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ZAGREB INDICES AND THE THERMAL BEHAVIOR OF STEROIDS: A QUANTITATIVE GRAPH-BASED STUDY

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ABSTRACT

In mathematical chemistry, graph theory provides a systematic and quantitative framework for understanding the relationship between molecular structure and the physicochemical properties of compounds. This study investigates the correlation between the first and second Zagreb indices and the melting points of a group of steroid compounds, bioactive molecules with significant pharmacological relevance. Ten steroid compounds were selected based on the availability of melting point data, and their chemical structures were modeled as molecular graphs. The Zagreb index values were calculated by analyzing the degrees of the vertices in each graph. Pearson correlation analysis and linear regression were employed to examine the relationship. The regression model for the first Zagreb index yielded an intercept of 245.77 with a coefficient of -0.1741 ($p = 0.317$), while the second Zagreb index produced an intercept of 224.92 with a coefficient of -0.091 ($p = 0.495$). Both analyses indicate weak and statistically insignificant negative correlations between Zagreb indices and melting points. These findings indicate that the Zagreb indices, in their current form, are insufficient to accurately capture variations in the melting points of steroid-based medicinal compounds. Nevertheless, this study underscores the potential of graph-based modeling in pharmaceutical chemistry.

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1. INTRODUCTION

Many fields use graphs as visual aids to analyze data, identify patterns, and convey information more clearly and efficiently. One application of this is in chemistry, where the properties of chemical compounds can be understood through an approach based on graph theory [1]. In this theory, chemical molecules are represented as graphs, which are mathematical structures consisting of vertices and edges. The atoms in a molecule are represented as vertices, while the bonds between atoms are described as edges connecting those vertices [2]. This approach enables the analysis of molecular structures in a systematic, mathematical, and measurable manner. One of the key concepts in graph theory is the topological index, a numerical descriptor that encodes specific features of a molecular structure. These indices are widely used to relate molecular architecture to various chemical and physical properties such as stability, reactivity, pharmacological activity, and other physicochemical attributes [3]. In chemical documentation, the use of chemical information derived from topological indices has proven useful for distinguishing isomers and determining correlations between structure and properties [4]. By employing topological indices, researchers can predict molecular behavior, including atomic connectivity and reactivity, with a high degree of accuracy.

With advances in scientific understanding, various topological indices have been developed to deepen our knowledge of the relationship between molecular structure and compound behavior. Several well-known topological descriptors in chemical graph theory include the Wiener index, Randić index, Hosoya index, and Zagreb indices, each capturing different aspects of molecular topology such as branching, connectivity, and distance relationships between atoms. Among these descriptors, the first Zagreb index and the second Zagreb index are classical indices that have been widely studied in mathematical chemistry [5]. In addition to these, researchers have increasingly focused on graph-energy concepts, which measure structural properties through the eigenvalues of a graph's associated matrices [6]-[9]. The First Zagreb Index is closely related to various important quantities in chemical graph theory, and its mathematical properties have been extensively studied [10]. This index was introduced by Gutman and Trinajstić in 1972. The Zagreb indices measure the branching pattern of a molecule based on the degrees of vertices in the molecular graph [11]. Their values have been linked to the distribution of π-electron energy, providing meaningful insights into the stability and reactivity of molecules, especially in organic compounds [12]. Due to their simplicity, strong theoretical foundation, and effectiveness in describing molecular branching and connectivity, the first and second Zagreb indices are frequently used as fundamental descriptors in chemical graph theory. Therefore, this study focuses on these two indices to investigate their relationship with the melting points of steroid compounds.

Steroid compounds represent a particularly important class of molecules for analysis. Belonging to the triterpenoid family, steroids are characterized by a core structure of four fused carbon rings: three cyclohexane rings and one cyclopentane ring, forming the cyclopentanoperhydrophenanthrene skeleton [13]. Steroids play essential roles in medicine and human physiology, with wide applications in pharmaceuticals, hormonal therapies, and disease treatment [13],[14],[15]. One of the critical physical properties of these compounds is their melting point, which serves as an indicator of thermal stability, intermolecular interactions, and molecular symmetry. Accurate prediction and understanding of melting points are crucial because this parameter plays a role in the initial identification and characterization of a compound, helps determine the purity level of a material through comparison with reference values, and forms the basis for the design of stable and effective drug formulations [16],[17].

