. The function f is said to be cordial labelling of G if $\left|\varphi_f(1) - \varphi_f(0)\right| \leq 1\ and\ \left|e_f(1) - e_f(0)\right| \leq 1$ where $e_f(t)$ and $\varphi_f(t)$ denote the number of edges and

vertices of G with label $t\ (=0\ or\ 1)$ respectively. The graph which admits cordial labelling is called cordial graph.

2. Incident of a vertex

G. P. Rathinabai et al. [15] defines a incident of a vertex $L_I(\varphi)$ as

$$L_I(\varphi) = \sum_{\forall \varphi \in V(G)} f(\varphi\omega)$$

where $f(\varphi\omega)$ is the label assigned to the edge $\varphi\omega$ i.e., incident of a vertex φ is the sum of all the labels of the edges that intersect with φ.

3. First and Second Zagreb Index

The first and second Zagreb indices were published in 1972 by Gutman and Trinajestic [16]. The Z-indices and total pi-electron energy were found to be related. Here's how these indices are calculated:

$$M_1(G) = \sum_{\forall \varphi\omega \in \mathrm{E(G)}} [\mathrm{L_I}(\varphi) + \mathrm{L_I}(\omega)]$$

and

$$M_2(G) = \sum_{\forall \varphi\omega \in \mathrm{E(G)}} [\mathrm{L_I}(\varphi) \times \mathrm{L_I}(\omega)]$$

The study of connected quasi-unicyclic network structures makes use of these indices [17]. Wei et al. [18] claim that the Z-indices are a great resource for understanding the properties of corona drugs.

4. Hyper Zagreb Index

In 2013, Shirdel proposed the Hyper Zagreb index [19]. The mathematical statement describing the HM index is as follows:

$$HM(G) = \sum_{\forall \varphi\omega \in E(G)} \big(L_I(\varphi) + L_I(\omega)\big)^2$$

There are numerous criteria to verify whether connected graphs are Hamiltonian. Simple graphs such as wheels, forests, and chemical graphs can have their Hamiltonian nature described by the HM-index [20]. According to Bommanahal et.al., [21], the HM-index can investigate intermediate graph aspects that are useful in network theory.

5. Reciprocal Randic index

Gutman [22] stated the reciprocal Randic index in 2014. Mathematically, the RR index is expressed as follows:

$$RR(G) = \sum_{\forall \varphi\omega \in E(G)} \sqrt{L_I(\varphi) \times L_I(\omega)}$$

6. Harmonic index

In 1987, Fajtlowicz proposed the harmonic index for the first time [23]. Being a computer engineer, he proposed this index for the networks of computers. Zhong [24] proposed an analogous degree-related for chemical graphs, particularly on trees, here is the definition of the H-index:

$$H(G) = \sum_{\forall \varphi\omega \in E(G)} \frac{2}{L_I(\varphi) + L_I(\omega)}$$

Hu and Zhang [25] state that the H-index is utilized to ascertain the extreme values of chemical trees about the order and number of molecular graphs.

7. Sum Connectivity index

The sum connectivity index originated in 2010 by Zhou and Trinajsti´ c [26]. It was suggested while presenting the H-index's generic form and it is defined as

$$SCI(G) = \sum_{\forall \varphi\omega \in E(G)} \frac{1}{\sqrt{L_I(\varphi) + L_I(\omega)}}$$

The boiling point and anti-tuberculosis drug enthalpy have a strong association (r = 0.957) that is influenced by the SC-index at [10].

8. Forgotten index

In 2015, Furtula and Gutman [27] created the Forgotten index to measure the characteristics of carbon compounds and they found a correlation between the F-index and some unique properties of the data set's octane isomers. The calculation goes like this:

$$F(G) = \sum_{\forall \varphi\omega \in E(G)} \{[L_I(\varphi)]^2 + [L_I(\omega)]^2\}$$

9. Hyper Forgotten index

Inspired by the Forgotten Index, the hyper Forgotten Index is a vertex degree-based index. The HF-index has the following mathematical definition:

$$F(G) = \sum_{\forall \varphi\omega \in E(G)} \{[L_I(\varphi)]^2 + [L_I(\omega)]^2\}^2$$

The characteristics of nanostar dendrimers can be explained by the Hyper Forgotten index [28]. Tree-like branches are joined to one another repeatedly by branching molecules called dendrimers, with a core component. Mahboob et al. [29] and Alam et al. [30] provide more information on chemical topological indices.

3. Techniques and Approaches

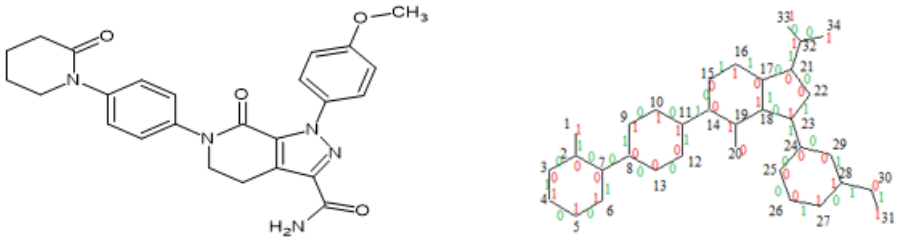
To determine the degree-related indices, three methods can be applied: edge partitioning, vertex partitioning, and degree counting. The topology of the relevant molecular graph of the underlying chemical is examined using graph theoretical methods. Prior to organizing the vertices based on degree, count each vertex individually. A line that connects two vertices forms an edge. In this case, a function $f: V(G) \to \{0,1\}$, and give the label $|f(\varphi) - f(\omega)|$ for each $\varphi\,\omega$. If $|\varphi_f(0) - \varphi_f(1)| \leq 1$ *and* $|e_f(0) - e_f(1)| \leq 1$ then the function f is considered as cordial label of G. where $e_f(t)$ and $\varphi_f(t)$ denote the number of edges and vertices of G with label t (= 1 *or* 0) respectively. Thus, the graph which admits cordial label is called cordial graph. The 2D structures of pharmaceuticals are depicted using the software chemSketch. Microsoft Excel may be used to create both correlation and line graphs. To make line graphs, you can utilize additional programs like Mathematica and Maple. Using the calculator, we were able to determine the values of the topological indices shown in Table 2. The physical and chemical properties and chemical structures of the heart attack medications were obtained from ChemSpider [31]. With SPSS software, we generated several regression models and used to compute topological indices to analyze the QSPR study.

4. Topological analysis of heart attack drugs structures

This study employs eight cordial label-based molecular descriptors to examine the twelve two-dimensional structures of heart attack medicines. While topological indices talk about the two-dimensional drug graphs, these structures are three-dimensional. Beyond heart attacks, these drugs are useful in the treatment of heart-related illnesses. Many medications are used to treat heart

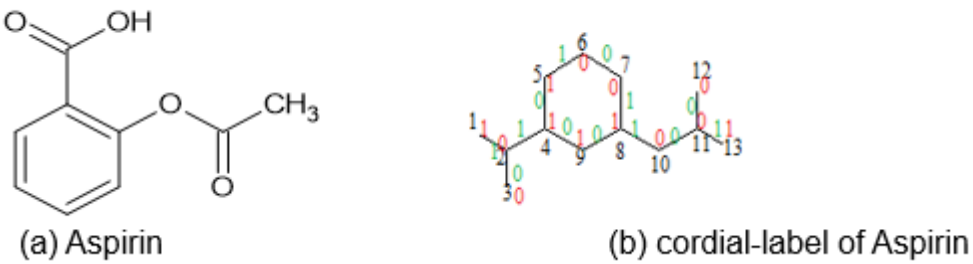
problems, such as warfarin, ticagrelor, quinapril, rivaroxaban, candesartan, captopril, carvedilol, dipyridamole, apixaban, ramipril, atenolol and aspirin. Overall, aspirin is the most significant drug. Aspirin serves as a preventive by stopping naturally occurring chemicals that cause fever, discomfort, stiffness, and blood clots from mixing. The molecular structures of these drugs are displayed in Figure 1. According to the QSPR study, there is a substantial correlation between the physical properties of drugs used to treat heart attacks and the topological indices as mentioned above.

