

CAC 2022



XVIII CHEMOMETRICS IN ANALYTICAL CHEMISTRY

29 AUGUST - 2 SEPTEMBER
ROMA



PROGRAM AT A GLANCE



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- **Olivier Devos** *University of Lille (France)*
- **Paolo Oliveri** *University of Genova (Italy)*

PRELIMINARY PROGRAM

Monday 29 August 2022

10:00-19:00 Registration of the participants

14:30-15:00 Conference opening

15:00-16:00 PL1: Harald Martens - Human-interpretable Machine Learning with an Eye for Causalities: *Making sense of modern measurement streams inside and outside chemistry*

16:00-16:30 Coffee break & Poster session

16:30-18:10 Contributed Session I: Big Data and Machine Learning

16:30-16:50 OL1: Davide Ballabio - Enhancing LC-MS/MS Spectral Searching With Multi-Task Neural Networks And Molecular Fingerprints

16:50-17:10 OL2: Gabriel Vivo-Truyols - On the use of Bayesian statistics for (big) data analysis: automation for both qualitative and quantitative chemometrics

17:10-17:30 OL3: Michael Soroohan Armstrong - Chemometrics with Amazon Web Services (AWS)

17:30-17:50 OL4: Jeroen Jansen - Process economy, efficiency and sustainability go hand in hand, how chemometrics can build a greener industry

17:50-18:10 OL5: Priyanka Kumari - QSRR for small pharmaceutical compounds in RPLC: A Machine learning approach

18:10-20:10 Welcoming cocktail

Tuesday 30 August 2022

09:00-10:00 PL2: Roy Goodacre - Lessons from large-scale metabolic phenotyping

10:00-11:00 Contributed Session II: Omics/ASCA and related methods I

10:00-10:20 OL6: Albert Menéndez Pedriza - Comparison of mid-level fusion strategies for the multi-omic analysis of toxicological data

10:20-10:40 OL7: Andrés Martínez Bilesio - Metabolomics-guided insights on Bariatric Surgery: a longitudinal chemometrics approach over 1H NMR spectra from serum samples

10:40-11:00 OL8: Sarah Malek - Evaluation of mid-infrared spectra of serum and synovial fluid in predicting early post-traumatic osteoarthritis in an equine model

11:00-11:30 Coffee break & Poster session

11:30-13:10 Contributed Session III: Applications I

11:30-11:50 OL9: Zuzana Małyjurek - Class-Modelling - Optimization, Validation and Application

11:50-12:10 OL10: Agnieszka Martyna - Likelihood ratio in forensic discrimination/classification tasks

12:10-12:30 OL11: Martina Foschi - Supervised and Unsupervised Chemometric Methods to deal with saffron aging and its Quality Control

12:30-12:50 OL12: Lorenzo Strani - Real time prediction of ABS properties through multiblock and local regression methods

12:50-13:10 OL13: Sebastian Orth - Spectral imaging - pre-harvest malting barley germination classification with sequential orthogonalised multiblock data fusion methodologies

13:10-14:30 Lunch & Poster session

- 14:30-15:00 KN1: Mathias Sawall - On the ambiguity underlying the spectral recovery problem and its analysis by the area of feasible solutions**
- 15:00-16:00 Contributed Session IV: Theory & algorithms I**
- 15:00-15:20 OL14: Sergey Kucheryavskiy - Procrustes cross-validation of multivariate regression models
- 15:20-15:40 OL15: Stephan Seifert - Opening the random forest black box with Surrogate Minimal Depth
- 15:40-16:00 OL16: Oxana Rodionova - Expansion of the DD-SIMCA concept
- 16:00-16:30 Coffee break & Poster session**
- 16:30-18:10 Contributed Session V: Multi-block/Multi-way/Multi-set I**
- 16:30-16:50 OL17: Paul-Albert Schneide - Speeding up PARAFAC2 dramatically
- 16:50-17:10 OL18: Isabelle Viegas - Coupled factorization of fluorescence data of proteins and quantum dots to assess their conjugation process
- 17:10-17:30 OL19: Oksana Mykhalevych - New tools for designing food ingredients structures
- 17:30-17:50 OL20: Maria Cairoli - Monitoring pollution pathways in river water by predictive path modelling using untargeted GC-MS measurements
- 17:50-18:10 OL21: Ivan Krylov - Fluorescence and scattering model estimation

