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RESEARCH ARTICLE

ABC Index Analysis: Physical Properties of Prenylated Xanthone

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Abstract: Xanthone is a heterocyclic compound with various substituents such as hydroxyl, prenyl, and methoxy groups, which contribute to its biological activities, including anticancer, antidiabetic, and antioxidant effects. This study aims to optimize the design of xanthone derivatives through a mathematical approach using Chemical Topological Graphs (CTG) and the Atom-Bond Connectivity (ABC) index. Three xanthone derivatives—1,7-dihydroxy-3-methoxy-2-(3-methylbut-2-enyl)xanthone (1), Gartanin (2), and Garcinone E (3)—were analyzed based on the number of prenyl substituents, and a literature review was conducted to identify their physicochemical properties, molecular structures, and potential biological activities. The results indicate that an increased number of prenyl substituents leads to higher ABC index values (32.186; 43.987; and 51.744, respectively), reflecting more complex molecular structures and enhanced bioactivity potential. A higher ABC index also correlates with increased boiling points, molecular stability, and bioactivity, along with reduced polarity and melting points, as evidenced by the melting point decreasing from 220°C to 152.5°C. However, these findings remain theoretical and require further validation through experimental studies.

Keywords: Xanthone, ABC Index, Prenyl, Chemical Topological Graph (CTG)

1. Introduction

Xanthone is a heterocyclic compound with various substituents (hydroxy, prenyl, geranyl, methoxy, halogen, and others) [1, 2]. The presence of these substituents imparts diverse biological activities, including anticancer, antidiabetic, and antioxidant properties [3]. Xanthone occurs naturally in various plants, including Garcinia mangostana, as well as in certain microorganisms and lichens. The biosynthesis of xanthone involves the shikimate-acetate pathway in plants and the acetate-malonate pathway in microorganisms, highlighting the flexibility of this molecule in ecological adaptation. Xanthone can be synthesized through the condensation of phenols and aromatic aldehydes, using nanoparticle-based catalysts such as Cu and $CuFe_2O_4$, which enhance the efficiency of the reaction [4]. This catalytic approach provides a more efficient and environmentally friendly synthesis method, yielding higher amounts of xanthone [5].

Isolation can be carried out from various natural sources or through chemical synthesis. Xanthones are commonly obtained through the condensation of phenols with aromatic aldehydes in chemical synthesis, while natural isolation is frequently conducted from the rind of Garcinia mangostana fruit, which contains xanthone derivatives such as gartanin and garcinone E [6]. Several studies have shown that xanthone derivatives, such as garcinone E and gartanin, exhibit significant anticancer activity, with IC50 values varying accordingly. Gartanin has an IC50 value ranging from 10–30 µM, while garcinone E shows an IC50 value of approximately 5–15 µM against cancer cells. Substituents like prenyl groups on xanthones can enhance their pharmacological potential by strengthening interactions with biological membranes, increasing hydrophobicity, and supporting their bioactivity in cancer treatment [7].

Xanthone compounds from mangosteen peel have a complex chemical structure, requiring analytical approaches capable of quantitatively and comprehensively describing their molecular properties. One method that can be utilized is the Chemical Topological Graph (CTG), which is a graphical representation of molecular structures where atoms and chemical bonds are converted into nodes and edges in a graph. Topological indices, such as the Atom-Bond Connectivity (ABC) index, have demonstrated utility in studies of heat formation in alkanes[8]. The ABC index has also been widely used to predict the physical, chemical, and pharmacological properties of molecules. The ABC index itself is defined as the sum over all adjacent vertex pairs in a graph, with each pair evaluated using the formula: $\sqrt{\frac{d_i+d_j-2}{d_i \cdot d_j}}$ where d_i represents the degree of vertex v_i [8]. Despite its usefulness, prior studies have shown several limitations in its application. For instance, the study by [9] on the supramolecular model of Fuchsine computed various topological descriptors without relating them to specific biological activities. Another study by [10] discussed extremal values of the ABC index on tree graphs but did not explore applications in real chemical systems. The development of the exponential variant of the ABC index by [11]remains at a purely mathematical characterization stage without validation against actual molecular structures. Furthermore, the study by [12] that analyzed topological indices on inverse graphs of generalized quaternion groups was entirely abstract and not connected to chemical or molecular biology contexts.

