

XVII CHEMOMETRICS IN ANALYTICAL CHEMISTRY

JUNE 25-29, 2018

HALIFAX • NOVA SCOTIA • CANADA



CONFERENCE PROGRAM

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Welcome

Four decades after the first CAC Meeting in Amsterdam, Halifax is proud to host the 17th CAC Conference. The CAC Permanent Committee and the Local Organizing Committee welcome you to CAC-2018, which has returned to Canada for the first time since 1992.

We are delighted to provide a forum to facilitate the interaction of leading international researchers in Chemometrics from about two dozen countries through oral and poster presentations, as well as a variety of social events. The conference features 16 invited speakers, including a special session in honour of Yizeng Liang. Posters will be highlighted with a social event on Wednesday afternoon and a number of awards will be presented to recognize achievements in the field.

Thank you for your participation in the conference. We hope that you enjoy your stay in Halifax and have a chance to explore the province of Nova Scotia, known as Canada's Ocean Playground.

Peter Wentzell
CAC-2018 Conference Chair

CAC Conference Sponsors



Committees

CAC Permanent Committee

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 Joaquim Jaumot, *University of Barcelona (Spain)*
 Hongmei Lu, *Central South University (China)*
 Marianna Lucio, *Helmholtz Zentrum München (Germany)*
 Edenir R. Pereira Filho, *Universidade Federal de São Carlos (Brazil)*
 Ronei Poppi, *University of Campinas (Brazil)*
 Åsmund Rinnan, *University of Copenhagen (Denmark)*
 Oxana Ye. Rodionova, *Semenov Institute of Chemical Physics (Russia)*
 Jean-Michel Roger, *IRSTEA, UMR ITAP (France)*
 Sarah C. Rutan, *Virginia Commonwealth University (USA)*
 Zhuoyong Zhang, *Capital Normal University (China)*

Committees

CAC Local Organizing Committee

Peter Wentzell (Dalhousie University) – Conference Chair
 Stephen Driscoll (Dalhousie University) – Web Management, A/V
 Jessica Nickerson (Dalhousie University) – Design/Communication/Registration
 Cannon Giglio (Dalhousie University)
 Danielle Spitzig (Dalhousie University)
 Chelsi Wicks (Dalhousie University)

Chris Brown (908 Devices) – Sponsorship
 Darren Andrews (Code the Solution) – Web Administration
 Anna de Juan (University of Barcelona) – Conference Planning
 Sarah Rutan (Virginia Commonwealth University) - Conference Planning

Chloe Wentzell - Volunteer
 Paige Fraser – Photographer
 Maynarhs da Koven - Consultant

Invited Speakers

Plenary Speakers

Rasmus Bro, *University of Copenhagen (Denmark)*
How to Utilize Machine Learning in Chemometrics

Steven D. Brown, *University of Delaware (USA)*
The Tao of Bruce: Bruce Kowalski and the Early Days of Chemometrics

Peter de B. Harrington, *Ohio University (USA)*
Cascading and Enhanced Restricted Boltzmann Machines for Feature Expansion of Spectra

Federico Marini, *University of Roma "La Sapienza" (Italy)*
PLS-DA: One, None, and a Hundred Thousand

Jean-Michel Roger, *IRSTEA (France)*
Orthogonal Projections in the Row and the Column Spaces

Keynote Speakers

Anna de Juan, *University of Barcelona (Spain)*
Data Fusion: What Else on Data Structures and Fusion Levels

Biao Huang, *University of Alberta (Canada)*
Advanced Data Analytics for Image Processing with Application in Oil-Water Interface Detection

Mohsen Kompany-Zareh, *Institute for Advanced Studies in Basic Sciences (Iran)*
Least Dependent Component Analysis: Miracle or Mirage

Marcelo Sena, *Federal University of Minas Gerais (Brazil)*
Combining Chemometrics and Paper Spray Mass Spectrometry for Forensic Analysis and Food Authenticity

Johan Westerhuis, *University of Amsterdam (The Netherlands)*
Variable Selection and Classification in the Presence of Observations Below the Detection Limit Using Error Rate p-Values

Elsevier Award Speaker

Joaquim Jaumot, *University of Barcelona (Spain)*
Chemometric Strategies for MS-Based Omics Data Analysis: From Chromatograms to Images

Invited Speakers

Liang Symposium Speakers

Philip Hopke, *Clarkson University (USA)*

Differential Probability Functions for Investigating Long-Term Changes in Local and Regional Air Pollution Sources

Hongmei Lu, *Central South University (China)*

Application of Chemometrics in Untargeted Metabolomics

Roma Tauler, *Institute of Environmental Assessment and Water Diagnostics (Spain)*


Characterization of Multivariate Curve Resolution Ambiguities

Beata Walczak, *University of Silesia (Poland)*

Working with log-Ratios

Hai-Long Wu, *Hunan University (China)*

Aspects of Recent Developments of Smart Multiway Calibration Methods in Analytical Chemistry



Analytica Chimica Acta and *Chemometrics and Intelligent Laboratory Systems* are proud to support the 2018 edition of CAC. You are invited to submit your manuscripts to either journal for publication.

Congratulations to Joaquim Jaumot for winning the 2018 *Chemometrics and Intelligent Laboratory Systems* Award.

You are invited to join the symposium to honor Prof. Liang, a former editor of *Chemometrics and Intelligent Laboratory Systems*.

General Information

Venue

The main conference activities will take place on the campus of Dalhousie University in Halifax, Nova Scotia. The location of the campus area relative to the conference hotels is shown below, with an expanded map on the following page.



- ① LORD NELSON HOTEL
- ② ATLANTICA HOTEL
- ③ HOWE HALL (CAMPUS RESIDENCE) – LUNCH ON THURSDAY, JUNE 28
- ④ LEMARCHANT PLACE (CAMPUS RESIDENCE)
- ⑤ MCCAIN ARTS AND SOCIAL SCIENCES BUILDING – ORAL SESSIONS
- ⑥ STUDENT UNION BUILDING – POSTER SESSIONS/LUNCH/BREAKS
- ⑦ DALHOUSIE ARTS CENTRE – OPENING RECEPTION
- ⑧ ROWE MANAGEMENT BUILDING – OPENING PLENARY LECTURE
- ⑨ BANK OF NOVA SCOTIA

General Information

Campus Map



Opening Reception

The Opening Reception will be held in the **Dalhousie Arts Centre Sculpture Court (7)** on Monday, June 26, 5:00-6:30 PM. Registration will be open and complimentary food and beverages will be provided.

The Opening Reception will be followed immediately by the Opening Plenary Lecture in the **Rowe Management Building Potter Auditorium (8)**.

Scientific Sessions

Oral presentations will be held in the Scotiabank Auditorium of the **McCain Arts and Social Sciences Building (5)**. Poster sessions, along with coffee breaks and lunches, will be in the McInnes Room of the **Student Union Building (6)**.

WiFi

On-campus wireless connection is provided through the **Dal-WPA2** and **eduroam** networks. You will be provided with an individual guest **NetID** and **password** in your registration package. These should be active June 23-30. Wired connection is not available unless you register your net address with the Computer Centre Help Desk (helpdesk@dal.ca).

Banquet Venue/Harbour Cruise

The Conference Banquet will be held at **Murphy's Restaurant** located on the Cable Wharf (1751 Lower Water Street). The banquet will be preceded by the Harbour Cruise, which will also depart from this location.

Guests should plan to be at the restaurant by 5:30 PM. The venue is within walking distance of the conference (~30 min) by proceeding down Spring Garden Road, turning left on Barrington Street and right at Duke Street. Bus #1 also follows this route (see below) up to Duke Street.



Public Transit

Conference attendees will be provided with **two bus passes** for Halifax Metro Transit, which are valid for regular routes and ferries (not including Airport). Regular fares (without pass) are \$2.50 (\$1.75 senior/child). More information on routes and fares can be found at www.halifax.ca/transportation/halifax-transit.

Financial/Medical Needs

ATMs are located in the Student Union Building (6) and the nearest bank is Scotiabank, located on the corner of Coburg and Robie (9). Emergency medical services are available at the Halifax Infirmary on Robie Street (see map) and a walk-in clinic is available opposite the bank on Robie Street.

Scientific Information

Oral Presentations

- Oral presentations (except PL-01) will take place in the Scotiabank Auditorium of the McCain Arts and Social Sciences Building.
- Duration of oral presentations (**including questions**):
 - Normal Oral Presentations: **15 min**
 - Plenary Lectures: **45 min**
 - Keynote Lectures: **30 min**
 - Liang Session: **20 min**
 - Flash Presentations: **3 min**
- All presenters **must remain in the allotted time** to keep the program on schedule. Session Chairs will be instructed to adhere to the schedule.
- All presenters are required to bring their presentation on a USB memory stick, which will be uploaded directly onto the Windows PC computer by the A/V assistant during a break prior to their session

Poster Presentations

- Poster presentations will take place in the McInnes Room of the Student Union Building.
- Dimensions of the display space are about 45 in x 45 in (114 cm x 114 cm). Posters may occupy more vertical space, but should not exceed the maximum width. Mounting hardware will be provided.
- Posters are not ordered by subject, but are assigned a number (e.g. P-01) and a colour code (see below) in the program. Posters should be mounted at the corresponding location as indicated by a label. Efforts have been made to co-locate posters by the same author.
- Posters will be available for viewing during all coffee breaks and lunches held in the McInnes Room. However, to allow poster authors freedom to leave their poster, they will only be expected to be present when their **colour code is "Active"**. The schedule of active posters is given on the following page and within the Scientific Program.
- Posters should be set up during or before the morning coffee break on Tuesday and taken down by the end of the morning coffee break on Friday.

