Visiting the 36th BMSS Annual Meeting 15th-17th Sept 2015
BMSS Introduction to Mass Spectrometry Course 14th & 15th Sept 2015
University of Birmingham – Edgbaston, UK

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The 36th British Mass Spectrometry Society (BMSS) Annual Meeting and Introduction to Mass Spectrometry Short Course was held at the University of Birmingham, Edgbaston, UK from 14th - 17th September 2016. The meeting, exhibition and short 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 historical attendances for the BMSS meetings, including smaller 2-day meetings that are held in the years of IMSC, are shown in *Table 1*. These numbers when compared to the declining membership numbers *(Table 2)* are very healthy and holding strong showing the obvious value and interest of the meeting.

Table 1. BMSS Annual Meeting Attendances

BMSS 2011	City Hall Cardiff - 264 delegates.
BMSS 2012	Astra Zeneca, Alderley Park (smaller 2 day, single session meeting) - 190 delegates.
BMSS 2013	Winter Gardens Eastbourne – 272 delegates.
BMSS 2014	Astra Zeneca, Alderley Park (smaller 2 day, single session meeting) - 180 delegates.
BMSS 2015	University of Birmingham - 275 delegates.

Table 2. BMSS Membership History

2010 – 719 members
2011 – 679 members
2012 – 631 members
2013 – 613 members
2014 – 577 members

The decline in BMSS members over the last five years is likely attributable to the decline of the pharmaceutical industry in the UK and the erosion of dedicated mass spectrometry facilities coupled with the adoption of the Mass Spectrometer as a universal detector in HPLC and other separation techniques. The current trend to simple push button operation mass spectrometers, no longer needing a specialist to perform and evaluate the sample analysis, potentially will be a continuing factor in the decline of members.

The symposia took place in the Elgar Concert Hall in the Bramall Building and the University's original, late-Victorian redbrick building, The Aston Webb building (pictured).

The Posters were positioned in two locations on the first floor foyer of the Bramall Building and in the first floor rotunda of the Aston Webb Building (pictured).

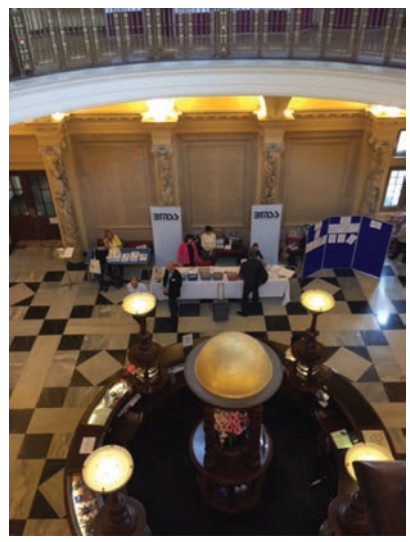
As usual, academia, industry and government were all well represented among the speakers and over 275 delegates were in attendance. The events were again accompanied by a one and a half day short course on 14th and 15th September which was designed, in keeping with the societies mantra to have a more 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.

The Aston Webb Building

Course Content

The course covered the fundamental aspects of mass spectrometry, assuming an undergraduate level of basic science, 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 used 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.



View of BMSS Annual Meeting Registration from the First floor rotunda of the Aston Webb Building

The BMSS Annual Meeting Conference

The aims of this BMSS annual meeting conference were to "of promoting knowledge and advancement in the field of mass spectrometry, and providing a forum for the exchange of views and information."

The conference was opened with a welcome from the current chair Colin Creaser who announced that "the format of the scientific programme this year is similar to that used for the last two annual meetings, including invited and contributed oral presentations, posters and panel discussions".

The meeting officially opened 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 Ron Heeren from the Maastricht Multi Modal Molecular Imaging Institute (M4I) on 'Molecular Pathology with MS: Towards Personalised Medicine' which, despite a short (10 minutes) technical issue with the slide presentation - which was handled very professionally, highlighted his groups roles as MS scientists embedded in a clinic. Along with the M4I fundamental research, innovative developments, and unique applications in multimodal imaging MS Professor Heeren feels his role is to build a bridge to solve clinical problems and follows the paradigm's of Dr Leroy Hood (Institute for Systems Biology (ISB), Seattle, WA, USA.) known as the 4 P's of modern medicine – Personalised, Preventative, Predictive and Participatory. The results shown have already demonstrated that rapid, direct tumour phenotyping is now reality and pointing the way towards patient side personalised diagnosis and therapy.

