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NOVEL MODIFIED TOPOLOGICAL INDICES OF ANTI-CANCER DRUGS

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Abstract

Chemical graph theory provides valuable tools for modelling and designing chemical structures and complex networks. It represents atoms as vertices and bonds as edges. Topological indices are numerical descriptors derived from molecular graphs of chemical compounds. These descriptors can be used to investigate structural features of molecules. It can be categorized as degree-based, distance-based, and spectral-based topological indices. Degree-based topological indices are the most investigated type of topological indices used in mathematical chemistry. Although these indices have proven useful, they sometimes fail to distinguish between non-isomorphic molecular graphs and capture subtle structural variations. In Quantitative-Structure Property Relationships (QSPR) studies, modifications to topological indices often enhance their statistical correlation with the physicochemical or biological properties of molecules, thereby improving predictive performance. Therefore, researchers develop and study modifications of existing topological indices. This research aims to modify the existing topological indices, introduce new indices, and validate these modified topological indices using the QSPR modelling approach. In the study, the novel modified topological invariants were formulated by modifying the existing indices, namely, Forgotten index, Atom-bond connectivity index, Sombor index, Nirmala index, Gourava indices, Randic index, Zagreb indices, Geometric-arithmetic index, Sum-connectivity index, and Symmetric division degree index. Then, to validate novel topological indices, the QSPR analysis was conducted. Moreover, the linear regression models were built to predict physical properties of the ten anti-cancer drugs for these modified topological indices. Also, we computed the correlation coefficients between the new modified indices and each of the physical properties of anti-cancer drugs. According to Randic's desirable attributes for topological indices, a topological index should have a good correlation with at least one property. These modified topological indices are strongly correlated with physicochemical properties of anti-cancer drugs. Therefore, these findings would be beneficial for designing effective anticancer drugs without conducting expensive and time-consuming laboratory experiments. Also, these novel modified indices can be used to forecast physicochemical properties of medicines for other types of diseases.

Keywords*:* *Topological Indices, QSPR Models, Anti-Cancer Drugs*