Wednesday 31 August 2022

- 09:00-10:00 PL3: Ingrid Måge - Industrial bioprocessing – an amusement park for chemometricians and analytical chemists**
- 10:00-11:00 Contributed Session VI: Multi-block/Multi-way/Multi-set II**
- 10:00-10:20 OL22: Jean-Michel Roger - N-CovSel, a new strategy for feature selection in N-way data
- 10:20-10:40 OL23: Mahdiyeh Ghaffari - Using Multi-Block Non-Negative Matrix Factorization for Multi-layer Plastic Sorting
- 10:40-11:00 OL24: Paul Gemperline - Combining ASCA and Tucker3 models to explain high-dimensional data
- 11:00-11:30 Coffee break & Poster session**
- 11:30-13:10 Contributed Session VII: Applications II**
- 11:30-11:50 OL25: Sabina Licen - Data fusion based on self-organizing map algorithm for the integration of different source/frequency instrumental data and spot sampling contextualization for environmental monitoring
- 11:50-12:10 OL26: Vicky Caponigro - Application of different chemometric approaches for MALDI-MSI data set of heterogeneous tissues. Case study: parotid tumour
- 12:10-12:30 OL27: Ewa Szymanska - Comprehensive chemometric strategy for the high-throughput screening of in-line spectroscopic sensors for milk composition traits
- 12:30-12:50 OL28: Maxime Ryckewaert - Combining hyperspectral imaging data with climate data to predict physiological variables of grapevine plants
- 12:50-13:10 OL29: Eleni Ioannidi - Using ATR FT-IR and MCR as a method to understand the crystal state of chocolates tempered under different conditions
- 13:10-14:30 Lunch & Poster session**

- 14:30-15:00 KN2: Hadi Parastar - Integration of handheld spectrometers and chemometrics for food authentication**
- 15:00-16:00 Contributed Session VIII: Spectroscopy & Imaging I**
- 15:00-15:20 OL30: Cristina Malegori - HSI-NIR and chemometrics for the quantification of collagen in bones: how chemical mapping can help in preserving archeological finds
- 15:20-15:40 OL31: Manuela Mancini - Spectroscopy and chemometrics for sorting waste wood material according to the best-suited application
- 15:40-20:30 Social activity (tours will start from the agreed meeting points at 17:00)**

Thursday 1 September 2022

- 09:00-10:00 PL4: Romà Tauler - Bilinear model factor decomposition: a general mixture analysis tool**
- 10:00-11:00 Contributed Session IX: Curve Resolution**
- 10:00-10:20 OL32: Martina Beese - An active constraint approach to identify essential spectral information in noisy data
- 10:20-10:40 OL33: Laureen Coic - A phasor view of Multivariate Curve Resolution
- 10:40-11:00 OL34: Anna De Juan - Trilinearity in Multivariate Curve Resolution: hybrid modeling and missing data
- 11:00-11:30 Coffee break & Poster session**
- 11:30-13:10 Contributed Session X: Spectroscopy & Imaging II**
- 11:30-11:50 OL35: Florent Abdelghafour - Combining spectral and spatial features extracted from hyperspectral images: Application on the detection of scab disease
- 11:50-12:10 OL36: Rodrigo Rocha de Oliveira - 2-D wavelet image decomposition and Multivariate Statistical Process Control for blending end-point detection
- 12:10-12:30 OL37: Valeria Tafintseva - Modelling and preprocessing of sparse infrared spectra
- 12:30-12:50 OL38: Nicola Cavallini - Tracing the identity of mountain product Parmigiano Reggiano PDO cheese using ^1H -NMR spectroscopy and multivariate data analysis
- 12:50-13:10 OL39: Paolo Oliveri - A combined chemometric strategy for a non-destructive age estimation of biological fluid stains
- 13:10-14:30 Lunch & Poster session**
- 14:30-15:00 KN3: Maria Cruz Ortiz - Analytical Quality by Design using a computational approach for the inversion of a PLS model**
- 15:00-16:00 Contributed Session XI: Omics/ASCA and related methods II**
- 15:00-15:20 OL40: Miguel De Figuereido - Rebalanced ASCA (RASCA) to handle unbalanced multifactorial designs
- 15:20-15:40 OL41: Michel Thiel - LMWiRe: an R package for Linear Modeling of Wide Responses based on ASCA family of methods
- 15:40-16:00 OL42: Claudia Beleites - An Experimental Design Perspective on Cross-Validation
- 16:00-16:30 Coffee break & Poster session**
- 16:30-17:50 Contributed Session XII: Spectroscopy & Imaging III**
- 16:30-16:50 OL43: Siewert Hugelier - Quantifying the Tau protein aggregation degradation process by classification of super-resolution fluorescence microscopy localizations
- 16:50-17:10 OL44: Erik Tengstrand - Calibration transfer of Near-Infrared and Raman models without using transfer samples

