

Mass Spectrometry & Spectroscopy

Visiting the 39th BMSS Annual Meeting 12th-13th September 2018 Introduction to Mass Spectrometry Course 10th & 11th September 2018 Churchill College, Cambridge, UK

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The 39th British Mass Spectrometry Society (BMSS) Annual Meeting and Introduction to Mass Spectrometry Course was held at the Churchill College, Cambridge, UK from September 10th to September 13th 2018. The meeting, exhibition and Introduction to Mass Spectrometry Course were organised by the BMSS.

History of BMSS

The formation of a specialist society formally began in 1964 after various iterations in the 1950's and 1960's under the names of the Hydrocarbon Research Group MS Panel and the Mass Spectroscopy Group; the latter was established to reflect the need of the growing mass spectrometry community for a society to cover all aspects of mass spectrometry.

The first formal conference of the BMSS took place in 1965 at University College, London and BMSS meetings have been held regularly every two years out of three since, in concert with the International Mass Spectrometry Conference (IMSC) which runs on the third year. BMSS has hosted the IMSC three times, in 1973 (Edinburgh), 1985 (Swansea) and 2003 (Edinburgh). A formal constitution for the BMSS was adopted in 1968. In the 1970s the Mass Spectrometry Discussion Group was established to further instrumental developments and fully incorporated with the Mass Spectroscopy Group as the 'British Mass Spectrometry Society'. In 1980 BMSS was registered with the UK Charity Commission, which required it to have a more educational emphasis.

The Venue

This year the BMSS Annual Meeting was hosted at Churchill College which is a constituent college of the University of Cambridge, England which boasts the largest college campus of 42 acres in Cambridge, a diverse student population and a track record of excellence, Churchill College, and to be one of the most forward-thinking academic institutions in the world following its motto – 'Forward' taken from the final phrase of Winston Churchill's first speech to the House of Commons as Prime Minister - his famous 'Blood, Toil, Tears and Sweat' speech - in which he said: "Come, then, let us go forward together."

Receiving its Royal Charter in 1960, Churchill College, is the national and Commonwealth memorial to Sir Winston Churchill. It is the embodiment of his vision of how higher education can benefit society in the modern age. Churchill College houses the Churchill Archives Centre the original purpose of which was to provide a home to Sir Winston's papers, since then it has become the home of papers from other prominent UK political figures including former Prime Ministers Margaret Thatcher and John Major, Churchill College has produced thirty-two winner of the Nobel Prize.

The venue, again an ideal geographic location with the University of Cambridge being the anchor point of the largest life science and (bio)pharma cluster in Europe, sadly was not conducive for an exhibition of 27 suppliers and sponsors as the exhibition was on multiple levels and different buildings, exhibitors isolated in small rooms - not easily visible to attendees. The parallel symposia sessions were held in the Wolfson and Colville Halls with the welcome reception, lunches and coffee breaks being held in the college dining hall.

The posters were positioned in multiple locations in two small rooms and a long corridor on the lower level. The number of communications in the programme were down compared to 2017 with around 48 oral presentations and 119 posters (2017 an anomalous year with around 52 oral presentations and 174 posters).

As usual, academia, industry and government were all well represented among the speakers and 278 delegates were in attendance, "and as fewer delegates were expected, as is normal in a year with an IMSC meeting which was held in Florence, the BMSS made a decision to secure a smaller venue and secured Churchill College," according to Gavin O'Connor the current chairperson who continued by stressing that "the registration for the 40th BMSS meeting opens in early January 2019 - so register early." In the light of BMSS cutting off registration early to cap the numbers for the past two meetings, readers should take heed or potentially be disappointed.



Figure 1. The 39th BMSS Annual Meeting Venue – Churchill College, Cambridge, UK.

The events were again accompanied by a one-and-a-half-day short course entitled Introduction to Mass Spectrometry Course on 10th and 11th September attended by 42 delegates which was designed, in keeping with the societies mantra to have a more educational emphasis, for novices to mass spectrometry who wanted to gain a solid understanding of the instrumentation, and who wanted to gain an awareness of the vast field of applications. For current mass spectrometry users, this provided an excellent refresher to the theory and a means to keep abreast of recent developments and advances in a rapidly changing field.

Course Content

The course covered the fundamental aspects of mass spectrometry, assuming an undergraduate level of basic chemistry, but required no previous practical experience or knowledge of the technique.

