QSPR ANALYSIS OF CERTAIN ANTI-HIV DRUGS

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Abstract: A broad spectrum of advanced medications appears yearly following the accelerated evolution of the chemical and pharmaceutical industry. In this paper, various degree-based and neighborhood degree sum-based topological indices of some anti-HIV drugs are explored applying the M-polynomial and NM-polynomial formulations. Moreover, QSPR analysis is carried out for the topological indices with regard to the physico-chemical properties of the anti-HIV drugs. The activity of nucleoside and non-nucleoside reverse transcriptase inhibitors is implemented as in drug configuration to manifest the significance of topological indices in the medicinal world. The procured outcomes affirm that topological indices being studied reflect effective correlation in accordance to physical and chemical properties of the anti-HIV drugs and consequently can assist in development of advanced and promising pharmaceutical for HIV medication.