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Modelling highly co-eluted peaks of analytes with high spectral similarity

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HIGHLIGHTS

- Modelling co-eluted peaks is key in curve resolution of chromatographic data
- Curve resolution may fail when the spectra of co-eluted peaks are highly similar
- Parallel factor analysis with linear dependence (PARALIND) is an option
- Two key cases are studied: L-proline derivatization and overlapping of fungicides

ABSTRACT

Modelling co-eluted peaks has always been a keystone in chemometric applications to chromatographic data. Multivariate Curve Resolution (MCR) and Parallel Factor Analysis 2 (PARAFAC2) have been widely used to solve the co-elution problem (among others), profiting from the uniqueness of the spectrum for each co-eluted analyte. Nevertheless, there are cases where these curve-resolution approaches may fail, when the same analyte gives two co-eluted peaks or when two analytes have highly correlated spectra. In this article, we put forward the usefulness of Parallel Factor Analysis with Linear Dependence (PARALIND) that is able to handle overlapping peaks when the spectral profiles of the analytes are highly correlated. To illustrate the problem, we study two different situations: first, the co-elution of two peaks, belonging to L-proline; and, second, an overlapped mixture of fungicides with high similarity in their spectra.

Keywords:
Chemometrics
Chromatography
Co-eluted peak
Co-elution
Curve resolution
Enantiomer
Multivariate Curve Resolution (MCR)
Parallel Factor Analysis with Linear Dependence (PARALIND)
Parallel Factor Analysis 2 (PARAFAC2)
Spectral similarity

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1. Introduction

The use of multi-channel detectors in chromatographic instruments [e.g., high-performance liquid chromatography with diode array detector (HPLC-DAD) or gas chromatography coupled to a mass detector (GC-MS)] generates a vast amount of information for a single sample (one complete spectral pattern for each elution time). To treat this data, powerful mathematical tools have been generated to extract the desirable information from the datasets and to solve the typical problems found in chromatographic runs [1,2]. Attending to the curve-resolution methods commonly used with coupled chromatographic data [1], it is worth highlighting the important role of multi-way and multi-set techniques {e.g., Parallel Factor Analysis 2 (PARAFAC2) [3–6] and Multivariate Curve

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