Attendees were introduced to the basic concepts and terminology of mass spectrometry and learned about the most important ionisation techniques in mass spectrometry such as electron ionisation, a range of atmospheric pressure ionisation techniques, some of the more recent ambient ionisation/direct analysis techniques and matrix-assisted laser desorption/ionisation. They also discovered how mass analysers work, including quadrupoles, ion traps, time-of-flight and Fourier transform mass spectrometers (Orbitrap and FT ICR), plus how hybrid mass spectrometers enable the design of the widest range of MS experiments to solve analytical problems: from compound characterisation to quantification.

Conference Schedule

<p>Session 1 - BMSS Fundamentals & Instrumentation. Each presentation 20 minutes, Keynote 30 minutes. <i>Chair: Professor Gareth Brenton</i></p>	<p>Session 2 - JPAG Impurity Profiling Regulatory & Overview. Each presentation 30 minutes. <i>Chair: Dr David Elder</i></p>
<p>Perdita Barran, University of Manchester, UK. Keynote: Variable Temperature Ion Mobility Mass Spectrometry Reveals Protein Microstates.</p>	<p>Elsbeth Gray, MHRA, UK. Regulatory Review on Control of Impurities.</p>
<p>Vincen Wu, Imperial College, UK. Desorption Electro-Flow Focusing Ionization (DEFFI) Parameter Optimization for Mass Spectrometry Imaging of Clinical Samples.</p>	<p>Mansoor Saeed, Syngenta, UK. Development of Analytical Methods Committee Guidance on Mass Spectrometry.</p>
<p>Stefania Maneta-Stavarakaki, Imperial College, UK. High-Throughput Lipidomics Analysis Directly on Cell Culture using Laser-Ablation Rapid Evaporative Mass Spectrometry.</p>	<p>David Elder, JPAG, UK. Why Increasing Sensitivity isn't always the Answer...</p>
<p>Stephan Rauschenbach, University of Oxford, UK. Electrospray Ion Beam Deposition for Imaging of Individual Biopolymers at Surfaces.</p>	

<p>Session 3 - BMSS Ion Mobility and Structure Each presentation 20 minutes, Keynote 30 minutes. <i>Chair: Dr Kostas Thalassinou</i></p>	<p>Session 4 - JPAG Impurity Profiling Case Studies and Applications. Each presentation 30 minutes. <i>Chair: Dr David Elder</i></p>
<p>Justin Benesch, University of Oxford, UK. Keynote: IM-MS of Protein Assemblies: in and Beyond Their Native State.</p>	<p>Alec Simpson, GSK, UK. Strategies for Structure Elucidation of Low-Level Impurities and Degradants: A Mass Spectrometric Journey.</p>
<p>R. Black, University of Manchester, UK. Combining Photoactivation and Ion Mobility Mass Spectrometry to Investigate structure and conformation.</p>	<p>Claudio Brunelli, Pfizer, UK. Quantification of Genotoxic Impurities in Active Pharmaceutical Ingredient Using LC-MS/MS.</p>
<p>Neil J. Oldham, University of Nottingham, UK. Chemical Modification and Collision Induced Unfolding using Native Ion Mobility-Mass Spectrometry Provides Insights into Protein Gas Phase Structure.</p>	<p>Sarah James, LGC, UK. Role of MS in Identifying/Quantifying Elemental Impurities (ICH Q3D).</p>
<p>Francisco Fernandez-Lima, Florida International University, USA. Current Trends in Trapped Ion Mobility Spectrometry - Mass Spectrometry.</p>	

<p>Session 5 - BMSS Cultural Heritage & Archaeology. Each presentation 20 minutes, Keynote 30 minutes. <i>Chair: Dr Chris Mussell</i></p>	<p>Session 6 - JPAG Impurity Profiling Novel Approaches. Each presentation 30 minutes. <i>Chair: Dr David Elder</i></p>
<p>Tamsin O'Connell, University of Cambridge, UK. Who Ate What Where & When? Mass spectrometry and the Study of Past Human Lives.</p>	<p>Mark Perkins, Anatune, UK. The Use of Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) as a Novel MS Approach to Impurities Profiling.</p>
<p>Simon Hammann, University of Bristol, UK. Palaeolipidomics - Gas chromatography Coupled to High Resolution Mass Spectrometry for the Detection of Dietary Cereal Processing in Archaeological Samples.</p>	<p>Andrew Ray, AstraZeneca, UK. Pharmaceutical Applications of Ion Chromatography/Mass Spectrometry.</p>
<p>James S.O. McCullagh, University of Oxford, UK. Mass Spectrometry Reveals Plant Polyphenols are Sequestered Into Growing Bone From the Diet and Preserved Over Archaeological Time.</p>	<p>Christopher J. Arthur. Data plotting strategies for the visualisation of complex datasets.</p>
<p>Giles Edwards, University of Manchester, UK. Development of a Novel Compact Carbon Dating Instrument Based on Collinear Resonance Ionisation Spectroscopy (CRIS).</p>	<p>Chris Nortcliffe, Sciex, UK. Characterization of Biological Impurities in Cell Derived Products.</p>