His lecture was followed by the welcome mixer and exhibition, which was held in the Great Hall. The Great Hall, now acting as the University's ceremonial hall used for significant events in the academic calendar including exams and graduation, is the University of Birmingham's most prestigious venue. It is hard to imagine that during World War One 1914-1919 it was a busy hospital ward of the Southern General Hospital where over the course of the war 130,000 patients were admitted

The Great Hall has also hosted televised events such as the 2010 UK General Election Leaders Debate and the BBC Antiques Road Show.

The welcome mixer, enjoyed by all, consisted of beer, wine, nuts and crisps, a venerable feast for the starving Mass Spectrometrists and exhibitors who had been busy all day.

The instrument and supplies exhibition, with a total of 31 vendors covered the 650 square meters of floor space available in The Great Hall and created the ideal forum to assess the state-of-the-art of modern mass spec instrumentation and vendors had the opportunity to go into detail about their new developments and products.

The two-day meeting started in earnest on Wednesday with a Plenary Lecture titled 'Hybrid Methods for Defining the Structure and Function of Cellular Machines' by Professor Brian Chait (Rockefeller University). Professor Chait was the recipient of 2015 American Society of Mass Spectrometry (ASMS) Award for a Distinguished Contribution in Mass Spectrometry.

Wednesday mornings two parallel sessions followed the plenary lecture and included the following oral presentations:

Session 1 - Complex Mixtures	**Session 2 - Small Molecules**
Chair: Dr Mark Barrow (University of Warwick)	Chair: Dr Jackie Mosely (Durham University)
Determination of Oilfield Additives using Separation Science and Mass Spectrometry	Development of an Interface for the Direct Analysis of Volatiles Using a Transportable Mass Spectrometer
By Elia Efstathios (University of Southampton)	By Dr Pilar Perez-Hurtado (Loughborough University)
Advanced Multi-modal Mass Spectrometry Applied to the Complexity of Lipid Imaging Analysis	Predicting collision-induced dissociation (CID) fragmentation: understanding the role of the mobile proton in small molecule fragmentation
By Jens Fuchser (Bruker UK Ltd)	By Dr Patricia Wright (University of Greenwich)
Enantiomer specific analysis of multi-component mixtures by correlated electron imaging–ion mass spectrometry	Determining relative binding affinities of integrin antagonists by ultrafiltration and liquid chromatography-mass spectrometry
By Professor Maurice Janssen (MassSpecpecD Ltd)	By Tshuma Nkazimulo (University of Nottingham)
Field asymmetric waveform ion mobility spectrometry combined with mass spectrometry for the analysis of anabolic steroids	Differentiation of Epimeric Oleanolic and Ursolic Acids and Related Pentacyclic Triterpenoids by Positive Mode Atmospheric Chemical Ionisation Mass Spectrometry
By Kayleigh Arthur (Loughborough University)	By Dr Martin William (University of Bradford)

Two particularly interesting presentations were:

Firstly Elia Estathios' discussion of how the internal corrosion of low-alloy steel transmission pipelines is a major concern in the oil and gas industry and how a model corrosion inhibitor formulation comprising of four quaternary amines, two AEEA imidazolines and two TOFA/DETA imazolines was prepared in methanol and used for qualitative and quantitative analysis using HPLC-MS, UHPLC-MS (/MS) and UHPSFC-MS (/MS). Use of UHPSFC as the methods of chromatographic separation, coupled with positive ion electrospray ionisation (+ve ESI) tandem mass spectrometry, which resulted in sub ppm (<0.5 ppm) detection limits for all corrosion inhibitors in neat solvent. The UHPSFC-MS method decreased the analysis times by a factor of 4 when compared to HPLC, eliminating any need of a sample preparation prior to analysis, especially in the case of crude oil.

The Great Hall housing the BSMM Annual Meeting exhibition.

Secondly Dr Martin William outlined a new and reliable method for distinguishing the equatorial and axial epimers of oleanolic and ursolic acids and related triterpenoids based primarily on the relative abundance of the [M+H]+ and [M+H-H2O]+ signals in their positive atmospheric pressure chemical ionisation (APCI+) mass spectra.

These sessions were followed by a thirty-minute coffee break, which was held in the exhibition area and permitted time to meet with vendors.

