

Symposium organised by the

## Royal Flemish Chemical Society (KVCV), Belgium and the

Royal Society of Chemistry (RSC), United Kingdom

Venue: Conference Centre Het Pand, Onderbergen 1, Ghent (Belgium)

















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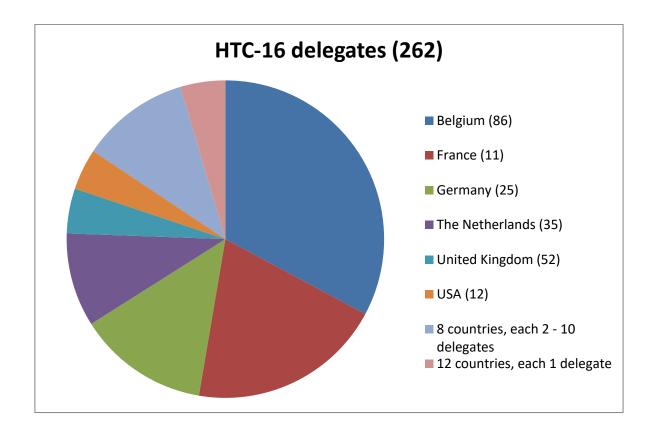
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## **DELEGATES**



## **SCIENTIFIC PROGRAMME**

## • SCIENTIFIC PROGRAMME OF HTC-16 IN A GLANCE

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#### **AWARDS**

#### **HTC - INNOVATION AWARD**

This award was created in 2017. The **LCGC Europe/HTC Innovation Award** replaced the 'Lifetime Achievement Award in Chromatography'.

The winner has been selected by the HTC-16 Scientific Committee and the HTC-16 Industry Board based on the following criteria:

- The winner has made an innovative contribution to the field of separation science by introducing new methodologies, new instrumentation, or new techniques in the field with a strong focus on applicability.
- The winner is a scientist under 45 years of age.





HTC INNOVATION AWARD 2020, Left to right Deirdre CABOOTER (KU Leuven), Ryan T. KELLY (Brigham Young University, USA) and Alasdair MATHESON (LC-GC Europe)

The 2020 HTC-Innovation Award recipient, presented at the HTC-16 Conference on 31 January 2020 is Professor **Ryan T. KELLY**, Department of Chemistry and Biochemistry at Brigham Young University, Utah, USA.

Title of the lecture by Prof. Kelly:

One Cell at a Time: 1D and 2D Separations for In-Depth Single-Cell and nanoscale Proteomics

## **HTC AWARD**

The most innovative oral presentation given during the conference received the **HTC Award**, sponsored by Elsevier. The winner was selected by the HTC-16 Scientific Committee and the HTC-16 Industry Board.



HTC-AWARD,
Left to right Deirdre CABOOTER (KU
Leuven),
Gert DESMET (VUB) and Award winner
André DE VILLIERS, Stellenbosch
University, South Africa

The HTC award was presented during the closing session of HTC-16 on 31 January 2020 to

Professor **André DE VILLIERS**, Stellenbosch University, South Africa.

Title of the Award winning lecture by prof. De Villiers:

Advantages and limitations of HILIC in the second dimension of comprehensive two-dimensional liquid chromatographic separations: A kinetic evaluation.

#### **POSTER AWARDS**

The three most innovative poster contributions received the **HTC-poster award**, sponsored by Analytical Science Advances (Wiley).

Selection criteria:

- Originality and novelty.
- Experimental effort.
- Visual and author's presentation.

#### FIRST POSTER AWARD



Sebastiaan EELTINK (left) and Ali **MOUSSA** 

#### **Ali MOUSSA**

Free University Brussels, Belgium

Numerical and Experimental Investigation of Sample Loss and Dispersion Occurring in Sample Loops Used in 2D-LC Setups (Poster MDLC-03)

Authors: Ali Moussa 1, Thomas Lauer 2, Dwight Stoll <sup>2</sup>, Gert Desmet <sup>1</sup> and Ken Broeckhoven <sup>1</sup> <sup>1</sup> Free University Brussels, Belgium; <sup>2</sup> Gustavus Adolphus College, Minnesota, United States

#### **SECOND POSTER AWARD**



Sebastiaan EELTINK (left) and Haibin LI

#### Haibin LI KU Leuven, Belgium

An experimental procedure for the in-depth evaluation of band broadening phenomena in capillary and nano-size columns (Poster FUN-04)

Authors: Haibin Li 1,2, Zhengjin Jiang 2 and Deirdre Cabooter 1

<sup>1</sup> KU Leuven, Belgium; <sup>2</sup> Jinan University, China

#### THIRD POSTER AWARD



Sebastiaan EELTINK (left) and Zhanyao HOU

Engineering, Belgium

#### Zhanyao HOU

Ghent University, Belgium

Polymerization of the Through-pores in HPLC Columns for Enhanced SEM Based Assessment of Packing Order

(Poster FUN-06)

Authors: Zhanyao Hou 1, Ken Broeckhoven <sup>2</sup>, Gert Desmet <sup>2</sup> and Frederic Lynen <sup>1</sup>

<sup>1</sup> Separation Science Group, Department of Organic and Macromolecular Chemistry, Ghent University, Belgium; <sup>2</sup> Free University Brussels, Department of Chemical

#### HTC TUBE SCIENTIFIC OUTREACH CONTEST

This first HTC-tube event offers a platform for scientists to present their own research related to Hyphenated Techniques in Chromatography in a short video format (not exceeding 3 minutes) during the conference. Although the format is free the jury will assess the video's in both in terms of scientific excellence and their ability to disseminate to work to a broader audience. An international jury has shortlisted the videos for the HTC-Tube which were presented during a plenary session on Thursday January 30th 2020. The winner, as well as the 2nd and 3rd place runners, will be chosen by a jury designated by the Scientific committee and will receive cash prizes. The HTC Tube was sponsored by Chromatographia.

#### **EXHIBITORS AND SPONSORS**

The organisers wish to express their appreciation to the sponsors. Their valuable contribution allowed the organisers to support the Early Career Speakers, and others, to attend to HTC.

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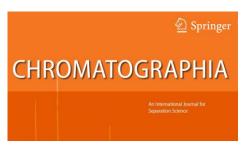
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## **ANNEX- Scientific programme**

### SHORT COURSES (Tuesday 28 January 2020)

## SHORT COURSE 1 - Multidimensional and Hyphenated Techniques in LC and GC

Tuesday January 28<sup>th</sup> 2020, 09:00 – 17:00

Speakers: Joeri Vercammen (Ghent University, BE), Dr. Dwight Stoll (Gustavus Adolphus College, USA), Dr. Davy Guillarme (University of Geneva, CH).

In the twenty years of its existence, GCxGC has evolved into a mature technique that enables comprehensive analysis of a complex samples in petrochemistry, food and environmental analysis. Nonetheless, the GCxGC footprint remains relatively small within the entire chromatography sphere. The goal of this training is to provide sufficient insight to convince those in doubt whilst at the same time provide new insights to its early adopters. Therefore, the following topics will be addressed: (a) Origins of GCxGC, (b) The concept of orthogonality, (c) Theory and basic principles, (d) Comparison of modulator technology, (e) Data handling challenges, (f) Recent applications, (g) Q&A. Each participant is encouraged to provide real life challenges he/she is confronted with during daily routine. These questions will be proactively incorporated into the training to make it even more relevant to everyone attending.

Two-dimensional liquid chromatography (2D-LC) is increasingly becoming recognized as a powerful and flexible analytical tool that can be used in a variety of applications areas, particularly when conventional one-dimensional (1D) separations are inadequate for some reason. Leveraging the potential of 2D-LC requires that users understand the underlying principles of the technique, and differences between 1D and 2D separations in method development. We will address several key concepts from a theoretical point of view, including undersampling, and the different types and modes of 2D separation (e.g., heartcutting and comprehensive separations). Then, we will use examples of contemporary separations of both small molecules (e.g., pharmaceutical impurity profiling) and larger biomolecules (e.g., peptides and proteins) to illustrate both what it is possible, and the steps in method development that are critical to successful separations. Finally, several practical topics will be discussed, including coupling to mass spectrometric detection, quantitation, and data visualization and analysis. We intend for the course to be practical in nature, with a solid theoretical foundation. We encourage attendees to bring any questions they have about separations they are currently doing, or plan to do, for discussion during the course.

#### **SHORT COURSE 2 - Cannabis Analysis**

Tuesday January 28<sup>th</sup> 2020, 09:00 – 17:00

Speakers: Dr. Barbara Paccheti (EMMAC) Dr. Gesa Schad, Dr. Allegra Leghissa, Dr. Xaver Monninghoff (Schimadzu), Dr. Hansjörg Majer (Restek), Dr. Flavio Franchina (University of Liège, BE).

Due to recent changes in legislation all over Europe, the medicinal cannabis market continues to grow, and CBD infused edibles, food supplements and cosmetic products are enjoying an unprecedented surge in popularity. Accurate cannabis analysis is required in order to ensure product quality and consumer safety. Cannabinoids are the primary active components of cannabis and the target compounds for potency testing. Terpenes influence the homeopathic effect, and contaminants such as pesticide residues and microbial contamination could cause serious harm, especially to immuno-compromised medicinal cannabis users.

This short course will cover the basics of cannabis and the industry, as well as the state-of-the-art testing methods currently available. In the first part, the basics of cannabis analysis and background on cannabis industry will be discussed. The second part handles basic testing for potency, moisture and mycotoxines, followed by advanced testing for terpenes, pesticides and chemical residues. In the final part of the short course, the analysis of (S)VOC compounds in cannabis is discussed. Speakers from academia (Flavio A. Franchina, Université de Liège), industry (Barbara Pacchetti - EMMAC) and experts from instrument manufacturers (Gesa Schad , Allegra Leghissa and Xaver Mönninghoff – Shimadzu; Hansjörg Majer - Restek), will cover these different topics.

#### **LECTURES**

**PL**: plenary lecture; **KL**: keynote lecture; **OC**: oral communication; **TU**: tutorial; **YES**: Young and Emerging Scientist presentation; **FP**: Poster Flash presentation

#### **WEDNESDAY 29 JANUARY 2020**

#### **HTC-16 OPENING CEREMONY**

Session Chair: Sebastiaan Eeltink (Vrije Universiteit Brussel, BE) and John Langley (University of Southampton, UK)

PL01 - UHPLC and prefractionation to increase metabolite identifications in metabolomics assays

Robert Kennedy

University of Michigan, USA

PL02 - Nano- and capillary LC separations using micro-pillar array columns for maximal efficiency and robustness

<u>Gert Desmet</u><sup>1</sup>, Jeff Op de Beeck<sup>2</sup>, Geert Van Raemdonck<sup>2</sup>, Kurt Van Mol<sup>2</sup>, Bo Claerebout<sup>1</sup>, Natalie Van Landuyt<sup>2</sup>, Paul Jacob<sup>2</sup>

<sup>1</sup>Department of Chemical Engineering, Vrije Universiteit Brussel, Brussels, Belgium;

#### **BIOPHARMACEUTICAL ANALYSIS**

Session Chair: Davy Guillarme (University of Geneva, CH)

KL01 - Expanding the analytical portfolio for the characterization of protein biopharmaceuticals

<u>Koen Sandra</u>, Liesa Verscheure, Jonathan Vandenbussche, Julie Storms, Shauni Detremmerie, Isabel Vandenheede, Emmie Dumont, Gerd Vanhoenacker, Ruben 't Kindt, An Cerdobbel, Pat Sandra

Research Institute for Chromatography

TU01 - HPLC analysis of biologicals in a cGMP environment Achim Treumann, KBI Biopharma bvba

OC01 - Enhanced peptide mapping and HCP analysis with Trapped Ion Mobility Spectrometry (TIMS) using a variety of LC flow regimes Stuart Pengelley, Bruker Daltonik GmbH, Fahrenheitstr. 4, 28359 Bremen, Germany

