



XI COLLOQUIUM
CHEMOMETRICUM
MEDITERRANEUM

27-30 JUNE 2023
PADOVA - ITALY

SPONSORS



UNIVERSITÀ
DEGLI STUDI
DI PADOVA



DIPARTIMENTO
DI INGEGNERIA
INDUSTRIALE



UNIMORE
UNIVERSITÀ DEGLI STUDI DI
MODENA E REGGIO EMILIA



UNIVERSITÀ DEGLI STUDI
DELL'INSUBRIA



Società Chimica Italiana



Let your data
flourish



TOPICS

Dear Colleagues, dear Friends

We are pleased to announce that the 11th Colloquium Chemometricum Mediterraneum (CCM XI 2023) will take place in Padova (Italy) from 27 till 30 June 2023.

In 1986, during an international conference, several French, Spanish and Italian chemometricians, each one speaking his own language, gathered and were able to share their own experiences on this topic. These facts were the seeds of the Colloquium Chemometricum Mediterraneum. The official languages of the conference are neo latin languages and English.

These Conferences have had a continuity over the years, starting in Barcelona (Spain, 1987), and following in San Miniato (Italy, 1991), Bastia (France, 1994), Burgos (Spain, 1998), Ustica (Italy, 2003), Saint Maximin La Sainte-Baume (France, 2007), Granada (Spain, 2010), Bevagna (Italy, 2013), Arles (France, 2017), Menorca (Spain, 2019).

The conference brings an outstanding and unique opportunity for exchanging knowledge on leading edge developments. The 11th Colloquium Chemometricum Mediterraneum welcomes all contributions on classical tools and new tools in Chemometrics. A non-limitative list of topics includes:

- Pattern Recognition and Calibration
- Experimental Design (DOE) and System Optimization
- Qualimetrics and Chemical Metrology
- QSAR/QSPR
- Image Analysis and hyperspectral imaging
- Process Analytical Technology (PAT)
- Multiway and Multiset analysis
- Teaching Chemometrics
- Recent Chemometrics developments
- Applications of Chemometrics in different domains: Cultural heritage, Environment, Food control, Omics sciences, Pharmaceuticals...

Following the tradition of previous editions, a Virtual Special Issue (VSI) on Chemometrics and Intelligent Laboratory Systems (Elsevier) will be published. (Further info [here](#))

The Organising Committee



COMMITTEES

SCIENTIFIC COMMITTEE

Prof. Marina Cocchi, Università di Modena e Reggio Emilia

Prof. Luis Cuadros, Universidad de Granada

Prof. Cyril Ruckebusch, Université de Lille

Prof. Riccardo Leardi, Università degli Studi di Genova

Prof. Federico Marini, Sapienza Università di Roma

Prof. Jean-Michel Roger, IRSTEA

Prof. Luis Sarabia, Universidad de Burgos

Prof. Michelle Sergent, Aix-Marseille University

Prof. Romà Tauler, IDAEA-CSIC

Prof. Roberto Todeschini, Università Milano - Bicocca

ORGANIZING COMMITTEE

Prof. Pierantonio Facco, Università di Padova

Prof. Davide Ballabio, Università di Milano – Bicocca

Dr. Eugenio Alladio, Università di Torino

Dr. Caterina Durante, Università di Modena e Reggio Emilia

Prof. Barbara Giussani, Università dell'Insubria

Prof. Paolo Oliveri, Università di Genova

Dr. Gianmarco Barberi, Università di Padova

Ing. Francesco Sartori, Università di Padova

VENUE

KEY LOCATIONS

The XI Colloquium Chemometricum Mediterraneum will take place at:

- **Centro Culturale Altinate - San Gaetano** ([via Altinate 71, Padova](#))
Reception desk, 27-29 June 2023
- **Aula Magna - Palazzo Bo** ([Via VIII Febbraio 2, Padova](#))
30 June 2023

The welcome cocktail and the conference dinner will take place at:

- **Caffè Pedrocchi** ([via VIII Febbraio 15, Padova](#))

MAP

The key locations of XI Colloquium Chemometricum Mediterraneum are in **red**.
Click on the map to get the Google Maps location.





VENUE

HOW TO REACH PADOVA

The city of Padova is easily reachable with all means of transport.

The city's closest airports are:

- Marco Polo Airport (Venice - Tessera)
- Antonio Canova Airport (Treviso)
- Valerio Catullo Airport (Verona)
- Guglielmo Marconi Airport (Bologna)

All these airports are connected to Padova rail station via busses or trains, which can be booked directly at the airport.