Table 1 displays the seven physicochemical experimental values of heart attack medications. Cordial label-based topological descriptors are used to generate the estimated values of these medications. The estimated and experimental values correlate, indicating the importance of topological indices. In Table 1, Six experimental parameters are utilized in the study of heart attack drugs namely boiling point, flash point, enthalpy, molar refraction, molar volume and surface tension. All the drug properties and two-dimensional structures displayed in Table 1 and Figure 1 and are derived from Pub Chem. The correlation coefficient calculations are based on the characteristics shown in Table 1. As stated in the following formulas, all of the topological indices are calculated utilizing the idea of a cordial label-based topological method. Eight cordial label-based topological indices are first and second Zagreb index, the Hyper Zagreb index, the Reciprocal Randic index, the Harmonic index, the Sum connectivity index, the Forgotten index, and the Hyper forgotten index are calculated to estimate the characteristics of heart attack medications. The values of the HF-index and H-index are highest and lowest, respectively, as Table 2 illustrates. The values of all the cordial label-based topological indices are given in Table 2.



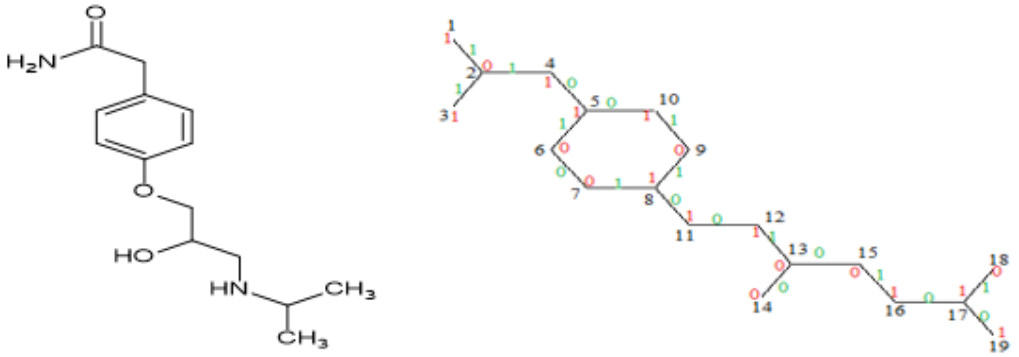
(a) Apixaban (b) cordial-label of Apixaban

Fig.1. Apixaban $[C_{25}H_{25}N_5O_4]$ has 34 atoms and 38 bonds and its cordial label consisting of $\varphi_f(1) = 17, \varphi_f(0) = 17$ *and* $e_f(1) = 19, e_f(0) = 19$



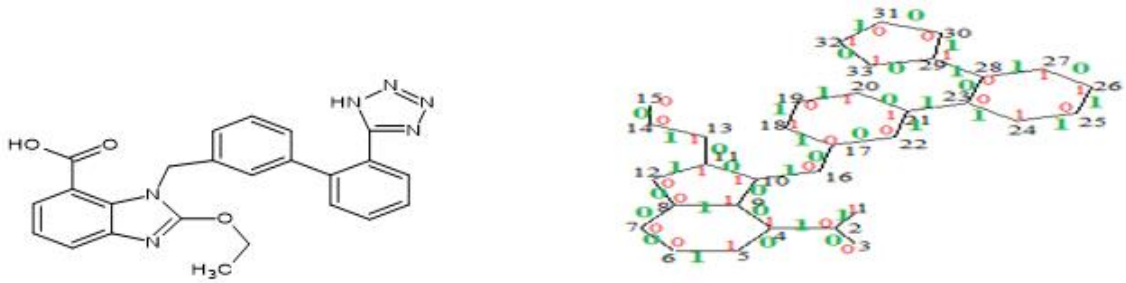
(a) Aspirin (b) cordial-label of Aspirin

Fig.2. Aspirin $[C_9H_8O_4]$ has 13 atoms and 13 bonds and its cordial label consisting of $\varphi_f(1) = 6, \varphi_f(0) = 7$ *and* $e_f(1) = 6, e_f(0) = 7$



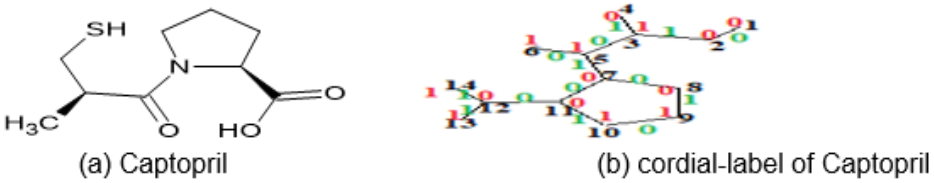
(a) Atenolol (b) Cordial-label of Atenolol

Fig.3. Atenolol $[C_{14}H_{22}N_2O_3]$ has 19 atoms and 19 bonds and its cordial label consisting of $\varphi_f(1) = 10$, $\varphi_f(0) = 9$ *and* $e_f(1) = 9, e_f(0) = 10$



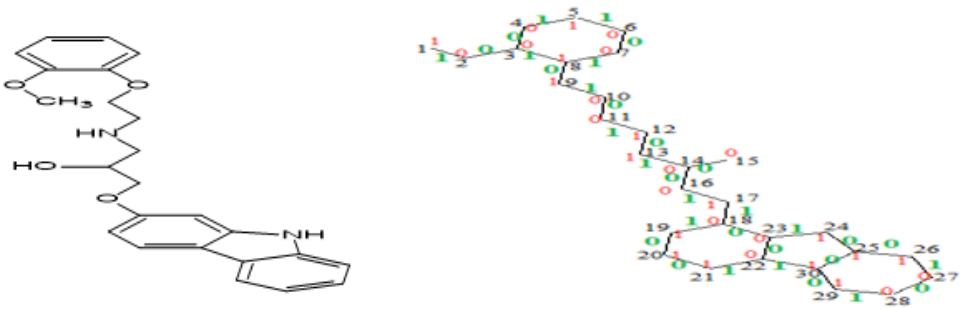
(a) Candesartan (b) Cordial-label of Candesartan

Fig.4. Candesartan $[C_{24}H_{20}N_6O_3]$ has 33 atoms and 37 bonds and its cordial label consisting of $\varphi_f(1) = 16$, $\varphi_f(0) = 17$ *and* $e_f(1) = 19, e_f(0) = 18$



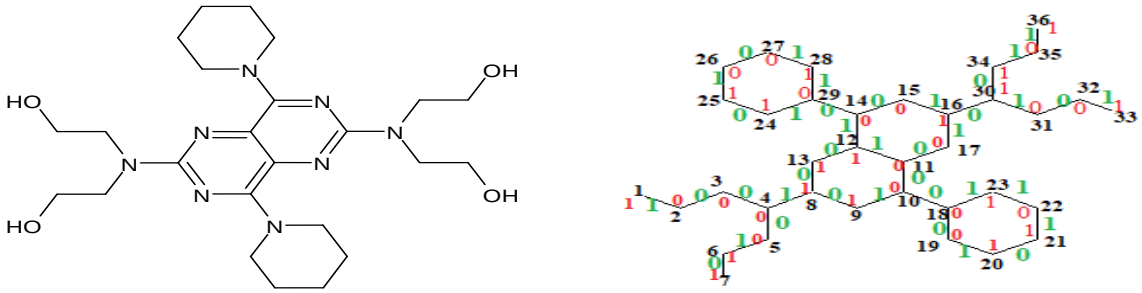
(a) Captopril (b) cordial-label of Captopril