The Wednesday morning two parallel sessions continued after the coffee break, before breaking for lunch with sessions on:

Session 3 - New Topics in Mass	**Session 4 - Quantitation**
Chair: Dr Anthony Bristow (AstraZeneca)	Chair: Dr Chris Mussell (LGC) and Dr Ken Brady (Agilent)
High-throughput picodroplet-based ESI-MS analysis of biosynthetic libraries	Development and validation of a candidate reference measurement procedure for the quantitation of total serum cortisol using liquid chromatography-tandem mass spectrometry.
Dr Clive Smith (Sphere Fluidics Limited)	James Hawley (University Hospital South Manchester)
LILBID: a soft mass-spectrometry method for non-covalently bound protein complexes in physiological environment	Measurement uncertainty in human sports drug testing.
Lieblein Tobias (University of Frankfurt)	Professor David Cowan (King's College London)
ETnoD IM-MS – how electrons alter the conformation of globular and disordered gas phase proteins.	Measurement uncertainty and mass spectrometry; basic concepts applicable to routine laboratories and lessons learnt from participation in National Metrology Institute laboratory intercomparions.
Jacquelyn Jhingree (University of Manchester)	Chris Mussell (LGC)
A novel atmospheric-pressure transmission-mode ion source for MALDI MS imaging	Determination of priority environmental pollutants in water treatment plant effluent: quantifying a drop (or two) in the ocean – depending on MS technique is used.
By Dr Rory Steven (National Physics Laboratory)	John Quick (ALS Environmental)

Of interest in these sessions were:

Rory Steven discussed how the majority of matrix-assisted laser-desorption-ionisation mass spectrometry (MALDI-MS) instrument designs employ reflection geometry; i.e. the laser irradiation and ion extraction take place on the same side of the sample. An alternative configuration, transmission geometry, involving laser irradiation from the backside of the sample, through a transparent support was discussed as was the construction and evaluation of an atmospheric pressure transmission mode MALDI-MS imaging source.

Chris Mussel discussed how metal-based Chemotherapeutics are highly effective and used to treat various strains of cancer; unfortunately patients experience a wide range of dangerous side effects. A new approach was described using the localised activation of an inert metallo-prodrug to ensure these compounds are only active where they are needed – near cancerous tissue. Less drug is wasted in other parts of the body, causing fewer side effects and translating into reduced dosages. Some drugs were shown to be an order of magnitude more potent than Cisplatin under comparable conditions.

After lunch the Wednesday afternoon was dedicated to a one and a half hour very lively and sometimes heated Panel Discussion/Workshop led by Dr Jerry Thomas (University of York) and Dr Tony Sullivan (Agilent) titled 'Should Proteomics be Standardized on a Single Platform?' This was followed by time to peruse and discuss the eighty poster which were presented by their author's.

A drinks reception and the conference dinner rounded off a full first day of the BMSS Annual Meeting and Conference.

Thursday morning started with two parallel sessions.

Session 5 - British Society for Proteome Research Joint Session – Protein Analysis	Session 6 - Metabolomics Society Joint Session - Metabolomics
Chair: Dr Tony Sullivan (Agilent)	Chair: Professor Mark Viant (University of Birmingham)
Keynote lecture: High-throughput screening of deubiquitylase (DUB) inhibitors by MALDI-TOF mass spectrometry.	Keynote lecture: In-situ mapping of microbial metabolism by ambient ionisation mass spectrometry.
Professor Matthias Trost (University of Dundee)	Dr Zoltan Takats (Imperial College London)
Detailed characterisation of photoactivatable metallodrug interactions with Peptides, Proteins, and DNA by high resolution tandem FT-ICR MS	Cholesterol metabolism during human CD4+ T cell activation
Christopher Wootton (University of Warwick)	Dr Yuqin Wang (Swansea University Medical School)
Release and isolation of O-glycans: towards a system for studying disorders of protein O-glycosylation	Physicochemical fractionation coupled with multiple-stage fragmentation for deep metabolome annotation of the NIH model organism, Daphnia magna (the water flea).
Kirsty Skeene (University of York)	Martin Jones (University of Birmingham)
Integrating native mass spectrometry into the structural biology workflow – exemplified by the structural analysis of a bacterial ferritin-like protein	Developing metabolomics strategies for the analysis of central energy metabolism using ion-chromatography coupled to mass spectrometry.
Dr David Clarke (University of Edinburgh)	Professor James McCullagh (University of Oxford)

These sessions were followed by a thirty-minute coffee break, which was held in the exhibition area and permitted time to meet with vendors.