Padova has also excellent rail connections, it is in fact reachable in 3 hours from Rome and in 2 hours from Milan.

PARTNER HOTELS

Details on partner hotels and discounted fees can be found in the CCM website ([here](#))

Additional information on Padova can be found in the CCM website ([here](#))

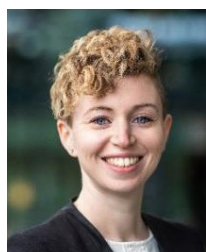
INVITED SPEAKERS



Josè Manuel Prats Montalbán

Universidad Politécnica de Valencia

José Manuel Prats-Montalbán is Full Professor at the Department of Applied Statistics, Operations Research and Quality of the UPV. He joined UPV in 2000, and defended his PhD thesis, "Statistical Process Control by Multivariate Image Analysis" in 2005. He is member of the Multivariate Statistics Engineering Group, where he is in charge of the MIA research line. He published in JCR journals, basically in the field of multivariate statistics and image analysis and he is involved in several projects dealing with the application and development of statistical models in multivariate statistical process control, computer vision and systems biology, such as the application of MIA on prostate cancer.



Francesca Grisoni

Eindhoven University of Technology

Francesca Grisoni is an Asst. Professor at the Eindhoven University of Technology, where she leads the Molecular Machine Learning team. After receiving her PhD in 2016 (University of Milano-Bicocca), Francesca worked as a data scientist and biostatistical consultant. Later, she joined the Univ. of Milano-Bicocca (2017) and ETH Zurich (2019) as a postdoctoral fellow, working on machine learning for drug discovery. Francesca received an ERC Starting Grant, and the Early Career Prize from the Dutch Royal Academy of Arts and Science. Her research focuses on AI for drug discovery, at the interface between computation and wet-lab experiments.



Sergey Kucheryavskiy

Aalborg University

Got a PhD degree in Physics and Mathematics in 2001 and after that took a break and was not active as a researcher. In 2004 started rebooting his carrier and decided to change research interests towards Chemometrics. He has been gradually developing his career as chemometrician since then. Current research interests include chemometrics (both theoretical and applied), image analysis and scientific programming. In his spare time Sergey works on pet-projects which result in various packages, apps, and toolboxes for using and learning chemometrics and related disciplines.



Marco S. do Reis

University of Coimbra

Marco S. Reis is an Associate Professor with Habilitation of Chemical Engineering at the University of Coimbra, Portugal. His research interests include process systems engineering, industrial data science, sensor fusion, hybrid modelling, fault detection/diagnosis/prognosis, predictive analytics, structured process improvement and chemometrics. He was President of the European Network for Business and Industrial Statistics (ENBIS) (2015-2017) and is currently an Honorary Member of this society. He was awarded with the Fulbright scholar fellowship (2020) and is the recipient of the Professor Almiro e Castro Award that distinguishes the scientific merit of a Portuguese researcher or faculty under 45 years old (2018).



Pierre Lebrun

PharmaLEx, University of Liège

Pierre Lebrun got his PhD at the University of Liège with a project to develop mathematical/statistical solutions to speed up in an accurate way the development of analytical methods in many field, such as chromatography and near infra-red spectrometry. He is now Director Statistics at PharmaLEx and a scientific collaborator with the University of Liège. His interest falls within different chemometric topics, such as quality by design, analytical development and validation, process analytical technologies (PAT) and process validation, bayesian statistics, design of experiments, multivariate calibration. He is author of several papers published in scientific peer reviewed journals.

PROGRAMME

	Tuesday June 27 <i>Centro Culturale Altinate San Gaetano</i>	Wednesday June 28 <i>Centro Culturale Altinate San Gaetano</i>	Thursday June 29 <i>Centro Culturale Altinate San Gaetano</i>	Friday June 30 <i>Aula Magna - Palazzo Bo</i>
09:00 - 09:20		PL02	PL04	PL05
09:20 - 09:40		Lebrun	Kucheryavskiy	Montalban
09:40 - 10:00		OR09	OR21	OR39
10:00 - 10:20		OR10	OR22	OR40
10:20 - 10:40		OR11	OR23	OR41
10:40 - 11:00		OR12	OR24	OR42
11:00 - 11:30		break + posters	break + posters	break
11:30 - 11:50		OR13	OR25	OR43
11:50 - 12:10		OR14	OR26	OR44
12:10 - 12:30		OR15	OR27	OR45
12:30 - 12:50		OR16	OR28	OR46
12:50 - 13:10		OR17	OR29	OR47
13:10 - 14:30	opening 14-14:30	lunch + posters	lunch + posters	lunch
14:30 - 14:50	PL01	PL03	awards	OR48
14:50 - 15:10	Reis	Grisoni	OR30	OR49
15:10 - 15:30	OR01	OR18	OR31	OR50
15:30 - 15:50	OR02	OR19	OR32	OR51
15:50 - 16:10	OR03	OR20	OR33	closure
16:10 - 16:30	OR04		OR34	
16:30 - 17:00	break + posters		break + posters	
17:00 - 17:20	OR05	social event	OR35	
17:20 - 17:40	OR06		OR36	
17:40 - 18:00	OR07		OR37	
18:00 - 18:20	OR08		OR38	
18:30 - 20:00	welcome cocktail			
20:00 - 24:00			social dinner	