- 17:10-17:30 OL45: Alisa Rudnitskaya - Characterization of microplastics from marine organisms using near infrared hyperspectral imaging
- 17:30-17:50 OL46: Jose Luis Aleixandre-Tudo - Spectral evaluation of fresh grapevine organs using self-organizing maps (SOM)
- 17:50-18:30 **Awards Ceremony (Elsevier Chemometrics and Intelligent Laboratory Systems Award & Lifetime Achievement Award)**
- 20:15-01:00 **Social dinner**

Friday 2 September 2022

09:00-11:00 Contributed Session XIII: Theory & algorithms II

- 09:00-09:20 OL47: Nematollah Omidikia - Infrared Ion Spectroscopy Peak Matching using Peak Annotation Technique
- 09:20-09:40 OL48: Sergio Oller Moreno - Peak matching across Gas Chromatography-Ion Mobility Spectrometry samples
- 09:40-10:00 OL49: Wouter Saeys - Multivariate monitoring and update strategies for calibration models
- 10:00-10:20 OL50: Sean Rozinski - What's UMAP Doing Anyway?
- 10:20-10:40 OL51: Ramin Nikzad-Langerodi - Does it Transfer? Assessing model generalization in domain adaptation with data fusion
- 10:40-11:00 OL52: Benjamin Mahieu - New developments around the VIP index

11:00-11:30 Coffee break & Poster session

11:30-12:50 Contributed Session XIV: Applications III

- 11:30-11:50 OL53: Dmitry Kirsanov - Chemometrics in spent nuclear fuel reprocessing
- 11:50-12:10 OL54: Joscha Christmann - Monitoring of fermentation processes by gas chromatography-ion mobility spectrometry (GC-IMS)
- 12:10-12:30 OL55: Martín Bravo - Development of an analytical platform for the identification of *Fusarium circinatum* in culture media, using VIS-NIR spectroscopy and chemometric methods
- 12:30-12:50 OL56: Tim Offermans - Retrospective Quality by Design (QbD) using Historical Process Data and Design of Experiments

