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Separation selectivity of liquid chromatographic columns: a comparison by nonparametric methods

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There are two legitimate aims for column selection: i) to determine similar ones to an existing one and ii) to find diverse (orthogonal) one(s) for optimal separation. Several different methods have already been elaborated to compare selectivity of chromatographic columns. All comparisons realize empirical approaches and based on measuring retention data of several well-chosen test compounds. Proper multivariate analyses can find similarities and differences in retention behavior of test compounds and stationary phases. As an illustration we adopted Wilson et al.'s data of 67 test compounds and 10 highly similar columns (C18-bonded silica stationary phases). The inherent characteristic groupings by physical properties were revealed with correct statistical tests and several independent methodologies. Generalized pair correlation method (GPCM)2 and sum of (absolute) ranking differences (SRD)3,4 unambiguously showed the same ranking pattern. The clustering by SRD is delivered to the reference. Therefore, all columns have been chosen as gold standard once and only once (comparison with one variable at a time). All lines of boxes correspond to an SRD ordering always with a different reference column (Figure 1). COVAT heatmaps show destroying the true pattern if the hydrophobic-subtraction model (HSM) evaluation is used. The ranking (clustering) pattern of chromatographic columns based on retention data (log k values) of 67 compounds and selectivity parameters of hydrophobic-subtraction model (HSM) provided various column groupings. Loss of information is inevitable for using the HSM data handling. Processing of retention data resulted in patterns that are consistent with differences in the columns' physicochemical parameters, whereas HSM results are deviating to a higher or lesser degree, depending on the particular chemometric approach. GPCM, SRD and COVAT procedures can be carried out on any data sets partially and on the whole to select the most similar and dissimilar columns, though our calculations were completed to the data set of Wilson et al.

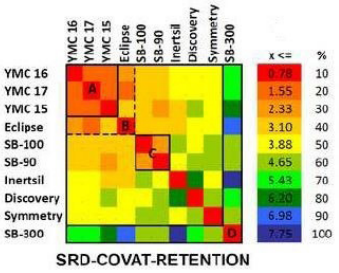

Figure 1. Heatmap plot of SRD analysis using primary retention data (67 test compounds) and comparison of one variable at a time.

Biography

Károly Héberger has completed his PhD, Cand. scient., DSc and t. Prof. In his early career, he investigated liquid phase oxidation (radical) processes and determined rate constants by kinetic ESR spectroscopy. Later, he studied quantitative structure activity (property) relationships like QSAR, QSPR and QSRR. Now, he deals with chemometrics such as multivariate data evaluation techniques, principal component analysis, stepwise linear regression, partial least squares regression, variable selection, model building and validation, pattern recognition (supervised and unsupervised), classification of food products, clustering, method comparison and ranking etc. His scientific results were presented in more than 160 papers (including book chapters) and has given more than 300 lectures (or posters) with h-index=34 and i-10 index=83 (Web of Science). The papers were cited above 3500 times.

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