The thermal behavior of a compound is closely related to its molecular structure, since structural characteristics influence intermolecular interactions, molecular packing, and overall stability in the solid state. Consequently, properties such as melting point can often be interpreted through structural descriptors derived from molecular graphs. In chemical graph theory, topological indices provide numerical representations of molecular topology, including aspects such as branching, connectivity, and distribution of atoms within a structure. These descriptors have been widely employed to develop quantitative structure–property relationships (QSPR), allowing researchers to investigate how variations in molecular topology influence physical properties. Therefore, establishing correlations between topological indices and melting points can provide valuable insight into the thermal behavior of compounds and enable predictive modeling of their physicochemical properties. To quantitatively evaluate this relationship, Pearson correlation analysis is employed to measure the strength and direction of the linear association between the variables, while linear regression analysis is used to model the predictive relationship between topological indices and melting points [18].

This study focuses on applying graph-theoretical approaches, particularly the Zagreb indices, to model and analyze the structural properties of steroid compounds. By establishing a quantitative relationship between topological descriptors and melting points, this work aims to support predictive modeling in drug development and molecular design. Such models can enhance early-stage pharmaceutical analysis, reduce trial-and-error in compound screening, and contribute to innovation in health-related chemistry and therapeutic compound development.

2. RESEARCH METHODS

2.1 Data Collection of Steroid Compounds

This study utilized data from ten steroid compounds with known melting points. The melting point data were obtained from reliable chemical databases and peer-reviewed literature to ensure data reliability. The primary sources used in this study include the PubChem database and previously published chemical reference works, which provide experimentally measured melting point values under standard laboratory conditions. The collected data were cross-checked to ensure consistency and accuracy before being used in the statistical analysis. The chemical structure of each compound served as the basis for calculating the first and second Zagreb indices. These compounds were selected due to their structural diversity and pharmacological relevance, contributing to the development of computational tools in drug screening and pharmaceutical research.

2.2 Molecular Graph Construction and Computational Workflow

Reproducibility of the analysis was maintained through a systematic workflow involving the construction of molecular graphs and the computation of Zagreb indices. Molecular structures of the steroid compounds used in this study were obtained from the chemical database PubChem in their standard structural form, and the melting point data were taken from the physicochemical property information available in the same database. Each molecule was represented as a molecular graph $G(V, E)$, where the set $V(G)$ represents atoms as vertices and the set $E(G)$ represents covalent bonds as edges. The degree of each vertex $d(v)$ was determined based on the number of bonds connected to the corresponding atom in the molecular structure. The first and second Zagreb indices were calculated according to their standard mathematical definitions once the molecular graph had been constructed. The resulting index values served as independent variables in the statistical analysis, while the melting point was treated as the dependent variable for modeling the relationship between molecular structure and its physical properties.

2.3 Zagreb Index Calculation

The first and second Zagreb indices were computed from the degrees of the vertices in the molecular graph representation of each steroid compound. In this representation, atoms correspond to vertices and chemical bonds correspond to edges. The molecular structure of each steroid compound was converted into a graph model following established conventions in mathematical chemistry. The degree of each vertex was determined based on the number of bonds connected to the corresponding atom in the molecular structure, and these vertex degrees were used to calculate the Zagreb index values using their standard mathematical formulas. Graph theoretical topological indices are widely used to investigate the relationship between molecular structure and physicochemical properties of chemical compounds, including melting points. In this study, the first Zagreb index and the second Zagreb index were selected because they describe the branching pattern and connectivity of atoms within the molecular graph, which may influence the physical properties of a compound. The definitions of these indices are given as follows:

Definition 1. [19] Suppose G is a graph, the first Zagreb index $M_1(G)$ of graph G are:

$$M_1(G) = \sum_{u \in V(G)} (\deg(u))^2 , \tag{1}$$

where $\deg(u)$ is degree of vertex u in $V(G)$.

