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Relationship between the Randić Index and Melting Points of Two Steroid Compounds with Hydroxyl Ketone Groups

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Abstract
Graph theory is an approach in mathematical chemistry used to represent and analyse molecular structures in a systematic and quantitative manner. In this approach, atoms are represented as vertices and chemical bonds as edges, enabling the application of topological indices to examine structure–property relationships of compounds. This study aims to analyse the relationship between topological indices, particularly the Randić index, and the melting points of two steroid compounds, namely Androstenedione and Estriol, which differ in their functional groups. The research method employed is a literature review using reliable scientific sources for molecular structure data and melting point values. Molecular graphs of both compounds were constructed and used to calculate the Randić index based on the degrees of connected vertices. The results show that Estriol has a higher Randić index value (19.43) than Androstenedione (17.66), reflecting a higher level of connectivity and structural complexity due to the presence of hydroxyl groups. This higher topological index is consistent with the higher melting point of Estriol compared to Androstenedione. These findings indicate a positive relationship between the Randić index and melting point and support the use of topological indices as an alternative approach for predicting the physical properties of steroid compounds.
Keywords: Randić index; steroid compounds; melting point; hydroxyl; ketone

Introduction

The graph theory approach in mathematical chemistry is used to represent molecular structures in a systematic and quantitative manner [1]. Molecular structures are visualized in the form of graphs, where atoms are represented as vertices and chemical bonds as connecting edges [2], [3]. This graph representation allows molecular structures to be analysed using measurable mathematical concepts and methods. This approach becomes particularly important, especially in the study of compounds with complex structures [4]. Through the application of graph theory, the relationship between molecular structure and the physical properties of compounds can be examined in a more objective and structured way [5].

Numerical parameters obtained from molecular graph representations are known as topological indices. Topological indices serve to describe the structural characteristics of a molecule, such as the degree of atomic connectivity and the complexity of the molecular network [6], [7]. Numerous studies indicate that topological indices correlate with various physical and chemical properties of compounds [8]. One physical property that is frequently studied in relation to topological indices is the melting point. The use of topological indices can serve as an alternative approach for predicting compound properties without relying entirely on experimental laboratory testing.

The Randić index is one of the topological indices widely used in studies of the relationship between structure and properties of chemical compounds [9], [10]. This index is calculated based on the degrees of vertices connected by each edge in a molecular graph. This calculation method makes the Randić index sensitive to the degree of branching and connectivity patterns within molecular structures. Its sensitivity to structural variations has led to its frequent application in the analysis of organic compounds. These characteristics make the Randić index relevant for studies that emphasize the relationship between molecular structure and physical properties [11].

Steroid compounds are a class of organic compounds with complex molecular structures and are widely utilized in the fields of chemistry and pharmacy. The basic framework of steroid compounds consists of four fused rings that form a relatively rigid structure. Variations in the physical and chemical properties of steroid compounds are influenced by the type and position of functional groups attached to this framework. Hydroxyl and ketone groups are functional groups commonly found in steroid compounds. Differences in these functional groups affect the types of intermolecular interactions and lead to variations in physical properties, including melting points.

This study aims to examine the relationship between the Randić index and the melting points of steroid compounds with different functional groups. Although numerous studies have investigated the relationship between topological indices and the physicochemical properties of organic compounds, studies specifically discussing steroid compounds containing hydroxyl and ketone functional groups remain limited. Steroid compounds possess complex molecular structures in which variations in functional groups may influence both covalent connectivity and intermolecular interactions. Understanding how these structural variations are reflected in topological indices and physical properties is therefore important for explaining structure–property relationships. In this study, the Randić index is employed to analyse two steroid compounds, namely Androstenedione and Estriol, which share a similar steroid backbone but differ in their functional groups. Through this analysis, the study aims to explore whether differences in molecular connectivity, as represented by the Randić index, are consistent with differences in the melting points of the selected steroid compounds.