Based on these gaps, this article aims to fill the research void by applying a mathematical approach using Chemical Topological Graph (CTG) and the ABC index directly to prenylated xanthone compounds, to evaluate their physical properties related to biological activity. By integrating graph theory and molecular chemistry, this study seeks to support the development of more efficient, data-driven drug design strategies, particularly for cancer therapy [13].

2. Method

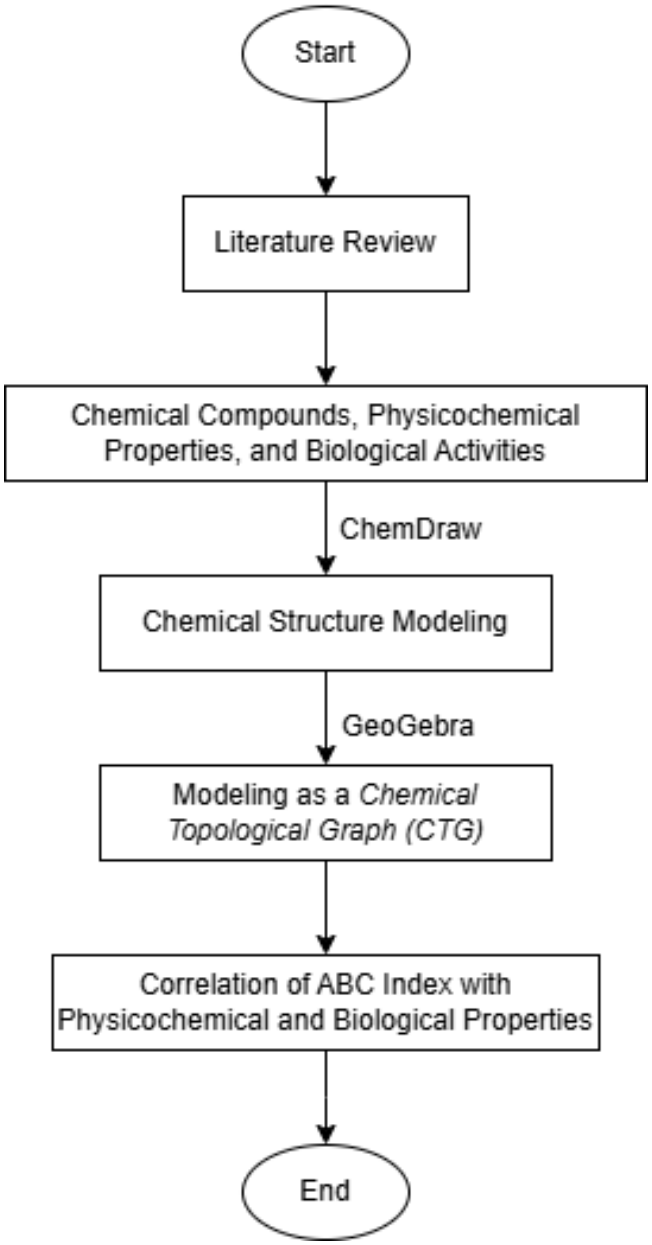

Figure 2.1: Research Flowchart

The stages carried out in this research are systematically structured and are explained in detail as follows:

1. The research begins with a literature review on Xanthone compounds, specifically 1,7-Dihydroxy-3-methoxy-2-(3-methylbut-2-enyl)xanthone ($C_{19}H_{18}O_8$), Gartanin ($C_{23}H_{24}O_6$), and Garcinone E ($C_{28}H_{32}O_6$). This review includes information on their physicochemical properties, biological activities, molecular structures, and potential applications in relevant fields. The literature study is conducted by examining scientific articles, reference books, and prominent chemical databases such as PubChem and Scopus.

2. After obtaining the molecular structures of the prenylated compounds, modeling is conducted in the form of a Chemical Topological Graph. In this stage, each atom in the molecule is represented as a node and each chemical bond as an edge in the graph.
3. The resulting topological graph is analyzed to calculate numerical values in the form of topological indices, with a particular focus on the Atom–Bond Connectivity (ABC) index. This index is calculated based on the degree of each atom involved in the bonds, representing the contribution of each pair of connected nodes within the chemical graph.
4. Finally, the calculated ABC index is then used to correlate the numerical properties of the chemical graph with the physical and biological properties of the studied compounds. This correlation aims to identify the relationship between molecular structure and compound characteristics.