12:50-13:30 Conference Closing

POSTER LIST

- P1: Fernanda Honorato - Authenticity of almond flour using handheld near infrared instruments and one class classifiers
- P2: Florent Abdelghafour - Unsupervised calibration transfer between spectrometer and hyperspectral camera: challenge proposed at the congress "Chimiométrie 2022"
- P3: Riccardo Aigotti - Odor concentration predictive model based on the odor activities of odorants produced by a municipal solid waste odor abatement scrubber
- P4: Ricard Boqué - ATR-MIR and MCR-ALS as a tool for monitoring wine alcoholic fermentation and detecting bacterial spoilage
- P5: Ricard Boqué - Prediction of beer shelf life using an HS-MS e-nose
- P6: Nicola Cavallini - The NIR side of lentil
- P7: Alessandro D'Alessandro - Exploiting pesto sauce by several analytical platforms: looking for most efficient information extraction and data fusion approach
- P8: Tiziana Forleo - Application of chemometric approaches to answer some archeological questions for the study of the Apulian Red-Figure Pottery
- P9: Gianmarco Gabrieli - Leveraging an integrated sensor array and machine learning to accelerate sensory evaluation of coffee
- P10: Barbara Giussani - Insights into multivariate data analysis for real-case fermentation process with miniaturized NIR spectroscopy
- P11: Klaudia Glowacz - Identification of metal ions with the use of quantum dots coupled with excitation-emission matrix fluorescence spectroscopy
- P12: Jule Hansen - Evaluation of preprocessing strategies for LCMS data using R
- P13: Christel Kamp - Spectral identification of therapeutic allergen products
- P14: Nicholas Kassouf - Comparison between colloidal and volatile profiles to create a chemometric model to classify different tomato sauce brands
- P15: Nicholas Kassouf - Multivariate analysis of colloidal and volatile profiles for class-modeling of different tomato sauce brands
- P16: Victor Cardoso - A comparison between artificial neural networks and partial least squares for coffee assessment by high-resolution mass spectrometry
- P17: Erwin Kupczyk - Benchmarking Machine Learning approaches for hit detection in High-Content Screening
- P18: Qicheng Wu - Robust quantitative analysis in Laser-Induced Breakdown Spectroscopy (LIBS) using artificial neural networks
- P19: Miguel De Figueiredo - Analyzing multifactorial designed data from multiple sources with a single model using AComDim
- P20: Giulia Gorla - Investigating sources of variance in miniaturized NIR spectroscopy: find clues and solve the riddle
- P21: Luis A. Sarabia - Logical analysis of the sample pooling results for qualitative analytical testing: a proof-of-concept study
- P22: Daniel Schorn-García - Acetic or lactic bacteria contamination? ASCA has the answer
- P23: María Julia Culzoni - A fluorometric photo-induced four-way calibration method for the determination of multiclass pesticides in citrus fruits
- P24: María Julia Culzoni - Chemometrically assisted high-throughput methotrexate sensing strategy based on a pH-switchable optical nanosensor
- P25: Hector Goicoechea - Multiway data modeling for enhancing classification performance: fluorescence data as case of study

- P26: Andrés Martínez Bilesio - Data fusion approach applied in chemometrics-assisted metabolomics analysis
- P27: Nicola Cavallini - Mapping Chemometrics with Chemometrics
- P28: Isabelle Viegas - Joint factorization of right-angle and front-face fluorescence data to improve PARAFAC pure profiles recovered from oil-in-water emulsions
- P29: Marc Marín García - Multivariate Curve Resolution of incomplete and partly multilinear multi-block data sets
- P30: Tobias Karakach - Low signal intensity, measurement errors and biological significance: a model for LC-MS proteomics
- P31: Reza Nafari - Quantitative evaluation of red meats in kebab loghmeh samples: fourier transform infrared data and chemometric methods
- P32: Justine Raeber - Fast and Convenient Authenticity Control of Natural Products using Mass Spectrometry and Chemometrics
- P33: Anastasiia Surkova - Aquaphotomics study of body fluids in cancer research
- P34: Soeren Wenck - Opening the Random Forest Black Box of the Asparagus Metabolome
- P35: Elianna Castillo - Relationship between cadmium availability and soil properties in cacao farms at Santander – Colombia
- P36: Abdelaziz Ait Sidi Mou - Application of multivariate data analysis coupled with spectroscopy to agroalimentaire investigation in Morocco: advancement and challenge
- P37: Matthias Rüdert - Chemometrics – a chemometric Python package
- P38: Rustam Guliev - Structuring and generalizing implementations of N-FINDR algorithm for unmixing hyperspectral data
- P39: Erik Johansson - Variable removal by logical blocks in OPLS predictions
- P40: John Kalivas - Rashomon effect and model interpretability: is it possible?
- P41: Lyle Lawrence - Diagnostic Plots to Aid Final Model Selection
- P42: Mansuk Oh - Bayesian Multivariate Receptor Modeling Software: BNFA and bayesMRM
- P43: Maria Sagrario Sánchez - Compliant class-models based on PLS2 to handle several categories encoded with error correcting output codes
- P44: Patrícia Valderrama - Are we there yet? efficient exploration and visualization of multivariate data with SCORXPLORE
- P45: Macarena Rojas - Chemical variation of sugar beet subjected to long-term storage by Vis-NIR spectroscopy, Hyperspectral Imaging and chemometric methods
- P46: Francesco Savorani - The NMR side of lentil: protein extraction and hydrolyzation, and a bit of data fusion
- P47: Marek Sikorski - Explorative study of strawberry juice from various fruit varieties using absorbance-transmission and fluorescence excitation-emission matrix technique
- P48: Sin Yong Teng - Chemsy: Simultaneous feature selection, pre-processing search, model selection, and hyper-parameter optimization in Python
- P49: Sonia Nieto Ortega - Reliable determination of the lipidic profile of oils extracted from fish by-products through near infrared spectroscopy and chemometrics
- P50: Claudete Pereira - A multivariate approach to quantify the enhancement effect on surface-enhanced spectroscopies
- P51: Beatriz Quintanilla-Casas - Virgin olive oil excitation-emission matrices: exploring their usefulness to predict taste attributes
- P52: Antonino Restivo - Multivariate Data Analysis and PAT in vaccines development: enabling multiple components quantification in complex formulations