AGENDA

TUESDAY 27th JUNE

Centro Culturale Altinate - San Gaetano
via Altinate n. 71, Padova

AFTERNOON

13:00 - 14:00 **Registration**

14:00 - 14:30 **Opening ceremony**

Chair: Marina Cocchi

14:30 - 15:10 **Plenary - Marco S. do Reis**

Toward the systematic development of hybrid models

15:10 - 16:30 **OR01 - Joan Borrás-Ferris (20 min)**

Multivariate Statistical Process Control via SMB-PLS

OR02 - Maria Cairoli (20 min)

Fingerprint-2-Footprint: dynamically reformulating animal feed production via NIR spectroscopy and life-cycle assessment

OR03 - Barbara Giussani (20 min)

A new approach to the Dissimilarity Index as a process control tool to detect deviations in alcoholic fermentation

OR04 - M. Sagrario Sanchez (20 min)

Partial Least Squares model inversion for intervals

16:30 - 17:00 **Coffee break + Posters**

Chair: Luis Sarabia

17:00 - 18:20 **OR05 - Anna de Juan (20 min)**

Multivariate Curve Resolution for incomplete multisets. Addressing the problem with a single factorization model

OR06 - Francesco Sartori (20 min)

An automated pre-processing framework for uneven-length multiphase batch processes

OR07 - Silvia Mas Garcia (20 min)

Benefits of multivariate curve resolution methods to analyze large-scale raw time-domain NMR data

OR08 - Issam Barra (20 min)

Soil Spectroscopy: use of the moment distance index for fine-tuning spectra acquisition and chemometric models improvement

18:30 - 20:00 **Welcome cocktail**

Caffè Pedrocchi, via VIII Febbraio 15, Padova

Centro Culturale Altinate - San Gaetano

via Altinate n. 71, Padova

MORNING

Chair: Michelle Sergent

09:00 - 09:40 **Plenary - Pierre Lebrun**

Application of DoE in pharmaceutical formulation development

09:40 - 11:00 **OR09 - Stefano Fornasaro (20 min)**

Characterization and optimization of a novel UV-C LED aerodynamic device for airborne microbe viability abatement

OR10 - Barbara Benedetti (20 min)

The power of DoE: how to solve complex analytical problems by multivariate optimization strategies

OR11 - Francesca Cenci (20 min)

Trade off between space exploration and information maximization in experimental design

OR12 - Sergio Garcia Carrion (20 min)

On the use of retrospective DOE for process optimization from historical data in Industry 4.0

11:00 - 11:30 **Coffee break + Posters**

Chair: Riccardo Leardi

11:30 - 13:10 **OR13 - Michelle Sergent (20 min)**

Quality by Design: principle and construction of proven acceptable independent range

OR14 - Lisa Rita Magnaghi (20 min)

DOE for sustainability: bioplastic films composition and preparation optimization for lab-scale production

OR15 - Emanuele Farinini (20 min)