Definition 2. [20] Suppose G is a graph, the second Zagreb index $M_2(G)$ of graph G are:

$$M_2(G) = \sum_{(u,v)\in E(G)} \deg(u) \cdot \deg(v), \tag{2}$$

where u and v denote the pair of vertices that are joined by the edge.

2.4 Correlation and Regression Analysis

Statistical relationships were analyzed by calculating Pearson correlation coefficients between each Zagreb index and the melting point. Simple linear regression models were constructed to evaluate the predictive capability of each index. Statistical significance was tested at a 95% confidence level. The Pearson correlation analysis was used to measure the strength of the linear relationship between the Zagreb index values and the melting point of steroid compounds. This method helps assess whether changes in one variable are proportionally related to changes in the other. The correlation coefficient was calculated using the following equation:

$$r = \frac{n\sum xy - (\sum x)(\sum y)}{\sqrt{[n\sum x^2 - (\sum x)^2][n\sum y^2 - (\sum y)^2]}}. \tag{3}$$

The Pearson correlation coefficient r represents the strength and direction of the linear relationship between two variables. In this study, x denotes the independent variable, while y represents the dependent variable, and n indicates the number of observed data points used in the analysis [21].

2.5 Melting Point Modeling

To further examine the predictive potential of the Zagreb indices, two simple linear regression models were constructed. Each model used one of the Zagreb indices as the independent variable and the melting point as the dependent variable [22]. The models were evaluated for their predictive accuracy and statistical significance. This modeling approach aims to explore the applicability of graph-based descriptors in predictive pharmacoinformatics, aligning with efforts to streamline early-stage compound evaluation in health-related chemical research.

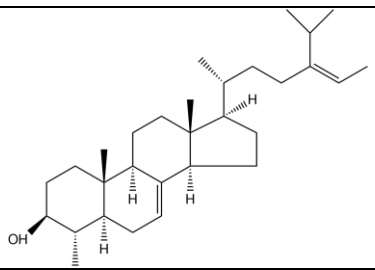
3. RESULTS AND DISCUSSION

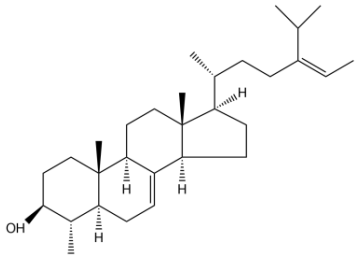
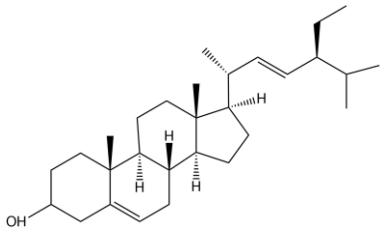
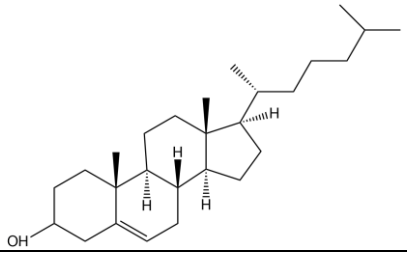
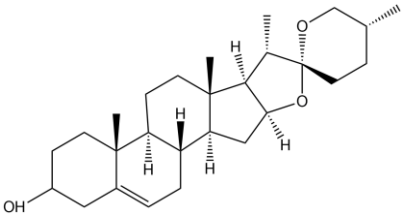
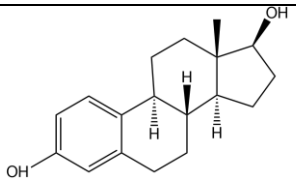
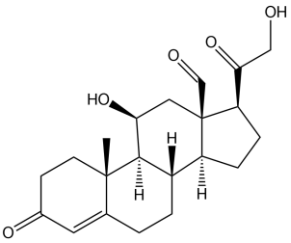
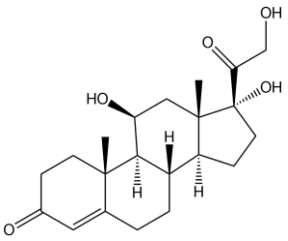
This section presents the results obtained from the calculation and data analysis of the Zagreb indices and the melting points of steroid compounds. Each finding is explained by emphasizing its relevance to the research objectives and is linked to the underlying theory to provide a clearer understanding of the relationship between molecular structure and the physical properties of the compounds.