Poster Schedule

Tuesday, June 26:

10:15-10:45 **YELLOW**
 12:30-13:00 **GREEN**
 13:00-13:30 **BLUE**
 15:00-15:30 **PINK**

Wednesday, June 27:

10:15-10:45 **GREEN, BLUE**
 12:45-13:15 **YELLOW**
 13:15-13:45 **PINK**

Publication

The *Journal of Chemometrics* will publish a special issue of the journal dedicated to CAC-2018. Conference participants are encouraged to submit their work to this issue for wider dissemination of research presented at the conference.

All submissions will be peer-reviewed. The deadline for submitted manuscripts is October 1, 2018. For more information, please consult the conference website.

Journal of
Chemometrics

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Program Schedule

	Monday	Tuesday	Wednesday	Thursday	Friday
8:30 AM		Opening Remarks	Keynote Lecture 3	Plenary Lecture 4	Plenary Lecture 5
8:45 AM	Morning Courses	Plenary Lecture 2	Oral Session E	Oral Session H	Oral Session K
9:15 AM		Oral Session A	Coffee Break	Coffee Break	Coffee Break
9:30 AM	Coffee Break	Coffee Break	Oral Session F	Oral Session I	Oral Session L
9:45 AM		Oral Session B	Plenary Lecture 3	Keynote Lecture 5	
10:00 AM	Lunch	Lunch	Lunch	Lunch	Closing Session
10:15 AM		Keynote Lecture 1	Keynote Lecture 4	Liang Symposium	
10:30 AM	Afternoon Courses	Oral Session C	Oral Session G	Coffee Break	
10:45 AM		Coffee Break	Flash Presentations (Awards)	Award Lecture	
11:00 AM		Keynote Lecture 2	Poster Mixer	Oral Session J	
11:15 AM		Oral Session D			
11:30 AM				Harbour Cruise	
11:45 AM				Banquet	
12:00 PM					
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4:30 PM	Opening Reception				
4:45 PM	Plenary Lecture 1				
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9:00 PM					

Scientific Program

MONDAY, JUNE 25: McCain Arts & Social Sciences Building
Dalhousie Arts Centre
Kenneth C. Rowe Management Building

08:00 REGISTRATION OPEN
McCAIN LOBBY

09:00-12:00 MORNING COURSES
McCAIN ARTS AND SOCIAL SCIENCES BUILDING

CR1A: Validation of Classification Models: Is your model right? And is it the right model?

Room: 2016

Instructor: Claudia Beleites (Chemometrics Consulting & Chemometrix GmbH)

CR2A: Advanced Preprocessing for Spectroscopic Applications

Room: 2017

Instructor: Neal Gallagher (Eigenvector Research Inc.)

CR3A: Analysis of Hyperspectral Data: How to maximise spatial and spectral information

Room: 2021

Instructors: Paolo Oliveri, Cristina Malegori (University of Genova)

CR6A: Chemometrics and Chromatography: Part 1

Room: 2190

Instructor: Sarah Rutan (Virginia Commonwealth University)

CR7A: Bayesian Statistics in Chemometrics: Why, when and how? (Part 1: Theory)

Room: 2198

Instructor: Gabriel Vivó-Truyols (Tecnometrix; University of Amsterdam)

Scientific Program: Monday, June 25

13:30-16:30	<p>AFTERNOON COURSES McCAIN ARTS AND SOCIAL SCIENCES BUILDING</p> <p>CR1P: Tools for Reproducible Research: Advanced Working Techniques in R and RStudio Room: 2016 Instructor: Claudia Beleites (Chemometrics Consulting & Chemometrix GmbH)</p> <p>CR3P: Advanced Approaches for One-class Modelling Room: 2021 Instructors: Paolo Oliveri, Cristina Malegori (University of Genova)</p> <p>CR6P: Chemometrics and Chromatography: Part 2 Room: 2190 Instructor: Sarah Rutan (Virginia Commonwealth University)</p> <p>CR7P: Bayesian Statistics in Chemometrics: Why, when and how? (Part 2: Applications) Room: 2198 Instructor: Gabriel Vivó-Truyols (Tecnometrix; University of Amsterdam)</p> <p>CR8P: ChemomeTRICKS Room: 2017 Instructor: Rasmus Bro (University of Copenhagen)</p>
17:00-18:30	<p>WELCOME RECEPTION SCULPTURE COURT, DALHOUSIE ARTS CENTRE REGISTRATION OPEN SPONSORED BY INFOMETRIX</p>
18:30-19:30	<p>OPENING PLENARY LECTURE POTTER AUDITORIUM, ROWE MANAGEMENT BUILDING PL-01: THE TAO OF BRUCE: BRUCE KOWALSKI AND THE EARLY DAYS OF CHEMOMETRICS Steven D. Brown (University of Delaware, USA) Chair: Peter Wentzell</p>

Scientific Program

TUESDAY, JUNE 26: McCain Arts & Social Sciences Building

08:00	<p>REGISTRATION OPEN McCAIN LOBBY</p>
08:30-09:00	<p>OPENING REMARKS SCOTIABANK AUDITORIUM</p>
09:00-09:45	<p>PLENARY LECTURE SCOTIABANK AUDITORIUM PL-02: PLS-DA: ONE, NONE AND A HUNDRED THOUSAND Federico Marini (University of Rome "La Sapienza", Italy) Chair: Paul Gemperline</p>
09:45-10:15	<p>ORAL SESSION A: CLASSIFICATION SCOTIABANK AUDITORIUM Chair: Paul Gemperline, East Carolina University</p>
09:45-10:00	<p>OA-01 SEMI-PARAMETRIC CLASSIFICATION OF FOREST-STRUCTURED GRAPHICAL MODELS <u>Cliff Spiegelman</u>¹, Mary Frances Dorn², Amit Moscovich³, Boaz Nadler⁴ ¹Texas A&M University, USA; ²Los Alamos National Labs, USA; ³Princeton University, USA; ⁴Weizmann Institute of Science, Israel</p>
10:00-10:15	<p>OA-02 ONLINE DISCRIMINATION OF CHEMICAL SUBSTANCES USING STANDOFF LASER INDUCED FLUORESCENCE SIGNALS <u>Marian Kraus</u>, Florian Gebert, Carsten Pargmann, Arne Walter, Frank Duschek German Aerospace Center, Institute of Technical Physics, Germany</p>
10:15-10:45	<p>COFFEE BREAK AND POSTER SESSION McINNES ROOM, STUDENT UNION BUILDING ACTIVE POSTERS: YELLOW (10:15:10:45)</p>

Scientific Program: Tuesday, June 26

10:45-12:15	<p>ORAL SESSION B: CLASSIFICATION AND FOOD ANALYSIS SCOTIABANK AUDITORIUM Chair: Neal Gallagher, Eigenvector Research</p>	12:15-13:30	<p>LUNCH AND POSTER SESSION McINNES ROOM, STUDENT UNION BUILDING SPONSORED BY CAMO ACTIVE POSTERS: GREEN (12:30-13:00) BLUE (13:00-13:30)</p>
10:45-11:00	<p>OB-01 FROM THE LAB TO THE FIELD: IDENTIFICATION OF NEW PSYCHOACTIVE SUBSTANCES (NPS) BY RAMAN SPECTROSCOPY AND CHEMOMETRICS <u>Jone Omar</u>, Boleslaw Slowikowski, Ana Boix European Commission, Directorate-General Joint Research Centre, Belgium</p>	13:30-14:00	<p>KEYNOTE LECTURE SCOTIABANK AUDITORIUM KL-01: ADVANCED DATA ANALYTICS APPROACHES FOR IMAGE PROCESSING WITH APPLICATION IN OIL-WATER INTERFACE DETECTION Biao Huang (University of Alberta, Canada) Chair: Cyril Ruckebusch</p>
11:00-11:15	<p>OB-02 ONE-CLASS RANDOM FOREST: AUTHENTICATION OF EVENING PRIMROSE OIL AND GROUND NUTMEG SAMPLES BY INFRARED SPECTROSCOPY <u>Felipe Bachion de Santana</u>¹, Waldomiro Borges Neto², Ronei J. Poppi¹ ¹University of Campinas, Brazil; ²Federal University of Uberlândia, Brazil</p>	14:00-15:00	<p>ORAL SESSION C: IMAGE ANALYSIS SCOTIABANK AUDITORIUM Chair: Cyril Ruckebusch, Université de Lille</p>
11:15-11:30	<p>OB-03 CHEMOMETRICS IN AUTHENTICATION OF VEGETABLE OILS <u>Liangxiao Zhang</u>^{1,3,5}, Zhe Yuan^{1,2}, Xinjing Dou^{1,2}, Peiwu Li^{1,3,4,5} ¹Chinese Academy of Agricultural Sciences, China; ²Key Laboratory of Biology and Genetic Improvement of Oil Crops, China; ³Laboratory of Quality and Safety Risk Assessment for Oilseed Products, China; ⁴Key Laboratory of Detection for Mycotoxins, China; ⁵Quality Inspection and Test Center for Oilseed Products, China</p>	14:00-14:15	<p>OC-01 WHEN HYPERSPECTRAL IMAGING MEETS TOPOLOGICAL DATA ANALYSIS <u>Ludovic Duponchel</u> Université de Lille, LASIR UMR CNRS, France</p>
11:30-11:45	<p>OB-04 IDENTIFICATION OF FRUITS WITH LEVELS OF THIABENDAZOLE ABOVE ALLOWED USING ONE-CLASS CLASSIFIERS AND SURFACE ENHANCED RAMAN SPECTROSCOPY <u>Carlos Alberto Teixeira</u>, Ronei Jesus Poppi State University of Campinas, Brazil</p>	14:15-14:30	<p>OC-02 ITERATIVE TARGET DETECTION FOR DETECTION AND CLASSIFICATION IN HYPERSPECTRAL IMAGES WITH AN APPLICATION TO A LANDSAT 8 IMAGE OF LAKE CHELAN, WA <u>Neal B Gallagher</u> Eigenvector Research, Inc., USA</p>
11:45-12:00	<p>OB-05 QUALITY ASSURANCE OF FOODS AND FUNCTIONAL INGREDIENTS USING QUANTITATIVE NMR METHODS AND CHEMOMETRICS <u>Fabrice Berrué</u>, Camilo Martinez-Farina, Ian Burton National Research Council of Canada, Canada</p>	14:30-14:45	<p>OC-03 IN SILICO INVESTIGATION INTO THE TARGETED ALGORITHMIC SEARCHING OF BIOMATERIAL SURFACE HETEROGENEITY <u>Ronan Dorrepaa</u>, Aoife Gowen University College Dublin, Ireland</p>
12:00-12:15	<p>OB-06 EXPERIMENTAL DESIGNS FOR SPECTROSCOPIC ASSESSMENT OF CACAO BEAN QUALITY <u>Claudia Beleites</u>^{1,2}, Fabian Tietz³, Sascha Rohn³, Andrea Krähmer¹ ¹Julius-Kühn-Institut, Germany; ²Chemometric Consulting and Chemometrix GmbH, Germany; ³University of Hamburg, Germany</p>	14:45-15:00	<p>OC-04 ANALYSIS OF STREET DRUGS USING NEAR INFRARED HYPERSPECTRAL IMAGING AND MULTIVARIATE CURVE RESOLUTION WITH ALTERNATING LEAST SQUARES (MCR-ALS) <u>William Francisco Cordeiro Dantas</u>¹, Larissa Elizabeth Cordeiro Dantas², Ronei Jesus Poppi¹ ¹University of Campinas, Brazil; ²Technical-Scientific Police Superintendence from Sao Paulo State, Brazil</p>

