
HANDLING OF MULTIVARIATE DATA FROM (HYPHENATED) CHROMATOGRAPHIC TECHNIQUES

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The data gathered from hyphenated chromatographic techniques is multivariate. However, chromatograms measured at, for instance, one UV detection wavelength also can be considered as multivariate analytical data. Instead of focussing on the information from a discrete peak to relate, for instance, to the concentration of a given compound, one can simultaneously use the information from several peaks or of the complete chromatogram or of the entire data matrix. In the latter cases one then has to extract information from this multivariate data set. Depending on the goal of the data analysis, different types of techniques can be applied. The main application fields are exploratory data analysis, curve resolution, pattern recognition, and multivariate calibration and modelling. In the exploratory data analysis one tries to see whether the data set has structure, i.e. whether groups of similar objects can be observed or whether outlying observations are present. The curve resolution techniques are applied to deconvolute overlapping peaks and to determine their concentration profiles. Pattern recognition methods are used to build models that allow distinguishing between samples of different classes and that allow predicting the class of newly measured samples. In multivariate calibration the multivariate signal is related to a quantitative aspect of the samples, e.g. concentration, activity (antioxidant, cytotoxic, antibacterial) Models again are built for predictive purposes. Within each type of analysis usually many different techniques can be applied.

During the tutorial some techniques applied in the different application fields shortly will be highlighted.