# HTC-15 (2018)

15<sup>th</sup> International Symposium on Hyphenated Techniques in Chromatography and Separation Technology 24 – 26 January 2018

Preceded by short courses on 23 January 2018

Symposium organised by the Royal Society of Chemistry (RSC), United Kingdom and the Royal Flemish Chemical Society (KVCV), Belgium supported by The British Mass Spectrometry Society and The Chromatographic Society \*\*\*

Venue: City Hall, Cardiff (Wales, United Kingdom)





HTC -15 24th - 26th January 2018 Cardiff, UK

15th International Symposium on

Hyphenated Techniques in Chromatography and Separation Technology







# **CONFERENCE COMMITTEES**

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Prof. John DEAN, Northumbria University, United Kingdom
Dr. Rudy SENTEN Royal Flemish Chemical Society KVCV, Belgium)



Scientific and Organising Committee of HTC-15 (partly) Left to right: John DEAN, Graham MILLS, Frederic LYNEN, Bob BOUGHFLOWER, Paul FERGUSON, Deirdre CABOOTER), Ruth GODFREY, Bas EELTINK, Tom LYNCH, Sam WHITMARSH and John LANGLEY **DELEGATES** 

# **DELEGATES/COUNTRY**



# **SCIENTIFIC PROGRAMME**

# • SCIENTIFIC PROGRAMME OF HTC-15 IN A GLANCE (details in annex)

| Activity                              |    |
|---------------------------------------|----|
| Plenary lectures                      | 5  |
| Keynote lectures                      | 16 |
| Oral presentations                    | 48 |
| Early Career Researcher presentations | 31 |
| Tutorials                             | 8  |
| Workshops                             | 1  |
| Short courses                         | 3  |
| Vendor seminars                       | 4  |
| Poster sessions                       | 3  |
| Poster Flash presentations            | 4  |
| Award ceremonies                      | 3  |

#### • **POSTERS**

| Poster category  | 64 |  |
|--|----|--|
| Advanced Analysis of Food and Beverages  | 2  |  |
| Advances in Clinical Analysis  | 3  |  |
| Analysis of Complex Energy Products  | 3  |  |
| Big Data Chemometrics and Method Development (In-Silico) (*)                   | 5  |  |
| BioPharma/Sample Prep & Automation   | 1  |  |
| Challenges in Quantitative Analysis  | 1  |  |
| Comprehensive Chromatography - The State of the Art                            | 10 |  |
| Energy & the Environment   | 4  |  |
| Exploiting Separation Science  | 6  |  |
| Food & Drink   | 10 |  |
| Fundamentals in Separation Science & Sample Prep                               | 4  |  |
| Fundamentals in Separation Science (*)   | 2  |  |
| Hyphenated Techniques for Comprehensive Analysis                               | 1  |  |
| Interfacing and Ionisation   | 1  |  |
| Ion Mobility - Mass Spectrometry (**)  | 4  |  |
| Microfluidics & flow process technology  | 1  |  |
| Quantitation, Pharma & Forensics   | 1  |  |
| (R)evolutions in Biopharmaceutical Analysis (*)                                | 1  |  |
| Other  | 4  |  |
| session organised by KVCV (*) and BMSS (British Mass Spectrometry Society, **) |    |  |

# **AWARDS**

## **HTC - INNOVATION AWARD**

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

The aim of the new award was to celebrate the work of a scientist who is innovatively evolving the field of hyphenated techniques in separation science. The award was open to any scientist under 45. The winner was selected by the HTC- scientific committee and received a 1.000 Euro Travel Grant, free registration and attendance to the social programme at HTC-15. Nominations from the readers of *LCGC Europe* were also considered by the judges.



The 2018 HTC-Innovation Award recipient, presented at the HTC-15 Conference on 25 January 2018 is Professor **Carolin HUHN**, University of Tübingen (Germany).

Title of the lecture by Prof. Huhn:

Multidimensional separations in the electric field – Instrumental innovations

## **KNOX MEDAL AWARD (RSC)**



The Royal Society of Chemistry (RSC) honours individuals deserving special recognition for their innovation or influential work in the field of Separation Science with the Knox Medal.

The 2018 Knox Medal recipient, presented at the HTC-15 Conference during the plenary opening session on 24 January 2018 is Professor **Peter MYERS**, University of Liverpool, UK,

Title of the plenary lecture by prof. Myers: Why do we still use silica ?

#### **POSTER AWARDS**

The most innovative poster contributions of HTC-15 received the HTC-15 Poster Award.

#### • FIRST POSTER AWARD

#### **Mathys BAERT**

Ghent University, Separation Science Group, Belgium

*Exploring the possibilities of temperature responsive columns in comprehensive two-dimensional liquid chromatography.* 

No co-authors.

#### <u>SECOND POSTER AWARD</u>

Kris WOLFS KU Leuven, Pharmaceutical Analysis, Belgium

#### Application of an Atmospheric Micro Hollow Cathode Discharge Set-up in a Novel GC-detector

Authors: Kris Wolfs, Niels van Boxtel, Juan Aspromonte, Ann van Schepdael and Erwin Adams

#### • THIRD POSTER AWARD



## Vincent PEPERMANS Free University of Brussels (VUB), Department of Chemical Engineering, Belgium

Enhancing detection limits in chromatography using solvent-assisted post-column refocusing

Authors: Vincent Pepermans, Jelle De Vos, Sebastiaan Eeltink and Gert Desmet

[the First and Second Award recipients were not present during the Poster Award session]

# **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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## ANNEX 1 – HTC-15 in the press

#### Top 10 reasons to register for HTC-15 today!

HTC-15 is almost here! And if you haven't already registered, here's a list of our top 10 reasons you should do so immediately:

- 1. The brilliant separation science: The conference programme speaks for itself - three days of great talks, posters, vendor exhibits, and all your favourite separation scientists under one (historic) roof.
- 2. The outstanding plenary lectures: Prof Peter Schoenmakers, Prof Rob Beynon, Prof Tuulia Hyotylainen, and Dr Eric Little will all be presenting plenary lectures, and we still haven't mentioned our Knox Medal winner...
- 3. The 2017 Knox Memorial Lecture (Prof Peter Myers!!!): As you may have heard, Prof Peter Myers was awarded the 2017 Knox Medal, and will be opening the conference with a plenary lecture entitled Why do we still use silica?, which we expect will be the usual scientific tour de force that we've come to expect of him.
- 4. The short courses: Three day-long short courses on SFC, biopharms and statistical analysis of chromatographic data, all led by experts and innovators in these fields.
- 5. The excellent posters: Poster presentations are a great way to discuss new research with the scientists who produced it, and HTC-15 has some great new research on show at the poster sessions. You can still submit late-breaking poster abstracts here.
- 6. The fabulous early-career researchers: The 24 ECR talks and many ECR posters are a heartening reminder that separation science continues to attract the best and brightest talent.
- 7. The vendor exhibits and seminars: Hear the latest news from all the big vendors and see how their products can help you do better science. And if that isn't enough, cough vendor freebies cough.
- 8. The networking opportunities: A gala conference dinner, a beer degustation event, and all those coffee breaks between sessions - that's plenty of time to strike up a conversation with that researcher you always meant to collaborate with, that ECR who you think would make a great new addition to your institution, or that keynote speaker whose work has always inspired you.
- 9. The venue: Did we mention that the venue is the historic, beautiful Cardiff City Hall, in the middle of the Welsh capital, home to this castle and this museum and this market? And that Great Western Railway offers discounted rail tickets to anyone travelling to Cardiff for a conference?
- 10. The fact that you really really want to: because HTC-15 is the premier analytical conference in the UK in 2018, and because reasons 1-9 are very persuasive. So don't wait, register now!

Website Royal Society of Chemistry, January 2018



# HTC Analytical Conference Comes to the UK

wned scientists. The meeting is being organised by the Royal ociety (KVCV), with support from the British Mass Spectrome



TC-15 will be pre ourses on 23 Janu



Chromatography Today, Buyer's Guide 2018

# **15th International Symposium on Hyphenated Techniques in Chromatography and Separation Technology (HTC-15)**

A preview of HTC-15, which will be held at Cardiff City Hall, Cardiff, United Kingdom, from 24–26 January 2018.



The 15th International Symposium on Hyphenated Techniques in Chromatography and Separation Technology (HTC-15) will be held at Cardiff City Hall, Cardiff, United Kingdom, from 24-26 January 2018. This is the second time the Hyphenated Techniques in Chromatography (HTC) conference has been held in the UK and the event is set to be a premier UK event for separation scientists in 2018, attracting national and internationally renowned scientists, with delegates from 15 different countries registered so far. The meeting is organized by the Royal Society of Chemistry Separation Science Group (RSC SSG) with the Royal Flemish Chemical Society (KVCV). Full meeting details can be found at www.htc-conference.co.uk The programme will include topics such as

Big Data, Fundamentals and Exploiting Separation Science, (R)evolutions in **Biopharmaceutical Analysis, Food and** Drink, Environmental, Comprehensive Chromatography, and much more. The

conference will include five plenary lectures, 16 keynote lectures, eight tutorial lectures, 48 oral presentations, and 24 early career researcher (ECR) presentations, as well as daily poster sessions

The plenary lectures will be given by Rob Beynon (University of Liverpool, UK), Tuulia Hyötyläinen (Örebro University, Sweden), Eric Little (Othus Inc), Peter Schoenmakers (University of Amsterdam, The Netherlands), and the recently announced Knox Medal winner, Peter Myers (University of Liverpool UK). An up-to-date speaker list can be viewed at www.htc-conference.co.uk. The oral programme is complete, with over 40% of presentations from abstract submissions. The full programme is now online and includes a dedicated ECR programme as one of the three parallel sessions.

Conference registration is open at www. ilmexhibitions.com/htc/registration/ Alongside the core scientific programme, the symposium is hosting an attractive

technical exhibition where leading companies

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# **ANNEX 2 – Scientific programme**

# SHORT COURSES (Tuesday 23 January 2018)

## **INTRODUCTION TO BIOPHARMACEUTICAL ANALYSIS**

#### Course Outline

- 1. Introduction to biopharmaceuticals contrasting with small molecules/traditional pharmaceuticals
- 2. Recent evolution of biopharmaceuticals and the biopharmaceutical market
- 3. The production of a biopharmaceutical
- 4. Critical performance characteristics common co- and post-translational modifications specific to biopharmaceuticals (emphasis on mAbs)
- 5. Overview of techniques employed in biopharmaceuticals analysis
- 6. Detailed review and application areas of the following techniques
  - o Reversed Phase (covering intact, fragments, peptides and amino acids)
  - HILIC (including glycan workflow's)
  - o lon exchange
  - o Size Exclusion Chromatography
  - Hydrophobic Interaction Chromatography
- 7. Course summary/conclusions

#### <u>Tutors</u> Dr. Koen Sandra

Research Institute for Chromatography (RIC), Kortrijk, Belgium

## Dr Szabolcs Fekete

University of Geneva, Switserland

#### Dr. Tony Taylor

Crawford Scientific and CHROMacademy, United Kingdom.