3. Results and Discussion

The Atom-Bond Connectivity index (ABC) is one of the most popular topological indices in chemical graph theory. A topological index is a number associated with the molecular structure and is used to predict the chemical and physical properties of the molecule. The ABC index is based on the degrees of the nodes in the graph.

Definition 1. Let G be a connected undirected graph. The ABC index is defined as

$$ABC = ABC(G) = \sum_{v_i v_j \in E(G)} \sqrt{\frac{d_{v_i} + d_{v_j} - 2}{d_{v_i} d_{v_j}}}$$

where $v_i \sim v_j$ indicates that nodes v_i and v_j are neighbors, d_{v_i} is the degree of node v_i, and d_{v_j} is the degree of node v_j [8]. Based on this definition, the following is an analysis of the ABC index values for several chemical compounds:

1. 1,7-Dihydroxy-3-methoxy-2-(3-methylbut-2-enyl)xanthone($C_{19}H_{18}O_8$)

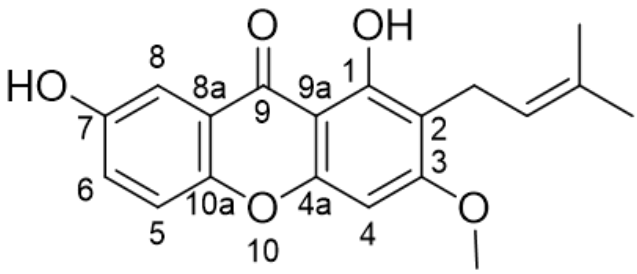

Figure 3.2: Chemical Structure of ($C_{19}H_{18}O_8$)

The representation of the compound in the form of a graph results in a structure as shown in the following illustration:

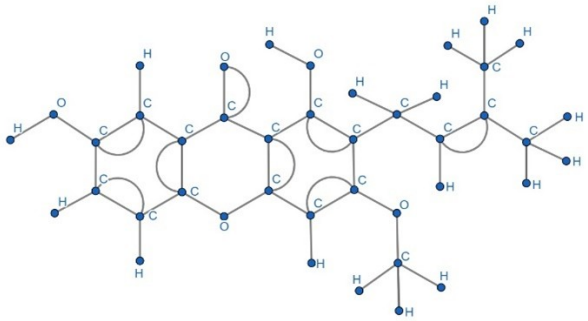

Figure 3.3: Graph Representation of ($C_{19}H_{18}O_8$)

1,7-Dihydroxy-3-methoxy-2-(3-methylbut-2-enyl)xanthone, with the chemical formula ($C_{19}H_{18}O_8$), when represented as a graph, will have several nodes: the C (Carbon) nodes are $C_1, C_2, ..., C_{19}$ with degree d(C) = 4, the H (Hydrogen) nodes are $H_1, H_2, ..., H_{18}$ with degree d(H) = 1, and the O (Oxygen) nodes are $O_1, O_2, ..., O_6$ with degree d(O) = 2. Next, the ABC index of this compound will be calculated, starting with the calculation of the types of edges between neighboring nodes: E(G) = (C, H), (C, C), (C, O), (O, H). The calculation of the ABC index for this compound is as follows:

$$
\begin{aligned}
ABC(G) &= \sum_{v_iv_j \in E(G)} \sqrt{\frac{d_{v_i} + d_{v_j} - 2}{d_{v_i} d_{v_j}}} \mathrm{ABC}_{C-H}(G) + \mathrm{ABC}_{C-C}(G) + \mathrm{ABC}_{C-O}(G) + \mathrm{ABC}_{O-H}(G) \\
&= \sum_{C_iH_j \in E(G)} \sqrt{\frac{d_{C_i} + d_{H_j} - 2}{d_{C_i} d_{H_j}}} + \sum_{C_iC_j \in E(G)} \sqrt{\frac{d_{C_i} + d_{C_j} - 2}{d_{C_i} d_{C_j}}} + \sum_{C_iO_j \in E(G)} \sqrt{\frac{d_{C_i} + d_{O_j} - 2}{d_{C_i} d_{O_j}}} \\
&\quad + \sum_{O_iH_j \in E(G)} \sqrt{\frac{d_{O_i} + d_{H_j} - 2}{d_{O_i} d_{H_j}}} \\
&= (16)\sqrt{\frac{4+1-2}{(4)(1)}} + (26)\sqrt{\frac{4+4-2}{(4)(4)}} + (2)\sqrt{\frac{2+1-2}{(2)(1)}} + (8)\sqrt{\frac{4+2-2}{(4)(2)}} \\
&= (16)\sqrt{\frac{3}{4}} + (26)\sqrt{\frac{6}{16}} + (2)\sqrt{\frac{1}{2}} + (8)\sqrt{\frac{4}{8}} \\
&= (16)\frac{1}{2}\sqrt{3} + (26)\frac{1}{4}\sqrt{6} + (2)\sqrt{\frac{1}{2}} + (8)\sqrt{\frac{1}{2}} \\
&= 8\sqrt{3} + \frac{13}{2}\sqrt{6} + \sqrt{2} + 4\sqrt{2} \\
&= 8\sqrt{3} + \frac{13}{2}\sqrt{6} + 5\sqrt{2} \\
&= 32.186
\end{aligned}
$$