OC02 - Polysorbate profiling and impurity quantitation in biotherapeutics formulations by HPLC with charged aerosol detection following on-line sample clean-up <a href="Frank Steiner">Frank Steiner</a>, Katherine S. Lovejoy<sup>1</sup>, Mauro De Pra<sup>1</sup>, Sara Carillo<sup>2</sup>, Ken Cook<sup>3</sup>, Paul H. Gamache<sup>4</sup>

<sup>1</sup>Thermo Fisher Scientific, Germering, Germany; <sup>2</sup>NIBRT, Dublin, Ireland; <sup>3</sup>Thermo Fisher Scientific, Hemel Hempstead, UK; <sup>4</sup>Thermo Fisher Scientific, Chelmsford, MA, USA

<sup>&</sup>lt;sup>2</sup>Pharmafluidics NV Technologiepark-Zwijnaarde 3, 9052 Gent, Belgium

#### **GC-MS AND GC×GC**

Session Chair: Hans-Gerd Janssen (Unilever, NL)

KL02 - In vitro characterization of lung inflammation mechanisms

<u>Jean-François Focant</u><sup>1</sup>, Delphine Zanella<sup>1</sup>, Florence Schleich<sup>2</sup>, Monique Henket<sup>2</sup>, Thibaut Dejong<sup>1</sup>, Renaud Louis<sup>2</sup>, Pierre-Hugues Stefanuto<sup>1</sup>

<sup>1</sup>Organic and Biological Analytical Chemistry Group, MolSys, University of Liège, Belgium;

KL03 - Learning the lessons from multidimensional separations

<u>Tadeusz Górecki</u><sup>1</sup>, Alshymaa A. Aly<sup>1</sup>, Hei-Yin Chow<sup>1</sup>, Magriet Muller<sup>2</sup>, Andre de Villiers<sup>2</sup>, Bob W.J. Pirok<sup>3</sup>, Peter Schoenmakers<sup>3</sup>

<sup>1</sup>University of Waterloo, Canada; <sup>2</sup>Stellenbosch University, South Africa; <sup>3</sup>University of Amsterdam, The Netherlands

OC03 - Problems and solutions related to calibration of thermal desorber – gas chromatography

Adissu Asfaw, Matthias Van der Veken, Kris Wolfs, Ann Van Schepdael, Erwin Adams KU Leuven, University of Leuven, Department of Pharmaceutical and Pharmacological Sciences, Pharmaceutical Analysis, Herestraat 49, O&N2, PB 923, B-3000 Leuven, Belgium

OC04 - Extending the Application Range of a GC×GC High-Resolution TOF-MS platform for Fuel Analysis by Hyphenation to Direct Inlet Thermal Analysis Techniques
Uwe Käfer¹, Thomas Groeger¹, Mohammed Saraji², Thomas Wilharm³, Ralf Zimmermann¹
¹Helmholtz Zentrum München GmbH/Univerity of Rostock, Germany; ²Photonion GmbH;
³ASG GmbH

#### **MAXIMIZING RESOLUTION**

Session Chair: Hamed Eghbali (DOW, NL)

TU02 - Maximising Resolution Through Hyphenation Tom Lynch Tom Lynch Analytical Consultancy, UK

YES01 - How to further increase the peak capacity of sub-hour on-line LC x LC separations? Soraya Chapel, Florent Rouvière, Sabine Heinisch Institut des Sciences Analytiques, UMR 5280, CNRS, Université Lyon 1, ENS Lyon, France

YES02 - Resolving power of high-porosity nanostructured monolithic columns in liquid chromatography for proteomic applications
José Luís Dores-Sousa, Sebastiaan Eeltink

Vrije Universiteit Brussel (VUB), Belgium

YES03 - High potential of a three dimensional approach (CPC×SFC/HRMS) to analyse HPAH in vacuum gas oil

Carole Reymond<sup>1</sup>, Agnès Le Masle<sup>1</sup>, Cyril Colas<sup>2</sup>, Nadège Charon<sup>1</sup>

<sup>1</sup>IFP Energies nouvelles, France; <sup>2</sup>Institut de Chimie Organique et Analytique, France

<sup>&</sup>lt;sup>2</sup>Respiratory Medicine, GIGA I3, CHU Sart-Tilman, University of Liège, Belgium

FP01 – Assessment of operating conditions affecting the peak capacity of intact protein bioanalysis in HIC

Raphael Ewonde Ewonde

Vrije Universiteit Brussels, BE

FP02 – The importance of sufficient chromatographic separation for identity confirmation Henk Gerritsen

Wageningen Food Safety Research, NL

FP03 – An experimental procedure for the in-depth evaluation of band broadening phenomena in capillary and nano-size columns

Haibin Li

KU Leuven, BE

FP04 – HPLC as a PAT tool featuring ballistic separations and direct process sampling Przemek Stasica
GSK, UK and University of Leeds, UK

#### **HIGH-RESOLUTION PROFILING**

Session Chair: Erwin Kaal (DSM Biotechnology Center, NL)

KL04 - Chiral separations and hyphenated techniques

<u>Michael Lämmerhofer</u>, Christian Geibel, Jeannie Horak, Ryan Karongo
University of Tübingen, Germany

KL05 - Miniaturized selective extraction devices for trace analysis in complex samples Thomas Bouvarel<sup>1</sup>, Stan Perchepied<sup>1</sup>, Audrey Combès<sup>1</sup>, Nathalie Delaunay<sup>1</sup>, Valérie Pichon<sup>1,2</sup>

<sup>1</sup>ESPCI Paris, France; <sup>2</sup>Sorbonne University

OC05 - Multidimensional performance assessment of micro pillar array column chromatography combined to ion mobility-mass spectrometry for proteomics research Cindy Nix, Gwenael Nys, Gael Cobraiville, Marianne Fillet University of Liège, Belgium

OC06 - Targeted metabolomics of the brain – the quest for sensitivity, selectivity and throughput

Ann Van Eeckhaut, Jana Bongaerts, Marie-Laure Custers, Liam Nestor, Anouk Pierre, Dimitri De Bundel, Ilse Smolders

Department of Pharmaceutical Chemistry, Drug Analysis and Drug Information, Research Group Experimental Pharmacology, Center for Neurosciences (C4N), Vrije Universiteit Brussel, Laarbeeklaan 103, 1090 Brussels, Belgium

#### **METHOD DEVELOPMENT**

Session Chair: Peter Van Broeck (Janssen Pharmaceutica, BE)

KL06 - Multi-dimensional chromatographic approaches to characterize protein biopharmaceuticals

<u>Davy Guillarme</u><sup>1</sup>, Valentina D'Atri<sup>1</sup>, Alexandre Goyon<sup>1</sup>, Alain Beck<sup>2</sup>, Sarah Cianferani<sup>3</sup>, Sabine Heinisch<sup>4</sup>, Dwight Stoll<sup>5</sup>, Jean-luc Veuthey<sup>1</sup>, Szabolcs Fekete<sup>1</sup>

<sup>1</sup>University of Geneva, Switzerland; <sup>2</sup>Center of Immunology Pierre Fabre, France; <sup>3</sup>University of Strasbourg, France; <sup>4</sup>University of Lyon, France; <sup>5</sup>Gustavus Adolphus College, MN, USA

KL07 - Impact of structural similarity on accuracy of retention time prediction: Theory and applications

Roman Szucs<sup>1,2,3</sup>

<sup>1</sup>Pfizer R&D UK, United Kingdom; <sup>2</sup>Commenius University, Bratislava, Slovakia; <sup>3</sup>University of Ghent, Ghent, Belgium

OC07 - Implementing principles of Analytical Quality by Design (AQbD) for method development in quality control environment

<u>Cedric Hubert</u> <sup>a</sup>, Riccardo Deidda <sup>a</sup>, Amandine Dispas <sup>a,b</sup>, Thomas Van Laethem <sup>a</sup>, Xuan Zhao <sup>a</sup>, Pierre Lebrun <sup>a,c</sup> and Philippe Hubert <sup>a</sup>

<sup>a</sup> University of Liege (ULiege), CIRM, Laboratory of Pharmaceutical Analytical Chemistry, Liege, Belgium. <sup>b</sup> University of Liege (ULiege), CIRM, Laboratory for the Analysis of Medicines, Liege, Belgium. <sup>c</sup> Pharmalex Belgium, Mont-Saint-Guibert, Belgium

OC08 - Development and qualification of a heartcutting 2D-LC method for determination of light-induced degradants of pediatric drug product delivered with liquid and soft foods Hans Thys, Ann De Nef, Willy Peys, An Van Cleempoel, Jean-Paul Boon, Kai Chen, Mario Hellings

Janssen Pharmaceutica, Belgium

#### SYSTEM DESIGN AND NOVEL COLUMN TECHNOLOGIES

Session Chair: Peter Schoenmakers (University of Amsterdam, NL)

TU03 - Extra-column broadening in modern UHPLC instrumentation Ken Broeckhoven

Vrije Universiteit Brussel, Belgium

YES04 - Characterization of proteins with in situ synthesis of miniaturized monolithic Immobilized Enzymatic Reactors coupled on-line with nano-liquid chromatography Stan Perchepied<sup>1</sup>, Nathalie Delaunay<sup>1</sup>, Valérie Pichon<sup>1,2</sup>

<sup>1</sup>Department of Analytical, Bioanalytical Sciences, and Miniaturization - UMR Chimie Biologie Innovation 8231, ESPCI Paris, PSL University, Paris, France; <sup>2</sup>Sorbonne University, Paris, France

YES05 - Nanofibrous sorbents: Promising newcomers in on-line biological sample handling Hedvika Raabova<sup>1</sup>, Lucie Chocholousova Havlikova<sup>1</sup>, Jakub Erben<sup>2</sup>, Jiri Chvojka<sup>2</sup>, Frantisek Svec<sup>1</sup>, Dalibor Satinsky<sup>1</sup> <sup>1</sup>The Charles University, Faculty of Pharmacy Hradec Kralove, Akademika Heyrovskeho 1203, 500 05 Hradec Kralove, Czech Republic; <sup>2</sup>The Technical University of Liberec, Faculty of Textile Engineering, Department of Nonwovens and Nanofibrous Materials, Studentska 1402/2, 460 01 Liberec 1, Czech Republic

YES06 - Evaluation of system performance in ultra-high-pressure operation mode Zhuoheng Zhou<sup>1</sup>, Mauro De Pra<sup>2</sup>, Frank Steiner<sup>2</sup>, Gert Desmet<sup>1</sup>, Sebastiaan Eeltink<sup>1</sup> Vrije Universiteit Brussel, Belgium; <sup>2</sup>Thermo Fisher Scientific, Germering, Germany

FP05 – Development of an improved protocol for the measurement of molecular diffusion coefficients of biopharmaceuticals

Donatela Sadriaj

University of Leuven, BE

FP06 – Design and evaluation of flow distributors for radially elongated hexagonal pillar arrays column using CFD modeling

Farideh Haghighi

Alzahra University, IR

FP07 – Numerical and Experimental Investigation of Sample Loss and Dispersion Occurring in Sample Loops Used in 2D-LC

Ali Moussa

Vrije Universiteit Brussel, BE

FP08 – Determination of the diffusion coefficients in SFC for a wide variety of samples and conditions

Vincent Pepermans

Vrije Universiteit Brussel, BE

#### **ADVANCES IN INDUSTRY**

Session Chair: Joeri Vercammen (Interscience and Ghent University, BE)

KL08 - Trends in analytics in Pharma Industry

Peter Van Broeck

Janssen Pharma, Belgium

Industry pitch - *Driving Proteomic NanoLC-MS to new crossroads, are we heading towards extra sensitive or increased throughput applications?* 

Robert van Ling, C. Mitterer, G. Jaouen, G. van Raemdonck, J. Op De Beeck PharmaFluidics, Belgium

Industry pitch - Experience the power of having a GC in your laptop: free modeling software to simulate GC separations

