

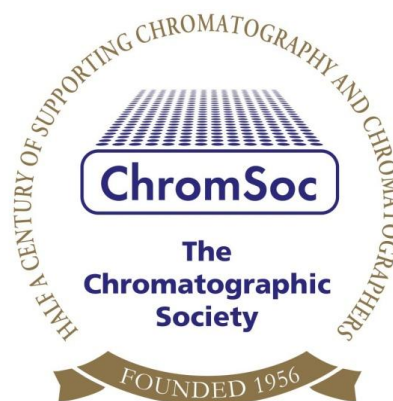
# “MATRIX CHALLENGING ANALYTICAL SCIENCE”



## BAT RESEARCH LABS

on 22nd & 23rd MAY 2013  
In “The New Auditorium”,

British American Tobacco, R & D Centre,  
Regents Park Road, Southampton, SO15 8TL,  
UK



**The Chromatographic Society** is an internationally connected organisation and UK registered charity devoted to the promotion and dissemination of knowledge on all aspects of chromatography and related separation techniques. The Chromatographic Society's AGM will feature as an integral part of this symposium.

The complex challenges that face today's analytical chemists will form the basis of this symposium.

A selection of some of the most challenging, diverse and difficult to analyse matrices and analytes has been selected for discussion. Successful methodological sample preparation approaches and associated state of the art instrumentation will be described by leading experts in their respective fields.

If you are a laboratory, industrial or forensic analyst faced with problems of selectivity, specificity and sensitivity, especially in matrices that are difficult to prepare and process, this is a *must attend* symposium for you.

If you are a manufacturer of analytical instrumentation or a contract analytical laboratory engaged in measurements and determinations in the forensic and environmental fields you will definitely benefit from attendance.

# **“MATRIX CHALLENGING ANALYTICAL SCIENCE”**

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**BAT RESEARCH LABS ON 22<sup>nd</sup> & 23<sup>rd</sup> MAY 2013**



**A TWO DAY SYMPOSIUM FOCUSING ON TODAY’S CHALLENGES TO SEPARATION SCIENCE POSED BY COMPLEX MATRICES.**

**Chromatographic and mass spectrometric analysis of body fluids, cadaveric tissues, vegetable matter, environmental pesticides, smoke aerosols, particulates and products of combustion will be explored by specialists from a variety of industries.**

**An exhibition of analytical instrumentation by leading manufacturers will form an important element of the symposium.**

## **Our Special Guest Speakers will include:**

**Prof. Dr. Ralf Zimmermann,**

Head of the “Joint Mass Spectrometry Centre” – JMSC @ University of Rostock and Helmholtz Zentrum München

*“On-line Monitoring of Complex Mixtures by Photoionisation Mass Spectrometry”*

**Prof. Jean-François Focant,**

University of Liege,

*“Chasing away the smell of death: GCxGC-TOFMS characterization of cadaveric VOCs”*

**Dr. Jasper van Heemst,**

BAT R&D labs Southampton,

*“Application of GC/HRTof for the identification and comparison of tobacco smoke constituents”*

**Dr. Peter Clayton ,**

BAT R&D labs, Southampton

*“Estimation of human smoke exposure by chromatographic analysis of spent cigarette filter extracts”*

**Dr. Greg Johnson,**

Thermo Fisher Scientific

*“Developments in GCMS/MS to achieve increased efficiency and accuracy in the analysis of complex matrices”*

**Dr. Tony Edge,**

Thermo Fisher Scientific

*“Removing Uncertainty by Removing Matrix Effects in Bio-analysis”*

**Prof. Dr. Ralf Zimmermann & Alec Kettle,**

LECO (Professor Ralf Zimmermann, speaking on behalf of LECO)

*“Gas chromatography coupled to fast high resolution TOF mass spectrometry (GC- and GCxGC-HRTOF) for analysis of highly complex mixtures”*

