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Chemometric QSRR Evaluation of Behavior of s-Triazine Pesticides in Liquid Chromatography

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Abstract : This study considers the selection of the most suitable in silico molecular descriptors that could be used for s-triazine pesticides characterization. Suitable descriptors among topological, geometrical and physicochemical are used for quantitative structure-retention relationships (QSRR) model establishment. Established models were obtained using linear regression (LR) and multiple linear regression (MLR) analysis. In this paper, MLR models were established avoiding multicollinearity among the selected molecular descriptors. Statistical quality of established models was evaluated by standard and cross-validation statistical parameters. For detection of similarity or dissimilarity among investigated s-triazine pesticides and their classification, principal component analysis (PCA) and hierarchical cluster analysis (HCA) were used and gave similar grouping. This study is financially supported by COST action TD1305.
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