

## **Multivariate Curve Resolution for quantitative first order calibration using a correlation constraint**

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Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS) is proposed for quantitative multivariate calibration of analyte mixtures in the presence of interferences. Using analyte concentrations in a set of calibration samples during the ALS optimization as a constraint, allow estimating its concentration in test samples, as well as estimating analyte and interferences spectral profiles. Since no information concerning the interferences is provided in calibration samples, the proposed approach can achieve the so-called second-order advantage in multivariate calibration, which is traditionally considered only to be present for more complex (higher order) instrumental data structures. The use of the proposed MCR-ALS method with a correlation constraint is shown for different experimental data sets including voltammetric analysis of mixtures (1), IR spectrometric analysis of agrofood samples (2), and characterization of pharmaceuticals in serum (3). Recent attempts to extend the same method to cope with more challenging problems will be discussed.

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1. M. C. Antunes, J. E. J. Simao, A. C. Duarte and R. Tauler, *Analyst*, 2002, 127, 809–817.
2. T. Azzouz and R. Tauler, *Talanta*, 2008, 74, 1201–1210.
3. H. C. Goicoechea, A. C. Olivieri, R. Tauler, *Analyst*, 2010, 127, 636-642.