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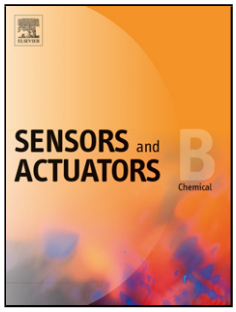

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Sliding Window Multi-Curve Resolution: Application to Gas Chromatography - Ion Mobility Spectrometry

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Abstract

Blind Source Separation (BSS) techniques aim to extract a set of source signals from a measured mixture in an unsupervised manner. In the chemical instrumentation domain source signals typically refer to time-varying analyte concentrations, while the measured mixture is the set of observed spectra. Several techniques exist to perform BSS on Ion Mobility Spectrometry, being Simple-to-use interactive self-modeling mixture analysis (SIMPLISMA) and Multivariate Curve Resolution (MCR) the most commonly used. The addition of a multi-capillary gas chromatography column using the ion mobility spectrometer as detector has been proposed in the past to increase chemical resolution. Short chromatography times lead to high levels of co-elution, and ion mobility spectra are key to resolve them. For the first time, BSS techniques are used to deconvolve samples of the gas chromatography - ion mobility spectrometry tandem. We propose a method to extract spectra and concentration profiles based on the application of MCR in a sliding window. Our results provide clear concentration profiles and pure spectra, resolving peaks that were not detected by the conventional use of MCR. The proposed technique could also be applied to other hyphenated instruments with similar strong co-elutions.

Keywords: Blind Source Separation; Multivariate Curve Resolution; Ion Mobility Spectrometry; Gas Chromatography; Hyphenated instrumentation; SIMPLISMA; co-elution

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