Scientific Program: Tuesday, June 26

- 15:00-15:30** **COFFEE BREAK AND POSTER SESSION**
McINNES ROOM, STUDENT UNION BUILDING
 ACTIVE POSTERS: **PINK** (15:00-15:30)
- 15:30-16:00** **KEYNOTE LECTURE**
SCOTIABANK AUDITORIUM
KL-02: VARIABLE SELECTION AND CLASSIFICATION IN THE
PRESENCE OF OBSERVATION BELOW THE DETECTION
LIMIT USING ERROR RATE P-VALUES
 Johan Westerhuis (University of Amsterdam, The Netherlands)
 Chair: Steven Brown
- 16:00-17:15** **ORAL SESSION D: VARIABLE SELECTION AND DATA**
PRE-PROCESSING
SCOTIABANK AUDITORIUM
 Chair: Steven Brown, University of Delaware
- 16:00-16:15** **OD-01** AUTOMATIC PRE-PROCESSING OF HYPERSPECTRAL
 IMAGES WITH A WAVELENGTH-SPECIFIC SHEARLET-BASED
 IMAGE NOISE REDUCTION METHOD
Puneet Mishra¹, Azam Karami², Alison Nordon¹, Douglas N. Rutledge³,
 Jean-Michel Roger⁴
¹University of Strathclyde, United Kingdom; ²Shahid Bahonar
 University of Kerman, Iran; ³AgroParisTech, INRA, Université Paris-
 Saclay, France; ⁴ITAP, Irstea, University Montpellier, France
- 16:15-16:30** **OD-02** SELECTIVE STANDARD NORMAL VARIATE
J-M. Roger¹, G. Rabatel¹, F. Marini², B. Walczack³
¹ITAP, Irstea Montpellier Centre, France; ²Univeristy of Rome "La
 Sapienza", Italy; ³Silesian University, Poland
- 16:30-16:45** **OD-03** CELL-WISE OUTLIER DIAGNOSTICS BASED ON
 PAIRWISE LOG-RATIOS
Jan Walach¹, Peter Filzmoser¹, Karel Hron², Stepan Kouril^{2,3}
¹TU Wien, Austria; ²Palacky University, Czech Republic; ³University
 Hospital Olomouc, Czech Republic
- 16:45-17:00** **OD-04** THE SIFT-MS FINGERPRINTING POWER FOR RAPID
 AUTHENTICATION OF EXTRA VIRGIN ARGAN OIL
Mourad Kharbach^{1,2}, Mohammed Alaoui Mansouri², Joeri Vercammen³,
 Abdelaziz Bouklouze², Yvan Vander Heyden¹
¹Vrije Universiteit Brussel (VUB), Belgium; ²University Mohammed V-
 Rabat, Morocco; ³Interscience, Belgium
- 17:00-17:15** **OD-05** BEER'S LINGUISTICS AND CHEMISTRY: AN
 INVESTIGATION
Nicola Cavallini^{1,2}, Rasmus Bro², Francesco Savorani³, Marina Cocchi¹
¹Università di Modena e Reggio Emilia, Italy; ²University of
 Copenhagen, Denmark; ³Politecnico di Torino, Italy

Scientific Program

WEDNESDAY, JUNE 27: McCain Arts & Social Sciences Building

08:30-09:00	<p>KEYNOTE LECTURE SCOTIABANK AUDITORIUM</p> <p>KL-03: LEAST DEPENDENT COMPONENTS ANALYSIS: MIRACLE OR MIRAGE</p> <p>Mohsen Kompany-Zareh (Institute for Advanced Studies in Basic Sciences, Iran and Dalhousie University, Canada) Chair: Sarah Rutan</p>	10:00-10:15	<p>OE-05 CONSTRAINTS OF MCR-ALS ON ANALYSIS OF HYPERSPECTRAL IMAGING BASED ON DIFFERENT SPECTROSCOPY</p> <p><u>Xin Zhang</u>, Zhuoyong Zhang Capital Normal University, China</p>
09:00-10:15	<p>ORAL SESSION E: MULTIVARIATE CURVE RESOLUTION SCOTIABANK AUDITORIUM</p> <p>Chair: Sarah Rutan, Virginia Commonwealth University</p>	10:15-10:45	<p>COFFEE BREAK AND POSTER SESSION McINNES ROOM, STUDENT UNION BUILDING</p> <p>ACTIVE POSTERS: GREEN, BLUE (10:15-10:45)</p>
09:00-09:15	<p>OE-01 SOFT CONSTRAINTS FOR IMPROVING THE QUANTITATIVE PERFORMANCE OF MULTIVARIATE CURVE RESOLUTION METHODS</p> <p><u>Paul J. Gemperline</u>¹, Mahsa Akbari Lakeh², Elnaz Tavakkoli², Hamid Abdollahi²</p> <p>¹East Carolina University, USA; ²Institute for Advanced Studies in Basic Sciences, Iran</p>	10:45-11:45	<p>ORAL SESSION F: CURVE RESOLUTION AND MULTI-WAY METHODS SCOTIABANK AUDITORIUM</p> <p>Chair: Philip Hopke, Clarkson University</p>
09:15-09:30	<p>OE-02 PEAK GROUP ANALYSIS: AN EXPLORATIVE TOOL IN FACPAC FOR THE ANALYSIS OF MULTIVARIATE DATA</p> <p><u>Henning Schröder</u>¹, Mathias Sawall¹, Denise Meinhardt^{1,2}, Klaus Neymeyr^{1,2}</p> <p>¹University of Rostock, Germany; ²Leibniz-Institute for Catalysis, Germany</p>	10:45-11:00	<p>OF-01 VISUALIZING THE RESOLUTION THEOREMS AND APPLICATION OF THE CORRESPONDENCE CONSTRAINT IN BILINEAR DECOMPOSITION OF MULTI-SET CHEMICAL DATA</p> <p><u>Masoumeh Alinaghi</u>, Hamid Abdollahi Institute for Advanced Studies in Basic Sciences, Iran</p>
09:30-09:45	<p>OE-03 IMAGE PROCESSING CONSTRAINTS IN MCR-ALS. NICE IMAGES, BETTER RESOLUTION?</p> <p><u>Siewert Hugelier</u>¹, Dario Cevoli¹, Raffaele Vitale^{1,2}, Cyril Ruckebusch¹</p> <p>¹Université de Lille, LASIR, France; ²KU Leuven, Belgium</p>	11:00-11:15	<p>OF-02 LOG-LINEAR MULTIVARIATE CURVE RESOLUTION</p> <p><u>Paul H. C. Eilers</u></p> <p>Erasmus University Medical Centre, The Netherlands</p>
09:45-10:00	<p>OE-04 A GENERALIZED CONSTRAINT FOR ACHIEVING THE UNIQUE SOLUTION IN SELF MODELING CURVE RESOLUTION METHODS BASED ON DUALITY PRINCIPLE</p> <p><u>Hamid Abdollahi</u>¹, Robert Rajko², Elnaz Tavakkoli¹, Mahsa Akbari Lakeh¹, Mahdiyeh Ghaffari¹, Nematollah Omidikia¹, Saeed Khalili¹</p> <p>¹Institute for Advanced Studies in Basic Sciences, Iran; ²University of Szeged, Hungary</p>	11:15-11:30	<p>OF-03 MULTILINEAR RESOLUTION OF ADVANCED FLUORESCENCE IMAGING DATA</p> <p><u>C. Ruckebusch</u>, S. Hugelier, T. Do, M. Sliwa Université de Lille LASIR CNRS, France</p>
		11:30-11:45	<p>OF-04 DISTRIBUTION OF FLUOROPHORES IN ARCTIC SEAS DETERMINED BY PARAFAC DECOMPOSITION OF EXCITATION-EMISSION FLUORESCENCE SPECTRA OF SEAWATER</p> <p><u>Ivan Krylov</u>^{1*}, Anastasia Drozdova², Timur Labutin¹</p> <p>¹Lomonosov Moscow State University, Russia; ²Shirshov Institute of Oceanology, Russian Academy of Sciences, Russia (*WSC-2018 Poster Awardee)</p>