## SUPERCRITICAL FLUID CHROMATOGRAPHY: FROM THEORY TO (INDUSTRIAL) APPLICATION

#### Course Outline

- Definition and properties of supercritical fluids
- SFC instrumentation
- Selection of stationary phases, organic modifiers and additives in SFC
- Selection of additives in SFC and analysis of basiccompounds
- How to use pressure and temperature in SFC?
- SFC method development strategy
- Applications of SFC in pharmaceutical, food, environmental, forensic, fragrance... (chiral/achiral, analytical/preparative)
- Kinetic performance and instrumental constraints of modernSFC (UHPSFC)
- Coupling SFC with MS and applications

• Industrial perspective and insights on the use of SFC

Tutors Prof. Caroline West University of Orleans, France Dr. Claudio Brunelli Pfizer Analytical Research and Development, United Kingdom Prof. Ken Broekhoven Free University of Brussels, Belgium

#### STATISTICAL ANALYSIS OF CHROMATOGRAPHIC DATA: A PRACTICAL GUIDE

#### Course Outline

1. Introduction.

- 1.1. Why do we need statistics to deal with chromatographic data?
- 2. Pre-processing methods
  - 2.1. Base-line correction
  - 2.2. Noise filtering
  - 2.3. Peak detection
  - 2.4. Peak detection in two-dimensional chromatography
  - 2.5. Peak tracking
  - 2.6. Chromatographic alignment
  - 2.7. Special topics with high-resolution mass spectrometry.
- 3. Curve resolution methods
  - 3.1. Raw data vs. peak tables.
  - 3.2. Curve resolution & peak fitting. Chromatographic peak models.
  - 3.3. Second-order methods: AMDIS, MCR-ALS.
  - 3.4. Third-order methods: PARAFAC, PARAFAC2
  - 3.5. Advanced methods.
- 4. Modelling & pattern recognition
  - 4.1. Exploration: PCA & HCA.
  - 4.2. Classification: SIMCA, PLS-DA, LDA, SVM.
  - 4.3. Multivariate modelling: PLS, RSVM.
- 5. Applications
  - 5.1. Food & pharma
  - 5.2. Oil & gas
  - 5.3. Forensics
  - 5.4. Chemicals & polymers
  - 5.5. Omics
- 6. Open discussion

<u>Tutor</u>

**Dr. Gabriel Vivo-Truyols** 

Tecnometrix, The Netherlands

# LECTURES and VENDOR SEMINARS, SOCIAL PROGRAMME

(Wednesday 24 – Friday 26 January 2018)

## PROGRAMME SCHEDULE

| Wednesday 24 January 2018   |                        |                        |  |
|---|------------------------|------------------------|--|
| Opening Ceremony followed by the plenary lecture 1 (Knox Award)   |                        |                        |  |
| keynote 1, session 1  | keynote 2, session 2   | Tutorial 1, session 3  |  |
| Vendor seminars 1 and 2   |                        |                        |  |
| keynote 3, session 4  | keynote 4, session 5   | Tutorial 2, session 6  |  |
| keynote 5, session 7  | keynote 6, session 8   | Tutorial 3, session 9  |  |
| Thursday 25 January 2018  |                        |                        |  |
| Breakfast Workshop  |                        |                        |  |
| Plenary lecture 2   |                        |                        |  |
| keynote 7, session 10   | keynote 8, session 11  | Tutorial 4, session 12 |  |
| Vendor seminars 3 and 4   |                        |                        |  |
| keynote 9, session 13   | keynote 10, session 14 | Tutorial 5, session 15 |  |
| keynote 11, session 16  | keynote 12, session 17 | Tutorial 6, session 18 |  |
| Friday 26 January 2018  |                        |                        |  |
| Plenary lecture 3   |                        |                        |  |
| keynote 13, session 19  | keynote 14, session 20 | Tutorial 7, session 21 |  |
| keynote 15, session 22  | keynote 16, session 23 | Tutorial 8, session 24 |  |
| Flash poster presentations  |                        |                        |  |
| Plenary lecture 4 and 5 followed by the Awards and Farewell Event |                        |                        |  |

## **PLENARY LECTURES**

- 1. Peter Myers, University of Liverpool (UK): Why Do We Still Use Silica ?
- 2. Eric Little, Osthus (USA): Big Data The Final Hyphen
- 3. Tuulia **Hyötyläinen**, Örebro University (S): *Hyphenated Techniques for comprehensive analysis of all metabolites in biological systems to describe metabolic changes caused by disease, environmental, nutritional, or genetic factors*
- 4. Rob Beynon, University of Liverpool (UK): Of mice, sex and mass spectrometry
- *5.* Peter **Schoenmakers**, University of Amsterdam (NL): *Multi-dimensional liquid chromatography of complex mixtures*



## **KEYNOTE LECTURES**

- 1. Hans Gerd **Janssen**, Unilever Research and University of Amsterdam (NL): *Separation science and its use for generating data, information and understanding*
- 2. Koen **Sandra**, Research Institute for Chromatography (B): *Recent advances in the analysis of protein biopharmaceuticals*
- *3.* Gert **Desmet**, Vrije Universiteit Brussel (B): *Recent Progress in the Development of Perfectly Ordered Separation Media*
- 4. Elizabeth **Want**, Imperial College London (UK): *UPLC-MS for Metabolic Phenotyping: Advantages, Assays and Applications*
- 5. Frederic **Lynen**, University of Ghent (B): *High temperature chromatography: the winning solution allowing both throughput and efficiency?*
- *6.* John **Langley**, University of Southampton (UK): *Supercritical Fluid Chromatography Mass Spectrometry: Robust, Reliable and Required*
- 7. Sebastiaan **Eeltink**, Vrije Universiteit Brussel (B): Advancing hydrophobic interaction chromatography methods to characterize biotechnology enzyme mixtures and to profile biotherapeutics
- 8. Michal **Holcapek**, University of Pardubice (CZ): *Clinical Lipidomic Quantitation Based on Mass* Spectrometry: Case Study of Pancreatic Cancer
- 9. Caroline West, University of Orleans (F): 50 shades of Green SFC
- *10.* Gabriel **Vivo Truyols**, Tecnometrix: *A paradigm shift for (big) data analysis in chromatography: on the use of Bayesian statistics*
- 11. Cris Lapthorn, GSK (UK): Ion mobility mass spectrometry leveraging rich data on the gas-phase ion to separate and assign
- 12. Barbara **Kasprzyk-Hord**ern, University of Bath (UK): Urban water profiling to inform the state of the environment and public health
- 13. Scott Summerfield, GSK (UK): Laboratory Automation: The Rise of the Machines
- 14. Peter **Tranchida** (replaced Luigi Mondello), University of Messina (I): *Flow Modulated Twodimensional Gas Chromatography Coupled to Tandem Mass Spectrometry for "Comprehensive" characterization of Complex Samples*
- 15. Thomas **Gröger**, Helmholtz Zentrum München GmbH (D): *Thermal Analysis in hyphenation with mass spectrometry as a versatile tool for the analysis of complex and high boiling petroleum products*
- 16. Peter **Tranchida** (replaced Paola Dugo), University of Messina (I): *Exploiting comprehensive twodimensional liquid chromatography in food analysis*