Development of eco-efficient cements by a multi-step Experimental Design

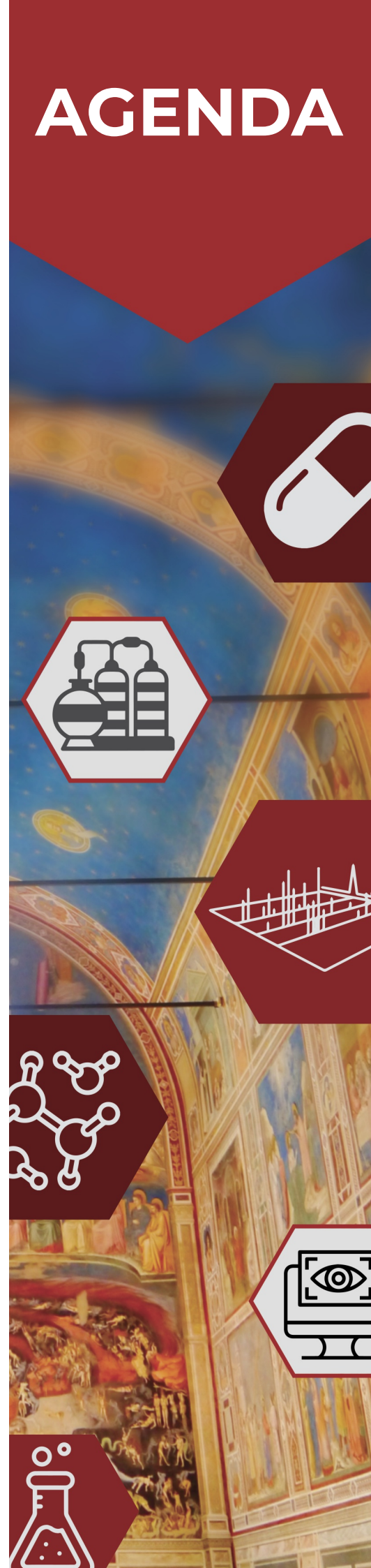
OR16 - Gloria Rovira (20 min)

Correction of the effect of seasonality through a data standardization strategy in the authentication of extra virgin olive oil

OR17 - Josè Camacho (20 min)

Comparison of VASCA, GASCA and its combined version G-VASCA

13:10 - 14:30 **Lunch + Posters**



AGENDA

WEDNESDAY 28th JUNE

Centro Culturale Altinate - San Gaetano

via Altinate n. 71, Padova

AFTERNOON

Chair: Roberto Todeschini

14:30 - 15:10 **Plenary - Francesca Grisoni**

Harnessing deep learning for drug discovery – challenges and opportunities

15:10 - 16:10 **OR18 - Davide Boldini (20 min)**

Practical guidelines for the use of gradient boosting for molecular property prediction

OR19 - Nicola Gambacorta (20 min)

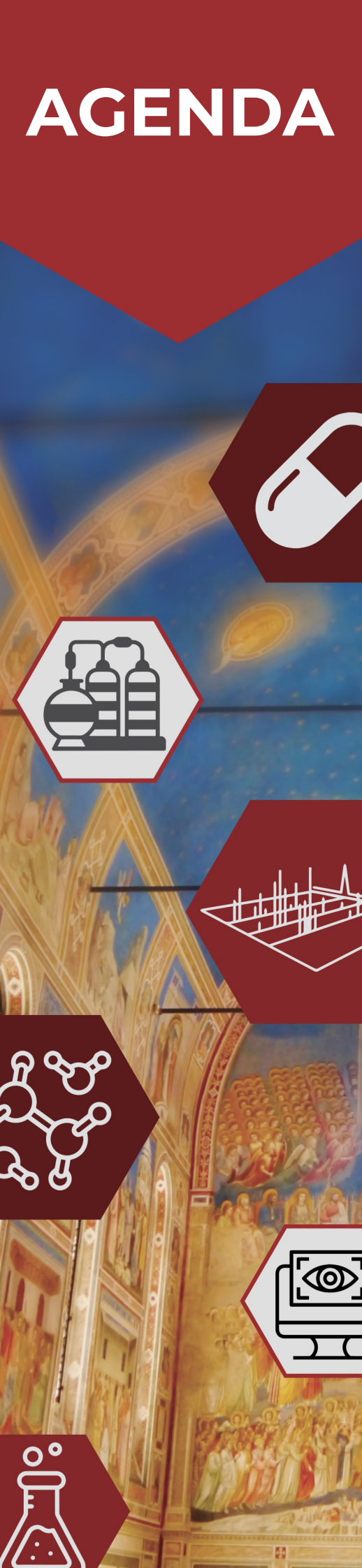
A multiple explainable machine learning framework for discriminating selective and unselective cannabinoid binders

OR20 - Rebecca Birolo (20 min)

Machine Learning Models for Making Cocrystallization More Sustainable

17:00 - 20:00 **Social Event**

Visit to the City of Padova and some historical buildings



THURSDAY 29th JUNE

Centro Culturale Altinate - San Gaetano

via Altinate n. 71, Padova

MORNING

Chair: Cyril Ruckebusch

09:00 - 09:40 **Plenary - Sergey Kucheryavskiy**

Unblind cross-validation

09:40 - 11:00 **OR21 - Jose Manuel Amigo Rubio (20 min)**

First evidence of Microplastics translocation in mussel tissues using Raman Imaging and Chemometrics

OR22 - Martina Beese (20 min)