Fig.5. Captopril $[C_9H_{15}NO_3S]$ has 14 atoms and 14 bonds and its cordial label consisting of $\varphi_f(1) = 7$, $\varphi_f(0) = 7$ *and* $e_f(1) = 7, e_f(0) = 7$



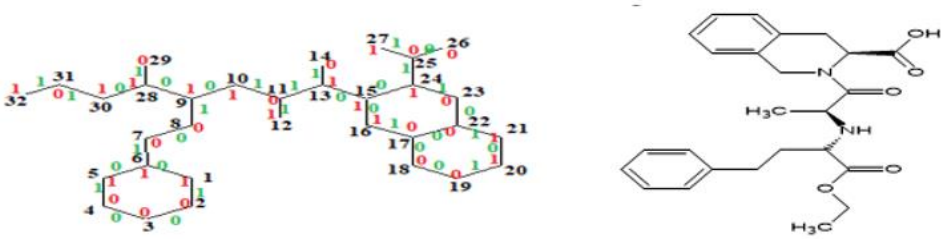
(a) Carvedilol (b) Cordial-label of Carvedilol

Fig.6. Carvedilol $[C_{24}H_{26}N_2O_4]$ has 30 atoms and 33 bonds and its cordial label consisting of $\varphi_f(1) = 15$, $\varphi_f(0) = 15$ *and* $e_f(1) = 16, e_f(0) = 17$



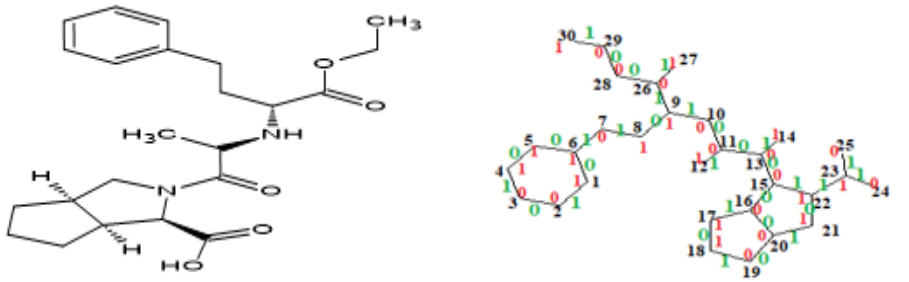
(a) Dipyridamole (b) cordial-label of Dipyridamole

Fig.7. Dipyridamole $[C_{24}H_{40}N_8O_4]$ has 36 atoms and 39 bonds and its cordial label consisting of $\varphi_f(1) = 18$, $\varphi_f(0) = 18$ *and* $e_f(1) = 20, e_f(0) = 19$



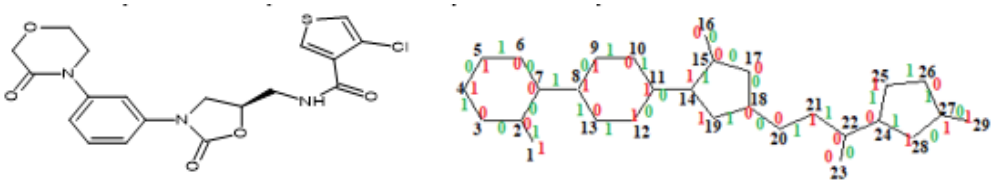
(b) Cordial-label of Quinapril (a) Quinapril

Fig.8. Quinapril $[C_{25}H_{30}N_2O_5]$ has 32 atoms and 34 bonds and its cordial label consisting of $\varphi_f(1) = 16$, $\varphi_f(0) = 16$ *and* $e_f(1) = 17, e_f(0) = 17$



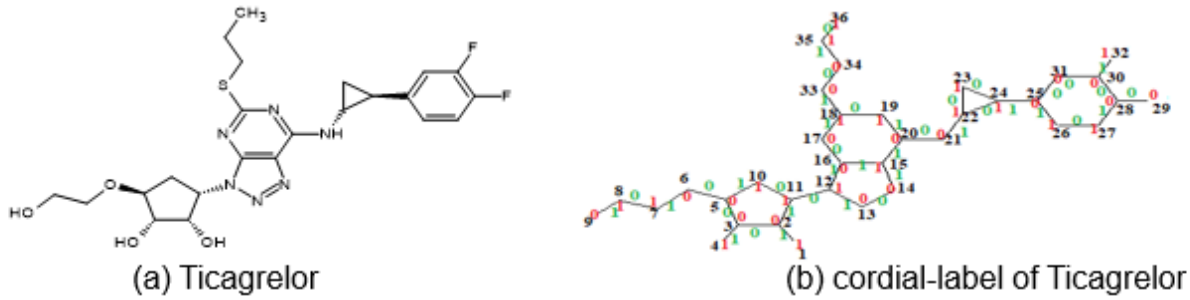
(a) Ramipril (b) cordial-label of Ramipril

Fig.9. Ramipril $[C_{23}H_{32}N_2O_5]$ has 30 atoms and 32 bonds and its cordial label consisting of $\varphi_f(1) = 15$, $\varphi_f(0) = 15$ *and* $e_f(1) = 16, e_f(0) = 16$



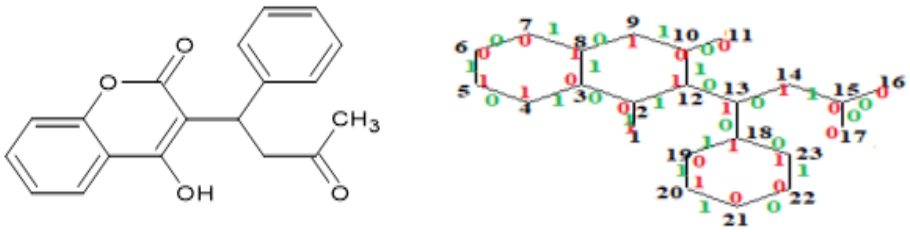
(a) Rivaroxaban (b) Cordial-label of Rivaroxaban

Fig.10. Rivaroxaban $[C_{19}H_{18}Cl\,N_3O_5\,S]$ has 29 atoms, 32 bonds and its cordial label consisting of $\varphi_f(1) = 14$, $\varphi_f(0) = 15$ *and* $e_f(1) = 16, e_f(0) = 16$



(a) Ticagrelor (b) cordial-label of Ticagrelor

Fig.11. Ticagrelor $[C_{23}H_{28}\,F_2N_6O_4\,S]$ has 36 atoms and 40 bonds and its cordial label consisting of $\varphi_f(1) = 18,\ \varphi_f(0) = 18\ and\ e_f(1) = 20, e_f(0) = 20$



(a) Warfarin (b) Cordial-label of Warfarin

Fig.12. Warfarin $[C_{19}H_{16}\,O_4]$ has 23 atoms and 25 bonds and its cordial label consisting of $\varphi_f(1) = 11,\ \varphi_f(0) = 12\ and\ e_f(1) = 13, e_f(0) = 12$

5. Regression models

Logical regression involves fitting a linear equation to observable data to model the relationship between two variables. While the second variable is thought to be dependent, and the first variable is thought to be independent. For each of the topological indices, the regression model can compute as follows:

$$Y = \alpha + \beta X;\ N, R^2, F\ [\text{Linear curve}]$$
$$Y = \alpha + \beta X + \gamma X^2;\ \ N, R^2, F\ [\text{Quadratic curve}]$$
$$Y = \alpha + \beta X + \gamma X^2 + \delta X^3;\ \ N, R^2, F[\text{Cubic curve}]$$
$$Y = \alpha + \beta \log X;\ \ N, R^2, F[\text{Logarithmic curve}]$$
$$Y = \alpha\, e^{\beta X};\ \ N, R^2, F[\text{Exponential curve}]$$

Where Y represents the dependent variable, while X is the independent parameter. Cordial label-based topological indices' estimated values are denoted by parameter X, whereas the physical or chemical characteristics of the medication used to treat heart attacks are represented by parameter Y. When X = 0, the intercept, or constant, parameter indicates the expected outcome. The slope parameter β indicates the expected rise in response for every unit change in X. In the regression model constant is represented by $'\alpha'$, while $'\beta','\gamma'\ and\ '\delta'$ represent the regression coefficients. Here N=12 be total number of samples of the drugs, 'R' be the correlation coefficients and 'F' is the Fisher's statistic [32, 33]. The best regression model was determined based on the maximum values of $R^2, R\ and\ F$.