Jaap de Zeeuw, HansJorg Maier

Restek Corporation, United States of America

Industry pitch - Meeting Customer's Needs: YMC New and Innovative Solutions for BioLC Daniel Eßer

#### YMC Europe GmbH, Germany

Industry pitch - Characterization of New MS-Compatible Mixed-Mode RP/AX HPLC Columns Thomas Henry Walter, Bonnie A. Alden, Melvin Blaze, Cheryl Boissel, Mathew DeLano, Jessica Field, Nicole L. Lawrence, Donna Osterman, Amit V. Patel Waters Corp, United States of America

Industry pitch - Gaining insights into the complex chemistry of cannabis aroma Laura McGregor<sup>1</sup>, Matthew Edwards<sup>1</sup>, Dave Bowman<sup>1</sup>, Claire Keller<sup>2</sup>

1 SepSolve Analytical, United Kingdom; 2 Markes International

#### **NEW TRENDS IN LC-MS**

Session Chair: Michael Lammerhofer (University of Tuebingen, DE)

KL09 - Utilising the power and selectivity of supercritical fluid chromatography and mass spectrometry to detect and quantify polymeric materials across a range diverse applications G. John Langley

University of Southampton, United Kingdom

OC09 - Advanced mass spectrometry in biomarker discovery for emerging contaminants Adrian Covaci

Toxicological Center, Department of Pharmaceutical Sciences, University of Antwerp Universiteitsplein 1, 2610 Wilrijk-Antwerpen, Belgium

OC10 - Development of IP-LC-MSMS methodology to monitor Tau phosphorylation around T217 in human CSF as biomarker read-out in clinical study samples of Alzheimer diseased patients

<u>Sebastiaan Bijttebier</u><sup>1</sup>, Clara Theunis<sup>2</sup>, Farid Jahouh<sup>1</sup>, Marc Verhemeldonck<sup>1</sup>, Dina Rodrigues Martins<sup>2</sup>, Marc Mercken<sup>2</sup>, Lieve Dillen<sup>1</sup>

<sup>1</sup>DMPK, Janssen Pharmaceutica, Turnhoutseweg 30, Beerse, Belgium; <sup>2</sup>R&D Neuro sciences, Janssen Pharmaceutica, Turnhoutseweg 30, Beerse, Belgium

OC11 - Exploring the Application of Liquid Chromatography-Ion Mobility-Mass Spectrometry for Targeted and Untargeted Metabolomics

John Walsby-Tickle, James S.O. McCullagh

Department of Chemistry, Chemistry Research Laboratory, University of Oxford, OX1 3TA

#### ANALYTICAL TECHNOLOGIES IN LIFE SCIENCE RESEARCH

Session Chair: Valérie Pichon (ESPCI Paris, FR)

TU04 - High throughput comprehensive lipid/protein composition of lipoproteins in normal and dyslipidemic patients

John R. Barr, Zsuzsanna Kuklenyik

Centers for Disease Control and Prevention, United States of America

YES07 - HILIC-MS/MS Analysis of Histamine and its Main Metabolites in Human Urine Samples in the Search of Novel Biomarkers for Irritable Bowel Syndrome

Maxim Nelis<sup>1</sup>, Lisse Decreacker<sup>2</sup>, Guy Boeckxstaens<sup>2</sup>, Patrick Augustijns<sup>3</sup>, Deirdre Cabooter<sup>1</sup> <sup>1</sup>KU Leuven, Laboratory for Pharmaceutical Analysis, Herestraat 49, 3000 Leuven, Belgium; <sup>2</sup>KU Leuven, Translational Research in GastroIntestinal Disorders (TARGID), Herestraat 49, 3000 Leuven, Belgium; <sup>3</sup>KU Leuven, Laboratory for Bio-pharmacy and Pharmaceutical Technology, Herestraat 49, 3000 Leuven, Belgium

YES08 - Approaches from Relative to Absolute Quantification in Untargeted Lipidomics by Surrogate Calibration

<u>Bernhard Drotleff</u>, Tomáš Pluháček, Michael Lämmerhofer University of Tuebingen, Germany

YES09 - Colorectal Cancer: Biomarkers and Effect Size

<u>Nicolas Di Giovanni</u><sup>1</sup>, Marie-Alice Meuwis<sup>2</sup>, Edouard Louis<sup>2</sup>, Jean-François Focant<sup>1</sup>

<sup>1</sup>Organic and Biological Analytical Chemistry Group, MS Lab, Université de Liège, Belgium;

<sup>2</sup>Translationnal Gastroenterology Unit, GIGA-R, CHU (University Hospital), Liège, Belgium

YES10 - Mimicking the blood-brain barrier by a biomimetic platform based on comprehensive two- dimensional liquid chromatography for drug diffusion studies.

Giacomo Russo, Frederic Lynen

Separation Science Group, Department of Organic and Macromolecular Chemistry, Ghent University, Krijgslaan 281, S4-bis, B-9000 Ghent, Belgium

#### **THURSDAY 30 JANUARY 2020**

#### PLENARY RSC SEPARATION SCIENCE GROUP SESSION

Session Chair: John Langley (University of Southampton, UK)

PL03 - What are the challenges faced by the separation scientists in environmental analysis today?

Leon P Barron

King's College London, United Kingdom

KL10 - Dealing with Earth's most complex mixtures

G. Trifiro, R. York, N.G.A. Bell

Department of Chemistry, University of Edinburgh, EH93FJ, Edinburgh, UK

#### **FOOD ANALYSIS**

Session Chair: Andre de Villiers (Stellenbosch University, SA)

KL11 - The importance of analytical chemistry and molecular knowledge in developing consumer-preferred food products

Hans-Gerd Janssen<sup>1,2</sup>, Boudewijn Hollebrands<sup>1</sup>, Herrald Steenbergen<sup>1</sup>, Ed Rosing<sup>1</sup>

<sup>1</sup>Unilever Research, Olivier van Noortlaan 120, 3133 AT Vlaardingen, The Netherlands; <sup>2</sup>Wageningen University, Lab. of Organic Chemistry, Stippeneng 4, 6708 WE Wageningen, The Netherlands

KL12 - Determination of enzyme activity using time resolved (LC-) Ion Mobility- Mass Spectrometry

<u>Erwin Kaal</u>, Emilie Usureau, Wim Bijleveld DSM Biotechnology Center, Netherlands

#### **HIGH-RESOLUTION TECHNIQUES**

Session Chair: Ken Broeckhoven (Vrije Universiteit Brussel, BE)

TU05 - Method development and optimization in analytical SFC Caroline West University of Orléans, France

KL13 - A Closer Study of Ion-Pair Chromatographic Separations of New Therapeutic Oligonucleotides

<u>Torgny Fornstedt</u><sup>1,2</sup>, Martin Enmark<sup>1,2</sup>, Jörgen Samuelsson<sup>1,2</sup>, Joakim Bagge<sup>1,2</sup>
<sup>1</sup>Department of Engineering and Chemical Sciences, Karlstad Universitet, Sweden; <sup>2</sup>The Fundamental Separation Science Group (FSSG.se)

#### SOFTWARE ADVANCES FOR MULTIDIMENSIONAL LC/GC

Session Chair: Jean-François Focant (Université de Liège, BE)

TU06 - Think Bayesian: old and new solutions for massive chromatographic data-analysis Gabriel Vivó-Truyols

Principal Scientist | Tecnometrix | C/ Maó, 30 | 07760 Ciutadella | Spain, Guest researcher | Analytical-chemistry group | University of Amsterdam | Science Park, 904. | 1098 XH Amsterdam | The Netherlands

YES11 - Establishing an Unique Open-Source Benchmark Dataset for the Comprehensive Evaluation of GC×GC Software

<u>Benedikt A. Weggler</u><sup>1</sup>, Lena M. Dubois<sup>1</sup>, Nadine Gawlitta<sup>2</sup>, Thomas Gröger<sup>2</sup>, John Moncur<sup>3</sup>, Luigi Mondello<sup>5</sup>, Stephen Reichenbach<sup>4</sup>, Peter Tranchida<sup>5</sup>, Zhijun Zhao<sup>6</sup>, Ralf Zimmermann<sup>2</sup>, Mariosimone Zoccali<sup>5</sup>, Jean-François Focant<sup>1</sup>

<sup>1</sup>University of Liège, MolSys - Organic and Biological Analytical Chemistry Group, Quartier Agora, Place du Six Août 11, B6c, 4000 Liège, Belgium; <sup>2</sup>Joint Mass Spectrometry Centre, Comprehensive Molecular Analytics, Helmholtz Zentrum München, Ingolstädter Landstr. 1, Neuherberg, 85764, Germany; <sup>3</sup>SpectralWorks Limited,The Heath Business and Technical Park, Runcorn, Cheshire, WA7 4QX, United Kingdom; <sup>4</sup>University of Nebraska-Lincoln, Lincoln, NE, USA; GC Image, LLC, Lincoln, NE, USA; <sup>5</sup>Dipartimento di Scienze Chimiche, Biologiche, Farmaceutiche ed Ambientali, University of Messina, Polo Annunziata, 98168 Messina, Italy; <sup>6</sup>J&X Technologies (Shanghai) Co., Ltd.

YES12 - Unlocking automated method development: new peak-tracking algorithm for very fast data analysis of (LCx)LC-MS and (GCx)GC-MS data

<u>Stef R.A. Molenaar</u><sup>1</sup>, Peter J. Schoenmakers<sup>1</sup>, Hans-Gerd Janssen<sup>1,2</sup>, Dwight R. Stoll<sup>3</sup>, Bob W.J. Pirok<sup>1</sup>

<sup>1</sup>University of Amsterdam, van 't Hoff Institute for Molecular Sciences, Analytical-Chemistry Group, Science Park 904, 1098 XH Amsterdam, The Netherlands; <sup>2</sup>Unilever Research and Development, P.O. Box 114, 3130 AC Vlaardingen, The Netherlands; <sup>3</sup>Department of Chemistry, Gustavus Adolphus College, St. Peter, Minnesota 56082, United States

#### RSC SEPARATION SCIENCE GROUP: SAMPLE PREPARATION AND INTRODUCTION

Session Chairs: Graham Mills (University of Portsmouth, UK) / Scott Fletcher (Hall Analytical, UK)

KL14 – Recent advances in sample preparation and sample introduction techniques: a view from Pharma

Rob Vreeken (Maastricht University, NE)

OC12 - The use of experimental design and automation for pharmaceutical solid oral dosage form sample preparation

Paul Ferguson

AstraZeneca, United Kingdom

OC13 - QuEChERS: a versatile tool for monitoring strategies in life science, environmental and manufacturing industries

<u>A Ruth Godfrey</u><sup>1</sup>, Geertje van Keulen<sup>1</sup>, Claire Desbrow<sup>2</sup>, Elena Jones<sup>3</sup>, Krzysztof Okonski<sup>1</sup>, Daniel Rees<sup>4</sup>, Roderick Thomas<sup>4</sup>, Rachel Townsend<sup>1</sup>

<sup>1</sup>Swansea University Medical School, Swansea, United Kingdom; <sup>2</sup>Biotage GB Limited, Hengoed, United Kingdom; <sup>3</sup>Hydro Industries Ltd, Carmarthenshire, United Kingdom; <sup>4</sup>Swansea University School of Management, Swansea, United Kingdom

OC14 - Comparison of OMCL methods for N-Nitrosamine impurities in Sartans- The ongoing challenges and wider issues

Mark William Harrison

AstraZeneca

#### INNOVATIONS AND APPLICATION IN INDUSTRY

Session Chair: Achim Treumann (KBI Biopharma, BE)

KL15 - Infrared ion spectroscopy (IR-IS): a promising tool for metabolite identification! Rianne van Outersterp², Jonathan Martens², Valerie Koppen¹, Giel Berden², Jos Oomens², Filip Cuyckens¹

<sup>1</sup>Drug Metabolism & Pharmacokinetics, Janssen R&D, Beerse, Belgium; <sup>2</sup>FELIX Laboratory, Radboud University, Nijmegen, The Netherlands; <sup>3</sup>van't Hoff Institute for Molecular Sciences, University of Amsterdam, The Netherlands

KL16 - Molecular Weight Distribution Characterization of Reactive Higher Ethyleneamines using Size-Exclusion Chromatography

<u>Hamed Eghbali</u><sup>1</sup>, Henk Hagen<sup>2</sup>, Marcel Van Engelen<sup>1</sup>, Willy Meertens<sup>1</sup>, Andreas Schweizer-Theobaldt<sup>3</sup>, David Meunier<sup>4</sup>

<sup>1</sup>Dow Benelux B.V., Core R&D Analytical Science, Terneuzen, 4530 AA, The Netherlands; <sup>2</sup>Dow Benelux B.V., Packaging and Specialty Plastics R&D, Terneuzen, 4530 AA, The Netherlands; <sup>3</sup>Dow Deutschland GmbH, Core R&D Analytical Science, 77836, Rheinmunster, Germany; <sup>4</sup>The Dow Chemical Company, Core R&D Analytical Science, Midland, MI, 48674, USA

OC15 - Is chromatography still at the heart of the future lab?

