

Abstract

Graph theory is a highly specialised and specific discipline of mathematics that elucidates the representation of any formed structure. Recently, it has garnered significant attention among academics because to its extensive applications in technology, electrical networks, linked networks, biological networks, and chemistry, among others. Currently, the rapidly expanding domain among academics is chemical graph theory, due to its extensive applications in technology, electrical and biological networks, linked systems, and chemistry, among others. Currently, chemical graph theory is a rapidly expanding domain among scholars. Topological descriptors are highly effective for predicting the physicochemical features and bioactivity of molecular graphs. In quantitative structure-activity relationships (QSAR) and quantitative structure-property relationships (QSPR), particularly within pharmaceutical research, a vast array of indices is examined in mathematical chemistry and drug development.

The study and calculation of topological descriptors of molecular graphs and networks is a significant issue in mathematics and computational chemistry. This thesis offers comprehensive details about many forms of TI's, including degree, distance, and counting-related polynomials. Molecular topological descriptors, as numerical invariants of a molecule's structure, are highly effective in predicting a molecule's bioactivity. Due to its applicability in several domains of mathematical chemistry, Research in this area has been greatly advanced by graph theory, which has also become quite popular among scholars. Numerous indicators are employed and studied in the fields of chemistry, pharmacology, drug manufacturing, and other associated disciplines. This thesis computes the eccentricity indices of a third-kind HDN networks and Polyhydroxyalkanoates (*PHA's*). To further explore the basic topologies of the network, we also provide analytically solved equations for these descriptors. These results enable us to understand the topology of significant networks or structures.