1. First Zagreb index $[M_1(G)]$

- Boiling point = $209.45 + 6.087[M_1(G)]$
- Flash point = $60.426 + 3.859[M_1(G)]$
- Enthalpy = $45.406 + 0.762[M_1(G)]$
- Molar refractivity = $19.403 + 1.204[M_1(G)]$
- Molar volume = $104.88 + 2.628[M_1(G)]$
- Surface tension = $41.413 + 0.234[M_1(G)]$

2. Second Zagreb index $[M_2(G)]$

- Boiling point = $270.43 + 8.726[M_2(G)]$
- Flash point = $102.9 + 5.439[M_2(G)]$
- Enthalpy = $53.18 + 1.089[M_2(G)]$
- Molar refractivity = $33.444 + 1.678[M_2(G)]$
- Molar volume = $141.83 + 3.509[M_2(G)]$
- Surface tension = $43.434 + 0.344[M_2(G)]$

3. Hyper Zagreb index $[HM(G)]$

- Boiling point = $261.95 + 2.015[HM(G)]$
- Flash point = $97.869 + 1.255[HM(G)]$
- Enthalpy = $52.077 + 0.252[HM(G)]$
- Molar refractivity = $31.397 + 0.39[HM(G)]$
- Molar volume = $136.57 + 0.821[HM(G)]$
- Surface tension = $43.336 + 0.078[HM(G)]$

4. Reciprocal Randic index $[RR(G)]$

- Boiling point = $225.237 + 13.22[RR(G)]$
- Flash point = $69.042 + 8.429[RR(G)]$
- Enthalpy = $47.292 + 1.658[RR(G)]$
- Molar refractivity = $22.915 + 2.603[RR(G)]$
- Molar volume = $113.271 + 5.658[RR(G)]$
- Surface tension = $41.528 + 0.525[RR(G)]$

5. Harmonic index $[H(G)]$

- Boiling point = $158.634 + 15.87[H(G)]$
- Flash point = $20.85 + 10.31[H(G)]$
- Enthalpy = $39.401 + 1.974[H(G)]$
- Molar refractivity = $5.99 + 3.252[H(G)]$
- Molar volume = $63.855 + 7.495[H(G)]$
- Surface tension = $41.422 + 0.545[H(G)]$

6. Sum connectivity index $[SCI(G)]$

- Boiling point = $166.058 + 22.58[SCI(G)]$
- Flash point = $26.662 + 14.62[SCI(G)]$
- Enthalpy = $40.104 + 2.82[SCI(G)]$
- Molar refractivity = $8.045 + 4.602[SCI(G)]$
- Molar volume = $70.59 + 10.51[SCI(G)]$
- Surface tension = $41.003 + 0.808[SCI(G)]$

7. Forgotten index $[F(G)]$

- Boiling point = $255.58 + 3.727[F(G)]$
- Flash point = $93.991 + 2.32[F(G)]$
- Enthalpy = $51.247 + 0.466[F(G)]$
- Molar refractivity = $29.59 + 0.727[F(G)]$
- Molar volume = $131.13 + 1.546[F(G)]$
- Surface tension = $43.424 + 0.141[F(G)]$

8. Hyper Forgotten index $[HF(G)]$

- Boiling point = $376.41 + 0.512[HF(G)]$
- Flash point = $172.5 + 0.312[HF(G)]$
- Enthalpy = $66.264 + 0.064[HF(G)]$
- Molar refractivity = $54.244 + 0.098[HF(G)]$
- Molar volume = $188.15 + 0.198[HF(G)]$
- Surface tension = $48.659 + 0.018[HF(G)]$

5.1. Computed Statistical parameters

This section makes use of multiple statistical parameters. A parameter is a helpful statistical analysis tool connected to the features that are used to characterize a certain population. It is employed to convey a certain characteristic shared by the whole population. The number of members in a sample is denoted by the letter "N". The values of N, which are not displayed in the table but are taken into account for the computation in Tables 3–11, are 12. "β" represents the slope value, while "α" is the constant. The correlation coefficient (r) is a statistical indicator of how well changes in one variable's value correlate to changes in another. R could be greater or less than zero. A positive number indicates a direct association between two items, while a negative value indicates an inverse relationship. Given that all of the correlation coefficients are positive, there is a significant direct link between them. The correlation coefficient ranges from $-1 \leq R \leq 1$. A P-value establishes the probability of reaching the observed outcomes in the case that the null hypothesis is correct. Every P-value in this article must be less than 0.05, signifying that each and every result is significant. Every property has a strong association, with the exception of surface tension. As the F-value rises, the variance between sample averages and within-sample variation also rises. It can be seen from the lower value of P that F is higher. With the use of the conventional first and second Zagreb index-indices, the properties of the anti-heart attack medications listed in Tables 7 and 8 were assessed quite well. Regarding the absolute values of R, we refer to them as R^2. R values can be either positive or negative depending on how two parameters are inversely and directly related. Table 3 shows how the six heart attack medicine characteristics and the first Zagreb index $[M_1(G)]$ correlate. The minimum and maximum correlations for the first Zagreb index are 0.614 and 0.963, respectively. Table 4 presents the significant values of P and all the parameters that form the second Zagreb index $[M_2(G)]$. The Hyper Zagreb index (HM-index) numerical results are shown in Table 5. Correlation values for the HM-index range from 0.601 to 0.934. The Reciprocal Randic index (RR-index) statistical parameter values are shown in Table 6. For the RR-index, the correlation coefficients range from 0.965 to 0.636. All P values for this RR-index are less than 0.03 and all F values are more than 6.796. The surface tension characteristic is not significant because its P-value is more than 0.05 in Table 7, which displays the harmonic index $[H(G)]$. The statistical parameter values range from 0.986 to 0.541. Except for surface tension, all P values for this $H(G)$-index are almost 0. The Sum connectivity index, or SC-index, has F-values ranging from 4.774 to 108.956 in Table 9. The SC-index has correlation coefficients ranging from 0.988 to 0.568 for all variables. Table 9 shows the parameters with correlation values greater than 0.9: Enthalpy (0.953), Molar refraction (0.988), Flash point (0.924), Molar volume (0.93), and Boiling point (0.957). Table 9 displays details on the Forgotten index. This measure has a correlation that varies from 0.584 to 0.929. The Hyper Forgotten index (HF-index) statistical variables are shown in Table 10. The range of correlation for this HF-index is 0.48 to 0.82. Tables 7, 8, and 10 contain the three unimportant numbers that are specifically related to the surface tension characteristic in the entire computation carried out in this paper. In Table 12 below, we compare the cordial label-based topological indices from our study (Study A) with the degree-based approach from Muhammad Waheed Rasheed et al. [12] (Study B).