Thorsten Teutenberg, D. Duisburg

Institut für Energie- und Umwelttechnik e. V. (IUTA), Bliersheimerstr. 58-60, 47229 Duisburg, Germany

OC16 - Automated preparation and analysis of haloacetic acids in water by GC/MS Mathias Vanlancker<sup>1,2</sup>, Joeri Vercammen<sup>1,2</sup>

<sup>1</sup>Interscience Expert Center, Avenue JE Lenoir 2, B-1348 Louvain-la Neuve, Belgium; <sup>2</sup>Ghent University, Faculty of Engineering and Architecture, Technologiepark Zwijnaarde 70A, 9052 Zwijnaarde, Belgium

#### **HYPHENATION AND MODULATION**

Session Chair: Paola Dugo (University of Messina, IT)

TU07 - Advances in two-dimensional liquid chromatography Bob W.J. Pirok

University of Amsterdam, Faculty of Science, Science Park 904, 1098 XH Amsterdam, The Netherlands

YES13 - Enhancing sensitivity in 2D-LC by hyphenating temperature-responsive phases with reversed phase liquid chromatography

<u>Kristina Wicht</u><sup>1</sup>, Mathijs Baert<sup>1</sup>, Sonja Krieger<sup>2</sup>, Norwin von Döhren<sup>3</sup>, André de Villiers<sup>4</sup>, Frederic Lynen<sup>1</sup>

<sup>1</sup>Department of Organic and Macromolecular Chemistry, Ghent University, 9000 Ghent, Belgium; <sup>2</sup>Agilent Technologies, Waldbronn, Germany; <sup>3</sup>Agilent Technologies, Middelburg, Netherlands; <sup>4</sup>Department of Chemistry, University of Stellenbosch, 7602 Matieland, South Africa

YES14 - Developing active-modulation interfaces for hyphenation of light-induced-degradation reactors with LC separations

Mimi den Uijl<sup>1</sup>, Bob Pirok<sup>1</sup>, Peter Schoenmakers<sup>1</sup>, Maarten van Bommel<sup>2</sup>

<sup>1</sup>Van 't Hoff Institute for Molecular Sciences, Faculty of Sciences, University of Amsterdam, The Netherlands; <sup>2</sup>Amsterdam School for Heritage, Media and Material Culture, Faculty of Humanities, University of Amsterdam, The Netherlands

YES15 - Application of evolutionary algorithms to optimise one- and two-dimensional gradient chromatographic separations

Bram Huygens, Gert Desmet

Vrije Universiteit Brussel, Department of Chemical Engineering

FP09 – Development of optimization strategies for heart-cut two-dimensional liquid chromatography

Denice van Herwerden

University of Amsterdam, NL

FP10 – A comparative study of UniSpray and Electrospray for the ionization of neuropeptides in LC-MS/MS

Jana Bongaerts

Vrije Universiteit Brussel, BE

FP11 – Deciphering the complex distributions of cellulose ethers by 2D-LC

Tijmen Bos

Vrije Universiteit Amsterdam, NL

FP12 – Optimization of an untargeted LC-MS method for metabolite profiling of restrictedvolume plasma samples

Karen Segers

Vrije Universiteit Brussel, BE

#### RSC SEPARATION SCIENCE GROUP: HIGH-THROUGHPUT ANALYSIS

Session Chair: Bob Boughtflower (University of Edinburgh, UK and GSK, UK)

KL17 - HTA and the clinical world

Lewis Couchman

Analytical Services International (ASI) Ltd., United Kingdom

KL18 - The Robot in your Lab; Friend or Foe?

Kathy Ridgway

Anatune Ltd.

OC17 - Will Bioanalysis surrender to the robotic army?

Arundhuti Sen

GSK

OC18 - Capillary Electrophoresis: Speed and Selectivity for High Throughput Analysis

Gordon Ross

Agilent Technolgies, UK

#### LC×LC(×LC) AND COUPLED COLUMNS

Session Chair: Frank Steiner (Thermo Fisher Scientific, DE)

KL19 - Advantages and limitations of HILIC in the second dimension of comprehensive twodimensional liquid chromatographic separations: A kinetic evaluation André de Villiers, Magriet Muller Stellenbosch University, South Africa

TU08 - Approaches Towards Method Development in Two-Dimensional HPLC Monika Maria Dittmann<sup>1</sup>, Stephan Buckenmaier<sup>2</sup>, Sascha Lege<sup>2</sup>

<sup>1</sup>Marxzell, Germany; <sup>2</sup>Agilent Technologies, Waldbronn, Germany

OC19 - Development of Microfluidic Chip Technology for Spatial Three-Dimensional Liquid Chromatography

<u>Jelle De Vos</u>, Thomas Themelis, Ali Amini, Sebastiaan Eeltink Department of Chemical Engineering, Vrije Universiteit Brussel, Belgium

OC20 - From batch to continuous processing: purification of a bioactive peptide by means of Multicolumn Countercurrent Solvent Gradient Purification (MCSGP)

Martina Catani¹, Chiara De Luca¹, Simona Felletti¹, Giulio Lievore¹, Alessandro Buratti¹, Antonio Ricci², Marco Macis², Walter Cabri², Massimo Morbidelli³, Alberto Cavazzini¹

Dept. Of Chemistry and Pharmaceutical Sciences, University of Ferrara, Ferrara, Italy;

Fresenius Kabi iPSUM, Villadose (Rovigo), Italy; Dept. of Chemistry and Applied Biosciences, Institute for Chemical and Bioengineering, ETH Zurich, Zurich, Switzerland

#### GAS CHROMATOGRAPHY AND DATA ANALYSIS

Session Chairs: Gabriel Vivo-Truyols (Tecnometrix, ES)

TU09 - Exotic fragrances of Namibia: Application of current fragrance analysis trends Stefan Louw<sup>1</sup>, Jacobina Sheehama<sup>1</sup>, Wencey Howaes<sup>1</sup>, Sabina Shikulo<sup>1</sup>, Celine Mukakalisa<sup>1</sup>, Theopolina Amakali<sup>1</sup>, Lydia Uusiku<sup>1</sup>, Renate Hans<sup>1</sup>, Karen Nott<sup>2</sup>, Amber Nott<sup>2</sup> <sup>1</sup>University of Namibia, Namibia; <sup>2</sup>Integrated Rural Development and Nature Conservation, Namibia

YES16 - Development of an untargeted and targeted multi-class method for cannabis products

<u>Flavio Antonio Franchina</u>, Lena Dubois, Jean-Francois Focant University of Liège, Belgium

YES17 - European lacquer in Context. Strategies to find THM-GC/MS resin biomarkers and application on historical lacquered objects.

<u>Louise Decq</u><sup>1,2</sup>, Steven Saverwyns<sup>1</sup>, Wim Fremout<sup>1</sup>, Delphine Steyaert<sup>3</sup>, Vincent Cattersel<sup>4</sup>, Emile Van Binnebeke<sup>3</sup>, Charles Indekeu<sup>4</sup>, Frederic Lynen<sup>2</sup>

<sup>1</sup>KIK-IRPA, Belgium; <sup>2</sup>Ghent University, Belgium; <sup>3</sup>Royal Museums of Art and History, Brussels, Belgium; <sup>4</sup>University of Antwerp, Belgium

YES18 - Optimization of untargeted screening workflow for the characterization of lung fluid samples

<u>Pierre-Hugues Stefanuto</u><sup>1</sup>, Delphine Zanella<sup>1</sup>, Florence Schleich<sup>2</sup>, Thibaut Dejong<sup>1</sup>, Monique Henket<sup>2</sup>, Renaud Louis<sup>2</sup>, Jean-François Focant<sup>1</sup>

<sup>1</sup>Organic and Biological Analytical Chemistry Group, MolSys, University of Liège, Belgium;

<sup>2</sup>Respiratory Medicine, GIGA I3, CHU Sart-Tilman, University of Liège, Belgium

FP13 – Revealing the reactivity of isomers of bio-oils by GC coupled to FTIC resonance mass spectrometry

Diana Catalina Palacio Lozano

University of Warwick, UK

FP14 – Multivariate Calibration of Chromatographic Fingerprints to Predict Antioxidant Potential in Argan kernels

Mourad Kharbach

Vrije Universiteit Brussel, BE

FP15 – KairosMS: A new tool for the processing of hyphenated ultrahigh resolution mass spectrometry data

**Hugh Jones** 

University of Warwick, UK

FP16 – Mass spectrometry with operation at constant ultrahigh resolution (OCULAR) Latifa AlOstad

University of Warwick, UK

#### FRIDAY JANUARY 31, 2020

#### HTC INNOVATION AWARD LECTURE AND DISCUSSION SESSION

Session Chairs: Alasdair Matheson (LC-GC) and Deirdre Cabooter (KU Leuven, BE)

KL20 – One Cell at a Time: 1D and 2D Separations for In-Depth Single-Cell and nanoscale Proteomics

Ryan T. Kelly (Brigham Young University, Utah, USA)

#### **HYPENATED TECHNIQUES**

Session Chair: František Švec (Charles University, CZ)

KL21 – Membrane-assisted solvent- and sorbent-phase microextraction of difficult liquid matrices

Hian Kee Lee (National University of Singapore, SG)

KL22 – *High-resolution two- (and three-) dimensional liquid chromatography* Peter Schoenmakers (University of Amsterdam, NL)

#### **COLUMN TECHNOLOGY**

Session Chair: John Langley (University of Southampton, UK)

KL23 - Porous polymer monolithic structures in hyphenated chromatographic techniques Frantisek Svec

Charles University, Czech Republic

KL24 - Shedding light on novel zwitterionic-teicoplanin chiral stationary phases for liquid chromatography: from fundamentals to innovative applications

<u>Alberto Cavazzini</u><sup>1</sup>, Francesco Gasparrini<sup>2</sup>, Simona Felletti<sup>1</sup>, Giulia Mazzoccanti<sup>2</sup>, Martina Catani<sup>1</sup>

<sup>1</sup>University of Ferrara, Italy; <sup>2</sup>quot; La Sapienza" University of Rome

#### **COUPLING TO MASS SPECTROMETRY**

Session Chair: Koen Sandra (RIC, BE)

YES19 - Detecting STAMPs of Microfluidic Separations by SERS and MALDI-MS

Pascal Breuer<sup>1</sup>, Freek Ariese<sup>2</sup>, Govert W. Somsen<sup>3</sup>, Peter J. Schoenmakers<sup>1</sup>

<sup>1</sup>University of Amsterdam, Faculty of Science, Van 't Hoff Institute for Molecular Sciences,
The Netherlands.; <sup>2</sup>Vrije Universiteit, Faculty of Science, Biophotonics and Medical Imaging,
The Netherlands.; <sup>3</sup>Vrije Universiteit, Faculty of Science, Biomolecular Analysis and
Spectroscopy, The Netherlands