Materials and methods

This section describes the methodological framework applied in this study, including the research approach, materials, data sources, and analytical procedures. A clear explanation of these aspects is necessary to ensure transparency in the research process and to provide a systematic basis for interpreting the results. The description of the methodology also clarifies how the molecular structures were represented and analysed using graph theory concepts. Through this framework, the procedures for constructing molecular graphs and calculating topological indices can be understood in a coherent and structured manner.

This study employs a theoretical analysis combined with a molecular graph modelling approach. In this approach, steroid compounds are represented as molecular graphs in which atoms are modelled as vertices and covalent chemical bonds are represented as edges. This representation enables the structural characteristics of the compounds to be analysed using mathematical concepts from graph theory. The use of graph models allows molecular structures to be examined quantitatively and facilitates the calculation of topological indices that describe molecular connectivity.

The materials analysed in this study consist of two steroid compounds, namely Androstenedione and Estriol. These compounds were selected because they share a similar steroid molecular backbone but differ in their functional groups. Androstenedione contains a ketone functional group, whereas Estriol contains hydroxyl groups attached to the steroid framework. The presence of different functional groups provides a basis for examining variations in molecular connectivity and their possible influence on the physical properties of the compounds.

The molecular structure data of Androstenedione and Estriol were obtained from reliable chemical literature and scientific databases. These sources provide well-established molecular structures that have been widely reported in chemical studies. Information regarding the melting point of each compound was also collected from the literature and used as a parameter in analysing

structure–property relationships. The use of reliable secondary data ensures the accuracy and consistency of the molecular information used in this study.

The analysis begins with illustrating the molecular structures of the selected compounds to obtain accurate structural representations. Each molecular structure is then transformed into a molecular graph, where atoms are represented as vertices and covalent chemical bonds as edges. This transformation allows the molecular structure to be analysed using graph-theoretical methods. Based on this representation, the Randić index is used as the main topological parameter to characterise the molecular graphs.

The Randić index is a well-known topological index that describes the connectivity between vertices in a molecular graph. This index is commonly used in mathematical chemistry to analyse the structural characteristics of chemical compounds. The calculation of the Randić index is based on the degrees of vertices connected by each edge in the graph. The definition of the Randić index used in this study is presented as follows.

Definition 1 [12] *Let $G = (V, E)$ be a molecular graph, where V is the set of vertices and E is the set of edges. The Randić index $R(G)$ is defined as*

$$R(G) = \sum_{uv \in E} \frac{1}{\sqrt{d_u d_v}} \tag{1}$$

where d_u *and* d_v *denote the degrees of vertices* u *and* v*, respectively.*

The obtained Randić index values are subsequently analysed descriptively and compared with the melting point data of Androstenedione and Estriol reported in the literature. This comparison is carried out to examine the relationship between the structural characteristics of molecular graphs and the physical properties of steroid compounds. Through this analysis, the study aims to identify whether differences in molecular connectivity are consistent with variations in melting point. The results of this comparison provide insight into the potential relationship between topological indices and physicochemical properties.

Results and discussion

This section presents the results of the study along with their corresponding discussion. The analysis begins with the structural representation of the steroid compounds investigated in this research. Understanding the arrangement of atoms and the connectivity between them is essential for constructing molecular graphs and performing further mathematical analysis. The molecular structures are first illustrated to provide an overview of the atomic arrangement within each compound, followed by their graph representations in which atoms are modelled as vertices and chemical bonds as edges. These graph models serve as the basis for calculating the Randić index. The obtained index values are then examined in relation to the melting points of the compounds in order to explore the relationship between molecular topology and physical properties.

Molecular Graph Representation of Steroid Compounds

The molecular structure of Androstenedione is presented in Figure 1 to illustrate the arrangement of atoms and chemical bonds forming the compound. This representation provides a comprehensive overview of the steroid molecular framework examined in this study. Information regarding atomic positions and bond types assists in understanding the structural characteristics of the compound in greater detail. Such structural understanding is required as an initial step prior to further mathematical analysis.