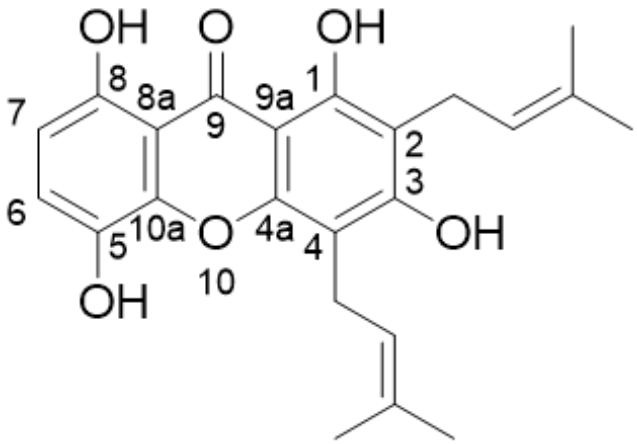

Figure 3.4: Chemical Structure of Gartanin ($C_{23}H_{24}O_6$)

The representation of the compound in the form of a graph results in a structure as shown in the following illustration.

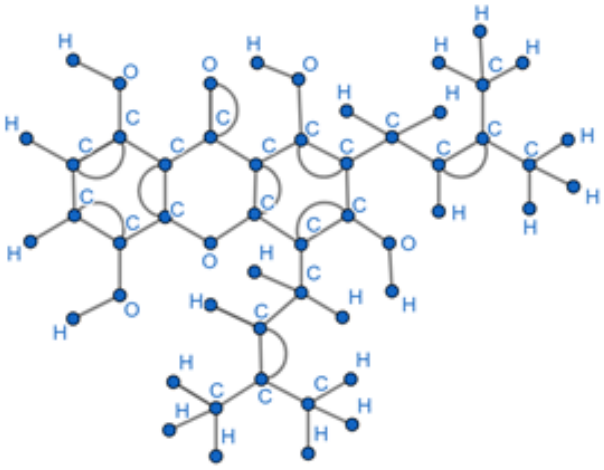

Figure 3.5: Graph Representation of Gartanin ($C_{23}H_{24}O_6$)

The chemical compound Gartanin ($C_{23}H_{24}O_6$), when represented as a graph, will have several nodes: the C (Carbon) nodes consist of $C_1, C_2, ..., C_{23}$ with degree d(C) = 4; the H (Hydrogen) nodes consist of $H_1, H_2, ..., H_{24}$ with degree d(H) = 1; and the O (Oxygen) nodes consist of $O_1, O_2, ..., O_6$ with degree d(O) = 2. Next, the ABC index of this compound will be calculated, starting with the computation of the types of edges between two adjacent nodes: $E(G) = \{(C, H), (C, C), (C, O), (O, H)\}$.

Here is the formatted calculation of the ABC index for the compound:

$$
\begin{aligned}
ABC(G) &= \sum_{v_iv_j \in E(G)} \sqrt{\frac{d_{v_i} + d_{v_j} - 2}{d_{v_i} d_{v_j}}} \mathrm{ABC}_{C-H}(G) + \mathrm{ABC}_{C-C}(G) + \mathrm{ABC}_{C-O}(G) + \mathrm{ABC}_{O-H}(G) \\
&= \sum_{C_iH_j \in E(G)} \sqrt{\frac{d_{C_i} + d_{H_j} - 2}{d_{C_i} d_{H_j}}} + \sum_{C_iC_j \in E(G)} \sqrt{\frac{d_{C_i} + d_{C_j} - 2}{d_{C_i} d_{C_j}}} + \sum_{C_iO_j \in E(G)} \sqrt{\frac{d_{C_i} + d_{O_j} - 2}{d_{C_i} d_{O_j}}} \\
&\quad + \sum_{O_iH_j \in E(G)} \sqrt{\frac{d_{O_i} + d_{H_j} - 2}{d_{O_i} d_{H_j}}} \\
&= (20)\sqrt{\frac{4+1-2}{(4)(1)}} + (32)\sqrt{\frac{4+4-2}{(4)(4)}} + (2)\sqrt{\frac{2+1-2}{(2)(1)}} + (8)\sqrt{\frac{4+2-2}{(4)(2)}} \\
&= (20)\sqrt{\frac{3}{4}} + (32)\sqrt{\frac{6}{16}} + (2)\sqrt{\frac{1}{2}} + (8)\sqrt{\frac{4}{8}} \\
&= (20)\frac{1}{2}\sqrt{3} + (32)\frac{1}{4}\sqrt{6} + (2)\sqrt{\frac{1}{2}} + (8)\sqrt{\frac{1}{2}} \\
&= 10\sqrt{3} + 8\sqrt{6} + \sqrt{2} + 4\sqrt{2} \\
&= 10\sqrt{3} + 8\sqrt{6} + 5\sqrt{2} \\
&= 43.987
\end{aligned}
$$

2. Garcinone E ($C_{28}H_{32}O_6$)

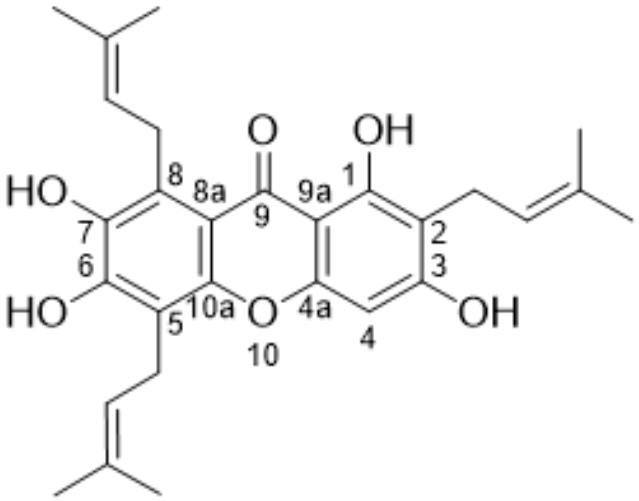

Figure 3.6: Chemical Structure of Garcinone E ($C_{28}H_{32}O_6$)

The representation of the compound in the form of a graph produces a structure as shown in the following illustration.

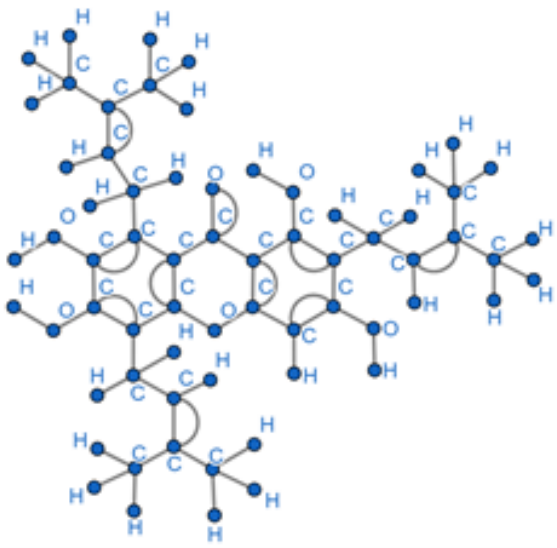

Figure 3.7: Graph Representation of Garcinone E ($C_{28}H_{32}O_6$)