YES20 - Unlocking the composition of gasoline gum content by application of GC-MS and UHPSFC-MS

<u>Andreas Panagiotopoulos</u><sup>1</sup>, Jim Barker<sup>2</sup>, Jacqueline Reid<sup>2</sup>, Julie Herniman<sup>1</sup>, G John Langley<sup>1</sup> <sup>1</sup>Chemistry, Faculty of Engineering and Physical Sciences, University of Southampton, UK; <sup>2</sup>Innospec Ltd, UK

YES21 - UHPSFC-MS to unravel complex PEG derivatives used in pharmaceutical formulation

<u>Sergio Cancho Gonzalez</u><sup>1</sup>, Paul Ferguson<sup>2</sup>, Sophie Bailes<sup>2</sup>, Julie Herniman<sup>1</sup>, G. John Langley<sup>1</sup>

<sup>1</sup>Chemistry, Faculty of Engineering and Physical Sciences, University of Southampton, UK; <sup>2</sup>PT&D Department, AstraZeneca, Macclesfield, Cheshire, UK

YES22 - Development and implementation of multi-dimensional LC-MS setup for a faster and more effective characterization of bio-therapeutic products

<u>Julien Camperi</u><sup>1</sup>, Lu Dai<sup>1</sup>, Davy Guillarme<sup>2</sup>, Cinzia Stella<sup>1</sup>

<sup>1</sup>Protein Analytical Chemistry, Genentech, 1 DNA Way, South San Francisco, CA, 94080, USA; <sup>2</sup>School of Pharmaceutical Sciences, University of Geneva, CMU, Rue Michel-Servet, 1, 1206 Geneva, Switzerland

#### RSC SEPARATION SCIENCE GROUP: DATA COMPLEXITY, MINING, AND CURATION

Session Chairs: Sam Whitmarsh (BP, UK) / Arun Sen (GSK, UK)

KL25 - The devils in the detail of our data processing David Kilgour Nottingham Trent University, United Kingdom

KL26 - Data Analytics: the journey from complexity to clarity

Camilla Liscio

Anatune, United Kingdom

OC22 - Extracting value from untargeted e-cigarette aerosol analysis: a metabolomics approach

Justin Frosina, Michał Brokl

OC23 - Non-targeted analysis of organic contaminants in complex environmental matrices-Applications of metabolomics data workflow

Ioannis Sampsonidis<sup>1,3</sup>, Thomas Aspray<sup>2</sup>, Umer Zeeshan Ijaz<sup>1</sup>, <u>Caroline Gauchotte-Lindsay</u><sup>1</sup> James Watt School of Engineering, University of Glasgow, Oakfield Avenue, Glasgow G12 8QQ, UK; <sup>2</sup>ERS ltd, Westerhill Road, Bishopbriggs, Glasgow, G64 2QH, UK; <sup>3</sup>Department of Nutritional Sciences, International Hellenic University, Sindos Campus, 574 00 Thessaloniki, Greece

#### **ADVANCES IN MULTI-DIMENSIONAL SEPARATIONS**

Session Chairs: Rudy Senten (Royal Flemish Chemical Society, Belgium)

KL27 - Recent Progress on the Simulation of Second Dimension Separations for 2D-LC, with Application to Biomolecule Separations

<u>Dwight Stoll</u><sup>1</sup>, Gabriel Leme<sup>1</sup>, Tyler Brau<sup>1</sup>, Thomas Lauer<sup>1</sup>, Gregory Staples<sup>2</sup>, Sarah Rutan<sup>3</sup> <sup>1</sup>Gustavus Adolphus College, United States of America; <sup>2</sup>Agilent Technologies, United States of America; <sup>3</sup>Virginia Commonwealth University, United States of America

KL28 - Exploiting Comprehensive Two-Dimensional Liquid Chromatography (LCxLC) for the Determination of Bioactive Compounds in Natural Products

Paola Dugo<sup>1,2</sup>, Francesco Cacciola<sup>1</sup>, Katia Arena<sup>1</sup>, Luigi Mondello<sup>1,2,3,4</sup>

<sup>1</sup>University of Messina, Italy; <sup>2</sup>Chromaleont s.r.l., Messina, Italy; <sup>3</sup>Unit of Food Science and Nutrition, Department of Medicine, University Campus Bio-Medico of Rome, Italy; <sup>4</sup>BeSep s.r.l., Messina, Italy

OC24 - Automated flexibility to implement two-dimensional and multiple LC-MS methods in a single instrument setup

Giorgia Greco<sup>1</sup>, Maria Gruebner<sup>1</sup>, Michael Witting<sup>2</sup>, Frank Steiner<sup>1</sup>

<sup>1</sup>Thermo Fisher Scientific, Germering, Germany; <sup>2</sup>Helmholtz Zentrum München, Research Unit Analytical BioGeoChemistry, Neuherberg, Germany

OC25 – Approaches towards multidimensional LC within the biopharmaceutical industry Isabelle François

#### **NEW ANALYTICAL METHODOLOGIES**

Session Chairs: Jelle De Vos (Vrije Universiteit Brussel, BE)

**T**U10 - Basic principles of analytical method validation Erwin Adams

KU Leuven, University of Leuven, Department of Pharmaceutical and Pharmacological Sciences, Pharmaceutical Analysis, Herestraat 49, O&N2, PB 923, B-3000 Leuven, Belgium

YES23 - Characterization of the Functionality-type x Molecular Weight Distribution of Complex Polyesters Using NPLCxSEC

Gino Groeneveld<sup>1</sup>, Andrea Gargano<sup>1</sup>, Robert Voeten<sup>2</sup>, Ron Peters<sup>1,3</sup>, Peter Schoenmakers<sup>1</sup> <sup>1</sup>University of Amsterdam, Van 't Hoff Institute for Molecular Sciences, Science Park 904 1098 XH Amsterdam, The Netherlands; <sup>2</sup>Vrije Universiteit Amsterdam, Amsterdam Institute for Molecules, Medicines and Systems, de Boelelaan 1083, 1081HV Amsterdam, The Netherlands; <sup>3</sup>DSM Coating Resins, Sluisweg 12, 5145 PE Waalwijk, The Netherlands

YES24 - Analysis of base oil mixtures with automated machine learning Samuel Ellick<sup>1</sup>, Paul J. Gates<sup>1</sup>, Christopher J. Arthur<sup>1</sup>, Christianne Wicking<sup>2</sup>, Thomas Hancock<sup>2</sup>, Samuel Whitmarsh<sup>2</sup>

<sup>1</sup>School of Chemistry, University of Bristol, Bristol, BS8 1TS, United Kingdom; <sup>2</sup>BP Technology Centre, Whitchurch Hill, Pangbourne, RG8 7QR

YES25 - Intelligent invertebrate toxicology (iNVERTOX): Linking metabolomics to behavioural changes in a freshwater invertebrate

<u>Thomas H Miller</u><sup>1</sup>, Keng Tiong Ng<sup>1</sup>, James I MacRae<sup>2</sup>, Nicolas R Bury<sup>3</sup>, Stewart F Owen<sup>4</sup>, Leon P Barron<sup>1</sup>

1: King's College London, London, SE1 9NH, UK; 2: The Francis-Crick Institute, London, NW1 1AT, UK; 3: University of Suffolk, Ipswich, UK; 4: AstraZeneca, Cheshire SK10 4TF, UK

YES26 - Monolithic molecularly imprinted polymer and nano-liquid chromatography for online miniaturized trace analysis in biological fluids

Thomas Bouvarel<sup>1</sup>, Nathalie Delaunay<sup>1</sup>, Valérie Pichon<sup>1,2</sup>

<sup>1</sup>Department of Analytical, Bioanalytical Sciences, and Miniaturization, UMR CBI 8231, ESPCI Paris, PSL University, 75005 Paris, France; <sup>2</sup>Sorbonne Université, 75005 Paris, France

#### **HTC-16 CLOSING SESSION**

Session Chairs: Frederic Lynen (Ghent University, BE) and Sebastiaan Eeltink (Vrije Universiteit Brussel, BE)

PL04 - Synthesis and functionalisation of nanostructured porous polymer materials for analytical applications

Emily F Hilder

University of South Australia, Australia

PL05 - Reflections on half a century of research in capillary gas chromatography
Pat Joseph Sandra

Research Institute for Chromatography, Belgium

#### **VENDOR SEMINARS**

#### SHIMADZU - Wednesday, 29 January 2020

Carotenoids and Apocarotenoids Determination by SFE/ SFC Triple Quadrupole Mass Spectrometry

Presenter: Prof. Paola Dugo (Food Chemistry, University of Messina, Italy)

#### AGILENT TECHNOLOGIES - Thursday, 30 January 2020

Mass Analysis Designed for Everyone

Presenter: Lilla Guricza (Agilent Technologies, Waldbronn, Germany)

#### AGILENT TECHNOLOGIES - Friday, 31 January 31 2020

Applying GCxGC to botanical flavour profiling in gin using SPME and Smart Connected GC - Using Self Aware systems to increase productivity

Presenters: Onno Kwast (JSB Netherlands) and Remko Van Loen (Agilent Technologies)

#### **POSTERS**

DATA-01 - Reinforcement Learning for the Optimization of Scouting Runs and Retention Modeling in Liquid Chromatography

<u>Alexander Kensert</u><sup>1</sup>, Gilles Collaerts<sup>1</sup>, Kyriakos Efthymiadis<sup>2</sup>, Gert Desmet<sup>3</sup>, Deirdre Cabooter<sup>1</sup>

<sup>1</sup>University of Leuven, Department of Pharmaceutical Sciences, Herestraat 49, Leuven, Belgium; <sup>2</sup>Vrije Universiteit Brussel, Department of Computer Science, Pleinlaan 9, 1050 Brussel, Belgium; <sup>3</sup>Vrije Universiteit Brussel, Department of Chemical Engineering, Pleinlaan 2, 1050 Brussel, Belgium

DATA-02 - KairosMS: A new tool for the processing of hyphenated ultrahigh resolution mass spectrometry data

<u>Hugh E. Jones</u><sup>1,2</sup>, Remy Gavard<sup>2</sup>, Diana Catalina Palacio Lozano<sup>1</sup>, Mary J. Thomas<sup>1,2</sup>, David Rossell<sup>3</sup>, Simon E. F. Spencer<sup>4</sup>, Mark P. Barrow<sup>1</sup>

<sup>1</sup>Department of Chemistry, University of Warwick, United Kingdom; <sup>2</sup>MAS CDT, Senate House, University of Warwick, United Kingdom; <sup>3</sup>Department of Economics & Business, Universitat Pompeu Fabra, Barcelona, Spain; <sup>4</sup>Department of Statistics, University of Warwick, United Kingdom

DATA-03 - Mass spectrometry with operation at constant ultrahigh resolution (OCULAR): advances for the analysis of complex mixtures

Molly Hayle<sup>1</sup>, Rory Downham<sup>1</sup>, Latifa AlOstad<sup>1</sup>, Diana Catalina Palacio Lozano<sup>1</sup>, Remy Gavard<sup>2</sup>, Mary J. Thomas<sup>1,2</sup>, David D. Stranz<sup>3</sup>, Enrique Mejia-Ospino<sup>4</sup>, Alexander Guzman<sup>5</sup>, Simon E. F. Spencer<sup>6</sup>, David Rossell<sup>7</sup>, Mark P. Barrow<sup>1</sup>

<sup>1</sup>Department of Chemistry, University of Warwick, Coventry, CV4 7AL, UK.; <sup>2</sup>Molecular Analytical Science Centre of Doctoral Training, University of Warwick Coventry, CV4 7AL, UK; <sup>3</sup>Sierra Analytics Inc., Modesto, California, USA; <sup>4</sup>Department of Chemistry, Universidad Industrial de Santander, Bucaramanga, Colombia; <sup>5</sup>Instituto Colombiano del Petroleo, Ecopetrol, Piedecuesta, Colombia; <sup>6</sup>Department of Statistics, University of Warwick,

