Multivariate Curve Resolution (MCR). Basic concepts and application to massive MS-based data

Introduction

Multivariate Curve Resolution is a mixture analysis methodology apt to explore data sets and retrieve the profiles that characterize the responses and contributions of the pure components present in the initial raw measurement.

The course will be divided in two parts:

a) an introductory description of the MCR methodology, with particular emphasis on the algorithm Multivariate Curve Resolution-Alternating Least Squares (MCR-ALS). This part will include a brief theoretical overview and a few simple hands-on examples and
b) a section focused on the treatment of massive separation data coupled with MS detection, using the adapted version of the MCR-ALS algorithm known as Region of Interest-MCR (ROIMCR), with both theory and practical explanations. ROIMCR is particularly well suited for massive MS-based data since it proposes a smart data compression without loss of m/z resolution.

Audience

The course is intended for a broad audience. Newcomers to the MCR field are welcome. The course will be especially suitable for practitioners working with data issued from separation techniques (chromatography and/or ion mobility) with MS or MS/MS detection.

Course plan

Part 1. MCR basics. Theory and hands-on work.

Part 2. MCR adapted to massive MS-based data. ROIMCR, theory and hands-on work.

Material

Course participants will receive slides with the theoretical explanations of the course. Freely available MATLAB-based GUIs will be used for the hands-on work.

Course conveners

Romà Tauler and Joaquim Jaumot (IDAEA-CSIC) and Anna de Juan (Universitat de Barcelona). The team in charge of the course has been responsible for the most relevant theoretical and practical implementations of the MCR-ALS algorithm over the past three decades.