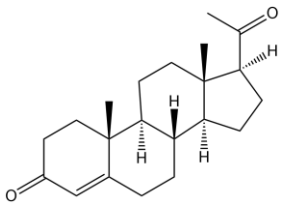
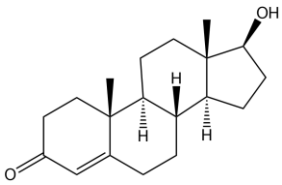
3.1 Steroid Compound Structure

Steroids are included in the triterpenoid group, which has a core structure of cycloplane perhydrophenanthrene. This steroid compound consists of three cyclohexane rings and one cyclopentane ring. The molecular structure and melting points of the ten compounds included in the steroid compounds will be calculated using the first Zagreb index and the second Zagreb index, as follows:

Table 1. Molecular Structure and Melting Point of Steroid Compounds

No.	Compound Name	Structure	Melting Point (°C)
1.	β-sitosterol		136

No.	Compound Name	Structure	Melting Point (°C)
2.	α-sitosterol		136
3.	Stigmasterol		136
4.	Cholesterol		150
5.	Diosgenin		225
6.	Estradiol		176
7.	Aldosterone		232
8.	Cortisol		215

No.	Compound Name	Structure	Melting Point (°C)
9.	Progesterone		131
10.	Testosterone		165

3.2 Calculation of Zagreb Indices for Steroid Compounds

This section will discuss the calculation of the first and second Zagreb indices for the steroid compound group. The Zagreb indices in the steroid compound group were computed from the degrees of the vertices in the molecular graph representation of each compound, where atoms correspond to vertices and chemical bonds correspond to edges. To simplify the calculation, the structure of the β-sitosterol compound will be depicted in graph form, which will be used as an example in finding the first and second Zagreb index values.