Table 1. Physicochemical characteristics of heart attack drugs

Medication name	Boiling Point [°Cat760mmHg]	Enthalpy [J]	Flash point [°C]	Molar refractivity [cm³]	Surface Tension [dyne/cm]	Molar volume [cm³]
Apixaban	770.5±60	112.2	419.8±3	125.6	61	323.4
Aspirin	321.4±25	59.5	131.2±16.7	44.5	49.9	139.6
Atenolol	508.0±50	81.9	261.1±30.2	74.3	45	236.7
Candesartan	754.8±70	115.4	410.3±35.7	122.5	59.6	310.5
Captopril	427.0±40	74.8	212.1±27.3	54.4	54.3	170.7
Carvedilol	655.2±55	101.4	350.1±31.5	119.6	53.9	325.1
Dipyridamole	806.5±75	122.9	441.5±37.1	139.4	81.6	373
Quinapril	662.0±55	102.3	354.1±31.5	119.5	52.3	360.1
Ramipril	616.2±55	96.1	326.4±31.5	111.4	50.2	346.8
Rivaroxaban	732.6±60	106.9	396.9±32.9	106.7	61	298.5
Ticagrelor	777.6±70	118.7	424.0±35.7	126.3	63.3	311.9
Warfarin	515.2±50	82.9	188.8±23.6	84.4	58.7	235.8

Table 2. Topological indices of heart attack drugs

Drug Name	$M_1(G)$	$M_2(G)$	HM(G)	RR(G)	H(G)	SCI(G)	F(G)	HF(G)
Apixaban	92	59	258	40.56	38.33	26.25	140	734
Aspirin	26	12	56	10.83	14.33	9.52	32	100
Atenolol	41	21	99	16.66	20.17	13.59	57	235
Candesartan	91	59	255	40.9	35.17	24.98	137	727
Captopril	30	17	76	13.49	13	8.99	42	172
Carvedilol	74	42	184	33.56	33.83	23.16	100	408
Dipyridamole	90	52	228	40.97	38	26.78	124	528
Quinapril	77	43	203	31.99	35.23	23.98	117	679
Ramipril	70	39	168	32.314	32.83	22.55	93	359
Rivaroxaban	75	46	199	34.14	32.17	22.17	107	503
Ticagrelor	98	62	276	44.02	38.47	27.13	152	916
Warfarin	63	41	183	26.9	24.17	16.91	101	559

Table 3. Data analysis for first Zagreb index $[M_1(G)]$

Characteristics	α	β	R	R^2	F	P	Indicator
Boiling point	209.445	6.087	0.961	0.924	121.216	0	Significant
Flash point	60.426	3.859	0.909	0.826	47.405	0	Significant
Enthalpy	45.406	0.762	0.959	0.92	114.423	0	Significant
Molar refractivity	19.403	1.204	0.963	0.927	126.799	0	Significant
Molar volume	104.881	2.628	0.867	0.751	30.194	0	Significant
Surface tension	41.413	0.234	0.614	0.377	6.063	0.034	Significant

Table 4. Data analysis for second zagreb index $[M_2(G)]$

Characteristics	α	β	R	R^2	F	P	Indicator
Boiling point	270.434	8.726	0.938	0.879	72.676	0	Significant
Flash point	102.901	5.439	0.872	0.76	31.611	0	Significant
Enthalpy	53.18	1.089	0.933	0.87	66.724	0	Significant
Molar refractivity	33.444	1.678	0.913	0.834	50.072	0	Significant
Molar volume	141.829	3.509	0.788	0.62	16.327	0.002	Significant
Surface tension	43.434	0.344	0.614	0.376	6.036	0.034	Significant

Table 5. Data analysis for Hyper zagreb index $[HM(G)]$

Characteristics	α	β	R	R^2	F	P	Indicator
Boiling point	261.946	2.015	0.934	0.873	68.807	0	Significant
Flash point	97.869	1.255	0.868	0.753	30.459	0	Significant
Enthalpy	52.077	0.252	0.93	0.865	64.328	0	Significant
Molar refractivity	31.397	0.39	0.915	0.838	51.599	0	Significant
Molar volume	136.566	0.821	0.795	0.632	17.137	0.002	Significant
Surface tension	43.336	0.078	0.601	0.362	5.667	0.039	Significant

Table 6. Data analysis for reciprocal Randic index $[RR(G)]$

Characteristics	α	β	R	R^2	F	P	Indicator
Boiling point	225.237	13.22	0.965	0.93	133.606	0	Significant
Flash point	69.042	8.429	0.917	0.841	52.804	0	Significant
Enthalpy	47.292	1.658	0.964	0.93	131.875	0	Significant
Molar refractivity	22.915	2.603	0.961	0.924	122.376	0	Significant
Molar volume	113.271	5.658	0.862	0.743	28.906	0	Significant
Surface tension	41.528	0.525	0.636	0.405	6.796	0.026	Significant

Table 7. Data analysis for Harmonic index $[H(G)]$

Characteristics	α	β	R	R^2	F	P	Indicator
Boiling point	158.634	15.87	0.95	0.902	92.229	0	Significant
Flash point	20.85	10.31	0.92	0.847	55.279	0	Significant
Enthalpy	39.401	1.974	0.942	0.887	78.749	0	Significant
Molar refractivity	5.99	3.252	0.986	0.972	344.964	0	Significant
Molar volume	63.855	7.495	0.937	0.878	71.977	0	Significant
Surface tension	41.422	0.545	0.541	0.293	4.143	0.069	Insignificant

Table 8. Data analysis for Sum connectivity index $[SCI(G)]$

Characteristics	α	β	R	R^2	F	P	Indicator
Boiling point	166.058	22.58	0.957	0.916	108.956	0	Significant
Flash point	26.662	14.62	0.924	0.854	58.527	0	Significant
Enthalpy	40.104	2.82	0.953	0.908	98.421	0	Significant
Molar refractivity	8.045	4.602	0.988	0.976	399.5	0	Significant
Molar volume	70.59	10.51	0.93	0.865	64.226	0	Significant
Surface tension	41.003	0.808	0.568	0.323	4.774	0.054	Insignificant

Table 9. Data analysis for Forgotten index [F(G)]

Characteristics	α	β	R	R^2	F	P	Indicator
Boiling point	255.58	3.727	0.929	0.863	63.085	0	Significant
Flash point	93.991	2.32	0.862	0.744	29.021	0	Significant
Enthalpy	51.247	0.466	0.926	0.857	59.881	0	Significant
Molar refractivity	29.59	0.727	0.917	0.841	53.051	0	Significant
Molar volume	131.13	1.546	0.805	0.648	18.398	0.002	Significant
Surface tension	43.424	0.141	0.584	0.341	5.18	0.046	Significant

Table 10. Data analysis for Hyper Forgotten index [HF(G)]

Characteristics	α	β	R	R^2	F	P	Indicator
Boiling point	376.41	0.512	0.82	0.673	20.601	0.001	Significant
Flash point	172.5	0.312	0.746	0.556	12.517	0.005	Significant
Enthalpy	66.264	0.064	0.82	0.672	20.488	0.001	Significant
Molar refractivity	54.244	0.098	0.792	0.627	16.836	0.002	Significant
Molar volume	188.15	0.198	0.664	0.441	7.888	0.019	Significant
Surface tension	48.659	0.018	0.48	0.231	3.001	0.114	Insignificant

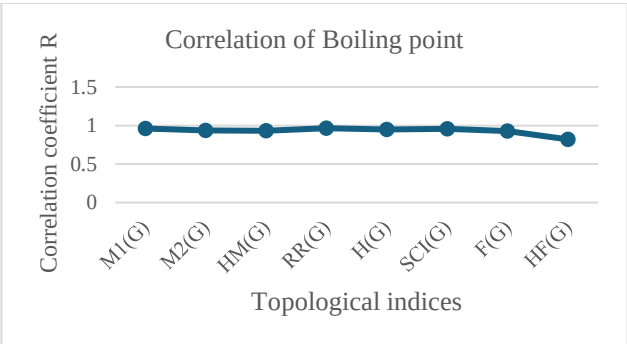
Table 11. Comparison of correlation coefficients for topological indices