Coventry, CV4 7AL, UK; <sup>7</sup>Department of Economics & Business, Universitat Pompeu Fabra, Barcelona 08005, Spain

FOOD-01 - Profiling of phenolic compounds using UPLC–MS for determining the geographical origin of green coffee beans from Ethiopia

Bewketu Mehari<sup>1</sup>, Mesfin Redi-Abshiro<sup>2</sup>, Bhagwan Chandravanshi<sup>2</sup>, Sandra Combrinck<sup>3</sup>, Robert McCrindle<sup>3</sup>, Minaleshewa Atlabachew<sup>4</sup>

<sup>1</sup>University of Gondar, Ethiopia; <sup>2</sup>Addis Ababa University, Ethiopia; <sup>3</sup>Tshwane University of Technology, South Africa; <sup>4</sup>Bahir Dar University, Ethiopia

FOOD-02 - The importance of sufficient chromatographic separation for identity confirmation Henk Gerritsen, Irma Bongers, Tina Zuidema Wageningen Food Safety Research, The Netherlands

FOOD-03 - Multivariate Calibration of Chromatographic Fingerprints to Predict Antioxidant Potential in Argan kernels: a Metabolomic Approach

Mourad Kharbach<sup>1,2</sup>, Johan Viaene<sup>1</sup>, Abdelaziz Bouklouze<sup>2</sup>, Yvan Vander Heyden<sup>1</sup>
<sup>1</sup>Department of Analytical Chemistry, Applied Chemometrics and Molecular Modelling,
CePhaR, Vrije Universiteit Brussel (VUB), Laarbeeklaan 103, B-1090 Brussels, Belgium;
<sup>2</sup>Pharmaceutical and Toxicological Analysis Research Team, Laboratory of Pharmacology
and Toxicology, Faculty of Medicine and Pharmacy, University Mohammed V- RabatMorocco

FOOD-04 - Analytical workflow for untargeted analysis: sampling, separation, detection, and data analysis methods to unravel aroma complexity

<u>Flavio Antonio Franchina</u>, Delphine Zanella, Pierre-Hugues Stefanuto, Jean-François Focant University of Liège, Belgium

FOOD-05 - Radiokitchen: Use of the 14C-radiodetector UPLC/HR-MS/MS approach to investigate the fate of pesticides during food processing

Mark Bücking<sup>1,2</sup>, Stephan Hennecke<sup>1</sup>, Bernd Göckener<sup>1</sup>

<sup>1</sup>Fraunhofer Institute for Molecular Biology and Applied Ecology IME-AE, Auf dem Aberg 1, 57392 Schmallenberg, Germany; <sup>2</sup>Monash University, School of Chemistry, 13 Rainforest Walk, Clayton, Victoria, 3800, Australia

FOOD-06 - Comparative study of various sorbents for determination of ochratoxin A and ochratoxin B in archive Tokaj wines using on-line SPE-HPLC

Aneta Kholová<sup>1</sup>, Ivona Lhotská<sup>1</sup>, Ivan Špánik<sup>2</sup>, Andrea Machyňáková<sup>2</sup>, Dalibor Šatínský<sup>1</sup>
<sup>1</sup>Department of Analytical Chemistry, Faculty of Pharmacy, Charles University, Czech
Republic; 2: The Institute of Analytical Chemistry, Faculty of Chemical and Food Technology,
Slovak University of Technology, Slovakia

FOOD-07 - Pushing the boundaries of hyphenation: Comprehensive aroma profiling of food and beverages

<u>Laura McGregor</u>, Bob Green, Aaron Parker, Anthon Buchanan SepSolve Analytical, United Kingdom FOOD-08 - Volatile profile of white wine with an easy-to-use GCxGC diverting flow modulator: towards the routine evaluation of the winemaking process

<u>Vakare Merkyte</u><sup>1,2</sup>, Edoardo Longo<sup>1,2</sup>, Daniele Fortuna<sup>1,2</sup>, Amanda Dupas de Matos<sup>1,2</sup>, Giulia Windisch<sup>1,2</sup>, Emanuele Boselli<sup>1,2</sup>

<sup>1</sup>Faculty of Science and Technology, Free University of Bozen-Bolzano, Piazza Università, 5, 39100 Bolzano, Italy; <sup>2</sup>Oenolab, NOITechPark Alto Adige/Südtirol, Via A. Volta, 13B - 39100 Bolzano, Italy

FOOD-09 - Rapid Separation of trans/cis Fatty Acid Methyl Esters with Agilent DB-FastFAME GC column

<u>Laura van Hoeve-Provoost</u><sup>1</sup>, Yun Zou<sup>2</sup>, Gustavo Serrano-Izaguirre<sup>3</sup>, Phil Stremple<sup>3</sup>
<sup>1</sup>Agilent Technologies, Middelburg, The Netherlands; <sup>2</sup>Agilent Technologies, Shanghai, China; <sup>3</sup>Agilent Technologies, Wilmington DE, USA

FOOD-10 - Simple, reliable determination of biogenic amines in wine. Direct analysis of underivatized biogenic amines by LC-ESI-MS

Giuliana Vinci, Laura Gobbi, Lucia Maddaloni

Department of Management, Sapienza University of Rome, Via del Castro Laurenziano 9, 00161 Rome, Italy

FOOD-11 - Chemical profiling of taste related compounds of various Eastern Scheldt seaweeds

<u>Tanja Moerdijk-Poortvliet</u>, Simona T. Popovici, Dylan de Jong, Roy Fremouw, Sandra de Reu, Geert Mol, Dorien Derksen

HZ University of Applied Sciences, Edisonweg 4, 4382 NW Vlissingen, The Netherlands

FUN-01 - Morphology optimization and assessment of the performance limits of nanostructured polymer monolithic columns for the analysis of intact proteins <u>José Luís Dores-Sousa</u>, Sebastiaan Eeltink Vrije Universiteit Brussel (VUB), Belgium

FUN-02 - Development of an improved protocol for the measurement of molecular diffusion coefficients of biopharmaceuticals

Donatela Sadriaj<sup>1</sup>, Huiying Song<sup>1</sup>, Gert Desmet<sup>2</sup>, Deirdre Cabooter<sup>1</sup>

<sup>1</sup>University of Leuven, Department of Pharmaceutical and Pharmacological Sciences, Herestraat 49, Leuven, Belgium; <sup>2</sup>Vrije Universiteit Brussel, Department of Chemical Engineering, Pleinlaan 2, 1050 Brussel, Belgium

FUN-03 - Determination of the Diffusion Coefficients in SFC for a Wide Variety of Samples and Conditions

<u>Vincent Pepermans</u>, Bart Degreef, Gert Desmet, Ken Broeckhoven Vrije Universiteit Brussel, Belgium

FUN-04 - An experimental procedure for the in-depth evaluation of band broadening phenomena in capillary and nano-size columns

Haibin Li<sup>1,2</sup>, Zhengjin Jiang<sup>2</sup>, Deirdre Cabooter<sup>1</sup>

<sup>1</sup>KU Leuven, Belgium; <sup>2</sup>Jinan University, China

FUN-05 - Design and evaluation of flow distributors for radially elongated hexagonal pillar arrays column using computational fluid dynamics modelling

Farideh Haghighi<sup>1,2</sup>, Zahra Talebpour<sup>1</sup>, Amir Sanati Nezhad<sup>2</sup>

<sup>1</sup>Department of Chemistry, Faculty of Physics and Chemistry, Alzahra University, Vanak, Tehran, Iran; <sup>2</sup>BioMEMS and Bioinspired Microfluidic Laboratory, Department of Mechanical and Manufacturing Engineering, University of Calgary, Alberta, Canada

FUN-06 - Polymerization of the Through-pores in HPLC Columns for Enhanced SEM Based Assessment of Packing Order

Zhanyao Hou<sup>1</sup>, Ken Broeckhoven<sup>2</sup>, Gert Desmet<sup>2</sup>, Frederic Lynen<sup>1</sup>

<sup>1</sup>Separation Science Group, Department of Organic and Macromolecular Chemistry, Ghent University, Krijgslaan 281 S4-Bis, Ghent, Belgium; <sup>2</sup>Free University Brussels, Department of Chemical Engineering, Pleinlaan 2, Brussel, Belgium

FUN-07 - Creating Monolithic Stationary Phases in Targeted Regions of 3D-printed Titanium Devices

<u>Marta Passamonti</u><sup>1</sup>, Suhas H. Nawada<sup>1</sup>, Sinéad Currivan<sup>2</sup>, Andrea Gargano<sup>1</sup>, Peter J. Schoenmakers<sup>1</sup>

<sup>1</sup>University of Amsterdam, The Netherlands; <sup>2</sup>Centre for Research in Engineering Surface Technology, Technological University Dublin, FOCAS Institute, Ireland

FUN-08 - Unraveling the molecular interactions driving retention and selectivity of a sphingomyelin-based stationary phase by QSPR interpreted through block relevance analysis

<u>Giacomo Russo</u><sup>1</sup>, Maura Vallaro<sup>2</sup>, Giulia Caron<sup>2</sup>, Frederic Lynen<sup>1</sup>

<sup>1</sup>Separation Science Group, Department of Organic and Macromolecular Chemistry, Ghent University, Krijgslaan 281, S4-bis, B-9000 Ghent, Belgium.; <sup>2</sup>CASSMedChem Research Group, Molecular Biotechnology and Health Sciences Department, University of Turin, Italy.

FUN-09 - *Evaluation of system performance in ultra-high-pressure operation mode*<u>Zhuoheng Zhou<sup>a</sup></u>, Mauro De Pra<sup>b</sup>, Frank Steiner<sup>b</sup>, Gert Desmet<sup>a</sup>, Sebastiaan Eeltink<sup>a</sup>

<sup>a</sup> Vrije Universiteit Brussel, Department of Chemical Engineering, Pleinlaan 2, B-1050,
Belgium; Thermo Fisher Scientific, Germering, Germany

GC(xGC)-01 - Development and application of PLOT GC columns on the Agilent Intuvo 9000 GC

<u>John Oostdijk</u><sup>1</sup>, Roy Lensen<sup>1</sup>, Abbey Fausett<sup>2</sup>, Gustavo Serrano-Izaguirre<sup>2</sup>

<sup>1</sup>Agilent Technologies Netherlands BV, The Netherlands; <sup>2</sup>Agilent technologies, Inc.