- P53: Elisa Robotti - Optimization of the parameters of a continuous annealing process in a steel producing company by multivariate statistics and Artificial Neural Networks
- P54: Laura Rolinger - Blend uniformity design space development and verification by PAT for minibatch blending
- P55: Carolina Silva - Application of class-modelling approaches for botanical and geographical origins of honey samples based on mineral content
- P56: Giacomo Squeo - Application of DoE and multivariate analysis for TXRF method development and data analysis. A case-study from the agri-food sector.
- P57: Mauro Tomassetti - A new survey for multicomponent analysis to solve problems linked to nano-compounds (case study)
- P58: Berta Torres - Discriminant classification models applied to hazelnut unsaponifiable fingerprint for geographical and varietal authentication
- P59: Patrícia Valderrama - Multivariate control chart based on PCA/Q residuals to evaluate Salmonella in meat-bone flour
- P60: Helene Halberg - Fluorescence spectroscopy of wine, a complex food system
- P61: Daniele Tanzilli - IMAGINE NIR to monitor Pesto sauce industrial production
- P62: Lucas F. Voges - Genotyping and statistical analysis of marzipan with DMAS-PCR
- P63: Andrea Junior Carnoli - Alternative approaches to untargeted LC/GC-MS data analysis
- P64: Cannon Giglio - Analysis of Pinot Noir Wines Using UV-Vis Spectroscopy
- P65: Milan Chhaganlal - Evaluation of the accuracy of NMR predictors for the prediction of fatty acid spectra
- P66: Mohamad Ahmad - An IDEL perspective on handling spatial correlation in hyperspectral imaging
- P67: Juan Araya - Identification of spectral patterns associated to different aggregation states of beta amyloid peptide in hyperspectral images through chemometric analysis
- P68: Juan Araya - Supervised pattern recognition using near infrared spectrum of serum for diagnosis of gestational diabetes mellitus
- P69: Issam Barra - Soil spectroscopy: use of chemometrics for fine-tuning spectra acquisition- case of scans number optimization
- P70: Katharina Beier - Classification of Horsetails using Machine Learning Methods on NIR Spectra
- P71: Irati Berasarte - Time-based colorimetric method for the simultaneous determination of calcium and magnesium ions with silver nanoparticles
- P72: Hooriyeh Borhani - Investigation of an innovative method for classifying nanostructures based on time series analysis and fuzzy logic in microscopic images
- P73: Ewa Sikorska - Multivariate models for prediction quality parametrs of berry beverages using FTIR-ATR spectroscopy
- P74: Jokin Ezenarro - Olive ripening assessment methodologies using digital image analysis
- P75: Davide Gattabria - An exploratory study on monitoring tomato plant growth by near infrared portable devices
- P76: Hector Goicoechea - Chemometric approaches to enhance the potential of new IR spectroscopic technologies
- P77: Hector Goicoechea - Feasibility of MCR-ALS to exploit the second-order advantage with first-order and non-bilinear second-order data. a systematic characterization
- P78: Ivan Krylov - Approximation of Martian rock emission spectra by multiparametric optimization