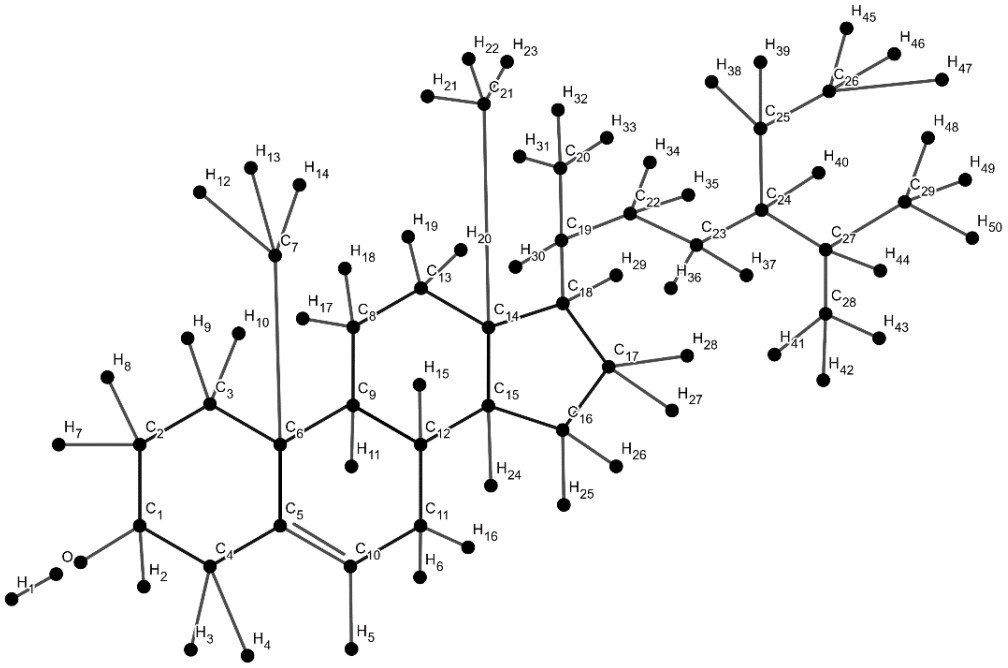


Figure 1. Graph Representation of The Structure of B-Sitosterol Compound

In the molecular graph shown in Fig. 1, the structure consists of 50 H atoms, 29 C atoms, and 1 O atom. Based on this atomic composition, the above equation can be used to calculate the first and second Zagreb indices as follows:

First Zagreb Index

$$M_1(G) = \sum_{u \in V(G)} (\deg(u))^2$$

$$= \sum_{H \in V(G)} (\deg(H))^2 + \sum_{C \in V(G)} (\deg(C))^2 + \sum_{O \in V(G)} (\deg(O))^2$$

$$= 50 \times (deg(H))^2 + 29 \times (deg(C))^2 + 1 \times (deg(O))^2$$
$$= 50 \times (1)^2 + 29 \times (4)^2 + 1 \times (2)^2$$
$$= 518$$

The above calculations show that the first Zagreb index value of the β-sitosterol compound is 518.

Second Zagreb Index

$$M_2(G) = \sum_{(u,v)\in E(G)} deg(u) \cdot deg(v)$$
$$= \sum_{(H,O)\in E(G)} deg(H) \cdot deg(O) + \sum_{(H,C)\in E(G)} deg(H) \cdot deg(C) + \sum_{(C,O)\in E(G)} deg(C) \cdot deg(O) + \sum_{(C,C)\in E(G)} deg(C) \cdot deg(C)$$
$$= 1[deg(H) \times deg(O)] + 49[deg(H) \times deg(C)] + 1[deg(C) \times deg(O)] + 30[deg(C) \times deg(C)]$$
$$= 1[1 \times 2] + 49[1 \times 4] + 1[4 \times 2] + 30[4 \times 4]$$
$$= 686$$

From the above calculation results, it can be seen that the second Zagreb index value of the β-sitosterol compound is 686.

The results of the calculation of the first Zagreb index and the second Zagreb index in other groups of steroid compounds are presented in Table 2. The table presents the values of the first and second Zagreb indices calculated from the vertex degrees of the molecular graph representation of each compound. This calculation provides an overview of the structural relationships and chemical properties of the steroid compounds analyzed, which will later be used to model the melting points of these compounds.

Table 2. Melting Point and Zagreb Index of Steroid Compound

Compound	Melting Point (℃)	First Zagreb Index	Second Zagreb Index
β-sitosterol	136	518	686
α-sitosterol	136	534	702
Stigmasterol	136	516	710
Kolestrol	150	482	670
Diosgenin	225	486	718
Estradiol	176	320	444
Aldosteron	232	384	532
Kortisol	215	386	534
Progesteron	131	374	520
Testosteron	165	340	478

3.3 Analysis of the Relationship of the First Zagreb Index to the Steroid Compound Group

The correlation analysis between the first Zagreb index and the group of steroid compounds can provide a clearer understanding of the relationship between the structure and chemical properties of these compounds. With this approach, we can explore how much influence the Zagreb index has on the chemical characteristics of steroid compounds. The following results present the correlation the results of the correlation analysis between the first Zagreb index and the group of steroid compounds that have been studied.

Table 3. Correlation Analysis of The First Zagreb Index with Melting Point

Pearson Correlation	Significance	N	Information
−0.353	0.317	10	Not Significant

Based on the results presented in Table 3, Pearson's correlation analysis shows a weak negative relationship between the first Zagreb index and the melting point, with a correlation coefficient of -0.353. This means that an increase in the index value tends to be followed by a decrease in the melting point, although the relationship is not strong. In addition, a significance value of 0.317 indicates that the relationship

is not statistically significant at a 95 percent confidence level. With a sample size of ten observations, it can be concluded that there is no significant relationship between the two variables based on the results of the calculations.

