



**School on Chemometric Strategies for Chromatographic Signal in targeted and untargeted Analysis - Modena, 2 – 5 February 2026**

# Preliminary Program

## Monday 2 February (optional)

AULA Informatica Unit 3 (piano -1)

This introductory day provides participants with the fundamental concepts and practical tools of chemometric data analysis. Through a combination of theory and hands-on exercises, attendees will learn how Principal Component Analysis (PCA) and Partial Least Squares–Discriminant Analysis (PLS-DA) are applied to explore, visualize, and classify chromatographic data. Emphasis will be placed on understanding the mathematical principles behind these techniques and their role in both targeted and untargeted workflows.

8:30 Registration

9:00 – 11:00 Principal Component Analysis (PCA) (L. Strani)

*11:00 – 11.15 coffee break*

11:15 – 13:00 Introduction to Classification (M. Cocchi - C. Durante)

*13:00 – 14:15 lunch*

14.15 – 16.00 Partial Least Squares-Discriminant Analysis (PLS-DA) (M. Cocchi – C. Durante)

*16.00 – 16.15 coffee break*

16.15 - 18.30 Lab Exercises: PCA and PLS-DA (C. Durante - L. Strani – S. Pellacani)

## Tuesday 3 February

Data quality and preprocessing are crucial steps for reliable chemometric interpretation. This session focuses on data pretreatment strategies — including normalization, scaling, baseline correction, and alignment — to prepare chromatographic signals for analysis. Participants will also be introduced to ANOVA–Simultaneous Component Analysis (ASCA), a powerful method to assess the influence of experimental factors on multivariate chromatographic data, combining the interpretability of ANOVA with the dimensionality reduction of PCA. ASCA is a particularly useful tool in metabolomics, foodomics, etc., since it most often deals with designed data where it is required to assess if treatments (factors) and their interactions have an effect, and which variables show significant variation when factor levels change.

8.30 Registration

9:00 – 10:30 Introduction and Data pretreatment (data alignment, baseline correction, etc.). (C. Durante – M. Cocchi)



10:30 – 10:50 *coffee break*

10:50 – 12:45 Data pretreatment – practical lab (C. Durante – S. Pellacani)

12:45 – 14:00 *lunch*

14:00 – 15:45 ASCA (F. Marini)

15:45 – 16:00 *coffee break*

16:00 – 18:30 ASCA – Practical Lab (F. Marini – L. Strani)

### **Wednesday 4 February**

The third day focuses on multiway data analysis with a deep dive into PARAFAC and PARAFAC2, a method particularly suited for handling chromatographic data with retention time shifts or evolving profiles. Attendees will learn how PARAFAC2 can model three-way datasets (samples  $\times$  time  $\times$  mass) to reveal consistent chemical structures across complex systems. Case studies will highlight applications in metabolomics, food chemistry, and environmental analysis, demonstrating how multiway approaches expand the analytical power of chemometrics.

9:30 – 11:00 Introduction to multiway data and multiway models: PARAFAC (B. Quintanilla-Casas)

11:00 – 11:15 *coffee break*

11:15 – 12:30 PARAFAC Practical Lab (B. Quintanilla-Casas - S. Pellacani)

12:30–13:30 *lunch*

13:30 – 15:30 Multiway model for shifted data: PARAFAC2 (B. Quintanilla-Casas)

15.30–15.45 *coffee break*

15.45–18.15 PARADISe for GCMS data Practical Lab (B. Quintanilla-Casas – S. Pellacani)

20:30 *Social Dinner*

### **Thursday 5 February**

The final day delves into advanced multivariate resolution techniques. Participants will explore Multivariate Curve Resolution–Alternating Least Squares (MCR-ALS) to decompose complex chromatographic signals into pure component profiles and concentration profiles. Furthermore, Region of Interest MCR (ROI-MCR) will be introduced as an evaluable method for matrix compression dimensionality, without losing information. Practical examples will demonstrate how these methods enable the extraction of chemical information from overlapping peaks frequently present in untargeted analysis.

9:30 – 11:00 Introduction to MCR-ALS (R.Tauler)

11:00 – 11:15 *coffee break*

11:15 – 12:30 MCR-ALS practical lab (R.Tauler – L.Strani, C.Durante)



12:30–13:30 *lunch*

13:30 – 15:30 ROI-MCR (R.Tauler)

15.30–15.45 *coffee break*

15.45–18.15 ROI-MCR Practical Lab (R. Tauler – C. Durante, L. Strani)

18:30 Question Time (Closure)