Scientific Program: Wednesday, June 27

11:45-12:30	<p>PLENARY LECTURE SCOTIABANK AUDITORIUM</p> <p>PL-03: CASCADING AND ENHANCED RESTRICTED BOLTZMANN MACHINES FOR FEATURE EXPANSION OF SPECTRA</p> <p>Peter de Boves Harrington (Ohio University, USA) Chair: Philip Hopke</p>	14:45-15:00	<p>OG-03 FUSION OF MULTIREOLUTION HYPERSPECTRAL AND FLUORESCENCE IMAGES FOR THE ANALYSIS OF SEDIMENT CORES</p> <p><u>Kévin Jacq</u>^{1,2}, Didier Coquin², Bernard Fanget¹, Yves Perrette¹, Pierre Sabatier¹, Fabien Arnaud¹, Ruth Martinez-Lamas^{3,4}, Maxime Debret³</p> <p>¹Université Grenoble Alpes, Université Savoie Mont Blanc, CNRS, France; ²Université Grenoble Alpes, Université Savoie Mont Blanc, Polytech Annecy-Chambéry, LISTIC, France; ³Normandie Université, UNIROUEN, UNICAEN, CNRS, France; ⁴IFREMER, Laboratory Géodynamique et Enregistrement Sédimentaire (LGS), France</p>
12:30-13:45	<p>LUNCH AND POSTER SESSION McINNES ROOM, STUDENT UNION BUILDING</p> <p>SPONSORED BY CAMO</p> <p>ACTIVE POSTERS: YELLOW (12:45-13:15) PINK (13:15-13:45)</p>	15:00-15:15	<p>OG-04 VARIETAL ORIGIN DISCRIMINATION OF THREE TUNISIAN VIRGIN OLIVE OILS BY MULTIBLOCK PARTIAL LEAST SQUARES - DISCRIMINANT ANALYSIS</p> <p><u>Astrid Maléchaux</u>¹, Rabia Korifi¹, Sonda Laroussi^{1,2}, Yveline Le Dréau¹, Jacques Artaud¹, Nathalie Dupuy¹</p> <p>¹Aix-Marseille Université, Université d'Avignon, CNRS, IRD, IMBE, France; ²Institut de l'Olivier, Unité Qualité et Technologie, Tunisia</p>
13:45-14:15	<p>KEYNOTE LECTURE SCOTIABANK AUDITORIUM</p> <p>KL-04: DATA FUSION: WHAT ELSE ON DATA STRUCTURES AND FUSION LEVELS?</p> <p>Anna de Juan (Universitat de Barcelona, Spain) Chair: Rasmus Bro</p>	15:15-15:30	<p>FLASH PRESENTATIONS SCOTIABANK AUDITORIUM</p> <p>Chair: Rasmus Bro</p>
14:15-15:30	<p>ORAL SESSION G: DATA FUSION SCOTIABANK AUDITORIUM</p> <p>Chair: Rasmus Bro, University of Copenhagen</p>		<p>FL-01 DATA FUSION FOR HYPERSPECTRAL IMAGING: A SCHEME FOR FUSING SPECTRAL AND TEXTURAL INFORMATION TO IMPROVE CLASSIFICATION MAPS (Poster: P-07)</p> <p><u>Puneet Mishra</u>¹, Alison Nordon², Mohd Shahrime Mohd Asaari²</p> <p>¹University of Strathclyde, United Kingdom; ²University of Antwerp, Belgium</p>
14:15-14:30	<p>OG-01 FUSED ADJACENCY MATRICES IN EXPLORATIVE DATA FUSION CONTEXT</p> <p><u>Marina Cocchi</u>¹, Nicola Cavallini^{1,2}, Caterina Durante³, Mario Li Vigni³, Rasmus Bro²</p> <p>¹Università di Modena e Reggio Emilia, Italy; ²University of Copenhagen, Denmark; ³ChemSTAMP s.r.l., Italy</p>		<p>FL-02 CHEMOMETRIC ANALYSIS OF FULL SCAN MASS SPECTRA COLLECTED FROM A MOBILE LAB WITH APPLICATION TO SOURCE IDENTIFICATION OF OUTDOOR AND INDOOR AIR CONTAMINANTS (Poster: P-20)</p> <p><u>Larissa C. Richards</u>^{1,2}, Nicholas G. Davey², Chris G. Gill^{1,2}, Erik T. Krogh^{1,2}</p> <p>¹University of Victoria, Canada; ²Vancouver Island University, Canada</p>
14:30-14:45	<p>OG-02 SO-CovSel, A NEW METHOD FOR VARIABLE SELECTION IN MULTI-BLOCK DATA</p> <p><u>Alessandra Biancolillo</u>¹, Federico Marini¹, Jean-Michel Roger²</p> <p>¹University of Rome "La Sapienza", Italy; ²ITAP, Irstea, Montpellier SupAgro, France</p>		<p>FL-03 CHARACTERIZATION OF SPATIAL VARIABILITY IN HYPERSPECTRAL IMAGES USING VARIOGRAM COMBINED WITH PCA (Poster: P-28)</p> <p><u>Jun-Li Xu</u>, Da-Wen Sun, Aoife A. Gowen University College Dublin, Ireland</p>

Scientific Program: Wednesday, June 27

FL-04 MULTIMODAL OPTICAL SPECTROSCOPY AND MULTIVARIATE DATA ANALYSIS FOR THE DEMARCATION OF HUMAN BRAIN TUMORS (Poster: **P-44**)

Mona Stefanakis, Edwin Ostertag, Anita Lorenz, Marc Brecht, Karsten Rebner

Reutlingen University, Germany

FL-05 PIXEL-BASED CHEMOMETRIC ANALYSIS OF LC-MS ANALYZED SAMPLES FROM AN INDUSTRIAL ENZYME PRODUCTION: CHARACTERIZATION OF DIFFERENT PRODUCTS AND INVESTIGATING IF THERE IS A LINK BETWEEN THE SMALL MOLECULE FINGERPRINT AND PRODUCT QUALITY? (Poster: **P-54**)

Sofie B. Knudsen^{1,2}, Nikoline J. Nielsen¹, Johan Qvist², Kim B. Andersen², Jan H. Christensen¹

¹University of Copenhagen, Denmark; ²Novozymes A/S, Denmark

15:30-17:30 **POSTER MIXER AND AWARD SESSION**
McINNES ROOM, STUDENT UNION BUILDING

15:45-16:15 **PRESENTATION OF AWARDS**

2018 Chemometrics and Intelligent Laboratory Systems Award to Joaquim Jaumot

Sponsored by Elsevier

Chair: Roma Tauler

2018 CAC Chemometrics Lifetime Achievement Award

Sponsored by CAC-2018

Chair: Lutgarde Buydens

16:15-17:30 **POSTER PRESENTATIONS AND SOCIAL HOUR**
SPONSORED BY 908 DEVICES

17:00 **CAC PERMANENT COMMITTEE MEETING**
Boardroom A

Scientific Program

THURSDAY, JUNE 28: McCain Arts & Social Sciences Building

08:30-9:15 **PLENARY LECTURE**
SCOTIABANK AUDITORIUM

PL-04: ORTHOGONAL PROJECTIONS IN THE ROW AND THE COLUMN SPACES

Jean-Michel Roger (ITAP, Irstea Montpellier Centre, France)

Chair: Geert Postma

09:15-10:15 **ORAL SESSION H: MULTIVARIATE CALIBRATION: THEORY**
SCOTIABANK AUDITORIUM

Chair: Geert Postma, Radboud University

09:15-09:30 **OH-01 INTERPRETATION OF PLS MODELS**

Åsmund Rinnan¹, José Camacho², Rasmus Bro¹

¹University of Copenhagen, Denmark; ²University of Granada, Spain

09:30-09:45 **OH-02 EXPLORING THE RESIDUAL SPACE WHEN INVERTING A PLS MODEL**

S. Ruiz, M.C. Ortiz, L.A. Sarabia, M.S. Sánchez

Universidad de Burgos, Spain

09:45-10:00 **OH-03 A NOVEL NONLINEAR PLS ALGORITHM TO CALCULATE ROBUST AND SIMPLE PREDICTIVE MODELS**

Francis B. Lavoie¹, Koji Muteki², Ryan Gosselin¹

¹Université de Sherbrooke, Canada; ²Pfizer Worldwide Research and Development, USA