On determining the factor ambiguity for incomplete data sets

OR23 - Rosalba Calvini (20 min)

Exploratory analysis of large hyperspectral datasets: coupling randomness and sparsity

OR24 - Vicky Caponigro (20 min)

Chemometric strategies for spatial and chemical analysis of maldi mass spectrometry imaging (MSI) of heterogeneous tissues. Case study: parotid tumour

11:00 - 11:30 **Coffee break + Posters**

Chair: Jean-Michel Roger

11:30 - 13:10 **OR25 - Cyril Ruckebusch (20 min)**

Calculating essential information in the fourier domain to accelerate hyperspectral imaging

OR26 - Enmanuel Cruz Muñoz (20 min)

Chemometrics coupled with Hyperspectral Raman Imaging for the characterization of pyrite weathering products

OR27 - Ruggero Guerrini (20 min)

Toward automatic clustering in MALDI imaging for a real unsupervised exploration of complex biological tissues

OR28 - Joaquim Jaumot (20 min)

Exploring sea bass multiomic images for spatially resolved transcriptomics and metabolomics

OR29 - Camilla Menozzi (20 min)

A smartphone-based device for in-vineyard monitoring of red grapes by multivariate analysis of RGB images

13:10 - 14:30 **Lunch + Posters**

AGENDA



AGENDA

THURSDAY 29th JUNE

Centro Culturale Altinate - San Gaetano

via Altinate n. 71, Padova

AFTERNOON

14:30 - 14:50 **Awards ceremony of the Italian Chemometric Group**
Lifetime Achievement Award 2023 and Young Researcher Award 2023

Chair: Federico Marini

14:50 - 16:30 **OR30 - Romà Tauler (20 min)**
Flexible implementation of multilinearity constraints in Multivariate Curve Resolution Alternating Least Squares (MCR-ALS)

OR31 - El Mostafa Qannari (20 min)
A new strategy of analysis for relating datasets

OR32 - Alejandra Arroyo Cerezo (20 min)
Study of the correction of spectral data obtained by SORS using chemometric blind signal separation (BSS)

OR33 - Nicolas Bernard (20 min)
Spectroscopic online and at-line monitoring of Anaerobic digestion at various process stages

OR34 - Luis Antonio Sarabia (20 min)
PLS class modeling using error correction output code matrices and nir spectroscopy to detect deficiencies in bakery doughs

16:30 - 17:00 **Coffee break + Posters**

Chair: Romà Tauler

17:00 - 18:20 **OR35 - Jean-Michel Roger (20 min)**
g-CovSel: covariance-oriented variable clustering

OR36 - Carolina Gastone (20 min)
Self-Optimizing High Shear Wet Granulation with DeepMPC

OR37 - Matthieu Lesnoff (20 min)
Averaging local PLSR models to predict chemical compositions and nutritive values of forages from spectral near infrared data

OR38 - Eugenio Sandrucci (20 min)
Monitoring the State of health (SOH) of green batteries (GreenBat)

20:00 - 24:00 **Conference dinner**
Caffè Pedrocchi, via VIII Febbraio 15, Padova

FRIDAY 30th JUNE

Aula Magna - Palazzo Bo

Via VIII Febbraio 2, Padova

MORNING

Chair: Paolo Oliveri

09:00 - 09:40 **Plenary - Josè Manuel Prats Montalbàn**
Last advances in the development of imaging biomarkers for breast cancer detection

09:40 - 11:00 **OR39 - Alessandra Olarini (20 min)**
Using data geometry to highlight the necessity of bridging the gap between clustering and spectral unmixing in complex samples

OR40 - Rodrigo Rocha de Oliveira (20 min)
NIR hyperspectral imaging combined with chemometrics for the monitoring of water patterns during dehydration of nonvascular epiphytic communities

OR41 - Raffaele Vitale (20 min)
The "black hole effect" in multivariate curve resolution based on alternating least squares: a comprehensive overview and two possible solutions to overcome it

OR42 - Eleonora Macchia (20 min)
Single-molecule bioelectronic sensor: improving reliability with chemometric approaches

11:00 - 11:30 **Coffee break**
Caffè Pedrocchi, via VIII Febbraio 15, Padova

Chair: Pierantonio Facco

11:30 - 13:10 **OR43 - Federico Marini (20 min)**
Revisiting the ROSA algorithm

OR44 - Adrian Gomez Sanchez (20 min)
Revisiting PCA for data sets with missing values

OR45 - Marion Brandolini-Bunlon (20 min)
PLSDA versus PCA on barycenters applied to metabolomics in a context of discrimination

