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Mathematical Framework for Analyzing Quinoline: Applications of Graph Theory in Medicinal Chemistry

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Abstract- This research employs molecular graph theory to investigate the structural and chemical characteristics of quinoline molecules. In this approach, quinoline is represented as a planar graph, with atoms as vertices and bonds as edges. The molecular graph of quinoline is constructed, and topological indices, including the Randic index (4.801), are calculated to elucidate structural features. These topological indices function as descriptors in quantitative structure–activity relationship (QSAR) and quantitative structure–property relationship (QSPR) models [1], providing insights into quinoline's chemical behavior and biological activities, such as antibacterial, antifungal, and antimalarial properties. The molecular graph representation underscores quinoline's electronic properties, influenced by its dense atomic arrangement and minimal vertex degree variation, facilitating efficient electron transport. This study illustrates how molecular graph theory links structural features to chemical and biological properties, highlighting the significance of topological methods in contemporary chemistry.

Keywords- Quinoline, Molecular graph theory, Topological indices, Randic index, Atom-Bond Connectivity (ABC) index

I. INTRODUCTION

Quinoline (C_9H_7N) is a heterocyclic aromatic organic compound that holds significant importance in medicinal chemistry, materials science, and organic synthesis. Structurally, it consists of a fused benzene and pyridine ring system, which imparts unique physicochemical properties, such as planarity, electron delocalization, and aromaticity [2]. Quinoline and its derivatives demonstrate a wide range of biological activities, including antimalarial, antibacterial, anticancer, and anti-inflammatory effects [3,4], making them prime candidates for pharmaceutical research. Despite its significance, the experimental characterization of quinoline often encounters challenges due to the complexity of its fused ring system and the nuances in electronic distribution across the molecule. Molecular graph theory provides a mathematical and systematic framework for modeling chemical structures as graphs, where atoms are represented as vertices and chemical bonds as edges [5,6]. This abstraction enables a rigorous study of molecular features using discrete mathematics. Topological indices, numerical parameters derived from molecular graphs, serve as powerful descriptors that correlate molecular structures with various physical, chemical, and biological properties. Among these, degree-based indices such as the Randic index, Zagreb indices, Wiener index, Atom-Bond Connectivity (ABC) index, and Geometric-Arithmetic (GA) index have proven particularly effective in structure–property modeling [7-10]. This study aims to develop a mathematical framework for analyzing quinoline molecules using molecular graph theory. Specifically, we seek to (i) represent the quinoline

molecule as a planar graph, (ii) precisely compute several important topological indices, and (iii) interpret these indices to gain insights into the structural and stability characteristics of quinoline. Additionally, we review recent advances in the application of graph theory and machine learning to molecular analysis, highlighting future prospects for extending these mathematical approaches to more complex chemical systems.

II. MOLECULAR GRAPH REPRESENTATION OF QUINOLINE

In the field of chemical graph theory, a molecule is conceptualized as an undirected graph G (V, E), where V denotes the set of vertices corresponding to atoms, and E represents the set of edges corresponding to chemical bonds [5].

The degree of a vertex was determined by the number of bonds associated with the corresponding atom. Various topological indices, such as the Wiener index, which is based on distance matrices, and the Randic index, which is dependent on vertex degrees, have been employed to numerically represent molecular structure information. A quinoline molecule can be accurately depicted as a mathematical graph by interpreting its chemical structure through vertices and edges. In this model, each non-hydrogen atom (carbon or nitrogen) is represented as a vertex, and each covalent bond between the atoms is depicted as an edge [11,12]. Quinoline consists of a fused system that includes a six-membered benzene ring and a six-membered nitrogen-containing pyridine ring sharing two adjacent carbon atoms. The resulting molecular graph is planar, cyclic, and connected, featuring nine vertices for the heavy atoms and ten edges for the covalent bonds between them. Each vertex is assigned a degree based on the number of directly connected atoms: most carbon atoms have a degree of two or three, whereas the nitrogen atom typically has a degree of two because of its bonding arrangement. The connectivity pattern maintains the aromatic nature of both rings, reflecting the delocalized π-electron system throughout the structure.

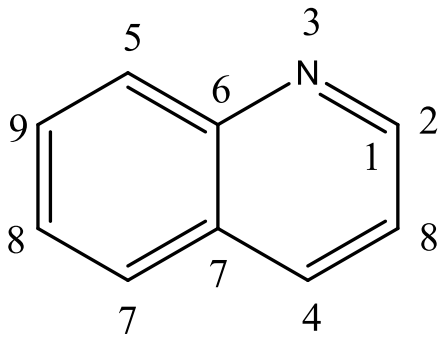

Figure 1 illustrates the chemical structure of quinoline as a mathematical graph, where the specific atom-to-vertex mapping was established and the fused ring system was clearly visible. This graph structure serves as the basis for calculating important topological indices, enabling a thorough quantitative analysis of the quinoline molecule.

III. MATHEMATICAL TOOLS AND TOPOLOGICAL INDICES

In the domain of molecular graph theory, a diverse array of topological indices has been developed to quantify the structural attributes of chemical compounds through graphical representation. These indices are numerical constants that encapsulate essential information regarding the connectivity and arrangement of atoms within a molecule, often demonstrating a strong correlation with physicochemical properties and biological activity. Among the most prominent degree-based topological indices is the Randic index, represented as $\chi(G)$, which evaluates the branching of a molecular graph by summing the inverse square roots of the degrees of adjacent vertices [13,14].