The compound Garcinone E ($C_{28}H_{32}O_6$), when represented as a graph, will have several nodes: the C (Carbon) nodes consist of $C_1, C_2, \ldots, C_{28}$ with a degree $d(C) = 4$; the H (Hydrogen) nodes consist of $H_1, H_2, \ldots, H_{32}$ with a degree $d(H) = 1$; and the O (Oxygen) nodes consist of $O_1, O_2, \ldots, O_6$ with a degree $d(O) = 2$. The ABC index of this compound will then be calculated, starting with the computation of each type of edge between two adjacent nodes: $E(G) = \{(C,H),(C,C),(C,O),(O,H)\}$.
Here is the formatted calculation for the ABC index of the compound:

$$
\begin{aligned}
ABC(G) &= \sum_{v_iv_j \in E(G)} \sqrt{\frac{d_{v_i} + d_{v_j} - 2}{d_{v_i} d_{v_j}}} \mathrm{ABC}_{C-H}(G) + \mathrm{ABC}_{C-C}(G) + \mathrm{ABC}_{C-O}(G) + \mathrm{ABC}_{O-H}(G) \\
&= \sum_{C_iH_j \in E(G)} \sqrt{\frac{d_{C_i} + d_{H_j} - 2}{d_{C_i} d_{H_j}}} + \sum_{C_iC_j \in E(G)} \sqrt{\frac{d_{C_i} + d_{C_j} - 2}{d_{C_i} d_{C_j}}} + \sum_{C_iO_j \in E(G)} \sqrt{\frac{d_{C_i} + d_{O_j} - 2}{d_{C_i} d_{O_j}}} \\
&\quad + \sum_{O_iH_j \in E(G)} \sqrt{\frac{d_{O_i} + d_{H_j} - 2}{d_{O_i} d_{H_j}}} \\
&= (30)\sqrt{\frac{4+1-2}{(4)(1)}} + (36)\sqrt{\frac{4+4-2}{(4)(4)}} + (4)\sqrt{\frac{2+1-2}{(2)(1)}} + (8)\sqrt{\frac{4+2-2}{(4)(2)}} \\
&= (30)\sqrt{\frac{3}{4}} + (36)\sqrt{\frac{6}{16}} + (4)\sqrt{\frac{1}{2}} + (8)\sqrt{\frac{4}{8}} \\
&= (30)\frac{1}{2}\sqrt{3} + (36)\frac{1}{4}\sqrt{6} + (4)\sqrt{\frac{1}{2}} + (8)\sqrt{\frac{1}{2}} \\
&= 15\sqrt{3} + 9\sqrt{6} + 2\sqrt{2} + 4\sqrt{2} \\
&= 15\sqrt{3} + 9\sqrt{6} + 6\sqrt{2} \\
&= 51.744
\end{aligned}
$$

The melting points of xanthone, gartanin, and Garcinone E show a decreasing trend as the number of prenyl groups increases. Xanthone has been reported to have a melting point of 220°C [14], gartanin 167°C [15], and Garcinone E 152.5°C [16]. Complete information on the

number of prenyl groups, melting points, and ABC index values of the three compounds is presented in Table 3.1.

Table 3.1: Compound ABC Index Values

Compound Name	Amount of Prenyl	Melting Point (°C)	ABC Index Value
1,7-dihydroxy-3-methoxy-2-(3-methylbut-2-enyl) xanthone ($C_{19}H_{18}O_6$)	1	220	32.186
Gartanin ($C_{23}H_{24}O_6$)	2	167	43.987
Garcinone E ($C_{28}H_{32}O_6$)	3	152.5	51.744

The results of this study demonstrate that an increase in the number of prenyl substituents on a molecular structure is directly proportional to an increase in the ABC index value. Quantitatively, the ABC index rose from 32.186 to 51.744 as the number of prenyl groups increased. The addition of prenyl groups enriches the molecular topology, which in turn contributes to the enhancement of the compound's biological activity [17].

In line with these findings, a higher ABC index has been shown to correlate positively with increased boiling point and molecular stability, while simultaneously contributing to decreased polarity and melting point. The decrease in melting point is evident from the observed reduction from 220°C to 152.5°C. These results indicate that the increase in the ABC index reflects the growing complexity of the chemical structure, which potentially contributes to enhanced stability, biological activity, and reduced polarity and melting point of the compound.

4. Conclusion

The calculation of the atom bond connectivity (ABC) index indicates that the addition of hydrophobic prenyl groups to xanthone derivatives contributes to increased molecular stability, enhanced biological activity, and reduced polarity and melting point. This is evidenced by a decrease in melting point from 220 °C to 152.5 °C. The increase in ABC index values reflects greater molecular complexity and higher bioactivity potential. This approach demonstrates potential as a predictive tool in the early-stage design of therapeutic compounds, particularly as candidates for anticancer and antidiabetic drugs. However, since the findings are theoretical and rely on topological mathematical models, further validation through experimental studies is necessary to confirm their effectiveness and applicability in real-world drug development.

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