The pair of Thursday morning parallel sessions continued after the coffee break - before breaking for lunch with sessions on:

Session 7 - Imaging in Mass Spectrometry	Session 8 - Ion Mobility and Instrumentation
Chair: Professor Malcolm Clench (Sheffield Hallam University)	Chair: Professor Perdita Barran (University of Manchester)
Measuring the performance of mass spectrometry imaging techniques.	Ion mobility mass spectrometry to investigate the stability of -crystallin dimers to increased oxidation and its significance to RP-MS / protein footprinting applications.
Dr Josephine Bunch (National Physical Laboratory)	Dr Simin Maleknia (University of New South Wales)
Mass spectrometric analysis of a three-dimensional hepatocarcinoma cell model to determine acetaminophen toxicity.	The effect of the charge model on in silico ion mobility calculations.
Ieva Palubeckaite (Sheffield Hallam University)	Lukasz Migaz (University of Manchester)
Analysis of nanoparticle-formulated anti-tumour drugs in preclinical models using multimodal mass spectrometry imaging	A Multi-pass Cyclic Ion Mobility Separator: Design and Performance
Nicole Strittmatter (AstraZeneca)	Dr Kevin Giles (Waters Corporation)
Combining MS and SRS Imaging for a Deeper View of Sample Chemistry.	Novel structural insights into cyclic AMP-dependent protein kinase (PKA) dynamics using ion mobility mass spectrometry IMS-MS.
Elizabeth Randall (University of Birmingham)	Dr Matthias Vonderach (University of Liverpool)

Ian Wright from the Dept. of Physical Sciences, Open University, Milton Keynes presented the BMSS Chair's Plenary Lecture titled 'Mass Spectrometry on Rosetta - Mission Accomplished' and

described the use of a combination of MEMS components, nanotechnologies and cold-EI (along with some more traditional pipes, valves, heaters, etc.) to successfully perform analytical measurements of materials from the surface of a comet. At the heart of the instrument, known as Ptolemy (included on the Philae Lander part of ESA's Rosetta space mission), is a miniaturised ion trap mass spectrometer. This was used to gather results from three discrete sets of analyses. The first was from solid organic particles collected at the first touchdown site, the second was after the lander came to rest and involved a series of measurements of the major volatiles, taken at intervals over a 45-hour period, and the third was from materials collected in one of our sampling ovens.

Late Thursday afternoon saw the presentation of various BMSS awards by the BMSS Chair Prof. Colin Creaser as part of the closing ceremony.

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 and the closing farewell.

Session 9 - Trapped Ion Instrumentation	Session 10 - Mass Spectrometry and Proteomics
Chair: Professor C. S. Creaser (Loughborough University)	Chair: Dr Jerry Thomas (University of York)
Two-dimensional Fourier transform ion cyclotron resonance mass spectrometry: from experimental curiosity to fully-fledged analytical method.	Improved efficiency of in situ tryptic proteolysis: from fingermarks to tissue
Dr Maria van Agthoven (University of Warwick)	Ekta Patel (Sheffield-Hallam University)
Comparison of dissociation methods for petroleum samples using Fourier transform ion cyclotron resonance mass spectrometry.	Similar or biosimilar: A batch-to-batch comparison of the therapeutic monoclonal antibody Herceptin; an ion-mobility and mass spectrometric insight into biosimilarity.
Dr Mark Barrow (University of Warwick)	Rosie Upton (University of Manchester)
Trapped Ion UVPD in an ion mobility enabled Q-ToF mass spectrometer.	Overcoming challenges during the development of a multiplexed SRM incretin method
Alina Theisen (University of Manchester)	James Howard (Loughborough University)
Systematic evaluation and optimisation of multi-stage fragmentation strategies for untargeted metabolite annotation.	Towards personalised medicine: Quantification of human drug metabolising enzymes and transporters using a QconCAT-based LC-MS/MS approach.
Dr Ralf Weber (University of Birmingham)	Dr Jill Barber (University of Manchester)

The prizes that were awarded were as follows:

The Barber Prize, sponsored by LGC, was awarded to the best new and upcoming researcher's oral presentation at the 2015 meeting. This year's awardee was Elizabeth Randall, University of Birmingham for her oral presentation titled 'Combining MS and SRS Imaging for a Deeper View of Sample Chemistry' which discussed how mass spectrometry imaging (MSI) provides chemical specificity and spatial information. A brief discussion of the current popular, if still problematic, techniques such as MALDI MSI and liquid extraction surface analysis (LESA) MS led to the work performed on Stimulated Raman Scattering (SRS) microscopy. Through combinations of these techniques on the same sample it was shown that it is possible to quantitatively and visually assess changes to the sample surface, which occur during laser ablation and liquid extraction. The combined workflows for the multimodal imaging of model and biological samples were presented with a view to better understanding mass spectrometry surface sampling processes.