## **ORAL PRESENTATIONS**

Session 1: Exploiting Separation Science (Chair: Tom Lynch)

- Florian **Füssl**, Thermo Fisher Scientific: Novel ways to introduce the traditional salt based chromatography technique of Ion Exchange Chromatography of biopharmaceutical proteins into High Resolution Mass Spectrometry
- Tung-Hu **Tsai**, National Yang-Ming University (Taiwan): *Hyphenated microdialysis and chromatography to monitoring protein free drug for pharmacokinetic study in rat*

• Erwin Adams, Pharmaceutical Analysis - KU Leuven (B): Analysis of Aromatic Substituted Quaternary Ammonium Salts using a Headspace Gas Chromatography Based Methodology

## Session 2: (R)evolutions in Biopharmaceutical Analysis (KVCV) (Chair: Deirdre Cabooter)

- Jelle **De Vos**, Free University of Brussel (B): *Prototyping of microfluidic multilayer modulator chip for multi-dimensional separations* (replaced Davy Guillarme, University of Geneva (CH): *From one to four comprehensive separation dimensions to characterize antibody drug conjugates*)
- Erwin Kaal, DSM (NL): Advancing the analytical toolbox using shotgun lipidomics for lipid modifying enzymes
- Michael Lämmerhofer, University of Tübingen (D): Lipidomics by UHPL-CQTOF-MS/MS with Data-Independent Acquisition and Clinical Applications

## Session 4: Fundamentals in Separation Science (KVCV) (Chair: Sebastiaan Eeltink)

- Ken **Broeckhoven**, Vrije Universiteit Brussel (B): Considerations for the use of ultra-high pressures in liquid chromatography for 2.1mm inner diameter columns
- Konstantin **Shoykhet**, Agilent Technologies: *Matching 1st and 2nd dimension chemistries in the 2D-LC. Active Solvent Modulation*
- Martina **Catani** (replaced Alberto Cavazzini), University of Ferrara (I): *Kinetics and mass transfer phenomena in modern chiral stationary phases*

## Session 5: Advances in Clinical Analysis (Chair: Dave Perrett)

- Lewis **Couchman**, Analytical Services International (ASI) Ltd (UK): *Opportunities for ultra-rapid LC-MS/MS in high-throughput bioanalysis*
- Claudio **Brunelli**, Pfizer (UK): From laboratory to patient: Implementation of SFC in pharmaceutical industry (replaced Zsuzsanna **Kuklenyik**, Centers for Disease Control and Prevention (USA): Apolipoproteins, non-polar lipids, polar lipids and lipoprotein particle numbers. Can we measure them all on large number of samples?
- Cancelled lecture by John Barr, Centers for Disease Control and Prevention (CDC) (USA): Detection and differentiation of botulinum neurotoxins for the diagnosis and prevention of botulism

## Session 7: High throughput versus High Efficiency Separations (CS) (Chair: Paul Ferguson)

- Monika Dittmann, Agilent Technologies: Strategies to Optimize Throughput in 2D-LC
- Tomas Leek, AstraZeneca (UK): Fast, efficient and selective: separation science for modern organic synthetic chemistry
- Bob **Boughtflower**, GSK (UK): Generic Reverse Phase Chromatography... Speed, performance... or both?

## Session 8: Exploiting Separation Science and Mass Spectrometry (Chair: Lewis Couchman)

- Szabolcs **Fekete**, University of Geneva (CH): *Possibilities of modern size-exclusion chromatography for therapeutic proteins; feasibility assessment for future mass spectrometry hyphenation*
- Joanne **Roberts**, Glasgow Caledonian University (UK): *Separation of isomeric metabolites of carbamazepine by liquid chromatography and high resolution accurate mass*

• Filip **Cuyckens**, Janssen R&D (B): *Quantitative drug metabolite profiling without authentic standards or radiolabels using LC-ICP-MS* 

## Session 10: SSG session (Chair: John Langley)

- Deirdre **Cabooter**, University Leuven (B): *Methodologies to determine b-term coefficients revisited*
- Frank **Steiner**, Thermo Fisher Scientific: *UHPLC quantitation and identity confirmation in drug development with a multi-detector approach*
- LCGC innovation award 2018: Carolin **Huhn**, University of Tübingen (D): *Multidimensional* separations in the electric field Instrumental innovations.

