

## MULTIVARIATE CURVE RESOLUTION (MCR). APPLICATION IN PROCESS ANALYSIS AND IMAGING

The course will be a combination of theoretical concepts and hands-on work around the topic of Multivariate Curve Resolution, particularly the description and the use of the MCR-Alternating Least Squares (MCR-ALS) algorithm. There will be explanations on how to work with single data sets and multiset structures (formed by several data tables together). Focus on recent variants of MCR incorporating hard-modeling information (e.g., kinetic laws,..) and calibration tasks (correlation constraint) will be also illustrated. Practical examples will be mainly processes and hyperspectral images, mostly collected with NIR spectroscopy. Some basics on the estimation of uncertainty (ambiguity) in the resolution results will also be introduced. Theory and hands-on work will be combined during the sessions. Documentation, software and data sets will be provided.

### Program

- MCR. Basic concept.
- Single data analysis.
- Multiset analysis.
- MCR variants: correlation constraint, hybrid hard- and soft-modelling.
- Assessment of ambiguity in MCR results.

**Requirements:** It is recommended that attendants have some basic background in multivariate data analysis. Since practical work will be done, bringing a laptop is necessary to follow adequately the course. No need for any preinstalled software is needed, since a compiled GUI interface (programmed in MATLAB environment) will be provided and used

### TRAINER PROFILE



**Anna de Juan**, associate professor at the Universitat de Barcelona. She has more than 20 years of experience developing and applying the MCR technique in very diverse areas. She has experience in teaching MCR in undergraduate and graduate programs at different international institutions and also in conferences and private companies.

**Joaquim Jaumot**, senior researcher at the Spanish Council of Research (CSIC) in Barcelona. He has worked as a professor at the Universitat de Barcelona and has a long experience in the MCR topic, particularly in the analysis of biochemical processes and -omic studies. He is the designer and main developer of the GUIs linked to the MCR algorithm.



**Schedule: 8 am – 12 am**  
**13:30 pm – 17:30 pm**  
(October 18, 2015)