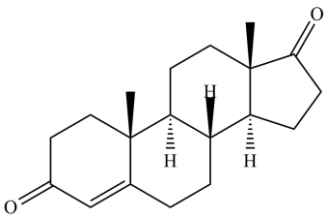

Figure 1 Molecular Structure of Androstenedione

The graph representation of the Androstenedione molecular structure is shown in Figure 2, where atoms are represented as vertices and chemical bonds as edges. This graph form simplifies the molecular structure into a mathematical model that can be easily analysed. Each interatomic relationship is systematically represented, allowing the connectivity pattern of the molecule to be clearly observed. This graph model serves as the basis for calculating the topological indices used to investigate the physical properties of the compound.

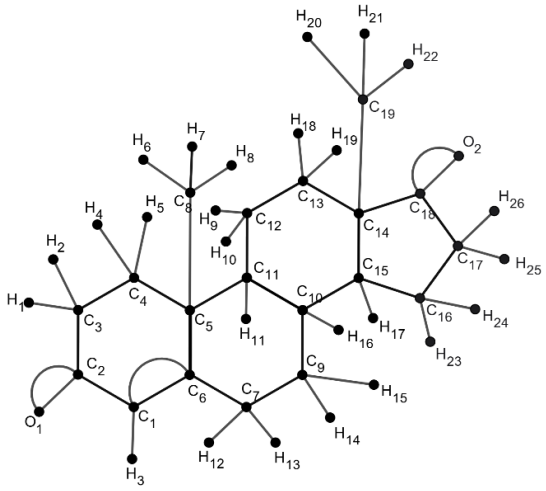

Figure 2 Graph Representation of the Structure of Androstenedione Compound

The molecular structure of Estriol is displayed in Figure 3 to show the arrangement of atoms and chemical bonds forming the compound. This visualization highlights the structural differences between Estriol and Androstenedione. Information on the number of atoms, bond types, and molecular configuration provides an initial understanding of the compound's structural complexity. This understanding is important as a foundation for graph representation and subsequent analysis.

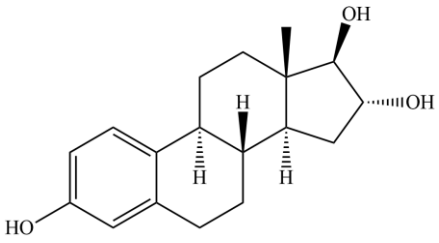

Figure 3 Molecular Structure of Estriol

The graph representation of the Estriol molecular structure is presented in Figure 4 using a molecular graph approach. Atoms in the molecule are represented as vertices, while chemical bonds are represented as edges. This representation enables systematic mathematical analysis of interatomic connectivity. The graph model is used as the basis for calculating topological indices and comparing the structural characteristics with those of other compounds.