Elizabeth Randall and Professor Colin Creaser (Photograph courtesy of BMSS)

Pui Yiu Lam and Professor Colin Creasey (Photograph courtesy of BMSS)

The Bordoli Prize, sponsored by Waters, awarded to the best new and upcoming researcher's poster presentation at the 2015 meeting. This year's awardee was Pui Yiu Lam, University of Warwick for her poster titled 'Molecular Clock of Islet Amyloid PolyPeptide: from Dimerization to Deamidation' which showed how aggregated islet amyloid polypeptide (IAPP) is toxic to pancreatic beta-cells which cause islet cell death and results in type 2 diabetes. The poster showed the use of ultrahigh resolution of FTICR MS to explore the linking positions between dimerised IAPPs and the deamidation sites of the IAPP. Also shown were the tandem mass spectra of CAD, IRMPD, and ECD of dimerised and deamidated IAPP which are used for sequencing the protein, and determining the binding and deamidation positions of the IAPPs. Quantitative mass spectra were also shown to demonstrate the aggregation rate of IAPP throughout the experiment. The relationship

Lucio Manzi and Professor Colin Creasey (Photograph courtesy of BMSS)

between dimerisation, polymerisation, and deamidation were linked through the time-point monitoring experiments. ECD was shown to be an important fragmentation method in the study of the binding between non-covalently bounded proteins.

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 AstraZeneca, provided an opportunity for all delegates of the BMSS Annual Meeting and Conference to vote for the best poster at the conference from any author.

The Delegates Choice Poster Prize was awarded to Lucio Manzi, University of Nottingham for his poster titled 'Mapping protein complexes by carbene footprinting' where he discussed how the interactions between proteins and their binding partners are vital in many biological processes and the use of a novel water soluble photolabelling reagent in combination with mass spectrometry to map protein complexes contact surfaces using a differential footprinting approach.

The technique was tested on a range of protein interactions, including the Lysozyme-NAG5 complex, an extensively characterised protein-ligand system. Liquid chromatography-tandem mass spectrometry (LC-MS/MS) analysis strategy was applied to labelled lysozyme to quantify site-specific incorporation of the reactive intermediate generated from the photolysis of the diazirine. The extent of the labelling exhibited by bound and unbound protein was compared. Variations in the labelling pattern reflected changes in solvent exposure resulting from binding.

To further test the technique, binding of USP5 to diubiquitin, a system whose structure is not completely known was also investigated. The results obtained were in good agreement with previous literature, demonstrating that the novel photolabelling reagent, in combination with LC/MS analysis, can provide high quality structural information for mapping protein-ligand and protein- protein interaction sites

BMSS Meetings Secretary Dr Anthony Sullivan, summarised the meeting saying:

"This year's Annual BMSS Meeting, held at the University of Birmingham for the first time, was in all aspects a resounding success." He continued: "achieving the overall aims of promoting knowledge and advancement in the field of mass spectrometry, and providing a forum for the exchange of views and information. A well-balanced scientific programme was constructed, addressing everything from instrument fundamentals and design to the latest developments in selected application areas. This year a theme of collaboration and connection ran through the programme, with three sessions devoted to the society's Special Interest Groups, one in collaboration with BSPR and another with the Metabolomics Society, reflecting BMSS's wish to share and engage.

"At the social level, the meeting provided plentiful opportunities to chat and share, over coffee or the inevitable beer. 160 delegates attended the Conference Dinner, and thoroughly enjoyed themselves in true BMSS tradition.

"The Vendor Exhibition was, as always, a critical component of the meeting – seeking to bring the vendors closer to the delegates, we moved away from the use of purpose-built shell structures to a more open layout in the beautiful Great Hall. The feedback was excellent, from delegates and exhibitors alike."

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 high 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.

The next BMSS annual meeting and conference will be returning to Eastbourne, the site of the 2013 meeting, and will take place from 12th-15th September 2016.

Acknowledgement: Thank you to Lisa Sage, BMSS administrator, for her assistance in providing the historical demographics and the awardee photographs.