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Analysis of the Relationship Between Second Zagreb Index Values and the Oxidation Levels of Terpenoid Derivatives

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A B S T R A C T

Terpenoids are a group of secondary metabolites composed of isoprene units containing five carbon atoms (C_5), synthesized from acetate through the mevalonate pathway. This research examines two triterpenoid derivatives, densiflorinic acid A and densiflorinic acid B. The second Zagreb index is applied to illustrate atomic interaction patterns—including H–C, C–O, O–H, and C–C—which serve as indicators of molecular structural complexity. The findings indicate that the second Zagreb index is a reliable measure for assessing the structural complexity and oxidation levels of triterpenoid derivatives that share the same core framework.

Keywords: Chemical Topological Graph, Second Zagreb index, densiflorinic, oxidation.

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1. Introduction

Secondary metabolites are chemical compounds produced by plants through the biosynthesis of primary metabolites. One important role of secondry metabolites is as a defense mechanism against pathogens. In general, the type of secondary metabolites commonly found in plants include alkaloids, flavonoids, saponins, tannins, phenols, steroids, and terpenoids [1]. Terpenoids themselves are a group of secondary metabolites composed of isoprene units with five carbon atoms (C_5) and are synthesized from acetate via the mevalonate pathway [2]. The dysoxylum plant from the milaceae is one type of plant that produces secondary metabolites in the form of terpenoids (Sumarya, 2020). Research conducted by Dharmayani et al. [3] identified two triterpenoid derivative compounds, namely densiflorinic acid A and densiflorinic acid B. These two compounds possess similar structural frameworks but differ only by one functional group; this variation leads to differences in their oxidation levels.

The degree of oxidation of a compound reflects the process of change in organic compounds, which is usually characterized by an increase in oxygen atoms or a decrease in hydrogen atoms. Changes in the oxidation state of a compound are typically accompanied by modifications in its physical and chemical properties. Alterations in chemical and physical properties are fundamentally reflected in changes in the functional groups of the compound. Such changes influence other chemical characteristics, including polarity and stability. Meanwhile, physical properties affected by oxidation include solubility and volatility [4].

Variations in oxidation levels that modify the chemical and physical properties of organic molecules also influence their bioactivity [5]. This is caused by differences in levels that meet functional groups in the structure, resulting in different interaction patterns when the compounds are tested for their bioactivity [6]. Densiflorinic acid A and densiflorinic acid B exhibit different bioactivities: densiflorinic acid A shows antibacterial activity against *Bacillus subtilis* with an activity value of 26.5 µM, whereas densiflorinic acid B demonstrates strong antibacterial activity against *Shigella dysenteriae* with a value of 53 µM [3].

Changes in the oxidation state of two triterpene-type terpenoid derivatives, namely densiflorinic acid A and densiflorinic acid B, can be explained by a Chemical Topological Graph (CTG). A chemical topological graph is a form of graphical representation of molecules in chemistry. Theoretically and computationally, CTG allows the depiction of atoms in a molecule [7]. Graph theory itself was first introduced by Leonhard Euler in 1736 and has developed into a branch of mathematics that is applicable in various aspects of life [8]. In mathematics, a graph is formed from a collection of objects and special relationship between these objects. Visually, objects in a graph are represented as points, circles, or vertices, while relationship between objects are depicted through connecting lines [9]. In addition, in graph theory, there is the concept of adjacency, where two vertices are said to be adjacent if they are connected by an edge. The vertex degree is defined as the number of edges incident to that vertex [10]. Graph theory has many applications, including in the field of chemistry, trough the use of topological indices [8].

Topological indices are used to represent the structure of a molecule, where vertices represent atoms or chemical elements, while edges represent the bonds connecting these atoms [11]. In a molecule, atoms are depicted as vertices, and bonds between atoms are shown as edges in the graph [12]. Topological indices have become an interesting field or study, one of which is the Zagreb index [13]. The Zagreb index is a topological parameter used in chemistry to describe the level of complexity of a molecule based on its graph. This index plays a role in predicting the physiochemical properties of molecules and is used in structural analysis, biological activity modeling, and structure-activity relationship studies in drug development. In general, the higher the Zagreb index value, the more complex the molecular structure being represented [14].

In this study, the analysis focuses on two terpenoid derivatives, namely densiflorinic acid A and densiflorinic acid B. The second Zagreb index is applied to represent the interaction patterns between atoms such as H–C, C–O, O–H, and C–C, thereby providing insights into the structural complexity of the molecules. Through this approach, this research aims to quantitatively examine variations in interaction patterns, which may serve as a foundation for further studies on compounds with similar characteristics.