OR46 - Nunzia Iaccarino (20 min)
Data fusion and multivariate curve resolution for evaluating the metabolic impact of different gadolinium-based contrast agents in mice

OR47 - Alessandra Biancolillo (20 min)
Authentication of PDO saffron of L'Aquila (*Crocus sativus* L.) by HPLC-DAD coupled with a discriminant multi-way approach

13:10 - 14:30 **Lunch**
Caffè Pedrocchi, via VIII Febbraio 15, Padova

AGENDA



AGENDA

FRIDAY 30th JUNE

Aula Magna - Palazzo Bo

Via VIII Febbraio 2, Padova

AFTERNOON

Chair: Davide Ballabio

14:30 - 16:10 **OR48 - Mattia Sozzi (20 min)**

Nuclear Magnetic Resonance and Chromatography Data Fusion approach for authentication and traceability of Italian hazelnuts

OR49 - Nicholas Kassouf (20 min)

Quantification of recycled PET in commercial bottles by IR spectroscopy and chemometrics

OR50 - Elena Cazzaniga (20 min)

NIR spectroscopy and chemometrics against food fraud: spotting Mechanically Separated Meat (MSM) in processed meat products

OR51 - Caterina Durante (20 min)

Comparative analysis of ROI-MCR and Compounds Discover protocols for preprocessing LC-MS signals in untargeted metabolomic studies of Parmigiano Reggiano cheese

16:10 - 16:30 **Closure**



POSTERS

- P01 Adrian Gomez Sanchez**
Adrian Trilinearity constraint for incomplete data sets
- P02 Aina Queral-Beltran**
MCR-ALS multiset incomplete data block analysis of the sulfamethoxazole degradation by chlorination, photodegradation, Cl/UV, and pyrolysis
- P03 Alessandro D'Alessandro**
Multivariate Curve Resolution (MCR) applied to hyperspectral images: case study on Pesto alla Genovese sauce
- P04 Alessandro Monari**
Novel electro-analytical approach for the detection and discrimination of cannabinoids in cannabis extracts
- P05 Alessandro Zappi**
Chemometrics in environmental chemistry: application of self-organizing maps for the study of Saharan dust events
- P06 Ana Maria Jimenez Carvelo**
Towards the creation of a global harmonised database and a single analytical multivariate method - tequila authentication as a case study
- P07 Andrea Balivo**
Authentication of milk from buffaloes fed with hydroponic barley forage using E-nose
- P08 Andrea Botton**
Virtual Sensor to Forecast the Mooney Viscosity in an Industrial Rubber Production Process
- P09 Andres Cruz Conesa**
Near-infrared spectroscopy (NIRS) to determine apparent metabolizable energy (AME) and apparent ileal phosphorus digestibility (AIDP) in broiler diets
- P10 Ane Bordagaray**
Determination of riboflavin, flavin adenine nucleotide and flavin mononucleotide produced by lactic acid bacteria by fluorescence spectroscopy
- P11 Beatriz Quintanilla-Casas**
Handling saturation in untargeted GC-MS data analysis
- P12 Berta Torres Cobos**
Nuttin' to hide: A showdown between Fingerprinting and PARADISe to uncover the secrets of hazelnut authenticity
- P13 Blanche Krieguer**
ESR investigation of polymer materials irradiated with gamma and X-rays with SIMPLISMA treatment
- P14 Claudia Scappaticci**
Development of non-destructive tools for the authentication of the typical Italian vegetable species Mugnoli di Pettorano sul Gizio
- P15 Consuelo Pizarro**
Rapid spectrochemical differentiation of amyotrophic lateral sclerosis and its progression based on ATR-FTIR coupled with chemometrics