Molecular descriptor	Boiling point	Flash point	Enthalpy	Molar refractivity	Molar volume	Surface tension
$M_1(G)$	0.961	0.909	0.959	0.963	0.867	0.614
$M_2(G)$	0.938	0.872	0.933	0.913	0.788	0.614
HM(G)	0.934	0.868	0.93	0.915	0.795	0.601
RR(G)	0.965	0.917	0.964	0.961	0.862	0.636
H(G)	0.95	0.92	0.942	0.986	0.937	0.541
SCI(G)	0.957	0.924	0.953	0.988	0.93	0.568
F(G)	0.929	0.862	0.926	0.917	0.805	0.584
HF(G)	0.82	0.746	0.82	0.792	0.664	0.48

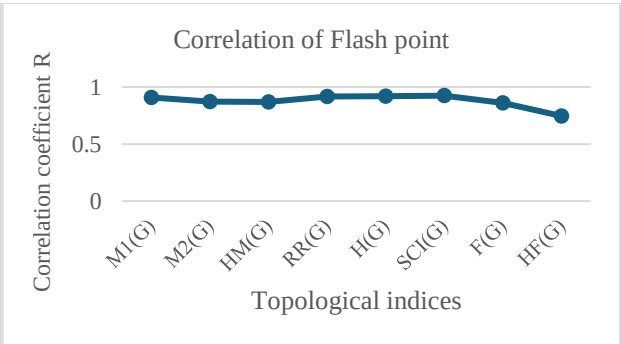
In Table 12 below, we compare the cordial label-based topological indices from our study (Study A) with the degree-based approach from Muhammad Waheed Rasheed et al. [24] (Study B).

Table 12. Comparison of cordial label based topological indices with degree-based approach.

	Study A	Study B	Study A	Study B	Study A	Study B	Study A	Study B	Study A	Study B	Study A	Study B
Molecular descriptor	Boiling point	Boiling point	Flash point	Flash point	Enthalpy	Enthalpy	Molar refractivity	Molar refractivity	Molar volume	Molar volume	Surface tension	Surface tension
$M_1(G)$	0.961	0.9464	0.909	0.9014	0.959	0.9446	0.963	0.933	0.867	0.864	0.614	0.68
$M_2(G)$	0.938	0.9627	0.872	0.9186	0.933	0.9623	0.913	0.968	0.788	0.883	0.614	0.66
HM(G)	0.934	0.962	0.868	0.9227	0.93	0.9467	0.915	0.94	0.795	0.871	0.601	0.635
RR(G)	0.965	0.9664	0.917	0.9253	0.964	0.966	0.961	0.978	0.862	0.903	0.636	0.656
H(G)	0.95	0.9263	0.92	0.8858	0.942	0.929	0.986	0.918	0.937	0.865	0.541	0.691
SCI(G)	0.957	0.9657	0.924	0.9297	0.953	0.9677	0.988	0.99	0.93	0.927	0.568	0.654
F(G)	0.929	0.9635	0.862	0.9196	0.926	0.9607	0.917	0.962	0.805	0.878	0.584	0.666
HF(G)	0.82	0.9401	0.746	0.8898	0.82	0.9374	0.792	0.92	0.664	0.809	0.48	0.689

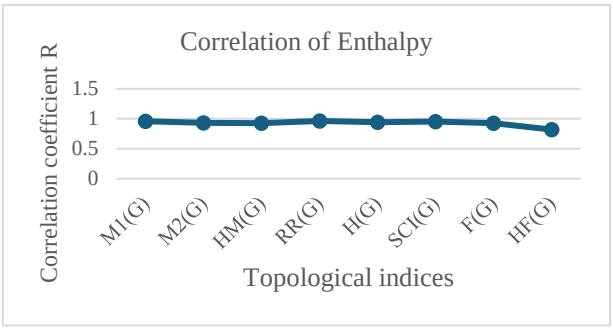


(a) Correlation between Topological indices



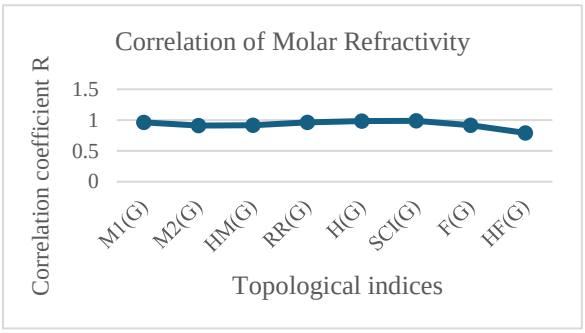
(b) Correlation between Topological indices

and Boiling point

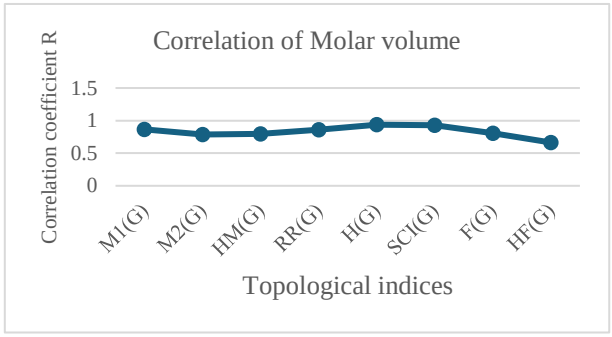


(c) Correlation between Topological indices and Enthalpy

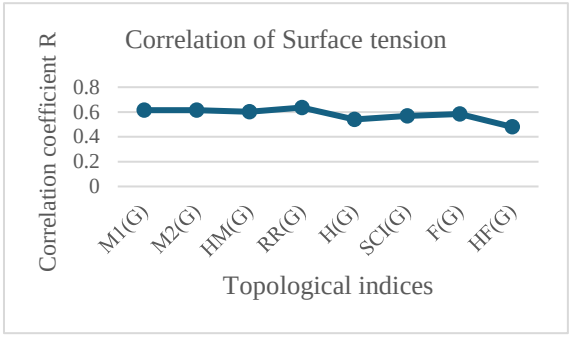
and Flash point



(d) Correlation between Topological indices and Molar Refractivity



(e) Correlation between Topological indices and Molar Volume



(f) Correlation between Topological indices and Surface Tension

Fig.13. Correlation between topological indices and all physicochemical properties

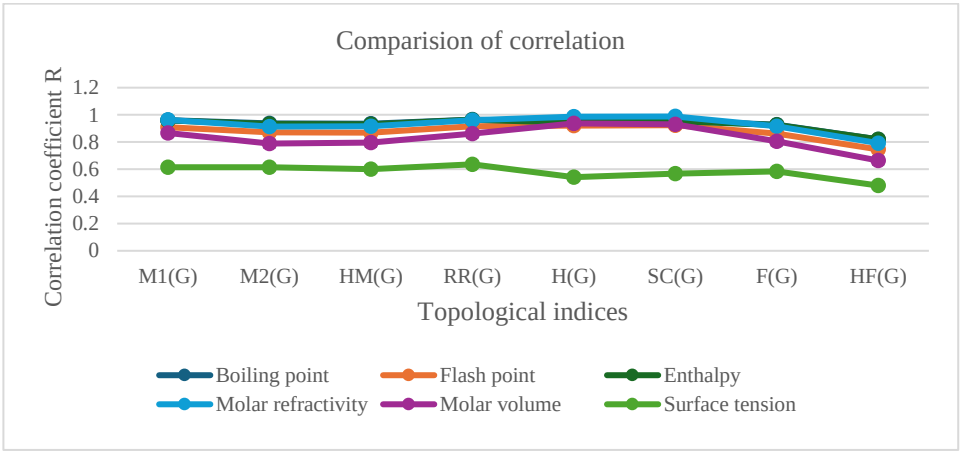


Fig.14. Correlation between Topological indices and all physicochemical properties