#### Session 11: Big Data - What do we do with it? (Chair: Arun Sen)

- Remy **Gavard**, University of Warwick (UK): *Replicates of Complex Mixtures in Ultra-High Resolution Mass Spectrometry Could Help Pave The Way to Big Data*
- Benjamin Woolford-Lim, GlaxoSmithKline (UK): Big Data When Less is More
- Phil **Kay**, JMP, SAS Institute (UK): *Looking Inside the Black Box of Machine Learning Methods: Applications in Analytical Chemistry*

#### Session 13: Green Separations (Chair: Paul Ferguson)

- Stephen Lock, Sciex (UK): Can CE-MS improve the detection of peptides and intact proteins and in biological samples?
- Julie Herniman, University of Southampton (UK): UHPSFC-MS of a Range of Steroidal Compounds
- Mariosimone **Zoccali**, University of Messina (I): Online extraction and determination of carotenoids from food sample by means of supercritical fluid extraction-supercritical fluid chromatography-mass spectrometry

# Session 14: Big Data Chemometrics and Method development (In-Silico) (KVCV) (Chair: Ken Broeckhoven)

- Yvan Vander Heyden, Vrije Universiteit Brussel (B): Chromatographic fingerprints: chemometrics and application in method development
- Kai **Chen**, Janssen Pharmaceutical Companies of Johnson & Johnson (B): Use of different computer-aided method development software in late stages across global sites in pharmaceutical industry
- Roman Szucs, Pfizer (UK): Structure driven prediction of retention :Improvement of accuracy

#### Session 16: Ion Mobility - Mass Spectrometry (BMSS) (Chair: Alison Ashcroft)

- Claire **Eyers**, University of Liverpool (UK): Understanding phosphorylation-mediated effects on NF-κB interactions using IM-MS
- Kevin Giles, Waters Corporation: An Advanced Cyclic Ion Mobility Mass Spectrometry System
- Helen **Cooper**, University of Birmingham (UK): *FAIMS mass spectrometry for the analysis of peptides and proteins*

#### Session 17: Screening Enviroment Pollutants, what can the data tell us? (Chair: Graham Mills)

- Leon **Barron**, King's College London (UK): Suspect screening of aquatic environmental matrices using high resolution analysis and in silico tools for broad scope tentative contaminant identification
- Anthony **Gravell**, Natural Resources Wales (UK): Screening of environmental passive sampling extracts using LC Q-TOF-MS in data-independent acquisition mode
- Lara **Kelly**, Markes International Ltd: *Combining high-capacity sorptive extraction with Thermal desorption pre-concentration for analysis of (S)VOCs in environmental samples*

#### Session 19: Automating Complex Sample Workflows (Chair: Bob Boughtflower)

- Camilla Liscio, Anatune: Automated sample preparation: the missing hyphen to hypernation
- Sheelan Ahmad, GlaxoSmithKline (UK): Solid Phase Micro-Extraction Breaking Free from Total Concentration Analysis
- An **Adams**, Dow (UK): Analytical developments in sample preparation to reliably measure the emission of volatiles from materials in a high-throughput fashion

## Session 20: Comprehensive Chromatography - The State of the art (Chair: Hans Gerd Janssen)

- Bob **Pirok**, University of Amsterdam (NL): Applicability of retention modelling in hydrophilicinteraction liquid chromatography for algorithmic optimization programs with gradient-scanning techniques
- Marco **Ruijken**, MsMetrix: All Ion Differential Analysis in Product Control Applications using GC/MS and Comprehensive GCxGC/MS
- John **Dean**, Northumbria University (UK): *Detection of bacteriologically produced hydrogen sulphide using SHS-MCC-GC-IMS*

## Session 22: Analysis of Complex Energy Products (Chair: Tom Lynch)

- Sam Whitmarsh, BP (UK): Direct infusion MS who needs hyphenation anyway?
- Laura **McGregor**, SepSolve Analytical: *Fast and efficient group-type analysis of hydrocarbons by GCxGC*
- James **Diekmann**, VUV Analytics: *Recent Advances in the Analysis of Petroleum-based Fuels using Gas Chromatography-Vacuum Ultraviolet Spectroscopy*

## Session 23: Advanced Analysis of Food and Beverages (Chair: Lewis Jones)

- Lewis **Jones**, Sensient Flavours: *Can Gas Chromatography Olfactometry Determine the Importance of Volatile Organic Chemical to Food and Beverage Odour?*
- Sara **Stead**, Waters Corporation: *Rapid evaporative ionization mass spectrometry for high throughput screening in food analysis: the case of boar taint*
- Natasha D. **Spadafora**, University of Calabria/Markes International: *Monitoring the effect of post*harvest storage on fruit quality by TD-GC×GC-TOF MS

## EARLY CAREER RESEARCHER PRESENTATIONS

## Session 3: Fundamentals in Separation Science (Chair: Paul Ferguson)

• José Luís **Dores-Sousa**, Vrije Universiteit Brussel (B): *Probing selectivity of mixed-mode reversedphase / weak-anion-exchange columns for small-molecule separations in liquid chromatography* 

- Vincent **Pepermans**, Vrije Universiteit Brussel (B): Understanding the possibilities of solventassisted post-column refocusing to enhance detection limits in 1-D and 2-D LC
- Mathijs **Baert**, Ghent University (B): *Investigating the potential for improved temperature responsive separations in liquid chromatography*

## Session 6: Interfacing and Ionisation (Chair: Ruth Godfrey)

- Gino **Groeneveld**, University of Amsterdam (NL): *Characterization of complex polyether polyols* using comprehensive two-dimensional liquid chromatography hyphenated with high resolution mass spectrometry (LCxLC-HRMS)
- Yannick **Van Wanseele**, Vrije Universiteit Brussel (B): *The comparison of Unispray and Electrospray for the ionization of neuropeptides*
- Alex **Hodgson** (replaced Dandan Yan), Unversity of Tasmania (Au): Sequential Three-Dimensional Gas Chromatography with Accurate Mass Spectrometry: A Novel Tool for High-Resolution Characterization of Multicomponent Samples

## Session 9: Microfluidics & Flow Process Technology (Chair: Sebastiaan Eeltink)

- Johannes **Höpfner**, Karlsruhe Institute of Technology (KIT) (D): Chemically Sensitive Online Detectors for SEC – current advances for SEC-MR-NMR and SEC-QCL-IR
- Nico **Apel**, Fraunhofer LBF (D): *Comprehensive Two-Dimensional Liquid Chromatography Coupled* to *Triple-Detection for Characterization of Branched Polymers*
- Elise Lemasson, Institut de Chimie Organique et Analytique(ICOA) (F): Chromatographic strategies combining RPLC, mixed-mode HPLC and SFC coupled to MS for impurity profiling of drugs candidates