**Sue Roach,**

Anatune

*“Chromatography of Challenging Matrices - automating the sample preparation of body fluids”*

**Tony Taylor**

Crawford Scientific

*“Screening Multiple Interaction Columns for Enhanced Selectivity in Separating Complex Mixtures”*

**Ken Brady,**

Agilent Technologies

*“Discovery and Quantitation of unknowns by Rapid High Resolution Accurate Mass (HRAM) GC/MS Analysis”*

**Antonio Ballisai**

Perkin Elmer

Poster Title to be provided

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**Laboratory tours for delegates organised by BAT : See PROGRAMME TIMETABLE**



## MATRIX CHALLENGING ANALYTICAL SCIENCE SYMPOSIUM TIMETABLE – 1<sup>st</sup> Day

### 22nd MAY 2013

10:30AM REGISTRATION FOR THE SYMPOSIUM & EXHIBITION SET UP

12:00 NOON LUNCH

1:00PM EXHIBITION OF ANALYTICAL EQUIPMENT OPENS

1:00 to 1:45PM BAT R&D LIVE Exhibition Open for Group A

1:00 – 1:30 BAT Lab Tour for Group B

2:30PM Welcome from BAT: Dr Chris Proctor (Chief Scientific Officer)

2:40PM Introduction to the symposium: The Chromatographic Society, Dr Chris Bevan

2:45PM Dr. Tony Edge,

Thermo Fisher Scientific

*“Removing Uncertainty by Removing Matrix Effects in Bio-analysis”*

3:15PM Sue Roach,

Anatune

*“Chromatography of Challenging Matrices - automating the sample preparation of body fluids”*

3:30PM Tony Taylor

Crawford Scientific

*“Screening Multiple Interaction Columns for Enhanced Selectivity in Separating Complex Mixtures”*

3:45PM Andrew Baker

Advion

*“I’m not putting that anywhere near my Mass Spec”*

4:00PM Peter Bridge

VWR Merck Hitachi

*"New range of HPLC instrumentation from VWR - Hitachi "*

4:15PM Nick Bukowski & Bob Green

ALMSCO International

*"Ultra-trace detection and quantitation of lachrymatory compounds in complex forensic samples"*

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**7:00PM Symposium Reception drinks and dinner at Holiday Inn, SO15 1HJ**

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## **MATRIX CHALLENGING ANALYTICAL SCIENCE SYMPOSIUM TIMETABLE -2<sup>nd</sup> DAY**

**23<sup>RD</sup> MAY 2013**

9:30AM WELCOME TO SYMPOSIUM **DAY 2**

9:45AM Prof. Jean-François Focant,

University of Liege,

*"Chasing away the smell of death: GCxGC-TOFMS characterization of cadaveric VOCs"*

10:45AM Prof. Dr. Ralf Zimmermann,

Head of the "Joint Mass Spectrometry Centre" – JMSC @ University of Rostock and Helmholtz Zentrum München

*"On-line Monitoring of Complex Mixtures by Photoionisation Mass Spectrometry"*

11:45AM Dr. Jasper van Heemst,

BAT R&D labs Southampton,

*"Application of GC/HRTof for the identification and comparison of tobacco smoke constituents"*

12:30PM LUNCH

1:30PM EXHIBITION OF ANALYTICAL EQUIPMENT OPENS

1:00 – 1:45PM BAT R&D LIVE Exhibition Open for Group B

1:00 – 1:30PM BAT Lab Tour for Group A

1:30PM **CHROMATOGRAPHIC SOCIETY AGM FOR CS MEMBERS ONLY**



2:30PM Dr. Peter Clayton ,

BAT R&D labs, Southampton

*“Estimation of human smoke exposure by chromatographic analysis of spent cigarette filter extracts”*

3:15PM Dr. Greg Johnson,

Thermo Fisher Scientific

*“Developments in GCMS/MS to achieve increased efficiency and accuracy in the analysis of complex matrices”*