GC(xGC)-02 - Chemical characterization and in vitro antioxidant activity of essential oil from Commiphora kraeuseliana resin

Wencey Howaes, Celine Mukakalisa, <u>Stefan Louw</u> University of Namibia, Namibia

GC(xGC)-03 - Turning up the heat on WAX GC columns without getting burned Laura van Hoeve-Provoost<sup>1</sup>, Vanessa Abercrombie<sup>2</sup>

<sup>1</sup>Agilent Technologies, Middelburg, The Netherlands; <sup>2</sup>Agilent Technologies, Folsom CA, USA

GC(xGC)-04 - Innovations in GCxGC software for characterisation of petrochemicals Nick Bukowski, Laura McGregor, Steve Smith, Aaron Parker SepSolve Analytical, United Kingdom

GC(xGC)-05 - The PHySICAL Project: Research Protocol Applied on a Japanese Buddha Statue

<u>Jonas Veenhoven</u><sup>1,2,4</sup>, Steven Saverwyns<sup>2</sup>, Delphine Mesmaeker<sup>3</sup>, Nathalie Vandeperre<sup>3</sup>, Maarten van Bommel<sup>4</sup>, Henk van Keulen<sup>5</sup>, Frederic Lynen<sup>1</sup>

<sup>1</sup>Ghent University, Belgium; <sup>2</sup>Royal Institute for Cultural Heritage (KIK/IRPA), Belgium; <sup>3</sup>Royal Museums of Art and History, Belgium; <sup>4</sup>University of Amsterdam, The Netherlands; <sup>5</sup>Cultural Heritage Agency of the Netherlands, The Netherlands

GC(xGC)-06 - Revealing the reactivity of isomers of bio-oils by gas chromatography coupled to Fourier transform ion cyclotron resonance mass spectrometry

Diana Catalina Palacio Lozano<sup>1</sup>, Hugh E. Jones<sup>1,2</sup>, Remy Gavard<sup>2</sup>, Mary J. Thomas<sup>1,2</sup>,
Claudia X. Ramirez<sup>3</sup>, Enrique Mejia-Ospino<sup>3,4</sup>, Matthias Witt<sup>5</sup>, Mark P. Barrow<sup>1</sup>

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Bucaramanga, Colombia; ⁴Centro de Materiales y Nanociencias (CMN), Universidad

Industrial de Santander, Bucaramanga, 678, Colombia; ⁵Bruker Daltonik GmbH, Bremen,

Germany

GC(xGC)-07 - Polymer Sequence investigations with pyrolysis-GC <u>Wouter Knol</u><sup>1</sup>, Till Gruendling<sup>2</sup>, Christiane Lang<sup>2</sup>, Bastiaan Staal<sup>2</sup>, Bob Pirok<sup>1</sup>, Ron Peters<sup>1,3</sup>, Peter Schoenmakers<sup>1</sup>

<sup>1</sup>Van 't Hoff Institute for Molecular Science (HIMS), University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands; <sup>2</sup>BASF, Carl-Bosch-Strasse 38, Ludwigshafen am Rhein, Germany; <sup>3</sup>DSM, Sluisweg 12, 5145 PE, Waalwijk, The Netherlands

GC(xGC)-08 - Thermal desorber – gas chromatography with offline and inline liquid calibration for the determination of residual solvents in drug loaded albumin Kris Wolfs, Adissu Asfaw, Ann Van Schepdael, Erwin Adams KU Leuven, Pharmaceutical Sciences, Belgium

GC(xGC)-09 - Total volatilization headspace gas chromatography for the determination of volatile methyl siloxanes in personal care products

<u>Juan Antonio Aspromonte</u><sup>1</sup>, Giulia Giacoppo<sup>1,2</sup>, Kris Wolfs<sup>1</sup>, Erwin Adams<sup>1</sup>

<sup>1</sup>KU Leuven, Belgium; <sup>2</sup>University of Messina, Italy

GC(xGC)-10 - Considerations on adsorbent materials for in vitro and ex vivo VOCs (bio-)sampling

<u>Flavio Antonio Franchina</u>, Delphine Zanella, Thibaut Dejong, Jean-François Focant University of Liège, Belgium

GC(xGC)-11 - Optimization of a multidimensional gas chromatographic separation. Classical steps toward a better characterization of the separation space

Meriem Gaida, Kinjal B. Bhatt, Benedikt A. Weggler, Flavio A. Franchina, Jean-François Focant

University of Liège, MolSys - Organic and Biological Analytical Chemistry Group, Quartier Agora, Place du Six Août 11, B6c, 4000 Liège, Belgium

GC(xGC)-12 - Can increased Instrumental Sensitivity Replace Extensive Sample Preparation?

<u>Kinjal B. Bhatt</u>, Meriem Gaida, Benedikt A. Weggler, Flavio A. Franchina, Jean-François Focant

University of Liège, MolSys - Organic and Biological Analytical Chemistry Group, Quartier Agora, Place du Six Août 11, B6c, 4000 Liège, Belgium

GC(xGC)-13 - Tackling challenges for the adoption of two-dimensional gas chromatography in Forensic Sciences

Lena M. Dubois<sup>1</sup>, Katelynn A. Perrault<sup>2</sup>, Jean-François Focant<sup>1</sup>

<sup>1</sup>University of Liège, MolSys - Organic and Biological Analytical Chemistry Group, Quartier Agora, Place du Six Août 11, B6c, 4000 Liège, Belgium; <sup>2</sup> Laboratory of Forensic and Bioanalytical Chemistry, Forensic Sciences Unit, Division of Natural Sciences and Mathematics, Chaminade University of Honolulu, Honolulu, HI 96816, USA

GC(xGC)-14 - Development of a new polymeric ionic liquid stationary phase for use in Hightemperature GC

Adriaan Ampe, Frederic Lynen

UGent, Belgium

HYP-01 - Double barrel ESI source and novel tandem nanoLC-MS setup enables 24/7 proteome profiling with close to 100% MS utilization

Runsheng Zheng<sup>1</sup>, Thomas Lanzinner<sup>2</sup>, Georg Völkle<sup>3</sup>, Christopher Pynn<sup>1</sup>, Jan Linnemann<sup>2</sup>, John Modrow<sup>2</sup>, <u>Wim Decrop</u><sup>1</sup>, Andreas Tebbe<sup>2</sup>, Peter Jehle<sup>1</sup>, Mauro De Pra<sup>1</sup>, Alexander Boychenko<sup>1</sup>

<sup>1</sup>Thermo Fisher Scientific, Dornierstr. 4, 82110 Germering, Germany; <sup>2</sup>Evotec (München) GmbH, Am Klopferspitz 19a, 82151 Martinsried, Germany; <sup>3</sup>Sonation GmbH, Alte Schulstr. 39, 88400 Biberach, Germany

HYP-02 - Hyphenated Method (LC-MS/MS-Fluorometric) for Determination of Nucleoside Triphosphates and Analogs in Peripheral Blood Mononuclear Cells (PBMCs)
Christos Kolaris<sup>1</sup>, Susan Zondlo<sup>1</sup>, Yuwen Zhao<sup>1</sup>, John Ling<sup>2</sup>, Deqing Xiao<sup>2</sup>, Brian Kearney<sup>2</sup>, Thomas L. Tarnowski<sup>2</sup>

<sup>1</sup>QPS, LLC, Newark, Delaware, USA; <sup>2</sup>Gilead Sciences, Inc., Foster City, CA,USA

HYP-03 - Characterization of Polymers by Hyphenating Pyrolysis with GPC-MS

<u>Eva Tudela Palomar</u><sup>1</sup>, Bart Otte<sup>1</sup>, Alex Konig<sup>1</sup>, Sebastian Hagenhoff<sup>2</sup>, Matthias Pursch<sup>2</sup>

1 Dow Benelux B.V, The Netherlands; 2 Dow Stade Produktions GMBH & CO. OHG

HYP-04 - A non-targeted analysis approach for screening of volatile and semi-volatile compounds by off-line sampling coupled to ATD-GC-MS (automated thermal desorption gas chromatography mass spectrometry)

Quentin Dutertre, Angelo Balsamo, Samuel Kleinhans, Anneke Glabasnia, Catherine Goujon-Ginglinger

Philip Morris, Switzerland

HYP-05 - Coupling of Thermal Gravimetric Analysis with Fast Gas Chromatographic Separation - Mass Selective Detection and its Applications for Material Testing An Adams, Wilco Hoogerwerf, Pascal Pijcke, Ron Bassie, Brian Dickie Dow Benelux

HYP-06 - Is my Decaffeinated Coffee Caffeine-Free? Engaging Chemistry Undergraduates with Mass Spectrometry and Chromatography

Julie Herniman, G John Langley

University of Southampton, United Kingdom

HYP-07 - Particle number and stoichiometric characterization of lipid-protein nanoparticle assemblies in biofluids by size fractionation and comprehensive quantitative LC-MS/MS analysis

Zsuzsanna Kuklenyik, John R. Barr

Centers for Disease Control and Prevention, United States of America

MDLC-01 - Complementary Dual LC as Alternative to Multi Heart-Cut LC for Samples of Medium Complexity resulting in improved precision, sensitivity and productivity Frank Steiner, Maria Gruebner, Mauro De Pra

Thermo Fisher Scientific, Germany

MDLC-02 - Development of optimization strategies for heart-cut two-dimensional liquid chromatography

<u>Denice van Herwerden</u>, Stef R.A. Molenaar, Andrea F.G. Gargano, Peter J. Schoenmakers, Bob W.J. Pirok

Van 't Hoff Institute for Molecular Science (HIMS), Analytical Chemistry group, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, the Netherlands

MDLC-03 - Numerical and Experimental Investigation of Sample Loss and Dispersion Occurring in Sample Loops Used in 2D-LC Setups

<u>Ali Moussa</u><sup>1</sup>, Thomas Lauer<sup>2</sup>, Dwight Stoll<sup>2</sup>, Gert Desmet<sup>1</sup>, Ken Broeckhoven<sup>1</sup>

<sup>1</sup>Vrije Universiteit Brussel, Belgium; <sup>2</sup>Gustavus Adolphus College, United States

MDLC-04 - Deciphering the complex distributions of cellulose ethers by 2D-LC <u>Tijmen S. Bos</u><sup>1,4</sup>, Jindra Purmova<sup>2</sup>, Leif Karlson<sup>2</sup>, Rob Haselberg<sup>1,4</sup>, Peter J. Schoenmakers<sup>3,4</sup>, Govert W. Somsen<sup>1,4</sup>

<sup>1</sup>BioAnalytical Chemistry, Amsterdam Institute for Molecules, Medicines and Systems, Vrije Universiteit Amsterdam, De Boelelaan 1108, 1081 HZ Amsterdam, The Netherlands; <sup>2</sup>Nouryon, Zutphenseweg 10, 7418 AJ Deventer, The Netherlands; <sup>3</sup>Van 't Hoff Institute for Molecular Science (HIMS), University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands; <sup>4</sup>Center for Analytical Sciences Amsterdam (CASA), The Netherlands

MDLC-05 - A 2D-LC-MS Method for Impurity Profiling of Synthetic Oligonucleotides

<u>Feiyang Li</u>, Ryan Karongo, Stefanie Bäurer, Michael Lämmerhofer Eberhard-Karls-University Tübingen, Germany

MDLC-06 - Development of peak-tracking algorithms for use in data analysis and method optimization in multi-dimensional liquid chromatography

<u>Stef R.A. Molenaar</u><sup>1</sup>, Dwight R. Stoll<sup>2</sup>, Ron A.H. Peters<sup>1,3</sup>, Govert W. Somsen<sup>4</sup>, Peter J. Schoenmakers<sup>1</sup>, Bob W.J. Pirok<sup>1</sup>

<sup>1</sup>Van 't Hoff Institute for Molecular Sciences, Analytical Chemistry Group, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands; <sup>2</sup>Department of Chemistry, Gustavus Adolphus College, Saint Peter, Minnesota 56082, United States; <sup>3</sup>DSM Coating Resins, Sluisweg 12, 5145 PE Waalwijk, The Netherlands; <sup>4</sup>Division of BioAnalytical Chemistry, Amsterdam Institute for Molecules, Medicines and Systems, Vrije Universiteit Amsterdam, De Boelelaan 1108, 1081 HZ Amsterdam, The Netherlands

MDLC-07 - Cold-Trap Modulated LCxLC for Polymer Analysis

<u>Leon E. Niezen</u><sup>1</sup>, Bastiaan B.P. Staal<sup>2</sup>, Christiane Lang<sup>2</sup>, Bob W.J. Pirok<sup>1</sup>, Peter J. Schoenmakers<sup>1</sup>

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MDLC-08 - 2D-LC-MS/MS for Bioanalytical Quantitation of Chiral Drugs Sonja Schipperges<sup>1</sup>, Lucas C. Harps<sup>2</sup>, Felix Bredendiek<sup>2</sup>, Maria K. Parr<sup>2</sup>, Bernhard Wuest<sup>1</sup>, Andreas Borowiak<sup>1</sup>

<sup>1</sup>Agilent Technologies, Germany; <sup>2</sup>Freie Universitaet Berlin, Germany

MDLC-09 - Enhancing the Application and Exploitation of Temperature Gradients in Temperature Responsive Liquid Chromatography