<p>Session 7 - BMSS Challenging Analytes and Analyses. Each presentation 20 minutes, Keynote 30 minutes. <i>Chair: Dr Mark Barrow</i></p>	<p>Session 8 - BMSS Metabolite Identification. Each presentation 20 minutes, Keynote 30 minutes. <i>Chair: Dr Dan Weston</i></p>
<p>Philippe Schmitt-Kopplin, Helmholtz Zentrum München, Germany. Keynote: The Holometabolome: High Resolution Tailored Metabolomics in Nutrition and Environmental Research.</p>	<p>Johanna Haglund, MetaSafe AB, Sweden. Keynote: Quantitative and Qualitative Applications for Analysis of Drugs and Their Metabolites In Vitro and In Vivo.</p>
<p>Emma K. Sisley, University of Birmingham, UK. Data Processing Tools for Native LESA TWIMS Mass Spectrometry Imaging.</p>	<p>Bela Paizs, University of Bangor, UK. Efficient Prediction of Metabolite Fragmentation Patterns for Searching Structural Databases.</p>
<p>Diana Catalina Palacio Lozano, University of Warwick, UK. Advanced analysis of bio-oils by gas chromatography coupled to Fourier transform ion cyclotron resonance mass spectrometry.</p>	<p>Stephen Wilkinson, AstraZeneca, Cambridge, UK. The use of the Liquid Extraction Sample Analysis (LESA)-PLUS Platform to Perform Localised Metabolite Identification From Tissue Samples.</p>
<p>Colin S. Creaser, Loughborough University, UK. Strategies for Targeted and Non-Targeted Profiling of Complex Samples Using Field Asymmetric Waveform Ion Mobility Spectrometry-Mass Spectrometry.</p>	<p>Simon Wood, Cyprotex Discovery, Macclesfield, UK. Identification of the Metabolites of Alicaforsen, a 20-mer Phosphorothioate Oligonucleotide, in Human Hepatocyte Samples: A Novel LC-MS Methodology Utilizing Targeted Pre-Cursor Ion Scanning.</p>

<p>Session 9 - BMSS Proteomics & Metabolomics. Each presentation 20 minutes, Keynote 30 minutes. <i>Chair: Professor Helen Cooper</i></p>	<p>Session 10 - Reid Answering the New Challenges in Small Molecule Quantification. Each presentation 20 minutes, Keynote 30 minutes. <i>Chair: Dr Timothy Sangster</i></p>
<p>Claire Eyers, University of Liverpool, UK. Keynote: The Expanding Landscape of Human Protein Phosphorylation.</p>	<p>Dr Graeme T. Clark, Concept Life Sciences, Manchester, UK. Keynote: Expanding Expectations Within Non-Regulatory Bioanalysis.</p>
<p>Richard J. A. Goodwin, AstraZeneca, Cambridge, UK. Defining drug delivery, metabolism and response through combined multimodal mass spectrometry imaging molecular (MALDI, DESI and imaging mass cytometry).</p>	<p>Glen Hawthorne, AstraZeneca, Cambridge, UK. Meeting the Bioanalytical Challenges of Novel Drug Delivery Initiatives.</p>
<p>Jana Havlikova, University of Birmingham, UK. Development of Liquid Extraction Surface Analysis Mass Spectrometry for Identification of ESKAPE Pathogens from Complex Substrates.</p>	<p>Amy Tym, LGC, Fordham, UK. Challenges of Validating Endogenous Analytes In Atypical Matrices by LC-MS/MS.</p>
<p>Albert Koulman, University of Cambridge, UK. Leptin Levels Potentially Regulate Modifications in the Lipidome 60 Years After Gestational Famine Exposure.</p>	<p>Patrizia Dragone, Angelini S.p.A., Rome, Italy. Bioanalytical Strategies to Overcome Discovery Challenges for GSK-3beta inhibitors.</p>