The results of the correlation analysis previously described provide an overview of the relationship between the first Zagreb index and the group of steroid compounds. The following table will show the value of the correlation coefficient, which shows how much influence the first Zagreb index has on the group of steroid compounds studied. These results provide a more detailed understanding of the relationship between molecular structure and chemical properties of steroid compounds.

Table 4. Regression Analysis of First Zagreb Index with Melting Point

Variable	B	Std.Error	Beta	*t*	Significant
Constant	245.77	71.865	-	3.420	0.009
First Zagreb Index Value	-0.1741	0.163	-0.353	-1.068	0.317

The regression model obtained from the analysis can be expressed as $MP = 245.77 - 0.1741M_1$. Based on the results shown in Table 4, linear regression analysis indicates that the constant (intercept) has a value of 245.77 with a significance level of 0.009, suggesting that the intercept is statistically significant. The regression coefficient for the first Zagreb index variable is -0.1741 with a significance value of 0.317. These results imply that each one-unit increase in the value of the first Zagreb index is associated with a decrease of approximately 0.174 units in the melting point. The regression model therefore indicates a negative relationship between the first Zagreb index and melting point. However, the coefficient is not statistically significant (p = 0.317), suggesting that the index does not provide reliable predictive power for melting point variation in this dataset. The coefficient of determination R^2 indicates that only a small portion of the variance in melting point can be explained by the first Zagreb index.

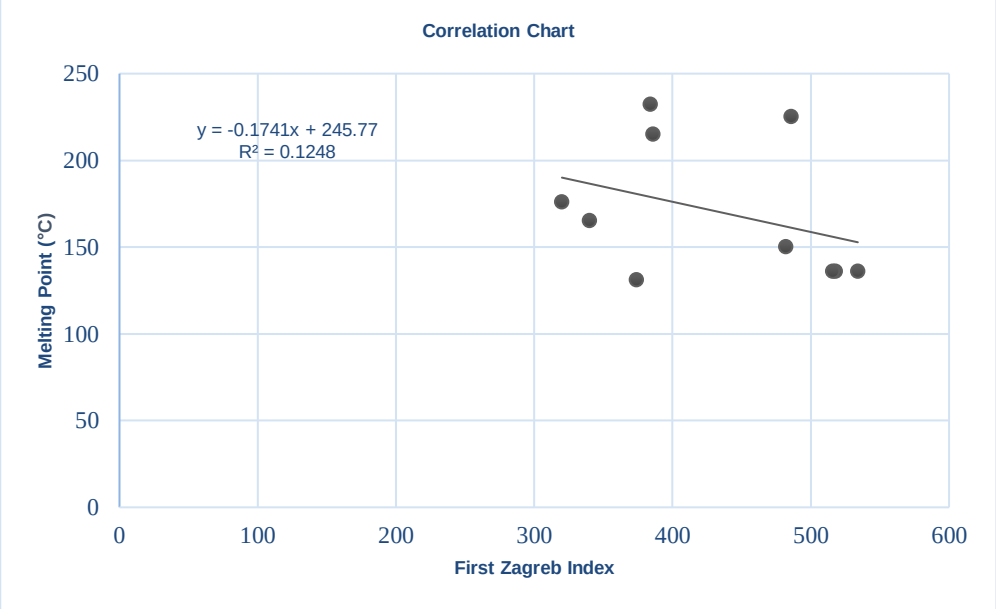


Figure 2. Relationship Between the First Zagreb Index and Melting Point

The relationship between the First Zagreb Index and the melting point in the form of a scatter plot is presented in Fig. 2. The First Zagreb Index is represented on the horizontal axis, while the melting point is plotted on the vertical axis, enabling a direct observation of their relationship. The distribution of the data points reveals a slight negative trend, as indicated by the regression line with the equation $MP = -0.1741M_1 + 245.77$. The coefficient of determination $R^2 = 0.1248$ indicates a weak correlation between the two variables. Several data points deviate from the regression line, suggesting that the variation in melting point cannot be fully explained by the First Zagreb Index alone. This observation implies that additional structural or physicochemical factors may contribute to the melting point of the compounds.

