



Chemometrics in Food Chemistry: Chapter 6. Multivariate Curve Resolution Methods for Food Chemistry (Data Handling in Science and Technology)

Anna de Juan, Silvia Mas

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The term multivariate curve resolution (MCR) designates a family of methods devoted to solving the mixture analysis problem in multicomponent samples. MCR provides the qualitative and quantitative contribution (profile) of each of the compounds in a sample from the sole information of the raw experimental data acquired. Food analysis is about knowing the qualitative and quantitative composition of foodstuffs and, hence, MCR fits very well in this scenario. Typical problems related to food analysis that can be solved by MCR are the identification and analytical determination of target compounds in the presence of unknown interferences/compounds, obtaining food fingerprint information to be used for authentication, adulteration or other purposes, and the interpretation of food processes. All these situations can be solved by handling measurements as simple as a data table with one spectrum (response) per sample or as complex as flexible multiset structures formed by several data tables (e.g. excitation/emission spectra, hyphenated separation techniques: high-performance liquid chromatography with diode array detection, liquid chromatography or gas chromatography–mass spectrometry, etc.), each of them related to a sample or to a particular food condition.

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