## Session 12: Separations by shape: Instrumentation (Chairs: Alison Ashcroft & Anton Calabrese)

- Christianne Wicking, BP (UK): FAIMS and fortune
- Corentin **Decroo**, Umons (B): *Topology discrimination of saponin ions by Hyphenated Mass* Spectrometry techniques and computational chemistry
- Alex **Hodgson**, VUV Analytics: Better Living Through (Flavor) Chemistry: *Vacuum Ultraviolet* Spectroscopy as a New Tool for GC Analysis of Terpenes in Flavors and Fragrances

## Session 15: Approaches to maximising analytical data (Chair: Scott Fletcher)

- Samuel **Ellick**, University of Bristol (UK): *Data to decision: efficient processing of complex petroleomics data*
- Ruben **Epping**, Bundesanstalt für Materialforschung und -prüfung (BAM) (D): *Characterization of Small Heterogeneities in Polymers by Analysis of UPLC/ESI-MS Reconstructed Ion Chromatograms*
- Jack **Rice**, University of Bath (UK): *Quantitative proteomics for molecular diagnostics of public health*

## Session 18: Separations by shape: Further applications of chromatography (Chair: Caroline West)

- Marion **Iguiniz**, Université de Lyon (F): *On-line coupling of RPLC and chiral SFC for the analysis of pharmaceutical compounds*
- Ravindra **Hegade**, Ghent University (B): Enhanced resolution of stereoisomers through Stationary phase optimized selectivity liquid and supercritical chromatography (SOS-LC and SOS-SFC)

• Felicity **Elder**, University of Bath (UK): *LC-MS/MS chiral analysis of chloramphencicol in the environment* 

## Session 21: Energy & the Environment (Chair: Sam Whitmarsh)

- Diana **Palacio**, University of Warwick (UK): *Fingerprint characterization of bio-oil from the pyrolysis of African palm and its esterification product*
- Rachel **Townsend**, Swansea University (UK): Mass Spectrometric Investigation of Compounds of Interest to the Chemical Investigation Programme (CIP) within Environmental Matrices: Homogenate Analysis
- Mary **Thomas**, University of Warwick (UK): *Petroleomic Depth Profiling of Staten Island Soil by GC and FT-ICR MS*

#### Session 24: Life science & pharma (Chair: Melissa Hanna-Brown)

- Angela **Taylor**, University of Birmingham (UK): *From GC-MS to LC-MS/MS: Further Advances in Adrenal Cancer Diagnosis*
- Aysegul **Dogan**, Hacettepe University: *Green Bioanalytical Analysis of Voriconazole and Tadalafil by HPLC*
- John **Walsby-Tickle**, University of Oxford (UK): *Improving Untargeted Metabolomics with Ion Chromatography-Mass Spectrometry*

## **WORKSHOP**

Dayna **Mason**, RSC CPD & outreach in Cardiff 5UK) and Deirdre **Cabooter**, Vrije Universiteit Brussel (B): *Professional development and careers* : breakfast workshop on Thursday morning 25 January 2018 at 08:00.

## **TUTORIALS**

- 1. James **Heaton**, Pfizer Ltd (UK): *Tutorial on the fundamentals of hydrophilic interaction chromatography (HILIC) for pharmaceutical analysis*
- 2. Julie Herniman, University of Southampton (UK): Interfacing LC to MS
- 3. Anna Slater, University of Liverpool (UK): Flow chemistry: A synthetic chemist's perspective
- 4. Antonio **Calabrese**, University of Leeds (UK): *Separation and characterisation by ion mobilitymass spectrometry*
- 5. Chris Hopley, LGC: Maximising analytical data by understanding the implications of uncertainty
- 6. Peter **Tranchida** (replaced Paola Dugo), University of Messina (I): *Analysis of food products using advanced analytical techniques*
- 7. John **Dean**, Northumbria University (UK): *Environmental health and well-being: diagnostics with hyphenated gas chromatography*
- 8. Ruth **Godfrey**, Swansea University (UK): *LC-MS small molecule quantitation: a short tutorial of best practice*

#### **VENDOR SEMINARS**

- 1. VRS Recruitment Lunch Seminar: Securing YOUR Perfect Job!
- 2. SCIEX Lunch Seminar: Mapping Protein Modifications Using Novel MS Strategies
- 3. ELLUTIA Lunch Seminar: MAX a new concept in GC-FTIR
- 4. SHIMADZU Lunch Seminar: Smart & Green Hyphenated Solutions



#### **POSTERS**

1. Yung-Yi **Cheng**, Institute of Traditional Medicine, National Yang-Ming University, Taipei, Taiwan, Republic of China: *An LC-MS/MS Method to Monitor Tamoxifen and its Metabolites in Rat for Pharmacokinetic Study* 

2. Marco **Ruijken**, MsMetrix, Netherlands: *Comparative Analysis in GCxGC/MS: Detection and Identification of Co-Eluting Unknowns* 

3. Aarif **El-Mubarak**, King Saud University, Saudi Arabia: *Development and validation of screening method for pesticides residues analysis in vegetables and fruits* 

4. John **Moncur**, SpectralWorks Limited, United Kingdom: *Quantitation of Dodecanoic Acid in Coconut Oil* 

5. Alan **Brailsford**, Kings College London, United Kingdom: *The analysis of steroid seizures from UK customs- Implications for Anti-Doping* 

61. Dima **AlMekdad**, LGC and King s College London, United Kingdom: *Development of micro-flow liquid chromatography mass spectrometry reference method for metanephrines in plasma* 