2. Research Methods

This research uses a literature study method, or library study, which is a research approach carried out by reviewing various books and other reading sources relevant to the topic determined by the researcher. The research was conducted by reading, observing, and understanding references

from books and reading sources, such as journals and papers containing information related to graph theory, topological indexes, structures, and properties of organic compounds, especially the compounds densiflorinic acid A and densiflorinic acid B [3]. Molecular structure data was obtained from trusted chemical literature, then drawn using ChemDraw software, and analysis was carried out by calculating the second Zagreb Index value and evaluating its relationship with the oxidation level of atoms in the compound molecule.

3. Result and Discussion

The Zagreb Index is one of the topological parameters used The research employed a literature study approach, also referred to as a library-based study, in which data is gathered by examining books and other relevant written sources related to the selected topic. This study was carried out by reading, reviewing, and interpreting information from books, journals, and scientific papers that discuss graph theory, topological indices, molecular structures, and the properties of organic compounds, particularly densiflorinic acid A and densiflorinic acid B [3]. The molecular structure data were obtained from reputable chemical literature, illustrated using ChemDraw software, and subsequently analyzed by calculating the value of the second Zagreb index and evaluating the oxidation levels of the atoms within the molecules.

Definition 3.1. *[15] Let G be a graph. The second Zagreb index $M_2(G)$ is defined as*

$$M_2(G) = \sum_{xy \in E(G)} \deg(x) \cdot \deg(y) \tag{1}$$

where x and y are vertices of the graph G, $E(G)$ denotes the edge set of G, and $xy \in E(G)$ represents an edge connecting the vertices x and y, while $\deg(x)$ and $\deg(y)$ denote the degrees of the vertices x and y, respectively.

In the study of terpenoid derivative compounds, the value of $M_2(G)$ can be associated with the oxidation state of the atoms comprising the compound. The oxidation state is influenced by the pattern of chemical interactions between atoms, and each interaction contributes to the total Zagreb index. To investigate this relationship, the calculation of the second Zagreb index is carried out by considering the following components.

1. The value $\sum_{HC \in E(G)} \deg(H) \times \deg(C)$ which represents the total contribution of interactions between hydrogen and carbon vertices, reflecting H–C bonds in the molecule.
2. The value $\sum_{CO \in E(G)} \deg(C) \times \deg(O)$ which represents the total interactions between carbon and oxygen vertices, corresponding to C–O bonds.
3. The value $\sum_{HO \in E(G)} \deg(H) \times \deg(O)$ which represents the total interactions between hydrogen and oxygen vertices, corresponding to H–O bonds.
4. The value $\sum_{CC \in E(G)} \deg(C) \times \deg(C)$ which represents the total interactions between carbon vertices, corresponding to C–C bonds.

In this study, we analyzed terpenoid derivative compounds.

a) Densiflorinic Acid Compound A.

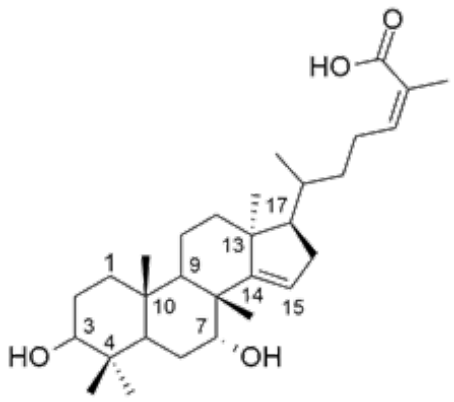

Figure 1. Densiflorinic acid compound A

If the compound is represented in the form of a graph, it will result in Figure 2.

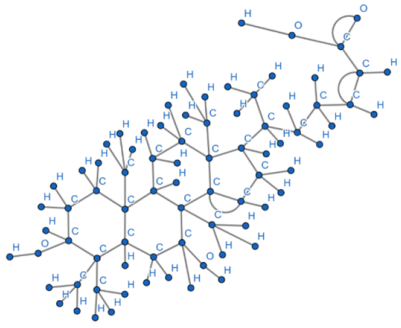

Figure 2. Graph representation of the densiflorinic acid A compound

Calculation of the second Zagreb Index for Densiflorinic.

$$\begin{aligned} M_2(G) &= \sum_{xy \in E(G)} \deg(x) \times \deg(y) \\ &= \sum_{HC \in E(G)} \deg(H) \times \deg(C) + \sum_{CO \in E(G)} \deg(C) \times \deg(O) \\ &\quad + \sum_{HO \in E(G)} \deg(H) \times \deg(O) + \sum_{CC \in E(G)} \deg(C) \times \deg(C) \\ &= 45(1 \times 4) + 5(4 \times 2) + 3(1 \times 2) + 34(4 \times 4) \\ &= 180 + 40 + 6 + 544 \\ &= 770. \end{aligned}$$

Thus, the total calculated value of the Zagreb Index for Densiflorinic Acid A is 770.

b) Densiflorinic acid compound B.