10:00-10:15 **OH-04 TRANSDUCTIVE CALIBRATION UPDATING**

Erik Andries¹, John H. Kalivas², Anit Gurung²

¹Central New Mexico Community College, USA; ²Idaho State University, USA

10:15-10:45 **COFFEE BREAK AND POSTER SESSION**
McINNES ROOM, STUDENT UNION BUILDING

Scientific Program: Thursday, June 28

10:45-11:30	<p>ORAL SESSION I: MULTIVARIATE CALIBRATION: APPLICATIONS SCOTIABANK AUDITORIUM Chair: Ronei Poppi, University of Campinas</p>	13:15-15:00	<p>SYMPOSIUM IN HONOUR OF YI-ZENG LIANG SCOTIABANK AUDITORIUM Chair: Peter Wentzell</p>
10:45-11:00	<p>OI-01 IMPROVEMENT OF NIR CALIBRATION MODELS AND THEIR VALUE FOR ANIMAL FOOD PRODUCERS <u>Mark Schoot</u>^{1,2}, Christiaan Kapper¹, Gijs van Kessel³, Jeroen Jansen² ¹Nutricontrol, The Netherlands; ²Radboud University, The Netherlands; ³Agrifirm Innovations Center, The Netherlands</p>	13:15-13:20	<p>OPENING REMARKS Peter Wentzell</p>
11:00-11:15	<p>OI-02 DETERMINING OXIDE LAYER THICKNESSES ON TECHNICAL COPPER BY PLS WITH OVERLAYED INTERFERENCE AND ABSORBANCE UV-VIS SPECTRA AND AES DEPTH PROFILES <u>Jan Stiedl</u>^{1,2,3}, Simon Green³, Thomas Chassé², Karsten Rebner¹ ¹Reutlingen University, Germany; ²University of Tuebingen, Germany; ³Robert Bosch GmbH, Automotive Electronics, Germany</p>	13:20-13:40	<p>YL-01 CHARACTERIZATION OF MULTIVARIATE CURVE RESOLUTION ROTATION AMBIGUITIES <u>Roma Tauler</u> Institute of Environmental Assessment and Water Diagnostic (IDEA-CSIC), Spain</p>
11:15-11:30	<p>OI-03 EXAMINING SOURCES OF VARIATION IN MID-IR SPECTROSCOPY OF LIQUID MILK <u>M.K. Nieuwoudt</u>^{1,2,4}, S.E. Holroyd³, C.M. McGovern^{1,4}, C.M. Triggs¹, M.C. Simpson^{1,2,4} ¹The University of Auckland, New Zealand; ²The MacDiarmid Institute for Advanced Materials and Nanotechnology, New Zealand; ³Fonterra Research & Development Centre, New Zealand; ⁴Dodd-Walls Centre for Photonics and Quantum Technologies, New Zealand</p>	13:40-14:00	<p>YL-02 APPLICATION OF CHEMOMETRICS IN UNTARGETED METABOLOMICS <u>Hongmei Lu</u>, Zhimin Zhang, Hongchao Ji, Pan Ma Central South University, China</p>
11:30-12:00	<p>KEYNOTE LECTURE SCOTIABANK AUDITORIUM KL-05: COMBINING CHEMOMETRICS AND PAPER SPRAY MASS SPECTROMETRY FOR FORENSIC ANALYSIS AND FOOD AUTHENTICITY Marcelo M. Sena (Universidade Federal de Minas Gerais and Instituto Nacional de Ciência e Tecnologia em Bioanalítica, Brazil) Chair: Ronei Poppi</p>	14:00-14:20	<p>YL-03 DIFFERENTIAL PROBABILITY FUNCTIONS FOR INVESTIGATING LONG-TERM CHANGES IN LOCAL AND REGIONAL AIR POLLUTION SOURCES <u>Phillip K. Hopke</u>^{1,2}, Mauro Masiol¹, Stefania Squizzato¹, Meng-Dawn Cheng³ ¹University of Rochester Medical Center, USA; ²Clarkson University, USA; ³Oak Ridge National Laboratory, USA</p>
12:00-13:15	<p>LUNCH HOWE HALL DINING ROOM</p> <p>POSTER AWARD COMMITTEE MEETING, McINNES ROOM</p>	14:20-14:40	<p>YL-04 WORKING WITH LOG-RATIOS <u>Beata Walczak</u>, Zuzanna Mayjurek University of Silesia, Poland</p>
		14:40-15:00	<p>YL-05 ASPECTS OF RECENT DEVELOPMENTS OF SMART MULTIWAY CALIBRATION METHODS IN ANALYTICAL CHEMISTRY <u>Hai-Long Wu</u> and Ru-Qin Yu Hunan University, China</p>
		15:00-15:30	<p>COFFEE BREAK AND POSTER SESSION McINNES ROOM, STUDENT UNION BUILDING</p>

Scientific Program: Thursday, June 28

- 15:30-16:00** **KEYNOTE LECTURE/AWARD LECTURE**
SCOTIABANK AUDITORIUM
KL-06: CHEMOMETRIC STRATEGIES FOR MS-BASED OMICS
DATA ANALYSIS: FROM CHROMATOGRAMS TO IMAGES
 Joaquim Jaumot (Institute of Environmental Assessment and Water Research – IDAEA, Spain)
 Chair: Beata Walczak
- 16:00-16:30** **ORAL SESSION J: SEPARATIONS**
SCOTIABANK AUDITORIUM
 Chair: Beata Walczak, University of Silesia
- 16:00-16:15** **OJ-01** A NOVEL NON-TARGETED APPROACH UTILISING
 SUPERVISED MACHINE LEARNING TO FIND KEY FEATURES
 FROM GC-MS RAW DATA
Kimmo Sirén, Ulrich Fischer, Jochen Vestner
 DLR Rheinpfalz, Institute for Viticulture and Oenology, Germany
- 16:15-16:30** **OJ-02** ON THE USE OF BAYESIAN STATISTICS FOR (BIG) DATA
 ANALYSIS
Gabriel Vivo-Truyols^{1,2}
¹Tecnometrix, Spain; ²University of Amsterdam, The Netherlands
- 17:30-19:30** **HARBOUR CRUISE**
Murphy's Restaurant at Cable Wharf (Boarding 17:45)
1751 Lower Water Street
SPONSORED BY EIGENVECTOR RESEARCH INC.
- 19:30** **CONFERENCE BANQUET**
Murphy's Restaurant at Cable Wharf
1751 Lower Water Street

Scientific Program

FRIDAY, JUNE 29: McCain Arts & Social Sciences Building

- 08:30-9:15** **PLENARY LECTURE**
SCOTIABANK AUDITORIUM
PL-05: HOW TO UTILIZE MACHINE LEARNING IN
CHEMOMETRICS
 Rasmus Bro (University of Copenhagen, Denmark)
 Chair: Johan Westerhuis
- 09:15-10:15** **ORAL SESSION K: APPLICATIONS IN HEALTH/MEDICINE**
SCOTIABANK AUDITORIUM
 Chair: Johan Westerhuis, University of Amsterdam
- 09:15-09:30** **OK-01** MULTIVARIATE ANALYSIS APPLIED TO MULTICOLOUR
 FLOW CYTOMETRY TO DETECT RARE CELL POPULATIONS
Geert Postma¹, Rita Folcarelli¹, Selma van Staveren^{2,3}, Gerjen
 Tinnevelt^{1,2}, Lutgarde Buydens¹, Leo Koenderman², Jeroen Jansen¹
¹Radboud University, The Netherlands; ²TI-COAST, The Netherlands;
³University Medical Center Utrecht, The Netherlands
- 09:30-09:45** **OK-02** EXPLAINING POSSIBLE RELATIONS BETWEEN
 MICROBIAL OTUS AND METABOLOME IN THE COMPLEX GUT -
 DIFFERENT STUDIES
Marianna Lucio¹, Tanja V. Maier¹, Alesia Walker¹, Dirk Haller², Janet
 Jansson^{3,4,5,6}, Philippe Schmitt-Kopplin^{1,2}
¹Helmholtz Zentrum München – Deutsches Forschungszentrum für
 Gesundheit und Umwelt GmbH, Germany; ²Technische Universität
 München, Germany; ³Pacific Northwest National Laboratory, USA;
⁴DOE Joint Bioenergy Institute, USA; ⁵University of California,
 Berkeley, USA; ⁶University of Copenhagen, Denmark
- 09:45-10:00** **OK-03** A NOVEL UNBIASED METHOD LINKS VARIABILITY OF
 CO-EXPRESSION BETWEEN MULTIPLE MARKERS ON SINGLE
 CELLS TO A CLINICAL PHENOTYPE
Gerjen H. Tinnevelt^{1,2}, Selma van Staveren^{2,3}, Kristiaan Wouters⁴, Bart
 Hilvering³, Rita Folcarelli¹, Leo Koenderman³, Lutgarde M.C. Buydens¹,
 Jeroen J. Jansen¹
¹Radboud University, The Netherlands; ²TI-COAST, The Netherlands;
³University Medical Center Utrecht, The Netherlands; ⁴Laboratory of
 Metabolism and Vascular Medicine, Maastricht, The Netherlands

Scientific Program: Friday, June 29

10:00-10:15	OK-04 OPTICAL MAPPING FOR DNA SUBSEQUENCE IDENTIFICATION: CONVOLUTING AND CROSS-CORRELATING VS LOCALIZING AND MATCHING <u>Raffaele Vitale</u> ^{1,2} , Arno Bouwens ^{2,3} , Jochem Deen ³ , Siewert Hugelier ¹ , Laurens D'Huys ² , Kris Janssen ² , Johan Hofkens ² , Cyril Ruckebusch ¹ ¹ Université de Lille, France; ² Katholieke Universiteit Leuven, Belgium; ³ Ecole Polytechnique Fédérale de Lausanne, Switzerland	11:45-12:00	OL-05 A SCORING METRIC FOR MULTIVARIATE DATA FOR PROFICIENCY TESTING IN VEHICLE EMISSIONS USING UNIVARIATE AND MULTIVARIATE METHODS <u>Werickson Fortunato de Carvalho Rocha</u> ¹ , Paulo Roque Martins Silva ¹ , Luiz Henrique da Conceição Leal ¹ , Valnei Smarçaro da Cunha ¹ , David A. Sheen ² ¹ National Institute of Metrology, Quality and Technology (INMETRO), Brazil; ² National Institute of Standards and Technology (NIST), USA
10:15-10:45	COFFEE BREAK AND POSTER REMOVAL McINNES ROOM, STUDENT UNION BUILDING	12:00-12:30	CLOSING SESSION SCOTIABANK AUDITORIUM Chair: Lutgarde Buydens POSTER AWARDS ANNOUNCEMENT OF NEXT CAC HOST
10:45-12:00	ORAL SESSION L: PROCESS ANALYSIS/CONTROL SCOTIABANK AUDITORIUM Chair: Lutgarde Buydens, Radboud University		
10:45-11:00	OL-01 EARLY DETECTION OF UNDESIRABLE DEVIATIONS IN MUST FERMENTATION BY USING FTIR-ATR SPECTROSCOPY AND MULTIVARIATE ANALYSIS <u>Ricard Boqué</u> ¹ , Julieta Cavaglia ¹ , Barbara Giussani ² , Olga Busto ¹ , Miquel Puxeu ³ , Montserrat Mestres ¹ ¹ Universitat Rovira i Virgili, Spain; ² Università degli Studi dell'Insubria, Italy; ³ VITEC, The Technology Park for the Wine Industry, Spain		
11:00-11:15	OL-02 COMPARING DIMENSION REDUCTION AND VARIABLE SELECTION-BASED METHODS FOR FAULT DIAGNOSIS IN HIGH DIMENSIONAL DATA <u>M. Koeman</u> ¹ , J. Engel ^{1,2} , J. Jansen ¹ and L. Buydens ¹ ¹ Radboud University, The Netherlands; ² Biometris, Wageningen UR, The Netherlands		
11:15-11:30	OL-03 "ALIGNMENT-FREE" MULTIVARIATE STATISTICAL PROCESS CONTROL FOR ONLINE MONITORING OF BATCH EVOLUTION <u>R.R. de Oliveira</u> ¹ , C. Avila ² , F. Mahdi ² , F. Muller ² , W. Sinclair ³ , A. de Juan ¹ ¹ Universitat de Barcelona, Spain; ² University of Leeds, United Kingdom; GlaxoSmithKline, United Kingdom		
11:30-11:45	OL-04 UNDERSTANDING CHEMICAL PROCESSES THROUGH PLS-PATH MODELS <u>Geert van Kollenburg</u> ¹ , Heleen Lanter ^{1,2} , Jeroen Jansen ² ¹ Radboud University, Netherlands; ² University of Applied Sciences Utrecht, Netherlands		