3:30PM Prof. Dr. Ralf Zimmermann & Alec Kettle,

LECO (Professor Ralf Zimmerman, speaking on behalf of LECO)

*“Gas chromatography coupled to fast high resolution TOF mass spectrometry (GC- and GCxGC-HRTOF) for analysis of highly complex mixtures”*

4:00PM Ken Brady,

Agilent Technologies

*“Discovery and Quantitation of unknowns by Rapid High Resolution Accurate Mass (HRAM) GC/MS Analysis”*

4:30PM CONCLUDING REMARKS, TEA AND FAREWELL

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## **ABSTRACTS RECEIVED**

### “On-line Monitoring of Complex Mixtures by Photoionisation Mass Spectrometry”

R. Zimmermann<sup>a</sup>, T. Streibel<sup>a</sup>, M. Sklorz<sup>a</sup>, R. Hertz<sup>a</sup>, C. Busch<sup>a</sup>, M. Saraji<sup>b</sup>, M. Bente<sup>b</sup>, A. Walte<sup>b</sup>



& b)



Resonance enhanced multi-photon ionisation–time-of-flight mass spectrometry (REMPI-TOFMS) using laser generated UV-photons is a sound method for selective analysis of aromatic species in complex gaseous matrices. Recently, improved electron-beam pumped excimer lamps (EBEL) and other incoherent VUV sources are used for the generation of VUV-light for single photon ionisation (SPI). SPI-TOFMS can additionally detect also aliphatic species. The latter mentioned techniques allow direct real-time monitoring of evolved gases from combustion and pyrolysis processes without fragmentation. Transfer of evolved gases to the TOFMS is carried out via heated sampling lines containing filters to account for the particle load and a deactivated quartz capillary. With these detection methods several applications in the field of monitoring of industrial and technical combustion and pyrolysis processes can be performed. This includes monitoring of car and truck exhausts, waste incineration plant effluents or products or gases from biomass pyrolysis or the industrial coffee roasting process. For example, primary organic products of biomass flash pyrolysis in a technical reactor at the KIT-Karlsruhe Institute of Technology (as part of the Biomass-to-Liquid process chain) were monitored in real time. The miscellaneous biomass feedstock (soft- and hardwood, wheat straw, coarse colza, miscanthus) showed distinguishable mass spectra with specific patterns. The main detectable components consisted of furan and phenol derivatives (cellulose and lignin decomposition products). It was possible to follow the chemical signature of the pyrolysis process gases as a function of e.g. process conditions or feed composition. In the contribution different applications are presented. Furthermore measurement concepts and examples for evolved gas analysis in thermal analysis (TA) and for on-line characterisation of tobacco smoke are considered.

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## “Chasing away the smell of death”

GCxGC-TOFMS characterisation of cadaveric VOCs

J.F. Focant et al



Soon after death, the decay process of mammalian soft tissues begins and leads to the release of hundreds of cadaveric VOCs into the surrounding environment. The study of post-mortem decomposition products is an emerging field of study in forensic science.

The complex processes of decomposition produce a variety of compounds as soft tissues and their component parts are broken down. These decomposition products include the VOCs responsible for the odour of decomposition. Human remains detection (HRD) dogs utilize this odour signature to locate human remains during police investigations and recovery missions in the event of a mass disaster. Currently, it is unknown which compounds or combinations of compounds are recognised by the HRD canines. Furthermore a comprehensive decomposition VOC profile remains elusive.

This presentation will illustrate recent advances in the characterization of human analogue decomposition VOCs using thermal desorption (TD) coupled to GCxGC, TOFMS. Decomposition headspace analyses of pig carcasses, grave soils, and HRD canine training solutions have been investigated. Several hundreds of post-mortem compounds have thus been identified.

It is believed these results will help to improve the design of the anato-chemistry and geo-forensic applications that could be of great value in forensic investigations.