3.4 Analysis of the Relationship of the Second Zagreb Index to the Steroid Compound Group

Correlation analysis between the second Zagreb index and the group of steroid compounds can provide a clearer understanding of the relationship between the structure and chemical properties of these compounds. With this approach, we can explore how much influence the Zagreb index has on the chemical characteristics of steroid compounds. The following will present the results of the correlation analysis between the second Zagreb index and the group of steroid compounds that have been studied.

Table 5. Correlation Analysis of The Second Zagreb Index with Melting Point

Pearson Correlation	Significance	N	Information
-0.245	0.495	10	Not Significant

Based on the results in Table 5, Pearson's correlation analysis shows that there is a weak negative relationship between the second Zagreb index value and the melting point value, with a correlation coefficient of -0.245. This means that an increase in index value tends to be followed by a decrease in melting point, although the relationship is not strong. In addition, the significance value of 0.495 indicates that the relationship is not statistically significant at the 95 percent confidence level. With a sample size of ten data points, it can be concluded that there is no significant relationship between the two variables based on the results of the calculations performed.

The results of the correlation analysis previously described provide an overview of the relationship between the second Zagreb index and the group of steroid compounds. The following table will show the value of the correlation coefficient, which shows how much influence the second Zagreb index has on the group of steroid compounds studied. These results provide a clearer picture of the relationship between molecular structure and chemical properties of steroid compounds.

Table 6. Regression Analysis of Second Zagreb Index with Melting Point

Variable	B	Std.Error	Beta	t	Significant
Constant	224.923	77.646	-	2.897	0.020
First Zagreb Index Value	-0.091	0.128	-0.245	-0.715	0.495

The regression model obtained from the analysis can be expressed as $MP = 224.92 - 0.091M_2$. Based on the results shown in Table 6, linear regression analysis indicates that the constant (intercept) has a value of 224.923 with a significance level of 0.020, suggesting that the intercept is statistically significant. The regression coefficient for the second Zagreb index variable is -0.091 with a significance value of 0.495. This result implies that each one-unit increase in the second Zagreb index is associated with a decrease of approximately 0.091 units in the melting point. The regression model therefore indicates a weak negative relationship between the second Zagreb index and melting point. However, since the significance value is greater than 0.05, the effect is not statistically significant. Consequently, the second Zagreb index alone cannot be considered a reliable predictor of melting point variation in the steroid compound dataset used in this study.