Poster Sessions

Posters will be available for viewing during all coffee breaks and lunches held in the McInnes Room of the Student Union Building. Posters are colour-coded to coordinate viewing with the presenting author.

Poster presenters are requested to be near their posters for discussion when the corresponding color code is designated as "ACTIVE" in the Scientific Program.

Tuesday, June 26:

10:15-10:45 **YELLOW**
 12:30-13:00 **GREEN**
 13:00-13:30 **BLUE**
 15:00-15:30 **PINK**

Wednesday, June 27:

10:15-10:45 **GREEN, BLUE**
 12:45-13:15 **YELLOW**
 13:15-13:45 **PINK**
 15:45-17:30 **POSTER SOCIAL EVENT**

Thursday, June 28:

10:15-10:45 **OPEN VIEWING**
 12:00-13:15 **NO POSTER VIEWING – LUNCH AT HOWE HALL**

Friday, June 29:

10:15-10:45 **POSTER REMOVAL**

Posters

P-01 Group: **GREEN**
 SOIL TEXTURE ANALYSIS USING COMPUTER VISION AND IMAGE PROCESSING
Anselmo E. de Oliveira¹, Pedro A. de O. Morais¹, Diego M. de Souza², Beata E. Madari²
¹Instituto de Química, UFG, Brazil; ²Embrapa Arroz e Feijão, Brazil

P-02 **GREEN**
 SOIL ORGANIC CARBON CONTENTS USING MULTIVARIATE IMAGE ANALYSIS
Anselmo E. de Oliveira¹, Pedro A. de O. Morais¹, Diego M. de Souza², Beata E. Madari², Anderson da S. Soares³
¹Instituto de Química, UFG, Brazil; ²Embrapa Arroz e Feijão, Brazil; ³Institute of Informatics, UFG, Brazil

P-03 **YELLOW**
 A MID-LEVEL DATA FUSION APPROACH FOR A SPECTROSCOPIC CHARACTERIZATION AND CLASSIFICATION OF PDO WINE VINEGARS
Rocío Ríos-Reina¹, Raquel M Callejón¹, Francesco Savorani^{2,3}, Jose M Amigo³, Marina Cocchi⁴
¹Universidad de Sevilla, Spain; ²Polytechnic University of Turin, Italy; ³University of Copenhagen, Denmark; ⁴Università di Modena e Reggio Emilia, Italy

P-04 **BLUE**
 AN ALTERNATIVE SIGNAL-CONSERVATIVE APPROACH FOR RAYLEIGH AND RAMAN SCATTER CORRECTION IN FLUORESCENCE LANDSCAPES
S. Azcárate, F.A. Chiappini, M.R. Alcaráz, H.C. Goicoechea
 Universidad Nacional del Litoral-CONICET, Argentina

P-05 Group: **BLUE**
 THREE-WAY DATA MODELLING ADVANTAGES TO SOLVE CLASSIFICATION ISSUES
Silvana M. Azcarate^{1,4}, Adriano de Araújo Gomes², José M. Camiña^{1,4} and Héctor C. Goicoechea^{3,4}
¹Universidad Nacional de La Pampa, and Instituto de Ciencias de la Tierra y Ambientales de La Pampa (INCITAP), Argentina; ²Universidade Federal do Sul e Sudoeste do Pará, Brazil; ³Universidad Nacional del Litoral, Argentina; ⁴Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Argentina

P-06 **PINK**
 SURFACTANT COMPOSITION ANALYSIS USING NIR SPECTROSCOPY: QUANTIFICATION OF MINOR IMPURITIES DURING CONTINUOUS SULFATION PROCESSES
S.E. Cunliffe^{1,2}, M.R. Baker², O. Mihailova², P.A. Martin¹, P.J. Martin¹
¹The University of Manchester, UK; ²Unilever Research and Development, UK

P-07 **GREEN**
 VALIDATION OF A METHODOLOGY FOR QUANTIFICATION OF SOIL ORGANIC MATTER USING A LARGE SPECTRA LIBRARY BY VISIBLE-NEAR INFRARED SPECTROSCOPY AND RANDOM FOREST
Felipe Bachion de Santana¹, André Marcelo de Souza², Ronei J. Poppi¹
¹University of Campinas, Brazil; ²Brazilian Agricultural Research Corporation (Embrapa Soils), Brazil

Posters

P-08 **YELLOW**

DATA FUSION FOR HYPERSPECTRAL IMAGING: A SCHEME FOR FUSING SPECTRAL AND TEXTURAL INFORMATION TO IMPROVE CLASSIFICATION MAPS
Puneet Mishra¹, Alison Nordon² and Mohd Shahrimie Mohd Asaari²

¹University of Strathclyde, United Kingdom; ²University of Antwerp, Belgium

P-09 Group: **BLUE**

ANALYSIS OF THE OXIDATION STATE OF COPPER OXIDES ON TECHNICAL SURFACES BY MCR USING UV-VIS AND AES SPECTRA

Jan Stiedl^{1,2,3}, Simon Green³, Thomas Chassé², Karsten Rebner¹

¹Reutlingen University, Germany; ²University of Tuebingen, Germany; ³Robert Bosch GmbH, Germany

P-10 **PINK**

APPLICATIONS OF CHEMOMETRICS IN PRECISION MEDICINE

Yingyi Hao¹, Yi Ran², Yu Liang¹, Yuan Liu¹, Fanfan Xie¹, Menglong Li¹, Zhining Wen¹, Li He²

¹Sichuan University, China; ²Biogas Institute of Ministry of Agriculture, China

P-11 **GREEN**

VARIABLE SELECTION AND DIMENSION REDUCTION APPLIED TO THE VARIETAL DISCRIMINATION OF EXTRA VIRGIN OLIVE OILS USING MIR, NIR AND RAMAN SPECTROSCOPIES

Astrid Maléchaux, Yveline Le Dréau, Pierre Vanloot, Nathalie Dupuy

Aix Marseille Univ, Univ Avignon, CNRS, IRD, IMBE, Marseille, France

P-12 **YELLOW**

MULTICHANNEL SENSORS BASED ON CHEMOMETRICS FOR COLORIMETRIC ANALYSIS OF METAL IONS AND METAL OXYANIONS

Zhuoyong Zhang, Xin Zhang, Lijuan Huang

Capital Normal University, China

P-13 **BLUE**

PROJECTION OF MCR-ALS AND MCR-BANDS SOLUTIONS ON THE AREA OF FEASIBLE SOLUTIONS

Xin Zhang¹, Zhuoyong Zhang¹, Roma Tauler²

¹Capital Normal University, China; ²Institute of Environmental Assessment and Water Diagnostic (IDEA-CSIC), Spain

P-14 **PINK**

HANDLING THE QUENCHING EFFECT IN THE DETERMINATION OF MIXTURES OF FOOD COLORANTS BY MEANS OF EXCITATION-EMISSION FLUORESCENCE DATA AND PARAFAC

L. Rubio, S. Sanllorente, L.A. Sarabia, M.C. Ortiz

University of Burgos, Spain

P-15 **GREEN**

CALIBRATION TRANSFER BETWEEN A FLUORIMETER BASED ON LIGHT-EMITTING DIODE AND OTHER WITH PULSED HIGH-PRESSURE XENON SOURCE

S. Sanllorente, L. Rubio, M.C. Ortiz, L.A. Sarabia

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P-16 Group: **YELLOW**

RAPID DISCRIMINATION OF FRAGRANCE CONTAMINATED WITH ALLERGENIC SUBSTANCE BY RAMAN SPECTROSCOPY AND CHEMOMETRICS METHODS

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P-17 **BLUE**

SUCCESSIVE SELECTION OF LEAST DEPENDENT VARIABLES IN SPECTROSCOPIC CLASSIFICATION AND QUANTIFICATION

Mohsen Kompany-Zareh^{1,2}, Wrya Farrokhi-Kurd², Saeed Bagheri², Peter Wentzell¹

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P-18 **BLUE**

PARTICLE SWARM OPTIMIZATION BASED DIAGONALIZATION OF FOURTH ORDER CUMULANTS TENSOR FOR ESTIMATION OF LEAST DEPENDENT COMPONENTS

Mohsen Kompany-Zareh^{1,2}, Peter D. Wentzell², Saeed Bagheri¹, Chelsi Wicks²

¹Institute for Advanced Studies in Basic Sciences, Iran; ²Dalhousie University, Canada

P-19 **PINK**

IMPLICATIONS OF MEASUREMENT ERROR STRUCTURE ON THE VISUALIZATION OF MULTIVARIATE CHEMICAL DATA

Chelsi C. Wicks¹, Peter D. Wentzell¹, Jez W.B. Braga², Liz F. Soares², Tereza C.M.