POSTERS

- P16 Davide Ballabio**
Chemometrics and molecular fingerprints to enhance LC-MS/MS spectral matching
- P17 Elia Arnese Feffin**
Estimation of null-space uncertainty in latent-variable model inversion: the case of correlated quality attributes
- P18 Elisa Robotti**
Identification of illicit storage treatment in fresh fish by a multi-omic approach coupled to chemometrics
- P19 Eloisa Bagnulo**
Chemometrics as a tool to answer to the challenges of the climate change and political situations on the consistency of cocoa flavour quality
- P20 Eneko Lopez**
Proper validation of classification models. A real-life example
- P21 Fabiola Pereira Verbi**
Non-invasive analysis and chemometrics for macronutrients determination in non-conventional food plants (PANC)
- P22 Flavia Bisozzi**
Application of PCA and classification method to prototype of fortified Piadina Romagnola
- P23 Flavio Montenegro de Andrade**
Characterization of Bio-oil samples obtained from Thermal liquefaction
- P24 Giacomo Squeo**
Application of doe and multivariate analysis for a txrf method development and data analysis. a case-study from the agri-food sector
- P25 Gianmarco Barberi**
Accelerating cell lines selection in biopharmaceutical process development through data-driven modeling on metabolomic dynamic information
- P26 Giulia Gorla**
Multivariate strategies for unlocking the potential of infrared spectra to enhance additive effects in historical mortars
- P27 Gorka Albizu Martinez**
Chemometrics to avoid systematic error in the control of nickel in electroless nickel plating processes by UV-Vis spectrophotometry
- P28 Harun Hano**
Comparison of Classification Models For Lung Cancer Detection Using Raman Spectroscopy
- P29 Henry Mac Keown**
Multivariate investigation on the interaction of two polymeric materials with emerging contaminants for sorptive extraction applications
- P30 Isabel Duran Meras**
3D fluorescence spectroscopy as a tool for discrimination of olive oils from traditional and superhigh-density olive groves



POSTERS

- P31 Jokin Ezenarro**
Studying nectarine ripening with near infrared spectroscopy
- P32 Jordi Cruz**
Comparison of different spectroscopic data and chemometric tools for determining citalopram content in pharmaceutical tablets
- P33 Jordi Riu**
Paper-based organic electrochemical transistor array for multi-analyte detection
- P34 Jordi Riu**
An insight into the problems of determining the adulteration of almond flour with low-cost miniaturised NIR instruments
- P35 Laurence Dujourdy**
Study of the resistance of *Bacillus subtilis* spores to UV light via Raman, FTIR and O-PTIR spectroscopy. Use of multiple co-inertia analysis (mCIA)
- P36 Lenka Halamkova**
Leveraging Machine Learning Approaches for Forensic Applications using the Attenuated total reflectance Fourier transform infrared (ATR-FTIR) Spectroscopy
- P37 Leonardo Sibono**
Multivariate statistics approach to infer metabolite profile variations in Pecorino Romano Cheese
- P38 Lorenzo Castellino**
Anomaly Detection in Production - Diagnostics and Insights from Data
- P39 Lorenzo Strani**
Chemometrics strategies to assess mountain products identity
- P40 Lorenzo Strani**
Assessment of iron nuclearity in mineral fibers by means of MCR-ALS
- P41 Manuela Mancini**
Hyperspectral near infrared imaging to investigate waste wood material characteristics
- P42 Martina Fattobene**
Evidence of the cultivation method of durum wheat by ICP-MS measurements of the elemental content in the seeds and flours
- P43 Martina Foschi**
ICP-MS and chemometrics for the characterization and discrimination of three different species of edible insects
- P44 Miriam Medina Garcia**
Multivariate analytical method based on liquid chromatographic fingerprinting and chemometrics to authenticate the geographical origin of tigernuts
- P45 Monica Casale**
A validated method for identifying mechanically separated meats by using multivariate analysis of 43 trace elements determined by ICP-MS



POSTERS

- P46 Nicola Caporaso**
Analysis of electronic nose data for the discrimination of volatiles from food-saliva interaction in individuals with different BMI
- P47 Nicola Cavallini**
Masters of PCA: The Evolution of Metallica Through the Years with Exploratory Data Analysis. An Invitation to Teaching PCA in a Different Way
- P48 Oliver Aleksandrei Polushkina**
Application of Variable-selection ANOVA Simultaneous Component Analysis in a longitudinal study on intrauterine growth restriction
- P49 Paolo Berzaghi**
Evaluation of Local approaches for processing Near-Infrared Spectroscopy for prediction of multi-products database
- P50 Raimundo Gargallo**
Chemometrics applied to the study of non-canonical DNA structures
- P51 Sabina Licen**
An instrumental data fusion technique based on Self-Organizing Map algorithm for contextualizing seawater sampling
- P52 Samuele Pellacani**
Development and optimization of an analytical method based on spme-arrow and chemometric techniques for the characterization of the aroma profile of bakery products
- P53 Sarah Curro**
Feasibility of a near-infrared spectroscopy system to estimate the microbial load of seafood products
- P54 Stefano Fornasaro**
Chemometrics strategies for the implementation of surface enhanced Raman scattering of crevicular fluid in periodontics and implantology
- P55 Stiufiuc Rares Ionut**
A new chemometric method for oral and oropharyngeal cancer detection based on multivariate analysis of Surface Enhanced Raman spectra of salivary exosomes
- P56 Tiziana Forleo**
A Raman-Based Chemometric study for the discrimination of tomatoes from agricultural techniques
- P57 Victor Hugo Cavalcanti Ferreira**
Improving convex-hull estimates to better explore LIBS images of biosamples by pre-processing the spectra
- P58 Luis Antonio Sarabia**
A proof-of-concept study on the logical analysis of sample pooling results for qualitative analytical testing
- P59 Magalie Claeys-Bruno**
Deep learning combined with experimental design to limit dependence on annotated data
- P60 Magalie Claeys-Bruno**
Prediction of supercritical CO₂ extraction kinetics of compounds of interest using experimental design



