Karoly Heberger, J Chromatogr Sep Tech 2018, Volume: 09
DOI: 10.4172/2157-7064-C2-043

Column Selection in Liquid Chromatography

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A lot of protocols have been elaborated for stationary phase selection, (further on column selection) in chromatography.[1-4]

One of the earliest developed procedure was the Tanaka system1: six selectivity parameters have characterized commercial packing column materials. Later, Euerby improved the system2 and defined the Column Difference Factor (CDF).[3] Snyder and Dolan have utilized five selectivity parameters and elaborated the so called hydrophobic-subtraction model with a cornerstone of column selectivity function (Fs).[4] Hoogmartens et al. have applied only four selectivity parameters and defined the *F*metric.[5] Their approach is known as KUL column selection system (CSS). All above approaches are empirical and all of them is based on measurement of some well-chosen reference compounds and calculation of Euclidean distance between the concerned and a reference column.

Our chemometric approach compares the column selection systems using some simple pattern recognition methods: (icon (polygon, radar or spider-web) plot and stacked plots. Ten similarity measures (Euclidean and Manhattan distance, Kendall tau, Spearman rho, Person's correlation coefficient, generalized pair correlation methods with various statistical test options as e.g. Williams' t test, conditional Fisher's exact test, McNemar test, etc. have shown some contradictory behavior, still their data fusion allows us to compare and rank the column ranking systems.

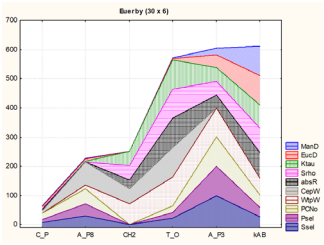

Figure 1. Stacked plot of ten column similarity measures (30 chromatographic columns and nine reference compounds.

A significant loss of information arises during the application of the hydrophobic-subtraction model.

We could not only rank and group the column classification protocols, but to select the most suitable similarity (or dissimilarity) measure for selection of the most similar and dissimilar i.e. orthogonal chromatographic system.

Work is under way to determine the smallest number of reference compounds responsible for all dominant interactions in chromatography and hence classification of chromatographic columns will be possible with the smallest efforts without having significant information loss.

Biography

Károly Héberger Ph.D., Cand. Sci., D.Sc., t.Prof.. in his early carrier he investigated liquid phase oxidation (radical) processes, and determined rate constants by kinetic ESR spectroscopy. Later he studied Quantitative - structure activity (property) relationships. QSAR, QSPR and QSRR. Now he deals with chemometrics: 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 more than 300 lectures (or posters). Hirsch index=34 and i-10=index 83 (Web of Sci). The papers were cited above 3800 times (without self - citations and cross - references).

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