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Computational Study of Chromatographic Behavior of a Series of S-Triazine Pesticides Based on Their in Silico Biological and Lipophilicity Descriptors

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Abstract : In this paper, quantitative structure-retention relationships (QSRR) analysis was applied in order to correlate in silico biological and lipophilicity molecular descriptors with retention values for the set of selected s-triazine herbicides. In silico generated biological and lipophilicity descriptors were discriminated using generalized pair correlation method (GPCM). According to this method, the significant difference between independent variables can be noticed regardless almost equal correlation with dependent variable. Using established multiple linear regression (MLR) models some biological characteristics could be predicted. Established MLR models were evaluated statistically and the most suitable models were selected and ranked using sum of ranking differences (SRD) method. In this method, as reference values, average experimentally obtained values are used. Additionally, using SRD method, similarities among investigated s-triazine herbicides can be noticed. These analysis were conducted in order to characterize selected s-triazine herbicides for future investigations regarding their biodegradability. This study is financially supported by COST action TD1305.

Keywords : descriptors, generalized pair correlation method, pesticides, sum of ranking differences
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