Pastore³, Vera T.R. Coradin³, Fabrice Davrieux⁴

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P-20 **GREEN**

CHEMOMETRIC APPROACHES FOR HANDLING PAPER VARIABILITY AND ESTIMATING THE DOCUMENT AGE

Carolina S. Silva¹, Maria Fernanda Pimentel¹, José Manuel Amigo^{1,2}, Carmen Garcia-Ruiz³, Fernando Ortega-Ojedad³

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³University of Alcalá, Spain

P-21 **YELLOW**

CHEMOMETRIC ANALYSIS OF FULL SCAN MASS SPECTRA COLLECTED FROM A MOBILE LAB WITH APPLICATION TO SOURCE IDENTIFICATION OF OUTDOOR AND INDOOR AIR CONTAMINANTS

Larissa C. Richards^{1,2}, Nicholas G. Davey², Chris G. Gill^{1,2}, Erik T. Krogh^{1,2}

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- P-22** **BLUE**
 ENHANCED INTRINSIC PEROXIDASE-LIKE ACTIVATED 3D GRAPHITIC PHASE C3N4 WITH DNA REGULATION AND APPLICATION FOR OXYTETRACYCLINE (OTC) DETECTION
Huimin Zhao, Yaofang Fan
 Dalian University of Technology, PR China.
- P-23** Group: **PINK**
 PHOTOCHEMICAL HARD-SOFT MCR FOR THE INVESTIGATION OF PHOTOCROMIC SYSTEMS
 O. Devos¹, J.P Placial², R. Métivier², M. Sliwa¹, C. Ruckebusch¹
¹Univ. Lille, CNRS, UMR 8516 - LASIR - Laboratoire de Spectrochimie et Raman, France;
²ENS Cachan, CNRS, UMR 8531 - PPSM - Laboratoire de Photophysique et Photochimie Supramoléculaires et Macromoléculaires, France
- P-24** **GREEN**
 MULTIVARIATE CLASSIFICATION OF SEVEN VARIETIES OF PRUNUS DULCIS WITH NEAR INFRARED SPECTROSCOPY, USING LEAVES AND WOOD OF NURSERY PLANTS
Sergio Borraz¹, Joan Simó^{1,3}, Ricard Boqué², Silvia Sans¹, Anna Gras¹
¹Universitat Politècnica de Catalunya, Spain; ²Universitat Rovira i Virgili, Spain; ³Fundació Miquel Agustí, Spain
- P-25** **YELLOW**
 PRELIMINARY STUDY ON DETERMINATION OF ORGANOLEPTIC TRAITS IN COOKED 'CALÇOTS' (*ALLIUM CEPA L.*) BY NEAR INFRARED SPECTROSCOPY
 Silvia Sans^{1,2}, Joan Ferré³, Ricard Boqué³, Joan Casals^{1,2}, Sergio Borraz¹, Joan Simó^{1,2}
¹Universitat Politècnica de Catalunya, Spain; ²Fundació Miquel Agustí, Campus Baix, Spain; ³Universitat Rovira i Virgili, Spain
- P-26** **BLUE**
 DEVELOPMENT OF A GC-FID METHODOLOGY BY MEANS OF MULTIVARIATE EXPERIMENTAL DESIGNS FOR DETERMINATION OF RESIDUAL SOLVENTS IN [11C]PK11195
Cassiano L. S. Costa, Daleska P. Ramos, Elias G. Vieira, Fernanda A. F. Almeida, Juliana B. Silva
 Nuclear Technology Development Center (CDTN), Brazil
- P-27** **BLUE**
 A NEW HPLC PROCEDURE FOR QUALITY CONTROL OF THE RADIOPHARMACEUTICAL [18F]FES
Cassiano L. S. Costa, Nicolly N. Santos, Juliana B. Silva, Soraya M. Z. M. D. Ferreira
 Nuclear Technology Development Center (CDTN), Brazil
- P-28** **PINK**
 BLENDING END-POINT DETECTION BY USING IMAGES AND HETEROGENEITY CURVES
Neirivaldo Cavalcante da Silva¹, Leandro de Moura França¹, José Manuel Amigo¹, Manel Bautista², Maria Fernanda Pimentel¹
¹Federal University of Pernambuco, Brazil; ²Novartis Pharma AG, Switzerland
- P-29** Group: **GREEN**
 CHARACTERIZATION OF SPATIAL VARIABILITY IN HYPERSPECTRAL IMAGES USING VARIOGRAM COMBINED WITH PCA
Jun-Li Xu, Da-Wen Sun, Aoife A. Gowen
 University College Dublin, Ireland
- P-30** **YELLOW**
 NOISEGEN - MEASUREMENT ERROR SIMULATION SOFTWARE
Stephen Driscoll, Peter Wentzell
 Dalhousie University, Canada
- P-31** **BLUE**
 DATA FUSION STRATEGIES FOR NIR-BASED BATCH PROCESS CONTROL AND END-POINT DETECTION
R.R. de Oliveira¹, A. Gómez-Sánchez¹, C. Avila², F. Muller², K. Pissaridi³, K. Krassa³, J. Ferré⁴, A. de Juan¹
¹Universitat de Barcelona, Spain; ²University of Leeds, United Kingdom; ³Megara Resins Anastasios Fanis S.A., Greece; ⁴Universitat Rovira i Virgili, Spain
- P-32** **PINK**
 A DATA FUSION MODEL MERGING NEAR INFRARED (NIR) AND TOTAL REFLECTION X-RAY FLUORESCENCE (TXRF) SPECTRA APPLIED TO QUANTIFY AND CHARACTERIZE THE COMPOSITION OF COFFEE BLENDS
 Camila Assis, Ednilton M. Gama, Clésia C. Nascentes, Leandro S. Oliveira, Marcelo M. Sena
 Universidade Federal de Minas Gerais, 31270-901 Belo Horizonte, MG, Brazil
- P-33** **GREEN**
 CHROMATOGRAPHIC METABOLIC PROFILING USING TWO FINGERPRINTING TECHNIQUES, UPLC-TOF-MS AND UPLC-DAD, FOR GEOGRAPHIC CLASSIFICATION OF MOROCCAN ARGAN OIL
Mourad Kharbach^{1,2}, Johan Viaene¹, Abdelaziz Bouklouze² and Yvan Vander Heyden¹
¹Vrije Universiteit Brussel (VUB), Belgium; ²University Mohammed V - Rabat, Morocco
- P-34** **YELLOW**
 CHROMATOGRAPHIC FINGERPRINTING OF CELLULAR RESPONSE TOWARDS FIVE BASIC TASTANTS
 Marcin Zabadał, Aleksandra Szuplewska, Michał Chudy, Patrycja Ciosek-Skibińska
 Warsaw University of Technology, Poland
- P-35** **BLUE**
 INFRARED SPECTROSCOPY COUPLED TO CHEMOMETRICS: A FAST APPROACH FOR CHARACTERIZING AND AUTHENTICATING LEBANESE HONEY
Rita El Hajj¹, Wadih Skaff², Nathalie Estephan¹
¹Holy Spirit University of Kaslik, Lebanon; ²ESIAM-Université Saint-Joseph, Lebanon