6. Geraint **Sullivan**, Swansea university, United Kingdom: *Application of gas chromatography-mass spectrometry (GC-MS) in the quantitative analysis of organic compounds generated in* 

gasification/pyrolysis coupled Fischer-Tropsch (FT) reactor: syngas clean up and hydrocarbon production

7. Benjami **Jenkins**, University of Cambridge, United Kingdom: *Novel method for determination of acylcarnitines* 

8. Stefan **Cretnik**, CTC Analytics, Switzerland: Automated combination of Purge & Trap with common GC-MS Injection techniques according to EPA Methods 524.2 and 8260 on the PAL automation platform

9. Phil **Kay**, JMP, SAS Institute, United Kingdom: *Looking Inside the Black Box of Machine Learning Methods: Applications in Analytical Chemistry* 

10. Marco **Ruijken**, MsMetrix, Netherlands: *MsCompare: An Untargeted GC/MS Metabolomics Platform for Quality Control, Precise Deconvolution and Data Analysis* 

11. Samuel **Ellick**, University of Bristol, United Kingdom: *Object orientated programming, a core skill for the modern analytical chemist?* 

12. Gitte **Coopmans**, VUB, Belgium: *Towards Multifactorial Method Development via Predictive Elution Window Stretching and Shifting* 

13. Tom Hancock, BP, United Kingdom: Oil analysis: an ensemble approach

14. Richard **Gillis**, University of Nottingham, United Kingdom: *Characterisation of insulin analogues* with SEC-MALS and complementary ultracentrifugation

15. Sophie **Inman**, LGC, United Kingdom: *Application of 2D-LC for the traceable quantification of human growth hormone in serum* 

16. Masahiro **Hashimoto**, JEOL(Europe)SAS, France: *GCxGC–HRTOFMS analysis of a complex lipid profile in human sebum* 

17. Thomas **Van de Velde**, Ghent University, Belgium: *Assessing 2-Dimensional Comprehensive Flow-Modulated Gas Chromatography for fingerprinting archaeological bitumen* 

18. Mathijs **Baert**, Ghent University, Belgium: *Exploring the possibilities of temperature responsive columns in comprehensive two-dimensional liquid chromatography* 

19. Peter **Russell**, Advanced Chemistry Development, Inc. (ACD/Labs), United Kingdom: *An informatics based approach to developing stability indicating methods* 20. Cancelled

21. Wen-Ya **Peng**, National Yang-Ming University, Taiwan, Republic of China: *Simultaneous determination of lovastatin and its metabolite in rat plasma by liquid chromatography tandem mass spectrometry* 

22. Alexandra **Harvey**, Defence Science and Technology Lab, United Kingdom: *Finding a needle in a haystack: analysis of GC x GC Data* 

23. Alan **Griffiths**, LECO UK, United Kingdom: *Comprehensive Analysis of Complex Environmental* Samples using Comprehensive Two-Dimensional GC with Ultra High Resolution Time-of-Flight Mass Spectrometry (GCxGC-HRMS)

24. Vincent **Pepermans**, Vrije Universiteit Brussel (VUB), Belgium: *Enhancing detection limits in chromatography using solvent-assisted post-column refocusing* 

25. Paul **Clarke**, Postnova Analytics, United Kingdom: *Molecule, particle, vesicle? - The new challenge for analytical separation technologies in polymer and protein characterisation* 

26. Tiffani Bouanati, UMons, Belgium: Microwave-assisted hydrolysis of Alginic Acid

27. Nesrete **Krasnici**, Rudjer Boskovic Institute, Croatia: *Thallium bioaccumulation and cytosolic distribution among biomolecules of different molecular masses in the liver of brown trout (Salmo trutta Linnaeus, 1758) from the Croatian river Krka* 

28. Laura **McGregor**, SepSolve Analytical, United Kingdom: *High-throughput GC×GC-FID for routine environmental analyses* 

29. Ravindra **Hegade**, Ghent University, Belgium: *Chiral Stationary Phase Optimized Selectivity Supercritical Fluid Chromatography (SOS-SFC): a novel approach for optimizing the separation of enantiomers* 

30. Juan **Aspromonte**, Pharmaceutical Analysis - KU Leuven, Belgium: *Characterization of Mesoporous Silica Used for Drug Delivery by Sorptive Interaction - Multiple Headspace Extraction -Gas Chromatography* 

31. Gesa **Schad**, Shimadzu Europa GmbH, Germany: *The power of selectivity and the strength to choose - Chiral Screening using an SFC / LC Switching System* 

32. Jiri **Salplachta**, Czech Academy of Sciences, Institute of Analytical Chemistry, Czech Republic: *Identification of Aspergillus spores by preparative IEF and MALDI-TOF MS* 

33. Luke **Whiley**, MRC-NIHR National Phenome Centre, Imperial College London, United Kingdom: *Stepwise HPLC Extraction and Purification of Endogenous Urinary Metabolites for Their Annotation and Identification in Large Scale Phenotyping Studies* 

34. Sebastiano **Panto**, LECO European Application & Technology Center, Germany: *Quantification of the extended list of suspected allergens in fragrance materials by GCxGC-TOFMS* 

35. João Micael **Leça**, Faculty of Exact Sciences and Engineering - University of Madeira, Portugal: *Underivatized LC-MS/MS determination of ethyl carbamate in wines* 

36. Andreia **Miranda**, University of Madeira, Portugal: *SPE-GC-MS screening of the volatiles from musts collected at different Madeira winemakers* 

37. Emilie **Descours**, ISIPCA, France: *Development of a new method of headspace analysis on flavored mineral waters* 

38. Jakub **Fibigr**, Charles University, Faculty of Pharmacy, Czech Republic: *Application of tandem UV/Charged aerosol detection in analysis of bioactive substances in food supplements* 

