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Topological indices of some anti-cancer molecular graphs and dendrimer structures

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Cancer disease are leading cause of death in the world as well as in Sri Lanka. Anticancer drugs and delivery dendrimers are one of the important medicine in curing cancers. Various experiments were performed to avoid the occurrence of the rapid growth of cancer cells. Because of that study of anti-cancer drugs and dendrimers are particularly important. Topological indices are molecular descriptors, which are numerical values associated with the physical properties of the chemical structure of a molecule. Finding the physical properties of a molecule in a laboratory is an expensive exercise as it requires many compounds, drugs and time. Therefore, by calculating topological indices, it is possible to get the necessary knowledge about molecules. The objective of this study is to compute the degree-based topological indices of some dendrimer structures that were not calculated earlier and predict the physical properties of selected anticancer drugs using linear regression models. In this work, various topological indices were defined on some anticancer drugs and dendrimer structures, which enable the researchers to know the physical, physicochemical, and chemical properties associated with them. Here the molecular structures were represented as hydrogen depleted molecular graphs considering the adjacency relationships among atoms as vertices corresponding to the atoms of the molecular graph and edges corresponding to chemical bonds. Zagreb and Randić indices are the commonly used indices around new drug design and improvement in this category. Therefore, in this study, degree-based topological indices such that Hyper Zagreb Index - HZ(G), Reduced Second Zagreb index - RM2(G), Augmented Zagreb Index - AZI(G), Forgotten Index - F(G), Inverse Sum Index - ISI(G) were calculated for Poly amidoamine (PAMAM), Polypropylene imine (PPI), Triazine drug delivery dendrimers. Considering the degree of the end vertices, topological indices were calculated for the dendrimer graph. The edge set of the whole graph was partitioned into several sets around on their degrees at the end vertices beginning from the dendrimer core unit. Finally, derived general formulas to find topological indices in the nth generation of a dendrimer. For anti-cancer drugs, fifteen drugs approved for Brain tumors, Testicular cancer, and Acute Lymphoblastic Leukemia were selected using the degree-based calculations, physical properties such as Boiling point, Melting point, Flashpoint, Molar Polarizability, Molar Volume, and Molar Refractivity were predicted. The most studied topological indices are vertex degree-based topological indices. For anti-cancer molecular graphs, selected Zagreb indices, Randic indices, Forgotten Index, Inverse Sum Index, Shigenhalli, and Kanabur Indices were calculated. Calculation of topological indices according to the edge partition is carried out and a MATLAB code was developed for the purpose. Finally, the linear regression model between the topological index and selected physical property was fitted using Minitab software. The significance of the study was predicted using the Pearson correlation coefficient. All calculated values were greater than 0.5 and most of them were greater than 0.75. Therefore values were highly positively correlated.

Keywords: Anti-cancer drug, Dendrimer, Topology Indices (TI)