Table 13. Logarithmic regression analysis for physicochemical properties verses topological indices

Characteristics	**Indices**	α	β	R^2	F	P	**Indicator**
Boiling point	First zagreb index $[M_1(G)]$	-734.288	328.167	0.904	94.475	0	Significant
Flash point		-527.873	205.64	0.79	37.523	0	Significant
Enthalpy		-71.515	40.788	0.887	78.657	0	Significant
Molar refractivity		-171.536	65.942	**0.936**	146.062	0	Significant

Molar volume		-333.062	149.032	0.813	43.524	0	Significant
Surface tension		9.159	11.653	0.314	4.579	0.058	Insignificant
Boiling point	Second zagreb index $[M_2(G)]$	-359.684	273.967	0.881	73.938	0	Significant
Flash point		-284.228	169.213	0.747	29.554	0	Significant
Enthalpy		-24.793	34.007	0.862	62.434	0	Significant
Molar refractivity		-92.372	53.973	**0.876**	70.857	0	Significant
Molar volume		-144.556	119.323	0.729	26.841	0	Significant
Surface tension		21.373	10.03	0.325	4.82	0.053	Insignificant
Boiling point	Hyper zagreb index [HM(G)]	-819.158	283.7	0.877	71.506	0	Significant
Flash point		-567.395	175.103	0.743	28.931	0	Significant
Enthalpy		-81.873	35.224	0.859	60.881	0	Significant
Molar refractivity		-183.884	56.085	**0.879**	72.558	0	Significant
Molar volume		-349.063	124.422	0.736	27.844	0	Significant
Surface tension		5.423	10.216	0.313	4.563	0.058	Insignificant
Boiling point	Reciprocal radic index [RR(G)]	-419.003	314.484	0.913	105.332	0	Significant
Flash point		-333.415	198.004	0.805	41.289	0	Significant
Enthalpy		-32.58	39.163	0.9	89.519	0	Significant
Molar refractivity		-107.279	62.921	**0.937**	149.121	0	Significant
Molar volume		-186.377	141.767	0.809	42.417	0	Significant
Surface tension		19.188	11.518	0.337	5.093	0.048	Insignificant
Boiling point	Harmonic index [H(G)]	-619.988	375.077	0.873	68.63	0	Significant
Flash point		-474.166	240.421	0.797	39.36	0	Significant
Enthalpy		-56.495	46.374	0.847	55.522	0	Significant
Molar refractivity		-155.673	77.502	**0.955**	213.402	0	Significant
Molar volume		-317.468	181.242	0.889	79.766	0	Significant
Surface tension		17.676	11.98	0.245	3.25	0.102	Insignificant
Boiling point	Sum connectivity index [SC(G)]	-461.058	368.488	0.887	78.642	0	Significant
Flash point		-370.138	235.469	0.806	41.423	0	Significant
Enthalpy		-37.232	45.691	0.866	64.79	0	Significant
Molar refractivity		-121.792	75.788	**0.962**	253.118	0	Significant
Molar volume		-234.986	176.136	0.884	76.083	0	Significant
Surface tension		21.537	12.181	0.267	3.643	0.085	Insignificant
Boiling point	Forgotten index [F(G)]	-681.657	290.48	0.869	66.476	0	Significant
Flash point		-482.38	179.254	0.736	27.883	0	Significant
Enthalpy		-64.832	36.073	0.851	57.267	0	Significant
Molar refractivity		-158.083	57.732	**0.88**	73.404	0	Significant
Molar volume		-295.589	128.909	0.746	29.435	0	Significant
Surface tension		11.383	10.237	0.297	4.231	0.067	Insignificant
Boiling point	Hyper Forgotten index [HF(G)]	-618.829	206.66	**0.779**	35.336	0	Significant
Flash point		-430.905	125.425	0.638	17.653	0.002	Significant
Enthalpy		-57.075	25.671	0.764	32.341	0	Significant
Molar refractivity		-141.354	40.37	0.762	32.086	0	Significant
Molar volume		-249.34	88.67	0.626	16.711	0.002	Significant
Surface tension		15.261	7.007	0.247	3.277	0.1	Insignificant

In Table 13, we observe that the coefficient of determination (R-squared) values is higher for molar refractivity, ranging from 0.876 to 0.962, indicating a strong positive correlation with physicochemical properties. Additionally, the P-values are close to 0 in most cases, except for surface tension, suggesting that the regression model is significant for all the physicochemical properties except for surface tension.

Table 14. Exponential regression analysis for physicochemical properties verses topological indices.

Characteristics	Indices	α	β	R^2	F	P	Indicator
Boiling point	First Zagreb index $[M_1(G)]$	285.142	0.011	0.906	96.301	0	Significant
Flash point		117.295	0.014	0.784	36.264	0	Significant
Enthalpy		53.495	0.008	**0.912**	103.83	0	Significant
Molar refractivity		36.377	0.014	**0.912**	103.359	0	Significant
Molar volume		128.491	0.011	0.773	34.028	0	Significant
Surface tension		43.2	0.004	0.417	7.154	0.023	Significant
Boiling point	Second Zagreb index $[M_2(G)]$	318.774	0.016	0.858	60.658	0	Significant
Flash point		137.411	0.02	0.713	24.87	0.001	Significant
Enthalpy		58.349	0.012	**0.861**	62.083	0	Significant
Molar refractivity		42.789	0.02	0.827	47.946	0	Significant
Molar volume		148.682	0.015	0.658	19.236	0.001	Significant
Surface tension		44.543	0.006	0.43	7.532	0.021	Significant
Boiling point	Hyper Zagreb index $[HM(G)]$	313.6	0.004	0.855	59.166	0	Significant
Flash point		134.755	0.005	0.709	24.387	0.001	Significant
Enthalpy		57.612	0.003	**0.859**	60.725	0	Significant
Molar refractivity		41.737	0.005	0.833	49.76	0	Significant
Molar volume		145.483	0.003	0.668	20.164	0.001	Significant
Surface tension		44.47	0.001	0.413	7.025	0.024	Significant
Boiling point	Reciprocal Randic index $[RR(G)]$	293.924	0.024	0.908	98.512	0	Significant
Flash point		121.2	0.03	0.795	38.884	0	Significant
Enthalpy		54.686	0.018	**0.919**	112.755	0	Significant
Molar refractivity		38.026	0.031	0.904	94.113	0	Significant
Molar volume		133.274	0.024	0.762	31.969	0	Significant
Surface tension		43.304	0.009	0.446	8.04	0.018	Significant
Boiling point	Harmonic index $[H(G)]$	259.254	0.029	0.892	82.469	0	Significant
Flash point		100.709	0.038	0.817	44.669	0	Significant
Enthalpy		49.902	0.022	0.887	78.853	0	Significant
Molar refractivity		31.119	0.038	**0.952**	197.473	0	Significant
Molar volume		109.721	0.031	0.875	70.266	0	Significant
Surface tension		43.356	0.009	0.316	4.612	0.057	Insignificant
Boiling point	Sum connectivity index $[SC(G)]$	263.124	0.041	0.903	92.597	0	Significant
Flash point		103.119	0.053	0.82	45.691	0	Significant
Enthalpy		50.36	0.031	0.904	94.46	0	Significant
Molar refractivity		31.923	0.054	**0.953**	204.212	0	Significant
Molar volume		112.694	0.044	0.865	64.023	0	Significant
Surface tension		43.061	0.014	0.348	5.328	0.044	Significant
Boiling point	Forgotten index $[F(G)]$	309.523	0.007	0.85	56.534	0	Significant
Flash point		132.573	0.008	0.705	23.843	0.001	Significant
Enthalpy		57.037	0.005	**0.853**	57.893	0	Significant
Molar refractivity		40.806	0.009	0.838	51.899	0	Significant
Molar volume		142.313	0.007	0.683	21.59	0.001	Significant
Surface tension		44.539	0.002	0.389	6.372	0.03	Significant

