QSPR Prediction for Nitrogen-Containing Heterocycles from Molecular Descriptors in HPLC

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Liquid chromatographic retention of 29 nitrogen-containing heterocycles has been predicted by quantitative structure property relationships (QSPR) methods based on simple- and multiple-linear regression analysis. In order to indicate the influence of different computed molecular descriptors on retention factors and well understand the important descriptors affecting the experimental values, simple- and multiple- linear models derived from two groups of different molecular descriptors (structural and physicochemical) were built. The proposed simple linear models gave the following results: the square of correlation coefficient, R_2, for the models physicochemical and structure molecular descriptors was in variety $0.80 \leq R_2 \leq 1.00$. The QSPR estimations of these nitrogen-containing heterocyclic compounds could be predicted with a multiple linear regression equation having the statistical index, $R_2=1.00$. The correlation equations and descriptors can be used for the prediction of the chromatographic retention for unknown structures.