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Application of Artificial Neural Network for Prediction of Retention Times of Some Secoestrane Derivatives

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Abstract : In order to investigate the relationship between retention and structure, a quantitative Structure Retention Relationships (QSRRs) study was applied for the prediction of retention times of a set of 23 secoestrane derivatives in a reversed-phase thin-layer chromatography. After the calculation of molecular descriptors, a suitable set of molecular descriptors was selected by using step-wise multiple linear regressions. Artificial Neural Network (ANN) method was employed to model the nonlinear structure-activity relationships. The ANN technique resulted in 5-6-1 ANN model with the correlation coefficient of 0.98. We found that the following descriptors: Critical pressure, total energy, protease inhibition, distribution coefficient (LogD) and parameter of lipophilicity (miLogP) have a significant effect on the retention times. The prediction results are in very good agreement with the experimental ones. This approach provided a new and effective method for predicting the chromatographic retention index for the secoestrane derivatives investigated.

Keywords : lipophilicity, QSRR, RP TLC retention, secoestranes
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