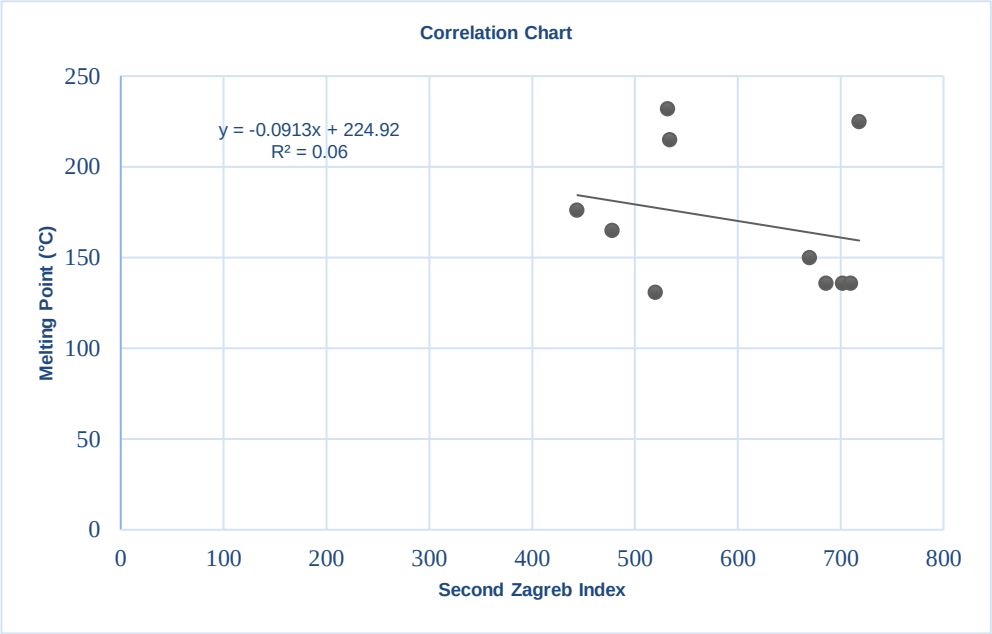


Figure 3. Relationship Between the Second Zagreb Index and Melting Point

The relationship between the Second Zagreb Index and the melting point is presented as a scatter plot in Fig. 3. The distribution of the data points indicates a very weak negative trend, as reflected by the regression equation $MP = -0.0913M_2 + 224.92$. The coefficient of $R^2 = 0.06$ suggests that the contribution of the Second Zagreb Index in explaining the variation in melting point is minimal. The relatively scattered distribution of points, along with noticeable deviations from the regression line, further indicates that the observed relationship is not statistically significant. This finding implies that factors other than the Second Zagreb Index play a more dominant role in influencing the melting point of the compounds.

The weak correlations observed between the Zagreb indices and the melting points of the steroid compounds indicate that the structural information captured by these topological indices may not fully represent the factors governing the thermal behavior of steroid molecules. Melting point is strongly influenced by intermolecular interactions such as hydrogen bonding, van der Waals forces, and crystal packing effects. While Zagreb indices effectively describe molecular branching and connectivity, they do not directly incorporate stereochemical configuration or intermolecular forces. Therefore, the limited predictive capability observed in this study suggests that additional molecular descriptors may be required to better model the melting point variation of steroid compounds.

4. CONCLUSION

This study aimed to examine the relationship between the first and second Zagreb indices and the melting points of steroid compounds using a graph-theoretical approach combined with correlation and regression analysis. The results indicate that both indices show weak negative correlations with melting point and do not exhibit statistically significant relationships. The regression model for the first Zagreb index produced an intercept of 245.77 with a coefficient of -0.1741 ($p = 0.317$), while the second Zagreb index produced an intercept of 224.92 with a coefficient of -0.091 ($p = 0.495$). These findings suggest that neither the first nor the second Zagreb index significantly influences the melting point values within the steroid compound dataset analyzed in this study.

These results highlight that the structural information represented by Zagreb indices, which mainly reflects molecular connectivity and vertex degree, is insufficient to explain variations in the thermal properties of steroid compounds. One limitation of this research is the relatively small dataset and the use of only two topological descriptors, which may not fully capture the complexity of intermolecular interactions affecting melting point values. Future research is therefore recommended to incorporate additional molecular descriptors, such as three-dimensional structural parameters, electronic descriptors, and quantum chemical

indices, as well as larger datasets, in order to develop more robust quantitative structure-property relationship (QSPR) models for predicting the physical properties of steroid compounds.

Author Contributions

Sarwa Hita: Data Curation, Formal Analysis, Investigation, Visualization, and Writing-Original Draft. I Gede Adhitya Wisnu Wardhana: Supervision, Conceptualization, Methodology, Validation, Funding Acquisition, and Writing—Review and Editing. Nguyen Dang Hoa Nghiem: Resources, Formal Analysis, Validation, and Writing—Review and Editing. Ni Komang Tri Dharmayani: Data Curation, Chemical Analysis, Resources, and Writing—Review and Editing. All authors discussed the results, provided critical feedback, and approved the final version of the manuscript.

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Declarations

The authors declare no competing interests.

Declaration of Generative AI and AI-assisted technologies

Generative AI tools (e.g., ChatGPT) were used solely for language refinement, including grammar, spelling, and clarity. The scientific content, analysis, interpretation, and conclusions were developed entirely by the authors. All final text was reviewed and approved by the authors.

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