Mathijs Baert<sup>1</sup>, Roman Szucs<sup>2</sup>, Filip Du Prez<sup>3</sup>, Ken Broeckhoven<sup>4</sup>, Frederic Lynen<sup>1</sup>

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MDLC-10 - Enhanced determination of pharmaceutical impurities through a temperature-responsive stationary phase in 2D-LC (TRLCxRPLC)

<u>Kristina Wicht</u><sup>1</sup>, Mathijs Baert<sup>1</sup>, Sonja Schipperges<sup>2</sup>, Norwin von Doehren<sup>3</sup>, André de Villiers4, Frederic Lynen<sup>1</sup>

<sup>1</sup> Department of Organic and Macromolecular Chemistry, Ghent University, 9000 Ghent, Belgium; <sup>2</sup> Agilent Technologies, Waldbronn, Germany; <sup>3</sup> Agilent Technologies, Middelburg, Netherlands; <sup>4</sup> Department of Chemistry, University of Stellenbosch, 7602 Matieland, South Africa

PHA-01 - Assessment of operating conditions affecting the peak capacity of intact protein bioanalysis in hydrophobic interaction liquid-chromatography

Raphael Ewonde Ewonde<sup>1</sup>, Daniel Eßer<sup>2</sup>, Sebastiaan Eeltink<sup>1</sup> Vrije Universiteit Brussels, Belgium; <sup>2</sup>YMC Europe, Germany

PHA-02 - *HPLC* as a *PAT* tool featuring ballistic separations and direct process sampling <a href="Przemek Stasica">Przemek Stasica</a><sup>1</sup>, Simon Watson<sup>1</sup>, Nicholas Holmes<sup>2</sup>, Richard Bourne<sup>2</sup> <a href="IGlaxoSmithKline">IGlaxoSmithKline</a>, Stevenage, SG1 2NY, UK; <sup>2</sup>Institute of Process Research and Development, School of Chemical and Process Engineering, University of Leeds, LS2 9JT, UK

PHA-03 - Optimisation of oligonucleotide separations using ion exchange chromatography - Focusing on the type of mobile phase counter ion

<u>Daniel Eßer</u><sup>1</sup>, Akiko Matsui<sup>2</sup>, Saoko Nozawa<sup>2</sup>, Noritaka Kuroda<sup>2</sup>

¹YMC Europe GmbH, Germany; ²YMC Co., Ltd., Japan

PHA-04 - Characterization of a GlyCLICK site-specific ADC using complementary middle-up LC-MS analysis

<u>Bastiaan Laurens Duivelshof</u><sup>1</sup>, Jonathan Sjögren<sup>2</sup>, Alain Beck<sup>3</sup>, Davy Guillarme<sup>1</sup>, Valentina D'Atri<sup>1</sup>

<sup>1</sup>Institute of Pharmaceutical Sciences of Western Switzerland, University of Geneva, Geneva, Switzerland; <sup>2</sup>Genovis AB, Lund, Sweden; <sup>3</sup>Center of Immunology Pierre Fabre, Saint-Julienen-Genevois, France

PHA-05 - A comparative study of UniSpray and Electrospray for the ionization of neuropeptides in LC-MS/MS

<u>Jana Bongaerts</u><sup>1,2</sup>, Yannick Van Wanseele<sup>1</sup>, Laurence Van Oudenhove<sup>3</sup>, Karen Segers<sup>1,2</sup>, Marijn Van Hulle<sup>3</sup>, Dimitri De Bundel<sup>1</sup>, Ilse Smolders<sup>1</sup>, Debby Mangelings<sup>2</sup>, Yvan Vander Heyden<sup>2</sup>, Ann Van Eeckhaut<sup>1</sup>

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PHA-06 - Advances in Biomolecule separation on small ID silica monoliths Petra Lewits, Benjamin Peters, Gisela Jung, Peter Knoell, Tom Kupfer Merck KGaA, Darmstadt, Germany

PHA-07 - Optimisation and standardisation of a breath biomarker discovery platform Laura McGregor<sup>1</sup>, Anthony Buchanan<sup>1</sup>, Bob Green<sup>1</sup>, Nick Bukowski<sup>1</sup>, Caroline Widdowson<sup>2</sup> <sup>1</sup>SepSolve Analytical, UK; <sup>2</sup>Markes International, UK

PHA-08 - Optimization of innovative MS-compatible mobile phases for the characterization of monoclonal antibody charge variants by CEX

Amarande Murisier<sup>1</sup>, Evelin Farsang<sup>2</sup>, Szabolcs Fekete<sup>1</sup>, Davy Guillarme<sup>1</sup>

<sup>1</sup>Institute of Pharmaceutical Sciences of Western Switzerland, University of Geneva, Geneva, Switzerland; <sup>2</sup>Department of Analytical Chemistry, University of Pannonia, Veszprém, Hungary

PHA-09 - Secondary column interactions between biopharmaceutical proteins and some recent size exclusion chromatography (SEC) columns in native SEC Annika Siölander

Novo Nordisk A/S, Denmark

PHA-10 - Factors that Influence the Recovery of Hydrophobic Peptides During LC-MS Sample Handling

Moon Chul Jung, Thomas Henry Walter

Waters Corp, United States of America

PHA-11 - Optimization of an untargeted LC-MS method for metabolite profiling of restrictedvolume plasma samples

<u>Karen Segers</u><sup>1,2</sup>, Kelsey Frederickx<sup>1,2</sup>, Johan Grech<sup>1,2</sup>, Jana Bongaerts<sup>1,2</sup>, Debby Mangelings<sup>1</sup>, Yvan Vander Heyden<sup>1</sup>, Ann Van Eeckhaut<sup>2</sup>

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SAM-01 - Advanced Automated Sample Preparation workflows for challenging GC-MS analyses

<u>Daniela Cavagnino</u><sup>1</sup>, Inge de Dobbeleer<sup>2</sup>, Cedric Wissel<sup>2</sup>, Martijn van den Hoven<sup>2</sup>, Tom Vercammen<sup>3</sup>

<sup>1</sup>Thermo Fisher Scientific, Italy; <sup>2</sup>Interscience, The Netherlands; <sup>3</sup>SampleQ, Interscience, Belgium

SAM-02 - Direct-connected GC headspace autosampler to extend the applicability of a clean, on-line solventless extraction technique for volatile impurities

<u>Daniela Cavagnino</u><sup>1</sup>, Manuela Bergna<sup>1</sup>, Cristian Cojocariu<sup>2</sup>

<sup>1</sup>Thermo Fisher Scientific, Italy; <sup>2</sup>Thermo Fisher Scientific, UK

STA-01 - Novel Polymer-based Stationary Phases for Temperature Responsive Liquid Chromatography

Mathijs Baert<sup>1</sup>, Filip Du Prez<sup>2</sup>, Frederic Lynen<sup>1</sup>

<sup>1</sup>Separation Science Group, Department of Organic and Macromolecular Chemistry, Faculty of Sciences, Ghent University, Krijgslaan 281-S4 Bis, B-9000 Ghent, Belgium; <sup>2</sup>Polymer Chemistry Research Group, Department of Organic and Macromolecular Chemistry, Faculty of Sciences, Ghent University, Krijgslaan 281-S4 Bis, B-9000 Ghent, Belgium

STA-02 - Fabrication of polymer monoliths in non-transparent 3D-printed polymer housings Noor Abdulhussain<sup>1</sup>, Sinéad Currivan<sup>1,2</sup>, Suhas Nawada<sup>1</sup>, Marta Passamonti<sup>1</sup>, Peter Schoenmakers<sup>1</sup>

<sup>1</sup>Van 't Hoff Institute for Molecular Science (HIMS), Faculty of Science, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands; <sup>2</sup>Centre for Research in Engineering Surface Technology (CREST), Technological University Dublin, FOCAS Research Institute, Camden Row, Dublin 8, Ireland

STA-03 - Advances in HPLC Separations using Graphitized Carbon Particles

<u>Petra Lewits</u><sup>1</sup>, Curtis W. Franz<sup>2</sup>, Cory E. Muraco<sup>2</sup>, William L. Maule<sup>2</sup>, Ken Espenschied<sup>2</sup>, Jay Jones<sup>2</sup>

<sup>1</sup>Merck KGaA, Darmstadt, Germany; <sup>2</sup>MilliporeSigma, Bellefonte, PA, US

STA-04 - Evaluation of New MS-Compatible Mixed-Mode RP/AX UPLC Columns

<u>Thomas Henry Walter</u>, Bonnie Alden, Melvin Blaze, Cheryl Boissel, Donna Osterman, Amit
V. Patel

Waters Corp, United States of America

STA-05 - A novel unique separation column for underivatized direct LC-MS analysis of amino acids and related compounds

Itaru Yazawa

Imtakt Corpoation, Japan

SFC-01 - Polyethylene Glycol (PEG) Characterisation by Supercritical Fluid Chromatography (SFC) with Evaporative Light Scattering and Mass Spectrometry Detection Rebecca Mott

AstraZeneca, United Kingdom

SFC-02 - Retention Modeling of Supercritical Fluid Chromatography Separations Mariyana Savova<sup>1,2</sup>, Stef R.A. Molenaar<sup>1</sup>, Bob W.J. Pirok<sup>1</sup>, Paul Ferguson<sup>3</sup>, Peter J Schoenmakers<sup>1</sup>

<sup>1</sup>van 't Hoff Institute for Molecular Sciences, Analytical Chemistry Group, University of Amsterdam, Science Park 904, 1098 XH Amsterdam, The Netherlands; <sup>2</sup>TI-COAST, Science Park 904, 1098 XH Amsterdam, The Netherlands; <sup>3</sup>AstraZeneca, Charter Way, Macclesfield SK10 2NA, United Kingdom

SFC-03 - Orthogonal Separation under Improved Sensitivity for Low Level Impurity detection by the Agilent 1260 Infinity II SFC/UHPLC Hybrid System Featuring an Agilent 1260 Infinity II Variable Wavelength Detector

<u>Susanne Stephan</u>, Edgar Naegele, Daniel Kutscher Agilent Technologies, Germany

SFC-04 - Development of a generic method to analyze flavonoids with unified chromatography-electrospray ionization mass spectrometry

Jérémy Molineau<sup>1</sup>, Manon Meunier<sup>1</sup>, Angéline Noireau<sup>1</sup>, Laëtitia Fougère<sup>1</sup>, Anne-Marie Petit<sup>2</sup>, Eric Lesellier<sup>1</sup>, Caroline West<sup>1</sup>

<sup>1</sup>University of Orléans, ICOA, CNRS UMR 7311, rue de Chartres, BP 6759; 45067 Orléans, France; <sup>2</sup>Technologie Servier, 25/27 rue Eugène Vignat, CS 11749, 45007 Orléans cedex 1, France

SFC-05 - Determination of mineral oil saturated and aromatic hydrocarbons in consumer products by supercritical fluid chromatography with flame ionization and UV detection Alan Rodrigo Garcia Cicourel<sup>1</sup>, Bas van de Velde<sup>1</sup>, Gerry Roskam<sup>1</sup>, Hans-Gerd Janssen<sup>1,2</sup> <sup>1</sup>University of Amsterdam, van't Hoff Institute for Molecular Sciences, Analytical Chemistry Group, Science Park 904, 1098 XH Amsterdam, The Netherlands; <sup>2</sup>Unilever Research and Development, Central Analytical Science, P.O. Box 114, 3130 AC Vlaardingen, The Netherlands

#### **SOCIAL PROGRAMME**

- Belgian Beer tasting event sponsored by Thermo Fisher Scientific on Wednesday evening 29 January 2020 in the poster room of the conference center Het Pand.
- Conference Dinner on Thursday evening 30 January 2020 in Monasterium Poortackere, Ghent.
- Farewell Drink sponsored by Shimadzu on Friday afternoon 31 January 2020.





HTC-16 Beer Tasting event, 29 January 2020





HTC-16 Conference dinner, 30 January 2020





HTC-16 Farewell Drink, 31 January 2020