

Symposium of Young Chemometrists

Bertinoro (FC)

February 3-6, 2025



The Chemometrics Group of the Analytical Chemistry Division of the Italian Chemical Society organizes the first edition of the **Symposium of Young Chemometrists in Bertinoro** (Forlì-Cesena) from **February 3 to 6, 2025**.

The symposium is dedicated to young researchers (PhD students and postdoctoral fellows) working in the field of chemometrics. Its aim is to motivate the young Italian chemometric community with activities aimed at improving advanced skills in chemometrics and enhancing networking opportunities for the younger members of the Chemometrics Group.

This first edition of the Symposium will focus on **data fusion** in combination with **variable selection** and **model validation** in chemometrics. The program will include activities related to these topics, such as **theoretical lectures, practical sessions, open discussions of chemometric case studies**, and a **data challenge**. These activities will be coordinated by the Chemometrics Group Board and **Prof. José Camacho**, Full Professor at the Department of Signal Theory, Telematics, and Communications of the University of Granada and PI of the Computational Data Science Laboratory (CoDaS Lab).

In particular, lectures given by Prof. José Camacho will cover the following topics:

- PCA and PLS: introduction, examples, interpretation and problems.
- Model Validation: general concepts and PCA CV
- PLS Validation: CV, dCV in PLS and PLS-DA, discussion on test-set validation
- Variable selection: general concepts, sparse PCA, group-wise PCA and interpretation
- PLS VS: sPLS and dCV
- Data Fusion: general concepts and low-level PCA fusion
- PLS DF: algorithms low-level and mid-level

Organizing Committee

Davide Ballabio
Eugenio Alladio
Caterina Durante
Barbara Giussani
Paolo Oliveri
Francesca Romano
Mattia Sozzi
Nicholas Kassouf
Martina Foschi
Lorenzo Strani

Sponsor



Società Italiana di Spettroscopia NIR

Monday, February 3rd

14:00	Bus transfer from <u>Forlì Railway Station</u>
14:30 – 15:00	Registration (<i>CEUB – Via A. Frangipane 6 – Bertinoro (FC)</i>)
15:00 – 15:15	Opening
15:15 – 15:30	<u>SISNIR</u> presentation (by <i>Rosalba Calvini</i>)

15:30 – 18:00 ICE BREAKING:

Presentation and open discussion of chemometric cases studies

15:30 – 16:00	<i>Ice Breaking 1 – Benedini Dario</i> : “Data fusion of two different handheld NIR spectrometers for milk analysis”
16:00 – 16:30	<i>Ice Breaking 2 – Lombardi Gabriele</i> : “Sourdough vs. Baker's Yeast Bread: NIR Spectroscopy and Chemometrics for Rapid Classification”
16:30 – 17:00	<i>Ice Breaking 3 – Romano Francesca</i> : “Multi-omics integration to investigate the biological activity of DNA G-quadruplex ligands in cancer cells”
17:00 – 17:30	<i>Ice Breaking 4 – Strani Lorenzo</i> : “Fusion of NIR spectra and process sensor data for the multivariate statistical process monitoring in industrial polymers production”
17:30 – 18:30	Guest presentation and Data Challenge introduction
20:00	<i>Dinner</i>

Tuesday, February 4th

09:30 – 18:00 Lectures by Prof. José Camacho

09:30 – 11:00 Theoretical and practical lessons on data fusion, variable selection and model validation

11:00 – 11:30 *Coffee Break*

11:30 – 13:00 Theoretical and practical lessons on data fusion, variable selection and model validation

13:00 – 14:30 *Lunch*

14:30 – 16:00 Theoretical and practical lessons on data fusion, variable selection and model validation

16:00 – 16:30 *Coffee Break*

16:30 – 18:00 Theoretical and practical lessons on data fusion, variable selection and model validation

18:00 – 19:00 Introduction of Young Chemometrists Group

20:00 *Dinner*

Wednesday, February 5th

09:30 – 18:00 Lectures by Prof. **José Camacho**

09:30 – 11:00 Theoretical and practical lessons on data fusion, variable selection and model validation

11:00 – 11:30 *Coffee Break*

11:30 – 13:00 Theoretical and practical lessons on data fusion, variable selection and model validation

13:00 – 14:30 *Lunch*

14:30 – 16:00 Theoretical and practical lessons on data fusion, variable selection and model validation

16:00 – 16:30 *Coffee Break*

16:30 – 18:00 Theoretical and practical lessons on data fusion, variable selection and model validation

18:00 – 19:00 Data Challenge organization

20:00 *Social Dinner*

Thursday, February 6th

09:30 – 12:45 DATA CHALLENGE

09:30 – 11:15 Team Data Challenge

11:15 – 11:45 *Coffee Break*

11:45 – 12:45 Data Challenge results

12:45 – 13:00 Closing

13:00 – 14:00 *Lunch*

14:30 Bus transfer to **Forlì Railway Station**