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A COMPUTATIONAL APPROACH TO PREDICTIVE MODELLING USING NM-POLYNOMIALS OF SOME ANTI-CANCER DRUGS

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Abstract. Cheminformatics integrates chemistry, computer science, and information technology to forecast chemical behaviors through quantitative structure–property relationships (QSPRs). This research enhances QSPR modeling by developing innovative connection-based graphical invariants, specifically tailored to improve the predictive accuracy of physicochemical properties (PCPs) in benzenoid hydrocarbons (BHs). Em-

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ploying NM-polynomials, we evaluate these invariants against established descriptors in modeling physico-chemical properties of coumarins. The results demonstrate that the NM-indices exhibit superior predictive performance. Additionally, we apply these methods to model the physicochemical properties of coumarin-related anti-cancer drugs, highlighting their potential in drug development. Statistical analysis indicates that the most accurate structure–property models are nonlinear in nature.