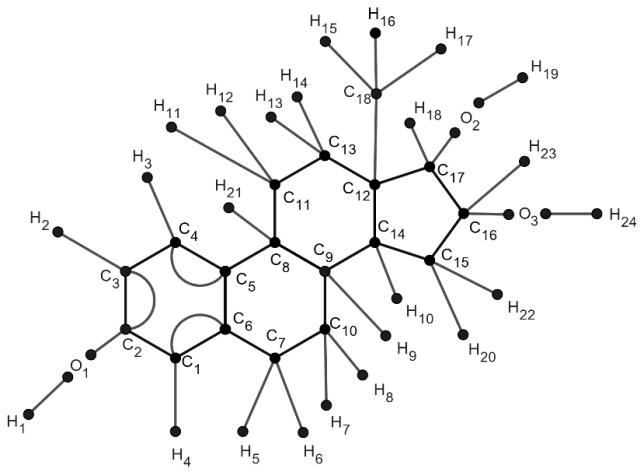

Figure 4 Graph Representation of the Structure of Estriol Compound

Calculation of the Randić Index

Based on Figure 2, each atom is represented as a vertex and each chemical bond as an edge. The molecular graph consists of oxygen–carbon (O–C), carbon–hydrogen (C–H), and carbon–carbon (C–C) bonds. For each edge $uv \in E(G)$, the contribution to the Randić index is determined by the degrees of the connected vertices u and v, denoted by $d_u$and d_v, respectively. Carbon atoms forming the steroid ring system and bonded to several neighbouring atoms generally exhibit higher vertex degrees, whereas oxygen and hydrogen atoms tend to have lower vertex degrees due to their valency limitations. This difference in vertex degrees reflects the variation in local connectivity within the molecular graph of Androstenedione.

Although the molecular graph contains 4 O–C bonds, 26 C–H bonds, and 13 C–C bonds, the Randić index is not determined solely by the number of bonds present in the structure. Instead, the index is calculated as the sum of the contributions$(d_u d_v)^{-1/2}$ over all edges in the graph, meaning that each bond contributes differently depending on the degrees of the vertices it connects. Consequently, the Randić index provides a quantitative description of the connectivity pattern and structural complexity of the Androstenedione molecular graph. Such structural information is important because variations in molecular connectivity may influence the physicochemical properties of the compound. According to Definition 1, the Randić index of the Androstenedione molecular graph is given as follows.

$$
\begin{aligned}
R(G) &= \sum_{uv \in E} \frac{1}{\sqrt{d_u d_v}} \\
&= 3\frac{1}{\sqrt{d_O d_C}} + 21\frac{1}{\sqrt{d_C d_H}} + 23\frac{1}{\sqrt{d_C d_C}} = 4\frac{1}{\sqrt{(2)(4)}} + 26\frac{1}{\sqrt{(4)(1)}} + 13\frac{1}{\sqrt{(4)(4)}} \\
&= 4\frac{1}{\sqrt{8}} + 26\frac{1}{\sqrt{4}} + 13\frac{1}{\sqrt{16}} \\
&= 17.66.
\end{aligned}
$$

The Randić index value obtained from the calculation for the Androstenedione compound is 17.66.

Based on the molecular graph constructed for the Estriol compound, the number of oxygen–carbon (O–C) bonds is 3, the number of oxygen–hydrogen (O–H) bonds is 3, the number of carbon–hydrogen (C–H) bonds is 21, and the number of carbon–carbon (C–C) bonds is 23. The number of each type of bond is used as the basis for calculating the Randić index by considering the degrees of the connected vertices. The calculation of the Randić index is expressed as follows.

Based on the molecular graph constructed for the Estriol compound, each atom is represented as a vertex and each chemical bond as an edge. The molecular graph comprises oxygen–carbon (O–C), oxygen–hydrogen (O–H), carbon–hydrogen (C–H), and carbon–carbon (C–C) edges. For each $uv \in$

$E(G)$, the contribution to the Randić index is determined by the degrees of the incident vertices $deg(u)$ and $deg(v)$. Carbon atoms forming the steroid ring system and bonded to multiple neighboring atoms generally exhibit higher vertex degrees, whereas oxygen and hydrogen atoms have lower vertex degrees due to their valency limitations. Accordingly, although the molecular graph contains 3 O–C bonds, 3 O–H bonds, 21 C–H bonds, and 23 C–C bonds, the Randić index is not computed solely based on the number of bonds, but rather as the sum of the contributions $(d_u d_v)^{-1/2}$ over all edges in the graph. This formulation ensures that the Randić index captures the local connectivity and structural complexity of the Estriol molecular graph. Based on Figure 4, the Randic index of the Estriol molecular graph is as follows.