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- P-36** Group: **PINK**
INSPEC: CHEMOMETRICS MEETS ADVANCED PROCESS CONTROL
Tim Offermans, Jeroen Jansen
Radboud University, The Netherlands
- P-37** **GREEN**
SINC: A NEW SOFTWARE FOR THE AUTOMATED AND SIMULTANEOUS PHASE AND BASELINE CORRECTION OF NMR DATA
Denise Meinhardt^{1,2}, Mathias Sawall¹, Henning Schröder¹, Klaus Neymeyr^{1,2}
¹University of Rostock, Germany; ²LIKAT, Leibniz-Institute for Catalysis, Germany
- P-38** **GREEN**
DESIGN OF EXPERIMENTS FOR THE REDUCTION OF THE ROTATIONAL AMBIGUITY IN MCR
Denise Meinhardt^{1,2}, Mathias Sawall¹, Christoph Kubis², Detlef Selent², Henning Schröder¹, Armin Börner², Klaus Neymeyr^{1,2}
¹University of Rostock, Germany; ²LIKAT, Leibniz-Institute for Catalysis, Germany
- P-39** **YELLOW**
CHARACTERIZATION OF FOOD-BORNE BACTERIA ON CULTURE MEDIA BY MULTIPLE MODALITIES OF HYPERSPECTRAL IMAGING
Ana Herrero-Langreo, Gauri Ravindra Chemburkar, Amalia G.M. Scanell, Aoife Gowen
University College Dublin (UCD), Ireland
- P-40** **BLUE**
THE USE OF MIR-FTIR COUPLED TO CHEMOMETRIC TOOLS TO DIFFERENTIATE BETWEEN DIESEL FUELS FROM DIFFERENT SUPPLIERS
A. Bouklouze, I. Barra, M. Alaoui, Y. Cherrah
University Mohammed V – Rabat, Morocco.
- P-41** **BLUE**
CLASSIFICATION OF FLUCONAZOLE API POLYMORPHIC FORMS IN PHARMACEUTICAL PRODUCTS BY ASSOCIATING FTIR, NIR AND RAMAN TO PLS-DA
Mohammed Alaoui Mansouri^{1,2}, Pierre-Yves Sacré¹, Eric Ziemons¹, Mourad Kharbach^{2,3}, Yahia Cherrah², Philippe Hubert¹, Abdelaziz Bouklouze², Roland Marini¹
¹University of Liege, Belgium; ²University Mohammed V - Rabat, Morocco; ³Vrije Universiteit Brussel, Belgium
- P-42** **BLUE**
RAPID DETECTION OF SMUGGLED NON-COMPLIANT DIESEL IN MOROCCAN MARKET USING MID INFRARED SPECTROSCOPY COUPLED TO A PLS-DA MODEL
Issam Barra¹, Mohammed Alaoui Mansouri^{1,2}, Yahia Cherrah¹, Abdelaziz Bouklouze¹
¹University Mohammed V – Rabat, Morocco; ²University of Liege, Belgium
- P-43** **PINK**
DUTCH SURFACE WATER QUALITY
André van den Doel^{1,2}, Geert van Kollenburg^{1,2}, Lutgarde Buydens¹ and Jeroen Jansen¹
¹Radboud University, The Netherlands; ²TI-COAST, Amsterdam, The Netherlands
- P-44** Group: **GREEN**
LOCAL VS. SVM-BASED STACKING APPROACH FOR PREDICTING PROPORTIONS OF COMPLEX BLENDS IN FOOD PRODUCTS
Beatriz Carrasco¹, Alberto Gil¹, José Ramón Quevedo², Elena Montañés², Guanghui Shen^{3,4}, Vincent Baeten⁴, Juan Antonio Fernández Pierna⁴
¹Blendhub, Murcia, Spain; ²Universidad de Oviedo, Spain; ³China Agricultural University, China; ⁴Walloon Agricultural Research Centre (CRA-W), Belgium
- P-45** **YELLOW**
MULTIMODAL OPTICAL SPECTROSCOPY AND MULTIVARIATE DATA ANALYSIS FOR THE DEMARCATION OF HUMAN BRAIN TUMORS
Mona Stefanakis, Edwin Ostertag, Anita Lorenz, Marc Brecht, Karsten Rebner
Reutlingen University, Germany
- P-46** **BLUE**
COMBINATION OF MCR-ALS AND K-MEANS INFORMATION FOR MASS SPECTROMETRY IMAGING DATA ANALYSIS
S. Mas¹, A. Torro², N. Bec², C. Larroque², P. Martineau², A. de Juan³, S. Marco¹
¹Signal and Information Processing for Sensing Systems, IBEC, Spain; ²Institut de Recherche en Cancérologie de Montpellier, France; ³Universitat de Barcelona, Spain
- P-47** **PINK**
MICROMETRIC MAPPING OF TOTAL ORGANIC CARBON IN LAKE SEDIMENT CORES COMBINING FUSION OF MULTIREOLUTION HYPERSPECTRAL IMAGES AND PLSR ANALYSIS
Kévin Jacq¹, Yves Perrette¹, Bernard Fanget¹, Didier Coquin¹, Pierre Sabatier¹, Fabien Arnaud¹, Ruth Martinez-Lamas^{2,3}, Maxime Debret²
¹University Grenoble Alpes, University Savoie Mont Blanc, France; ²Normandie Univ, UNIROUEN, UNICAEN, France; ³IFREMER, France
- P-48** **GREEN**
FLEXIBLE VARIABLE SELECTION USING ELASTIC NET REGRESSION
Cannon Giglio¹, Steven D. Brown²
¹Dalhousie University, Canada; ²University of Delaware, USA
- P-49** **YELLOW**
EVALUATION OF ACID STRENGTHS ON ELECTRONIC GROUND AND EXCITED STATES OF 2-(2'-HYDROPHENYL)BENZOTHAZOLE USING EXCITATION-EMISSION FLUORESCENCE MATRIX AND MULTIVARIATE CURVE RESOLUTION WITH ALTERNATING LEAST SQUARES (MCR-ALS)
Willian Francisco Cordeiro Dantas¹, Luis Gustavo Teixeira Alves Duarte¹, Fabiano Severo Rodembusch², Teresa Dib Zambon Atvars¹, Ronei Jesus Poppi¹
¹University of Campinas, Brazil; ²Federal University of Rio Grande do Sul, Brazil

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- P-50** **BLUE**
 EXPLORATIVE STUDY OF THE RED FRUIT JUICES FLUORESCENCE USING
 EXCITATION-EMISSION SPECTROSCOPY AND CHEMOMETRICS
Ewa Sikorska, Katarzyna Włodarska
 Poznań University of Economics and Business, Poland
- P-51** **BLUE**
 EVALUATION OF CHEMICAL PROPERTIES OF APPLE JUICES RELATED TO TASTE
 USING NEAR INFRARED SPECTROSCOPY AND CHEMOMETRICS
Ewa Sikorska, Katarzyna Włodarska
 Poznań University of Economics and Business, Poland
- P-52** **PINK**
 CHEMOMETRIC PROFILING OF CANNABIS STRAINS TO EVALUATE THEIR
 PHYTOCHEMICAL DIVERSITY
Elizabeth M. Mudge^{1,2}, Susan J. Murch¹, Paula N. Brown^{1,2}
¹University of British Columbia, Canada; ²BC Institute of Technology, Canada
- P-53** **GREEN**
 USE OF MOVING WINDOW PCA OF CHEMICAL PROFILES FOR AUTHENTICATION
 OF BOTANICAL PRODUCTS
 Jamie Finley, Paula Brown
 BC Institute of Technology, Canada
- P-54** **YELLOW**
 PIXEL-BASED CHEMOMETRIC ANALYSIS OF LC-MS ANALYZED SAMPLES FROM AN
 INDUSTRIAL ENZYME PRODUCTION: CHARACTERIZATION OF DIFFERENT
 PRODUCTS AND INVESTIGATING IF THERE IS A LINK BETWEEN THE SMALL
 MOLECULE FINGERPRINT AND PRODUCT QUALITY?
Sofie B. Knudsen^{1,2}, Nikoline J. Nielsen¹, Johan Qvist², Kim B. Andersen², Jan H.
 Christensen¹
¹University of Copenhagen, Denmark; ²Novozymes A/S, Denmark
- P-55** **BLUE**
 CHEMICAL IMAGE PROCESSING BY DISCRETE GABOR TRANSFORM COMBINED
 WITH GAUSSIAN APODIZATION FACTOR ANALYSIS FOR RESOLUTION OF THE
 EMBEDDED PEAKS IN COMPLICATED HYPER SPECTRAL DATA
Amir Hossein Alinoori
 Iranian Space Research Center and University of Kashan, Iran
- P-56** Group: **BLUE**
 GAUSSIAN APODIZATION FACTOR ANALYSIS FOR RESOLUTION OF THE
 EMBEDDED PEAKS IN ION TRAP TIME OF FLIGHT ION MOBILITY SPECTROMETRY
Amir Hossein Alinoori, Saeed Masoum
 University of Kashan, Kashan, Iran
- P-57** **PINK**
 FOUR-DIMENSIONAL QUANTITATIVE STRUCTURE-ACTIVITY ANALYSIS OF 1,4-
 NAPHTHOQUINONES DERIVATIVES TESTED AGAINST HL-60 HUMAN
 PROMYELOCYTIC
Márcia Miguel Castro Ferreira, Maria Cristina Andreatza Costa, Pedro Oliveira Mariz
 Carvalho
 University of Campinas, Brazil
- P-58** **PINK**
 MULTIVARIATE ACCELERATED SHELF-LIFE TESTING FOR DETERMINING THE
 SHELF-LIFE OF PAINTS
Márcia Miguel Castro Ferreira¹, Nelson Mituo Matsumoto²
¹University of Campinas, Brazil; ²PPPG Industrial do Brasil Tintas e Vernizes Ltda, Brazil
- P-59** **GREEN**
 A PIGMENT-BASED TAXONOMIC DISCRIMINATION ANALYSIS FOR THE IN-SITU
 CLASSIFICATION OF (HARMFUL) ALGAL BLOOMS
S.E. Zieger, G. Mistlberger, L. Troi, I. Klimant
 Graz University of Technology (TU Graz), Austria
- P-60** **YELLOW**
 HIGH-THROUGHPUT AUTHENTICATION OF CANNABIS EXTRACTS BY ULTRAVIOLET
 MICROPLATE READER AND MULTIVARIATE CLASSIFIERS
Peter Harrington, Zewei Chen
 Ohio University, USA
- P-61** **BLUE**
 NIR-HYPERSPECTRAL IMAGING TO VISUALIZE THE WETTING AND DRYING CYCLE
 IN CYANOLICHENS
Cristina Malegori, Paola Malaspina, Paolo Oliveri, Paolo Giordani, Monica Casale
 University of Genoa, Italy
- P-62** **PINK**
 HOW SIGNAL PRE-PROCESSING AFFECTS INTERPRETATION OF CHEMOMETRIC
 PROCEDURES – REMARKS AND SUGGESTIONS
Paolo Oliveri, Cristina Malegori, Monica Casale
 University of Genova, Italy
- P-63** **GREEN**
 CONTRAST ENHANCEMENT AND TOTAL VARIATION: A COMPARISON BETWEEN
 TWO SPATIAL CONSTRAINTS IN MCR-ALS OF HYPERSPECTRAL IMAGES
 Dario Cevoli¹, Raffaele Vitale^{1,2}, Siewert Hugelier¹, Cyril Ruckebusch¹
¹Université de Lille, France; ²Katholieke Universiteit Leuven, Belgium
- P-64** Group: **YELLOW**
 PENALTY OPTIMIZATION IN SPARSE DECONVOLUTION OF SUPER-RESOLUTION
 FLUORESCENCE IMAGES
Siewert Hugelier¹, Mohamad Ahmad¹, Raffaele Vitale^{1,2}, Cyril Ruckebusch¹
¹Université de Lille, France; ²Katholieke Universiteit Leuven, Belgium