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## “Application of GC/HRTof for the identification and comparison of tobacco smoke constituents”

Jasper van Heemst et al



Most extracts of plant-derived materials present analytical chemists with matrices that are particularly challenging to analyse. These extracts contain numerous compound classes with large variations in solubility, reactivity, stability and other chemical and physical properties. Furthermore, the abundances of compounds in these extracts vary widely from high concentrations to trace levels.

Tobacco extracts and smoke condensates' chemical composition increases in complexity as a result of curing, combustion and thermal degradation processes. Tobacco smoke is a very complex aerosol which contains over 5600 identified compounds and suggestions that the total number may approach 100,000.

Part of this research is focussed on understanding the processes driving the formation of smoke constituents. In order to understand these processes better, there is a need to characterise fully the compounds present in tobacco and smoke. This requires a non-targeted screening approach coupled with the capability to identify subtle differences in chemical profiles between samples. GC x GC - ToF approaches have been explored for the separation and identification of components in tobacco smoke and currently methods are being developed in which gas chromatography is coupled to high-resolution time-of-flight mass spectrometry to enable comparison of chromatographic data from different tobacco smoke samples.

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## “Estimation of human smoke exposure by chromatographic analysis of spent cigarette filters”

Peter Clayton



The presentation will explain the analytical measurements required to conduct the methodology and will detail some of the results published by BAT GR&D. A particular emphasis of the presentation will be the estimation of the mouth-level exposure to tobacco-specific nitrosamines a number of which are categorised as priority toxicants in smoke.

The Filter Analysis Method allows the estimation of ‘tar’ and nicotine yields obtained by individual smokers smoking their own cigarette in their everyday environment. It is a measure of the mouth-level exposure, the maximal exposure of tar, nicotine and other selected toxicants obtained by the smoker rather than the dose to a specified tissue.

The technique is based on the analysis of spent (smoked) cigarette filter tips which are extracted and related to smoking machine derived spent filter tips where, additionally, the mainstream smoke yields are known. The advantages of the approach include that no direct assumptions are made regarding the smoking behaviour of consumers; individual human smoke yields are estimated based on the amounts of constituents (namely nicotine, solanesol, UV absorbing species) deposited on a portion of the filter tip. The technique is non-invasive, allows for the characterisation of the natural smoking behaviour of large numbers of study participants.

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## “Removing Uncertainty by Removing Matrix Effects in Bio-analysis”

Dr. Tony Edge,



Starting the method development procedure for a complex biological fluid is often fraught with many decisions on;

- What sample preparation technique to use?
- How do we optimise recovery?

- How do we reduce the matrix effects?
- How to choose the correct column?

How these questions are answered will have a considerable bearing on how long it takes to develop the method and how robust the method is likely to be. This presentation will look at how to approach method development for a variety of different sample types ranging from impurity studies, environmental analysis, analysis of biological fluids. It will highlight how information regarding the chemical structure of the molecule can actually aid in what approaches to sample preparation need to be considered to ensure that the sample clean-up is effective.

Data will be presented on a quick and simple methodology for the optimisation of an extraction procedure and how this can affect the performance of the assay. This will be assessed by looking at key matrix components to determine the qualitative effect that optimisation of the extraction can have both in terms of the analysis of the individual sample but also in terms of the chromatographic stability of the analytical system. Repeat injections of an aqueous blank sample subsequent to the analysis of a biological extracts demonstrates that the use of correct sample preparation is key to have robust data. An investigation will also be presented which looks at the contribution the extraction technique itself adds to the matrix components has, and how this can be reduced by judicious use of the correct technology.

Finally the use of orthogonal chromatography to separate the interfering components from the analyte of interest will be discussed. The use of fingerprinting techniques will be discussed to differentiate between different molecular interactions with a range of column chemistries, as well as where to obtain this information. A real example will then be given of how this approach can be successfully applied to a routine bio-analytical assay.