Boiling point	Hyper Forgotten index $[HF(G)]$	385.293	0.001	0.662	19.562	0.001	Significant
Flash point		176.644	0.001	0.521	10.881	0.008	Significant
Enthalpy		67.45	0.001	**0.667**	20.066	0.001	Significant
Molar refractivity		54.532	0.001	0.633	17.233	0.002	Significant
Molar volume		180.117	0.001	0.481	9.278	0.012	Significant
Surface tension		48.518	0	0.282	3.921	0.076	Insignificant

In Table 14, we observed that the R-squared values are higher for Enthalpy and molar refractivity, indicating a strong positive correlation with the physicochemical properties. Additionally, the P-values are close to 0 in most cases, suggesting that the regression model is significant for all the physicochemical properties except for surface tension.

6. Analyzing correlation coefficients graphically

A graph is an incredibly powerful visual aid because it can swiftly communicate information, allow for comparisons, and display a variety of patterns and relationships within the data, including correlations, changes over time, frequency distribution, relative proportion of the whole, and other topics. Graphs can be classified into a variety of forms based on the sort of data they represent, including bar, line, area, scatter, pie, bubble, pictograph, and column charts. Six-line graphs illustrate the association between the qualities and topological indices in Figure 13. In Figure 14, all the associations are compared. Individual data points connected by lines form the basis of a line graph. The terms “line plot” and” line chart” are occasionally used to describe it. Line graphs in different colors are created to help differentiate between the correlations of the different elements. The topological index names are listed on the x-axis, and the correlation values are displayed on the y-axis. A strong correlation is indicated by the boiling point correlation graph, which is blue in color and has a value between 0.8 and 1.0. Every graph has a positive x-axis because topological indices (estimated values) and attributes (experimental values) are directly correlated.

A moderate correlation is shown by the surface tension correlation coefficient graph, which is colored green and spans from 0.4 to 0.6. While the other graphs in Figure 2 show extremely significant correlation values for all topological indices, the surface tension graph is moderate. These line graphs are produced using Microsoft Excel. The scatter plot can be useful for analyzing the correlation coefficients. Table 11 provides a comparison of correlation coefficient values for each. Table 11 displays numerical figures that indicate the variance in the correlation coefficients’ values. Graphs offer a clear and easy way to compare and comprehend data fluctuations. By using the indices mentioned above, it is simple to determine that parameters like enthalpy and boiling point have virtually the same correlation coefficient, and that all of the values for molar refractivity and flash point have correlation coefficients that are almost greater than 0.7.

7. Topological index applications

Topological indices have found wide applications in a wide range of scientific fields, such as network theory, chemistry, and pharmacology. The first molecular descriptor was created by chemist Wiener [5], and it was a distance-based index for evaluating the characteristics of the various classes of organic compounds. His work provided inspiration for the creation of cordial label-based indices, which have many applications in the world of chemistry. Example of the Zagreb indices, which are used to understand the structures of trees. Any of the above-mentioned indices can be used to characterize the physical properties of heart attack drugs. With the aid of indexes, eight characteristics of pharmaceuticals are investigated. Medication boiling points are calculated using

the Reciprocal Randic index, according to the correlation coefficient (r = 0.965). The harmonic index has the strongest association with Molar refractivity (r = 0.986). Although this correlation value is not particularly good, it is useful in the context of surface tension estimates. The following values are computed using the Sum Connectivity Index: molar refractivity (0.988), molar volume (0.93), flash point (0.924), enthalpy (0.953), and boiling point (0.957). This index is the most effective index since the values of the relationships between its five features are highest.

8. Conclusion and discussion

This approach uses several cordial label-based topological indices associated with numerical descriptors for each treatment to investigate the medications used to treat heart attacks. Fifteen cordial label-based topological index criteria have been used to evaluate twelve different heart attack drugs. The cordial label-based topological indices values and their correlations are displayed in Tables 2, 11, and Figure 2. Any novel medication needs to have specific structural properties, which can be identified using topological indices and QSPR modeling. In this work, we employ topological indices to recover topological information economically and efficiently from a structure. Several inferences can be made using the data for the designated cordial label-based topological indices in Tables 3-11.

Moreover, the QSPR study of the reciprocal Randic index (RR-index) indicates that it is a good predictor of pharmaceutical boiling points, with a correlation coefficient value of r = 0.965. The sum connection index shows a strong correlation with the heart attack medication's enthalpy (0.953), flash point (0.924), molar refractivity (0.988), and molar volume (0.93). The strongest correlation between this score and the four physical-chemical features of medications makes it the most effective. Tables 3 and 4 clearly show that all the properties have a good correlation with the Zagreb indices, except for surface tension (0.614). For the Zagreb indices, the correlation ranges are 0.788 to 0.963. The forgotten index and hyper forgotten index, with the exception of surface tension, exhibit great correlations with all properties; nevertheless, they do not have the highest correlation values with any particular attribute.

Related to Table 12, Muhammad Waheed Rasheed et al. [12] conducted research and analysis on the chemical structures of anti-heart attack medications. Our method for cordial label-based topological indices shows a higher correlation coefficient than their degree-based topological indices for the harmonic index [H(G)], except in the case of Surface tension. Similarly, the correlation coefficient values for all other topological indices such as the forgotten index F(G), the hyper-forgotten index HF(G), the reciprocal Randic index RR(G), the second Zagreb index M2(G), and the hyper-Zagreb index HM(G)-are higher with our cordial label-based method. Table 12. Provides a comparison of correlation coefficients between our findings and those of Muhammad Waheed Rasheed et al. [12]. We also obtained quadratic and cubic regression models for the topological indices versus physicochemical properties. However, since the linear regression is more significant, we are not presenting those regression analyses here. Only the logarithmic and exponential regression models showed significant results; therefore, the corresponding analyses are presented in Tables 13 and 14.

In QSPR studies, these parameters might be used as predicting factors. The physicochemical properties of drugs used to treat heart attacks are investigated in order to assess the predictive power of these markers. The results show that the topological indices, boiling point, enthalpy, molar volume, and molar refractivity all have a strong positive linear relationship. Also, each and every result is quite significant.

8.1. Limitations

The wide variety of topological indices that have been devised to convey information about chemical graphs and computer networks still does not allow one to determine all the features of substances. Thus, for a more theoretical and direct method to determine the features of chemical structures, particularly those related to heart attack medications, more molecular descriptors are required.

8.2. Future work

Our objective will also include examining the chemical and physical characteristics of drugs used to treat lung cancer, diabetes, and a few other serious illnesses. This will be accomplished by using a recently created index, which will yield more accurate findings than chemical graphs. Working on three-dimensional and geometric pharmacological descriptors is our second motivation.

Data Accessibility. There were no data used in this article.
Statement of funding. There was no funding for this research.

Conflicts of Interest. The authors assert that their personal relationships or known financial conflicts had no bearing on the findings of the study presented in this work.

Author Contributions:

I, Nandish, am the first and corresponding author of the work titled" Estimation of Heart Attack" under the guidance of Dr. Usha P. I am responsible for the research concept, experimental work, and validation and verification of the study. Dr. Usha P. was responsible for the critical review and supervision of the work. Dr. Ramananda H. S. was responsible for data collection and experimental analysis. Dr. Sandeep R. was responsible for drafting the manuscript in Microsoft word, reviewing and editing the manuscript.

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