Prediction of Chromatographic Retention of Nucleic Acids based on QSPR Model

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QSPR (quantitative structure property relationship) model is used to solve the problem for the prediction of physicochemical property of the special compound. The QSPR also provides a promising method for estimation of retention indices of organic compounds based on the descriptors derived solely from the molecular structure to fit experimental data. A variety of different types of descriptors can be used.

The goal of this work was to search for the correlation relationships between physicochemical properties and the chromatographic retention factor of nucleic acids. The correlation factors of nucleic acids were established by the empirical equations. The various descriptors were divided into physicochemical, geometrical, electronic, thermodynamic, and topological descriptors. Higher value of correlation coefficient of the empirical equation was obtained. as a results, the experimental data and the theoretical values have good agreement.