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Molecular Topology and TLC Retention Behaviour of s-Triazines: QSRR Study

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Abstract : Quantitative structure-retention relationship (QSRR) analysis was used to predict the chromatographic behavior of s-triazine derivatives by using theoretical descriptors computed from the chemical structure. Fundamental basis of the reported investigation is to relate molecular topological descriptors with chromatographic behavior of s-triazine derivatives obtained by reversed-phase (RP) thin layer chromatography (TLC) on silica gel impregnated with paraffin oil and applied ethanol-water (φ = 0.5-0.8; v/v). Retention parameter (RM0) of 14 investigated s-triazine derivatives was used as dependent variable while simple connectivity index different orders were used as independent variables. The best QSRR model for predicting RM0 value was obtained with simple third order connectivity index (3χ) in the second-degree polynomial equation. Numerical values of the correlation coefficient (r=0.915), Fisher's value (F=28.34) and root mean square error (RMSE = 0.36) indicate that model is statistically significant. In order to test the predictive power of the QSRR model leave-one-out cross-validation technique has been applied. The parameters of the internal cross-validation analysis (r2CV=0.79, r2adj=0.81, PRESS=1.89) reflect the high predictive ability of the generated model and it confirms that can be used to predict RM0 value. Multivariate classification technique, hierarchical cluster analysis (HCA), has been applied in order to group molecules according to their molecular connectivity indices. HCA is a descriptive statistical method and it is the most frequently used for important area of data processing such is classification. The HCA performed on simple molecular connectivity indices obtained from the 2D structure of investigated s-triazine compounds resulted in two main clusters in which compounds molecules were grouped according to the number of atoms in the molecule. This is in agreement with the fact that these descriptors were calculated on the basis of the number of atoms in the molecule of the investigated s-triazine derivatives.

Keywords : s-triazines, QSRR, chemometrics, chromatography, molecular descriptors
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