SHARENE BUNGAY, Memorial University of Newfoundland, St. John's, Newfoundland
Topological Indices for Chemical Structure Identification

Chemical structures (often represented as graphs) have a number of identifying properties, the most obvious being atoms (vertices) and bonds (edges). Although humans can easily determine whether two structures are the same or similar visually, computational chemical structure identification has proven to be a difficult task. With advances in technology resulting in a drastic increase in the number and rate of structures that are computed, the creation of databases with advanced search capabilities has become a necessity. Consequently, tools that allow for the identification of points of interest and the determination of levels of similarity between multiple structures are becoming increasingly important. Existing chemical structure representation schemes will be discussed in the context of our own topological indices which assign, based on its chemical environment (nearest neighbours), numerical values to each atom and bond in a structure. Such topological indices allow identification of functional groups (specific groups of atoms within a structure that exhibit characteristic chemical behaviour) and will be used to develop substructure search algorithms as used in the pharmaceutical industry to identify drug candidates. Further, easily computed properties of chemical structures have been seen to be useful in assessing similarity.