
Mutual peak matching in a series of HPLC/DAD mixture analyses

Взаимное отнесение пиков в серии HPLC/DAD хроматограмм одной и той же смеси.

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Abstract.

One of the largest challenges in HPLC (high performance liquid chromatography) method development is the necessity for tracking the movement of peaks as separation conditions are changed. Peak increments are then used to build a mathematical model capable of minimizing the number of experiments in an optimization circuit. Method optimization for an unknown mixture is, moreover, complicated by the absence of any *a priori* information on component properties and retention times when direct signal assignment is not possible. On the contrary, achievement of the maximum separation becomes an important factor for successful identification or quantitation. In this case, the optimization may be based on assigning peaks of the same component chosen from different experiments to each other. In other words, mutual peak matching between the HPLC runs is required.

A new method for mutual peak matching in a series of HPLC/DAD (HPLC with diode array detector) analyses of the same unknown mixture acquired at varying separation conditions has been developed. This approach, called MAP (Mutual Automated Peak matching), does not require any prior knowledge of the mixture composition. Applying abstract factor analysis (AFA) and Iterative Key set Factor Analysis (IKSFA) on the augmented data matrix, the algorithm detects the number of mixture components and calculates the retention times of every individual compound in each of the input chromatograms. Every candidate component is then validated by target testing for presence in each HPLC run to provide quantitative criteria for the detection of "missing" peaks and non-analyte components as well as confirming successful matches. The matching algorithm by itself does not perform full curve resolution. However, its output may serve as a good initial estimate for further modeling. A common set of UV-Vis spectra of pure components can be obtained, as well as their corresponding concentration profiles in separate runs, by means of Alternating Least-Square Multivariate Curve Resolution (ALS MCR), resulting in reconstruction of overlapped peaks.

The algorithms were programmed in MATLAB® and tested on a number of sets of simulated data. Possible ways to improve the stability of results, reduce calculation time, and minimize operator interaction are discussed. The technique can be used to optimize HPLC analysis of a complex mixture without preliminary identification of its components.

Keywords: peak matching, multivariate data analysis, self-modeling curve resolution, HPLC