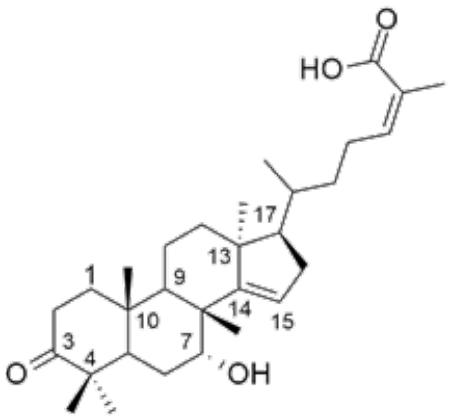

Figure 3. Densiflorinic acid compound B

If the compound is represented in the form of a graph, it will result in Figure 4.

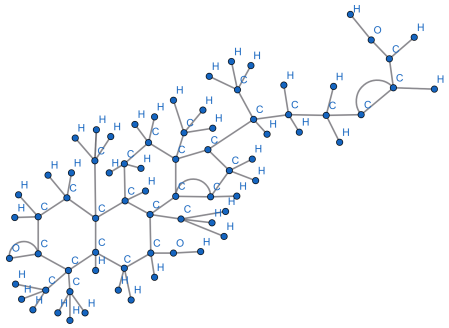

Figure 4. Graph representation of the densiflorinic acid B compound

Calculation of the second Zagreb Index for Densiflorinic Acid B.

$$\begin{aligned} M_2(G) &= \sum_{xy \in E(G)} \deg(x) \times \deg(y) \\ &= \sum_{HC \in E(G)} \deg(H) \times \deg(C) + \sum_{CO \in E(G)} \deg(C) \times \deg(O) \\ &\quad + \sum_{HO \in E(G)} \deg(H) \times \deg(O) + \sum_{CC \in E(G)} \deg(C) \times \deg(C) \\ &= 44(1 \times 4) + 6(4 \times 2) + 2(1 \times 2) + 34(4 \times 4) \\ &= 176 + 48 + 4 + 544 \\ &= 772 \end{aligned}$$

Thus, the total calculated value of the Zagreb Index for Densiflorinic Acid B is 772.

Table 1. Zagreb Index values of Densiflorinic Acid A and B

Compound	H and C	C and O	O and H	C and C
Densiflorinic Acid A	180	40	6	544
Densiflorinic Acid B	176	48	4	544

The results of the calculations indicate that the comparison of the second Zagreb index values for each bond type in densiflorinic acid A and densiflorinic acid B is presented in Table 1. The second Zagreb index for the C−H interactions in the two compounds differs, with values of 180 for densiflorinic acid A and 176 for densiflorinic acid B. This decrease reflects the reduced number of $C\breve{}H$ interactions in densiflorinic acid B, caused by the absence of a hydrogen atom at carbon atom number 3.

Furthermore, this missing hydrogen contributes to an increase in the (C – O) interaction value, where densiflorinic acid A has a (C – O) interaction value of 40, while densiflorinic acid B has a value of 48. This suggests a greater(C – O) interaction strength and bond density in densiflorinic acid B, consistent with the structural change resulting from the removal of the hydrogen atom.

Judging from the study of the structure of organic compounds, densiflorinic acid B has a higher oxidation level than densiflorinic acid A. This difference can be observed from the change in the $\sum O-H$ interactions. In densiflorinic acid A, the alcohol functional group (C – O – H) at carbon atom 3 is converted into a ketone functional group (C = O) , leading to a higher (C – O) interaction value and density in densiflorinic acid B.

Additionally, the total Zagreb index for the –C−H bonds in densiflorinic acid B is 180, which is lower than the value of 176 in densiflorinic acid A. This difference arises because the ketone group (C = O) contributes a greater bond density compared to the alcohol group (C – O – H), thus affecting the distribution of interactions within the molecule. From the results of this analysis, it can be concluded that the second Zagreb Index compound for each C−H, C−O, C−C bond interaction can be used as a parameter to compare the structural complexity and oxidation level between triterpenoid derivative compounds or other compounds with the same basic structure.

4. Conclusions

This study demonstrates that the second Zagreb index can serve as an effective parameter for comparing the structural complexity and oxidation levels of triterpenoid derivative compounds that share a similar basic framework. The calculation results indicate that the second Zagreb index value of acid (1) is 770, which is higher than that of acid (2), with a value of 772. The decrease in the index value is caused by variations in the interaction values of the C–H, C–O, and O–H reactants. Densiflorinic acid B exhibits a higher oxidation level compared to densiflorinic acid A, as reflected by the differences in the functional groups present in the two compounds.

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