- P79: Saeedeh Mohammadi Tanouraghaj - An assessment of the potential of different vibrational spectroscopic techniques in classification of various types of liquid milk by using multivariate chemometric methods
- P80: Arsenio Muñoz De La Peña - Discriminant analysis of three and four-way fluorescence data for classification issues
- P81: Alessandra Olarini - Hyperspectral imaging data: clustering or spectral unmixing?
- P82: Nicholas Pedge - Update of Transmission Raman Spectroscopy Calibration Models using Dynamic Orthogonal Projection (DOP)
- P83: Jordi Riu - Classification of bitter and sweet almonds using NIR miniaturized instruments
- P84: Mohamad Ahmad - A solution based on sample weighting to the leverage problem in Multivariate Curve Resolution-Alternating Least Squares
- P85: Gorka Albizu - Different chemometric strategies to control PTFE in Ni-P/PTFE electroless coating baths by UV-VIS
- P86: Tomass Andersons - Pure component recovery for rank-deficient problems
- P87: Cristian Fuentes - Application of a segmented analysis by MCR-ALS on ¹H-NMR spectroscopy for the identification of adulterations in brown sugars
- P88: Adrián Gómez-Sánchez - Unmixing exponential signals by Kernelizing
- P89: Jan Hellwig - Multi-Layer modeling of time series of NMR spectra
- P90: Nunzia Iaccarino - Exploring the dynamic equilibria of non-canonical DNA structures by Multivariate Curve Resolution and 2D correlation spectroscopy
- P91: Paulo Henrique Março - Pseudo-univariate calibration through MCR-ALS applied to electrochemical data to determine different amino acids simultaneously
- P92: Nematollah Omidikia - On the Visualization of Bayesian Nonnegative Factor Analysis
- P93: Nazanin Saburouhvahid - Application of PARAFAC for curve resolution of fluorescence lifetime imaging data
- P94: Aina Queral Beltran - UV absorption spectrophotometry and LC-DAD-MS coupled to chemometrics analysis of the degradation of sulfamethoxazole drug by UV/chlorine advanced oxidation processes
- P95: Carlos Pérez López - The potential of the ROIMCR methodology for sewage water sample characterization in environmental proteomics
- P96: Eugenio Sandrucci - Monitoring the State of Health (SOH) of green batteries (GreenBat)
- P97: Claudia Scappaticci – SIMCA framework for multi-block class modeling
- P98: Alessandra Biancolillo - ICP-OES analysis coupled with chemometrics for the characterization and the discrimination of high added value Italian Emmer samples
- P99: Juan Araya - Gestational diabetes mellitus, preterm birth and macrosomia early prediction using multivariate analysis on clinical and biochemical data
- P100: Michel Rocha Baqueta – Chemometrics-assisted microNIR spectroscopy for large-scale classification and authentication of high-quality Brazilian Canephora coffees

USEFUL INFORMATION

All the conference activities (except for the social program) will take place in the Cannizzaro Building (CU014) of the Chemistry Department of Sapienza University of Rome, which is located in the main University campus (main entrance is in Piazzale Aldo Moro 5). You can see how to access the Cannizzaro building from the main entrance in the map below:



The main lecture hall is **Aula La Ginestra**, which is located on the first floor of the building (signs will guide you through the access), while the poster boards will be mounted in the space outside the main entrance of the Chemistry building, where coffee breaks and lunches will also be served.

Registration

The registration desk is located in the main entrance hall of the Chemistry building and will be open throughout the conference.

A cash point is available next to the registration desk for on-site registrations, refunds and/or purchase of optional tours and additional conference dinner tickets.

When signing in at the registration desk, you will receive your conference badge and a conference bag with the conference material. Please make sure to wear your badge at all times while attending the conference.

Instructions for speakers

Presenting authors are encouraged to upload their presentations (directly on the computer located in Aula La Ginestra) as early as possible and, anyway, not later than the coffee break/lunch interval before their session.

Virtual Special Issue

Analytica Chimica Acta and Chemometrics and Intelligent Laboratory Systems journals are asking for the submission of review and research papers to the virtual special issue (VSI) dedicated to the subject: *Chemometrics: Intelligent data analysis for Analytical Chemistry*.

Accepted papers will be considered for publication in either one of the two journals. Details about the submission procedure to this VSI will be sent to all CAC2022 participants just after the conference has finished.

CAC2022 will be an environmentally friendly event promoting social solidarity: thanks to the Food for Good project endorsement, we will collect the surplus food at the end of the Conference meals and deliver it to charitable organizations such as family homes, soup kitchens and refugee centers, in accordance with applicable hygiene regulations and in compliance with Italy's Good Samaritan law (Law 155/2003)



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