<p>Session 11 - BMSS Environmental. Each presentation 20 minutes, Keynote 30 minutes. <i>Chair: Mr Dan Carrier</i></p>	<p>Session 12 - Reid Large Molecule Quantitation. Each presentation 20 minutes, Keynote 30 minutes. <i>Chair: Dr Richard Houghton</i></p>
<p>Marvin Shaw, University of York, UK. Keynote: Evaluation of Selected Ion Flow Tube Mass Spectrometry for VOC concentration and emission determination in Beijing - Automation and Calibration considerations.</p>	<p>Mohammed Abrar, BioApp Solutions Ltd, UK. Keynote: Bioanalytical Overview (Quantification of Peptides & Proteins) by LC-MS.</p>
<p>John Quick, ALS Environmental, UK. Exploring the Advantages of Automated Sample Preparation and High Sensitivity GC-MS for SVOC and Pesticide Analysis in Environmental Waters.</p>	<p>Robert Wheller, LGC, UK. Diversifying the Bioanalytical Toolkit for Protein LC-MS: Improving Selectivity with 2D-LC and HR-MS.</p>
<p>Peter J. Baugh, BMSS, UK. An Historic Perspective of Applications of Chromatography Mass Spectrometry to Environmental Matrix Analysis.</p>	<p>Richard G. Kay, MRC/University of Cambridge, UK. Biomarkers of Pancreatic Neuroendocrine Tumours Identified Through Plasma Peptidomics.</p>
<p>Mary J. Thomas, University of Warwick, UK. Petroleomic Depth Profiling of Contaminated Staten Island Soil by GC and FT-ICR MS.</p>	<p>Carmen González-Tejedo, CRUK/ University of Cambridge, UK. Antibody-Independent Targeted Quantification of KRAS Mutations by Parallel Reaction Monitoring Mass Spectrometry in Pancreatic Cancer Cells.</p>

The BMSS Annual Meeting Conference

Gavin O'Connor opened the meeting "Thanking all the sponsors and exhibitors, acknowledging that without them the meeting wouldn't happen and welcoming a delegation of scientists from the Chinese Mass Spectrometry Society, led by Professor Yi Chen (CMSS Vice President)."

The format of the scientific programme with two parallel sessions was similar to that of previous meetings, the major scientific themes of BMSS39 being focused on life sciences and (bio)pharma. The scientific program on Wednesday 12th September was organised in collaboration with the Joint Pharmaceutical Analysis Group (JPAG) who ran three sessions and two sessions on Thursday were organised by Reid Bioanalytical Forum.

The meeting commenced with the Maccoll Lecture, honouring the memory of Alan Maccoll, a pioneer of mass spectrometry and a founding father of what is now the BMSS which was presented by Professor Catherine E. Costello (Departments of Biochemistry, Biophysics and Chemistry Center for Biomedical Mass Spectrometry Boston University School of Medicine, Boston, MA USA). The lecture entitled 'Divide & Conquer Strategies for Glycan Structural Determinations' explained the biological role of glycans and other carbohydrate structures and how they were dependent on their structures. Cathy continued to explain that the determination of the molecules of interest present more challenges than are encountered for biopolymers with linear structures since they are in limited quantity and occur as components of complex mixtures with multiple closely related structures, often contain branches and labile modifications, and change with ageing (time), growth and the environment. Cathy explained why existing analytical techniques were unsatisfactory and laid the groundwork for explaining her approaches to structural studies through the optimisation of separation strategies and clarification of the mechanisms driving fragmentation, and how she and her co-workers use various combinations of these approaches on time-of-flight, Orbitrap and FT-ICR MS instruments.

Her lecture was followed by the welcome mixer (sponsored by Leco) and exhibition, which was held in the college dining hall.

The welcome mixer, enjoyed by all, consisted of a beer selection, red and white wine and nuts and crisps, a venerable feast for the starving Mass Spectrometrists and exhibitors who had been busy all day. Upon the conclusion, rather than an off-site social event, the organiser's planned to hold a barbecue (sponsored by Anatune) in the college grounds, which sadly was thwarted by poor weather, and the barbecue was held in the dining hall after the reception.

The two-day meeting started in earnest on Wednesday with the Robinson Lecture, a lecture to recognise the contribution to Mass Spectrometry of Professor Carol Robinson. The lecture was titled 'Using Proteomics to Probe the Spatial Proteome and Transcriptome' and was given by Professor Kathryn S. Lilley, (Cambridge Centre for Proteomics, Department of Biochemistry, University of Cambridge, Cambridge UK).

Wednesday mornings two parallel sessions followed a one-hour coffee break which took place after the Robinson Lecture, permitting delegates to review the even numbered posters, and included oral presentations from sessions one and two.

These sessions were followed by a lengthy two-hour lunch break at 12.10, which was held in the exhibition area and permitted attendees time to network with vendors, view posters and attend the Bruker Lunch Seminar (12.45 - 14.00).