39. Ivona **Lhotská**, Charles University, Faculty of Pharmacy in Hradec Králové, Department of Analytical Chemistry, Czech Republic: *On-line solid phase extraction coupled to liquid chromatography using column-switching system for mycotoxin analysis in beer* 

40. Stephen Lock, Sciex, United Kingdom: Polar pesticide analysis by CESI-MS

41. Laura **McGregor**, SepSolve Analytical, United Kingdom: *Flavour profiling of milk using high-capacity sorptive extraction and TD–GC×GC–TOF MS* 

42. Jani **Koponen**, National Institute for Health and Welfare (THL), Finland: *Dioxin, PCB, PBDE and PFAA concentrations in Baltic salmon during the 2000's* 

43. Camilla **Liscio**, Anatune Ltd, United Kingdom: *Sample Preparation Options for determination of Volatile compounds in Food* 

44. Dana **Moravcova**, Czech Academy of Sciences, Institute of Analytical Chemistry, Czech Republic: *Separation of amino acids and aromatic carboxylic acids on silica monolithic capillary columns* 

45. José Luís **Dores-Sousa**, Department of Chemical Engineering, Vrije Universiteit Brussel, Belgium: *Selectivity and mixed-mode retention mechanism of small-molecules in liquid chromatography using a reversed-phase / weak-anion-exchange stationary phase* 

46. Benjamin **Summers**, Purolite Ltd., United Kingdom: *Synthetic polymeric resins in downstream processing for food, fine chemicals and pharmaceuticals* 

47. Gesa **Schad**, Shimadzu Europa GmbH, Germany: *SFC-MS compared to LC-MS in the analysis of small molecules* 

48. Hansjoerg **Majer**, Restek Corp, United States: *Gas Chromatographic Computer Modeling Software for Optimized Method Development and Education* 

49. Erwin Adams, Pharmaceutical Analysis - KU Leuven, Belgium: Analysis of Aromatic Substituted Quaternary Ammonium Salts using a Headspace Gas Chromatography Based Methodology
50. Kris Wolfs, Pharmaceutical Analysis - KU Leuven, Belgium: Application of an Atmospheric Micro Hollow Cathode Discharge Set-up in a Novel GC-detector

51. Emilie **Halin**, UMONS, Belgium: *Primary and secondary structures of peptoids as probed by Ion Mobility Mass Spectrometry* 

52. Alex Ttofi, BP, United Kingdom: From clear liquids to clear solutions!

53. Liz **Bevan**, Agilent Technologies, United Kingdom: Understanding the dynamics of ion suppression caused by column bleed

54. Jane **Cooper**, Waters Corporation, United Kingdom: *The Analysis of Extractable and Leachable Components from Common Packaging Material using Ion-Mobility-Mass Spectrometry : Monitoring System Performance* 

55. Peter **Kusch**, Bonn-Rhein-Sieg University of Applied Sciences, Germany: *Application of Headspace* – Solid-Phase Microextraction Coupled with Gas Chromatography/Mass Spectrometry for the Characterization of Polymeric Materials

56. Stefan **Cretnik**, ETH Zürich, Switzerland: *Direct Coupling of Solid Phase Microextraction to an* Active Capillary Plasma Ionization Source for High-Throughput Trace Analysis in Solid and Liquid Matrices

57. Dovile **Lingaityte**, University of Southampton, United Kingdom: *The Analysis of Complex Methylene Diphenyl Diisocyanate (MDI) Oligomers using UHPSFC-APPI+ MS* 

58. Laura **Provoost**, Agilent Technologies, Netherlands: *Extending Thermal Stability and Column Lifetime of WAX GC Columns* 

59. Emmanuel **Colson**, UMONS, Belgium: *Characterisation and biological evaluation of Chilean quinoa saponin* 

60. Jani **Koponen**, National Institute for Health and Welfare (THL), Finland: *Novel method for simultaneous determination of perfluoroalkyl acids, parabens and cotinine from a low volume human serum sample* 

62. Lara **Kelly**, Markes International Ltd, United Kingdom: *Combining high-capacity sorptive extraction with Thermal desorption pre-concentration for analysis of (S)VOCs in environmental samples* 

63. Alan McKeown, Advanced Chromatography Technologies Ltd, United Kingdom: Highly Sensitive and Selective Quantification of Microcystin Toxins in Drinking Water By UHPLC-MS/MS
64. Alan McKeown, Advanced Chromatography Technologies Ltd, United Kingdom: A Practical, Selectivity Based Hydrophilic Interaction Liquid Chromatography (HILIC) Method Development Protocol

#### **FLASH POSTER PRESENTATIONS**

The following young scientists were nominated to give a poster flash presentation:

- Mathys **BAERT**, Ghent University, Separation Science Group, Belgium: *Exploring the possibilities* of temperature responsive columns in comprehensive two-dimensional liquid chromatography.
- Kris WOLFS, KU Leuven, Pharmaceutical Analysis, Belgium: Application of an Atmospheric Micro

Hollow Cathode Discharge Set-up in a Novel GC-detector

- Vincent **PEPERMANS**, Free University of Brussels (VUB), Department of Chemical Engineering, Belgium: *Enhancing detection limits in chromatography using solvent-assisted post-column refocusing*
- José Luís **Dores-Sousa**, Department of Chemical Engineering, Vrije Universiteit Brussel, Belgium: Selectivity and mixed-mode retention mechanism of small-molecules in liquid chromatography using a reversed-phase / weak-anion-exchange stationary phase

#### SOCIAL PROGRAMME

- Mixer sponsored by Leco on Wednesday afternoon 24 January 2018
- Beer Degustation Evening at The Yard, St. Mary Street, Cardiff on Wednesday evening 24 January 2018
- **Gala Dinner** in the National Museum, Cardiff on Thursday evening with visit of the museum collection followed by the dinner and the appearance of the *Blaenavon Male Voice Choir*