$$
\begin{aligned}
R(G) &= \sum_{uv \in E} \frac{1}{\sqrt{d_u d_v}} \\
&= 3\frac{1}{\sqrt{d_O d_C}} + 3\frac{1}{\sqrt{d_O d_H}} + 21\frac{1}{\sqrt{d_C d_H}} + 23\frac{1}{\sqrt{d_C d_C}} \\
&= 3\frac{1}{\sqrt{(2)(4)}} + 3\frac{1}{\sqrt{(2)(1)}} + 21\frac{1}{\sqrt{(4)(1)}} + 23\frac{1}{\sqrt{(4)(4)}} \\
&= 3\frac{1}{\sqrt{8}} + 3\frac{1}{\sqrt{2}} + 21\frac{1}{\sqrt{4}} + 23\frac{1}{\sqrt{16}} \\
&= 19.43.
\end{aligned}
$$

The Randić index value obtained from the calculation for the Estriol compound is 19.43.

Relationship between the Randić Index and Melting Point of Steroid Compounds

The relationship between the Randić index and the melting point of steroid compounds can be observed through a comparison of molecular topological data and the physical properties of each compound. This information is summarized in Table 1, which presents the Randić index values and melting points of Androstenedione and Estriol as the basis for analysing the relationship between the two. According to data reported in the PubChem database, the melting point of Androstenedione is approximately 173 °C, whereas Estriol exhibits a significantly higher melting point of about 282 °C. These melting point values are obtained from reliable chemical data sources and are used in this study to examine the relationship between molecular connectivity, represented by the Randić index, and the physical properties of steroid compounds [13],[14].

Table 1: Randić Index Values and Melting Points of Steroid Compounds

Compounds	Randić Index Values	Melting Points (ºC)
Androstenedione	17,66	173
Estriol	19,43	282

The Randić index value of Androstenedione is 17.66, which is lower than that of Estriol, which reaches 19.43. This difference reflects variations in the covalent bonding connectivity patterns in the molecular graphs of the two compounds. In molecular graph modeling, atoms are represented as vertices and only covalent bonds are included as edges; therefore, the Randić index is determined solely by the distribution of vertex degrees and the connectivity between atoms within the molecule. The molecular graph of Androstenedione, although it contains a ketone group (C=O) with a covalent double bond, does not exhibit a substantial increase in branching or connectivity, resulting in a lower Randić index value.

The molecular graph of Estriol is influenced by the presence of three hydroxyl (–OH) groups, which increase the number of covalent O–C and O–H bonds within the molecule. The addition of these covalent bonds increases the degrees of certain vertices and enhances local connectivity in the

molecular graph. This increased complexity of covalent connectivity is reflected in the higher Randić index value of Estriol. This interpretation is strictly based on the molecular graph representation and does not involve hydrogen bonding in the calculation of the graph index.

The difference in melting points between the two compounds can be explained from a chemical perspective by considering intermolecular interactions. Estriol has a melting point of 282 °C, whereas Androstenedione melts at 173 °C. The hydroxyl groups in Estriol enable the formation of strong intermolecular hydrogen bonds, which enhance crystal lattice stability and increase the energy required for melting. Intermolecular interactions in Androstenedione are dominated by dipole–dipole forces associated with the ketone group, resulting in a lower melting point. Accordingly, the Randić index describes the complexity of covalent bonding within the molecular structure, while hydrogen bonding serves as a complementary chemical explanation for differences in physical properties, particularly melting point.

Conclusion

The Randić index values obtained in this study indicate that graph theory can be used as an appropriate mathematical framework for representing the molecular structures of steroid compounds. Molecular graph representation allows the description of covalent bonding connectivity patterns and the calculation of the Randić index as a measure of structural complexity. The results show that Estriol has a Randić index value of 19.43 with a melting point of 282 °C, while Androstenedione has a Randić index value of 17.66 with a melting point of 173 °C, reflecting differences in covalent connectivity within their molecular structures. The difference in index values is qualitatively consistent with the difference in melting points of the two compounds, although melting behavior is also influenced by intermolecular interactions that are not included in the calculation of the graph index. These findings provide an initial indication of consistency between molecular graph complexity and physical properties, while broader generalization requires further analysis involving a larger set of compounds.

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