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## “Developments in GCMS/MS to achieve increased efficiency and accuracy in the analysis of pesticides in complex matrices”

Greg Johnson



Laboratories working in the areas of food safety and environmental analysis often need to build efficient, low cost, high throughput methods for the analysis of those pesticides that are amenable to Gas Chromatographic separation. Furthermore, these analytical methods must deliver results that are compliant for official reporting. In recent years, Triple Quadrupole GC-MS/MS has emerged as an essential tool to power these methodologies in a routine environment. The sensitivity and selectivity of GC-MS/MS provides excellent detection limits combined with high matrix tolerance.

Customization and maintenance of analytical methods in order to match the requirements of a specific organization requires time that may detracts from the main function of the laboratory which is result generation. GC-MS/MS systems performing routine pesticide analysis face dealing with high numbers of samples and a high matrix load. Cumulative deterioration of column performance is inevitable, although techniques such as back flushing can mitigate this to some degree. Retention time drift due to matrix effects, column trimming or replacement requires frequent method updates which can be both laborious and time consuming.

This presentation will discuss how customized implementation can be made practical and also how GC-MS/MS software and hardware can work together to enable users to both efficiently develop and also maintain these complex analytical methods.

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## “Screening Multiple Interaction Columns for Enhanced Selectivity in Separating Complex Mixtures”

Tony Taylor



The separation of complex mixtures often requires enhanced selectivity and the ability to retain and separate analytes with widely varying physico-chemical properties.

So called ‘mixed mode’ stationary phases offer the ability to differentiate between such analytes and therefore to analyse very complex mixtures in a single analysis. However these phases can often be considered difficult to work with, especially when the dominant interactions responsible for separation are not well understood.

Recent developments in mixed mode bonded phase ligands, particle morphologies and screening regimes have made these phases ever more attractive for the routine use of mixed mode phases for the analysis of complex mixtures.

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## “Discovery and Quantitation of unknowns by Rapid High Resolution Accurate Mass (HRAM) GC/MS Analysis”

Ken Brady



A discussion of the strengths and limitations of traditional GC/MS approaches with non-selective sample preparation techniques. Applying Fast Acquisition HRAM GCQToF to the discovery, identification, profiling and quantitation of complex samples analyses and the use of multivariate software to determine the unknowns of importance.

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## “I’m not putting that anywhere near my Mass Spec”

Andrew Baker



New developments to produce smaller cheaper Mass Spec Instruments mean that it is now possible to consider using this technique for analyses that previously would not have been considered. This short presentation will show how the Advion Expression CMS has been used in a variety of applications to make Mass Spec accessible in new ways and for new possibilities.

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## "New range of HPLC instrumentation from VWR - Hitachi "

Peter Bridge



The HPLC team at VWR has been working with Hitachi for nearly 30 years, starting as a Merck-Hitachi cooperation. During this time the robustness and reliability of the Hitachi HPLC instruments has helped to build and develop a strong partnership. Hitachi High Technologies is one of the leading manufacturers of high precision fluidic control and optical detection instruments. In May 2013, VWR will launch the new VWR-Hitachi UHPLC system which has been designed to enhance the separation and detection of related substances as well as improving laboratory productivity. This brief talk will give an overview of what to expect from this partnership.

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## Ultra-trace detection and quantitation of lachrymatory compounds in complex forensic samples

Nick Bukowski & Bob Green



ALMSCO International, Gwaun Elai Medical Science Campus, Llantrisant, RCT, UK.

Tear gas is commonly used in riot control or as a self-defence agent, thus the presence of tear gas constituents on a suspect's clothing can aid police in the justice process. The application of comprehensive two-dimensional gas chromatography coupled with time-of-flight mass spectrometry (GCxGC-TOFMS) to the analysis of solvent-extracted clothing samples will be presented. The enhanced separation provided by this technique offers the potential to 'fingerprint' the chemical composition of a tear gas, allowing it to be linked to a particular source. Separation of the complex matrix was achieved, allowing ultra-trace quantitation of lachrymatory compounds, such as capsaicin and dihydrocapsaicin, to sub-ppb levels. In addition, various data mining techniques, for the simplification of complex sample analysis, were applied in this study and will be presented.