The two parallel Wednesday sessions continued after the lunch break with sessions three, four, five and six. This session was broken at 15.40 for a 30-minute tea break and more time to peruse the exhibition and posters.

A drinks reception and the conference dinner at St. John's College, Cambridge rounded off a full first day of the BMSS Annual Meeting and Conference.

Thursday morning started with two parallel sessions, seven and eight. These sessions were followed by a one-hour coffee break, which was held in the exhibition area.

The pair of Thursday morning parallel sessions continued after the coffee break with sessions nine and ten before a break of one hour for lunch, during which the BMSS Annual General Meeting took place, preceded the afternoon sessions, the BMSS Chairs Plenary Lecture, prize presentations and the closing farewell.

The final lecture, the Plenary BMSS Chair's Lecture, was given by Professor E. N. Clare Mills (University of Manchester, UK) on 'From Detection of Allergens in Foods to Qualifying Foods as Drugs - the Role of Protein Mass Spectrometry'.

Late Thursday afternoon saw the presentation of various BMSS awards by the BMSS Chair Dr Gavin O'Connor as part of the closing ceremony.

The prizes that were awarded were as follows:

The Barber Prize, sponsored by Ionoptika, was awarded to the best new and upcoming researcher's oral presentation at the 2018 meeting in honour of Mickey Barber who had a dislike of giving oral presentations. This year's awardee was **Mary Thomas - University of Warwick** for her Thursday morning oral presentation titled '**Petroleomic Depth Profiling of Contaminated Staten Island Soil by GC and FT-ICR MS**' which discussed how the New York/New Jersey estuary, with a high population density and with many industrial upstream waste sources, was one of the highest contaminated waterways in the USA. Samples from five sampling depths of the sediment core were extracted followed by direct infusion atmospheric pressure photoionization (APPI) fourier transform ion cyclotron resonance (FT-ICR) MS and GC atmospheric pressure chemical ionisation (APCI) FT-ICR MS resulting in new compound classes being identified.



Mary Thomas - University of Warwick and Dr Gavin O'Connor (Photograph courtesy of BMSS).

The Bordoli Prize, sponsored by Waters in honour of Bob Bordoli is awarded to the best new and upcoming researcher's poster presentation at the 2018 meeting. This year's awardee was **Stephanie Rankin Turner - University of Loughborough** for her poster titled '**Rapid In-Situ Monitoring of the Compositional Changes in Fingerprint Residues with a Direct Sampling Probe**' which described the development of in-situ analysis methods for use at crime scenes to reduce the time and cost associated with police forensic analysis. Various studies have attempted to develop a methodology to establish the age of a fingerprint discovered at a scene, which is essential in establishing its relevance to the investigation time line, however so far there are no established techniques.



Stephanie Rankin Turner - University of Loughborough and Dr Gavin O'Connor (Photograph courtesy of BMSS).

Entrants for these two prizes must be current BMSS members with less than 5 years' experience in mass spectrometry, including MS oriented PG research but not including career breaks.

The Delegates' Choice Poster Prize Competition, sponsored by SS Scientific, provided an opportunity for all delegates of the BMSS Annual Meeting and Conference to vote for their choice as the best poster at the conference from any author.

The **Delegates Choice Poster Prize**, was awarded to **Robert Bradley - University of Durham** for his poster titled '**Development of UniSpray Mass Spectrometry**' where he discussed a novel ionisation source, UniSpray developed by Waters to overcome limitations faced by Electrospray Ionisation, such as the reduced desolvation efficiency at high flow rates. The key innovation of UniSpray is the presence of a charged, cylindrical target rod onto which the analyte solution is sprayed, increasing the desolvation efficiency



Robert Bradley - University of Durham and Dr Gavin O'Connor (Photograph courtesy of BMSS).

This extremely valuable meeting covered everything from basic principles to fundamental aspects, method developments and applications of the various uses and analyses performed utilising mass spectrometry. The quality of the poster contributions and the novelty of the scientific content of the presentations, describing all aspects of mass spectrometry and associated separation techniques, were of tremendous value for both novices and experts.

At the social level, the meeting provided plentiful opportunities to chat and share, over coffee or the inevitable beer. Many of the delegates (~200) attended the Conference Dinner, and thoroughly enjoyed themselves in true BMSS tradition. The Vendor Exhibition was, as always, a critical component of the meeting.

The next BMSS annual meeting and conference, its 40th, will held at the Royal Northern College of Music, Manchester, UK and will take place between 2nd and 5th September 2019. Updated details may be found at www.bmss.org.uk.

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