POSTERS

- P61 Maria Cruz Ortiz**
AQbD using a d-optimal design and parafac in an automatic spe system coupled to HPLD-FLD
- P62 Raffaele Emanuele Russo**
Optimization lithium recovery from LiFePO₄ batteries based on agri-food wastes through experimental design
- P63 Tommaso Paravano**
When DoE goes Untargeted: optimization and validation of an extraction procedure for emerging contaminants monitoring in a complex matrix
- P64 Adrian Venegas-Reynoso**
Quantitative Structure-Property Relationships for the prediction and understanding of liquid phase oxidation in hydrocarbons
- P65 Fabrizio Mastrolorito**
TIRESIA, a friendly XAI website for the assessment of developmental toxicity
- P66 Benoit Jaillais**
Texture analysis and chemometrics of hyperspectral images of bread
- P67 Daniele Tanzilli**
When do heterogeneous samples really need hyperspectral imaging techniques?
- P68 Giorgia Sciutto**
Identification and localization of dehydrated biological fluids in forensic evidences: the role of chemometric strategies in the processing of multiblock hyperspectral data
- P69 Paolo Oliveri**
Exploiting the correlation between different spectral blocks in a multiplatform hyperspectral imaging system
- P70 Pier Lorenzo Rolando**
Monitoring the colour of strawberry yoghurt purée: a combined approach of mixture design and multivariate image analysis
- P71 Pietro Bertani**
WHIM Descriptors for Medical Images Analysis
- P72 Veronica Ferrari**
Application of NIR-Hyperspectral imaging for the management of the Brown Marmorated Stink Bug (BMSB) pest
- P73 Arsenio Muñoz de la Pena**
An upgrade of MVC2, a MATLAB graphical user interface for second-order multivariate calibration
- P74 Edenir Rodrigues Pereira Filho**
Calcium, magnesium, and potassium determination in soy and corn leaves combining laser-induced breakdown spectroscopy (LIBS) direct analysis and partial least squares (PLS)
- P75 Eduardo Caballero Saldivar**
GC-IMS chromatogram alignment using the retention indexes of Analytical Standards



POSTERS

- P76 Giorgia Foca**
NIR spectroscopy and chemometrics for the identification of adulterated oregano samples
- P77 Jokin Ezenarro**
J-Score: a new joint parameter for PLSR model performance evaluation
- P78 Jokin Ezenarro**
expertPLS: a MATLAB toolbox for spectral preprocessing selection
- P79 José Antonio Cayuela-Sánchez**
NIRS measurement of soil organic carbon by using a compositional data method. an approach to avoid moisture interference
- P80 Josè Luis Gonzalez Solís**
Drug expiration study using raman spectroscopy and super-paramagnetic clustering
- P81 Jose Maria Gonzalez-Saiz**
Emerging FTIR-chemometric approach for ALS patients' discrimination based on selected spectra biomarkers
- P82 Kateryna Tkachenko**
Identification of lipidomic traits in plasma samples for the discrimination of patients affected by Parkinson's disease: UPLC-MS untargeted approach
- P83 Kurt Varmuza**
Adjusted Pareto scaling
- P84 Maria Suliany Rodriguez Barrios**
Establishing applicability limits of regression neural networks using decoders. Application to predict diesel properties using infrared spectra
- P85 Marina Cocchi**
Developing a Local RoBoost PLS framework
- P86 Roberto Todeschini**
Extended multivariate comparison of validity indices for cluster analysis
- P87 Gaelle Bordes**
Raman technology implementation PAT for Cell culture development: Chemometrics Raman models for accelerated and easier new process development
- P88 Lorenza Broccardo**
Calibration Transfer to Facilitate Knowledge Sharing and Speed Deployment
- P89 Qiang Zhu**
Quality prediction with sequential-orthogonalized PLS: an explorative method to capture process topology
- P90 Riccardo Voccio**
Automated Exploratory Analysis of Spectroscopic Data for Raw Material Identification (RMID) in the Tyre Industry