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### ABSTRACTS EXPECTED FROM:

Professor Ralf Zimmerman,(Speaking on behalf of LECO)



*“Gas chromatography coupled to fast high resolution TOF mass spectrometry (GC- and GCxGC-HRTOF) for analysis of highly complex mixtures”*

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Sue Roach,

*“Chromatography of Challenging Matrices - automating the sample preparation of body fluids”*

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Marco Koenen



*“GCXGC TOFMS”*

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Antonio Ballisai **PerkinElmer** POSTER PRESENTATION

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The registration fees include meals and refreshments supplied at the Symposium.

In order to encourage social networking between delegates, presenters and exhibitors, a pre-dinner mixer with canapés and sparkling wine in the Lyndhurst Bar followed by Dinner with wine in the Hamble Suite, Holiday Inn, Southampton, has been organised for the evening of 22<sup>nd</sup> May.

BAT will offer delegates a laboratory tour and open their dedicated R&D LIVE exhibition attraction to all attendees during the symposium.

**Sponsoring, Lecturing & Exhibiting Companies currently include:**



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**TO DISCUSS YOUR SPONSORSHIP LEVEL AND/OR YOUR LECTURE CONTENT PLEASE CONTACT**

Dr. Chris Bevan at: [chris.anne.bevan@gmail.com](mailto:chris.anne.bevan@gmail.com)

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Table top exhibition stand & 10 mins lecture time integrated into the programme

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**BRONZE LEVEL SPONSORSHIP £750**

Table top exhibition stand and 1 free delegate admission place

**DELEGATE ADMISSION PRICES:**

CHROMATOGRAPHIC SOCIETY MEMBER = £ 250

NON-MEMBER RATE = £ 300

NOTE: MEMBERS OF THE BMSS OR THE RSC MAY APPLY AT CHROMSOC MEMBERS' RATES

NOTE: VAT at 20% is additionally charged on all prices

**TO REGISTER AS A DELEGATE, BOOK YOUR EXHIBITION STAND AND SPONSORSHIP PLEASE USE THE FOLLOWING ELECTRONIC SECURE WEB LINK:**

<https://www4.eventsinteractive.com/mm/getdemo.ei?id=170252&s= 4RW0VZ7SI>

**OR CONTACT:**

Matthew Gilmour , Senior Conference Executive,

Meeting Makers

Block 4, Unit 4, Kelvin Campus

West of Scotland Science Park

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Email: [matthew@meetingmakers.co.uk](mailto:matthew@meetingmakers.co.uk) or [chromsoc@meetingmakers.co.uk](mailto:chromsoc@meetingmakers.co.uk)

**Please note:**

“**Chromsoc Bursaries**” are available for bona-fide students to assist them financially to attend this symposium.

Applications via E-Mail to: [The Chromatographic Society](mailto:chromsoc@meetingmakers.co.uk) at [chromsoc@meetingmakers.co.uk](mailto:chromsoc@meetingmakers.co.uk)



The Chromatographic Society website [www.chromsoc.com](http://www.chromsoc.com) will publish future updates of the symposium programme as it develops and reserves the right to make changes to the programme as necessary.

Notes: The Hotel for the Social Mixer Conference Dinner on the evening of 22<sup>nd</sup> May is the:

**Holiday Inn Hotel, Southampton**

**Herbert Walker Ave,**

**Southampton, SO15 1HJ, United Kingdom**

Should you wish to reserve yourself accommodation ring Hotel Reservations : 020 33 499 169

**Southampton is well served by rail, road and bus transport from most cities and airports in the UK.**



