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Evaluation of QSRR Models by Sum of Ranking Differences Approach: A Case Study of Prediction of Chromatographic Behavior of Pesticides

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Abstract : The present study deals with the selection of the most suitable quantitative structure-retention relationship (QSRR) models which should be used in prediction of the retention behavior of basic, neutral, acidic and phenolic pesticides which belong to different classes: fungicides, herbicides, metabolites, insecticides and plant growth regulators. Sum of ranking differences (SRD) approach can give a different point of view on selection of the most consistent QSRR model. SRD approach can be applied not only for ranking of the QSRR models, but also for detection of similarity or dissimilarity among them. Applying the SRD analysis, the most similar models can be found easily. In this study, selection of the best model was carried out on the basis of the reference ranking ("golden standard") which was defined as the row average values of logarithm of retention time (logtr) defined by high performance liquid chromatography (HPLC). Also, SRD analysis based on experimental logtr values as reference ranking revealed similar grouping of the established QSRR models already obtained by hierarchical cluster analysis (HCA).

Keywords : chemometrics, chromatography, pesticides, sum of ranking differences
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