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 Sorochan 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: Belal Gaci - 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 Achiement 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 r(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 evalution 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 spetroscopy: 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: Sin Yong Teng - High-Frequency Renewable Energy Reconciliation in Power Substations using Domain Adaptation for Zero-Shot Learning in Sequence
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 agroalimenaire investigation in Morocco: advancement and challenge
P37: Matthias Rüdt - 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 interpretabiltiy: 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 SCORXPLOR
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 Helath (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