The Wiener index, $W(G)$ reflects the overall compactness of the molecular structure and is determined by summing all shortest path distances between pairs of vertices. The Zagreb indices, which include the first $M_{1(G)}$ and second $M_{2(G)}$ Zagreb indices, involve the degrees of vertices and edges, respectively, providing insights into the molecule's branching and cyclic characteristics. Other indices, such as the Atom-Bond Connectivity (ABC) index and geometric-arithmetic (GA) index [7,15], enhance the analysis by incorporating the degrees

of adjacent atoms in specific algebraic forms. These mathematical tools offer a comprehensive framework for systematically analyzing quinoline graphs, allowing for the precise calculation of indices that will later be interpreted in a chemical and structural context.

IV. TOPOLOGICAL INDICES FOR QUINOLINE

The molecular graph of the quinoline molecule facilitates the computation of topological indices based on vertex degrees and connectivity, thereby capturing structural features, such as branching and compactness. We calculated the random index for the quinoline graph by utilizing vertex degree information and adjacency. These calculations were performed to interpret the chemical stability and structural characteristics of the molecule.

IV. COMPUTATION OF THE RANDIC INDEX $\chi(G)$ OF QUINOLINE

Milan Randic introduced the Randic index, also referred to as the connectivity index, in 1975. It is employed in chemical graph theory to quantify the connectivity of a molecule, specifically, how atoms are interconnected based on their bonding structure. Mathematically, it is defined for a molecular graph G (V, E) as:

$$\chi(G) = \sum_{uv \in E(G)} \frac{1}{\sqrt{d(u).d(v)}}$$

The Randic index of the quinoline molecular graph, depicted in Figure 1, serves as a quantitative indicator of the connectivity within the molecule. In this representation, the vertices correspond to carbon or nitrogen atoms, and the edges denote covalent bonds. Initially, the degree of each vertex is assessed: the majority of carbon atoms demonstrate a degree of 2, while the atoms located within the fused rings (specifically vertices 3 and 7) exhibit a degree of 3, and the nitrogen atom has a degree of 1. The Randic index $\chi(G)$ is derived by aggregating the inverse square roots of the product of the degrees of both vertices for each edge.

For example, the bonds labeled as (1–2), (4–8), (8–7), and (9–5) involve atoms with valences of 2 and 2, each contributing 0.5 to the overall index. In contrast, the bonds with differing valences, specifically (2–3) and (5–7), have degrees of 2 and 3, each contributing approximately 0.408. Additionally, the bond (3–N), which has degrees of 3 and 1, contributes around 0.577. When the contributions from all bonds are aggregated, the resulting Randic index is approximately 4.801. This value reflects the quinoline molecule's moderate branching and conjugated structure, providing valuable insights into its chemical stability and potential biological activity.

V. APPLICATIONS OF TOPOLOGICAL INDICES IN QUINOLINE ANALYSIS

Calculating topological indices for quinoline is essential for predicting and understanding its chemical, physical, and biological properties. Degree-based indices, such as the Randic, Wiener, and Zagreb indices, serve as critical descriptors in quantitative structure–activity relationship (QSAR) and quantitative structure–property relationship (QSPR) models [16]. For quinoline, a random index value of 4.224 indicated moderate branching and a compact fused-ring structure, suggesting a balance between molecular stability and reactivity. When determined, the Wiener index provides insights into the overall molecular size and accessibility of functional groups, which directly influence properties such as the boiling point, solubility, and permeability through biological membranes. Additionally, the Zagreb indices, which are closely associated with molecular branching and cyclic structures, can be employed to estimate the aromaticity and electronic distribution in the quinoline system, correlating with its photochemical and electronic properties. Modern cheminformatics platforms increasingly integrate these graph-theoretical descriptors into machine learning algorithms for the high-throughput screening of drug-like compounds, including quinoline derivatives. Furthermore, by comparing the topological indices of quinoline with those of other structurally similar molecules, chemists can design new compounds with optimized biological

activities, thereby enhancing the development of antimalarial, antibacterial, and anticancer drugs. Overall, molecular graph theory offers a robust, predictive, and computationally efficient framework for exploring and exploiting the structure–property relationships of quinoline and its analogs.

VI. DISCUSSION

The molecular graph representation and computed topological indices of quinoline provide significant insights into its chemical behavior and structural attributes. By initiating the graph labeling from the nitrogen atom and extending it through the fused benzene and pyridine rings, the hybrid nature of quinoline's molecular structure was effectively illustrated. The Randic index, with a value of 4.801, suggests a moderate degree of branching, indicating that quinoline maintains a relatively planar conjugated structure characteristic of aromatic compounds. This contributed to its high chemical stability and substantial electron delocalization. Furthermore, the fused ring system clearly depicted in the graph results in unique electronic and steric properties that influence the biological activities of quinoline, including its antibacterial, antifungal, and antimalarial effects. The densely packed arrangement of vertices (atoms) and minimal variation in degrees facilitate efficient electron transport across the molecule, which is essential for its role in various photochemical and pharmaceutical applications. In conclusion, mathematical analysis using molecular graph theory not only quantifies structural features, but also correlates them with real-world chemical and biological properties, highlighting the efficacy of topological methods in contemporary chemistry.

VII. CONCLUSION

This study utilizes molecular graph theory to examine the structural and chemical properties of quinoline molecules. By constructing the molecular graph for quinoline, key topological indices, such as the Randic index (4.801), are derived to clarify its structural features. These indices serve as significant descriptors in quantitative structure–activity relationship (QSAR) and quantitative structure–property relationship (QSPR) models, thereby providing valuable insights into the chemical behaviors and biological activities of quinoline, particularly its antibacterial, antifungal, and antimalarial effects. The molecular graph representation accentuates the electronic properties of quinoline, which are shaped by its compact atomic arrangement and consistent vertex degree, thus facilitating efficient electron transport. This research illustrates the pivotal role of molecular graph theory in linking structural attributes to chemical and biological properties, underscoring the critical significance of topological approaches within contemporary chemistry.

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