Visiting the 37th BMSS Annual Meeting 13th-15th September 2016
BMSS Introduction to Mass Spectrometry Course 12th & 13th September 2016

The Winter Gardens, Eastbourne, UK
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The 37th British Mass Spectrometry Society (BMSS) Annual Meeting and Introduction to Mass Spectrometry Short Course was held at the Winter Gardens, Eastbourne, UK from 12th to 15th 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 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.
BMSS 2016 – Eastbourne Winter Garden – Attendance not available at press time

Table 2. BMSS Membership History

2010 – 719 members
2011 – 679 members
2012 – 631 members
2013 – 613 members
2014 – 577 members
2015 – 620 members

The Venue

This year the BMSS Annual Meeting returned to a very sunny, warm and pleasant Eastbourne at the same venue as the 2013 Annual Meeting. The Winter Gardens a Grade II listed building in Eastbourne, was designed in 1875 by Henry Currey and built by the seventh Duke of Devonshire as part of the Devonshire Park complex, together with the Devonshire Park Theatre and the Indian Pavilion. This historic building consists of two main parts - the Floral Hall, originally used as a skating rink in winter and concert hall in summer, and the Gold Room.

Both parts are now used for performances, cabaret style events, dinner dances and as a conference venue. The Congress Suite, utilised by BMSS, links the Floral Hall and the Congress Theatre providing undercover access for delegates. The parallel symposia sessions were held in the Gold Room and the Congress Suite with the welcome reception, exhibition, lunches and coffee breaks being held in the Floral Hall.

Figure 1. The 37th BMSS Annual Meeting Venue – The Winter Gardens in Eastbourne from the better side. (Photograph courtesy of BMSS)

The Posters were positioned in a single location in the Devonshire Park Hall that provided ample viewing space and time for discussions with poster presenters.

Figure 2. The 37th BMSS Annual Meeting Poster Session.

As usual, academia, industry and government were all well represented among the speakers and around 225 delegates were in attendance. The events were again accompanied by a one-and-a-half-day short course on the 12th and 13th 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.

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.

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' and was opened with a brief welcome from the current chair Dr Christine Eckers. The format of the scientific programme this year was similar to that of previous meetings, with invited and contributed oral presentations and posters, but this year BMSS also decided to include keynote speakers for the sessions, designed to provide an in-depth view of their work.

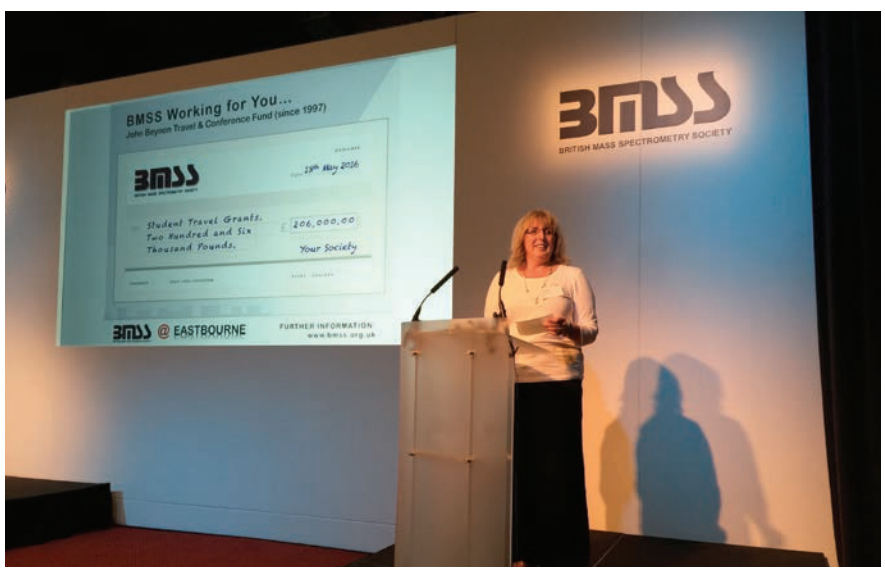

Figure 3. Christine Eckers opening the BMSS annual meeting. (Photo courtesy of BMSS)

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 Renato Zenobi from Department of Chemistry and Applied Biosciences, ETH Zurich, Switzerland. The lecture entitled 'Exhalomics by Ambient Mass Spectrometry' explained how exhaled breath contains important information on the state of a person's health and that Mr Zenobi's vision is to employ real-time non-invasive chemical analysis of exhaled breath for applications such as patient diagnosis, the treatment and monitoring of diseases, drug compliance/drug abuse, pharmacokinetics, and others. He proceeded to show in a very interesting lecture that the technique could be used in medical diagnosis, by showing examples of the detection of novel biomarkers for diseases such as obstructive sleep apnea (OSA) and chronic obstructive pulmonary disease (COPD). The methodology used to analyse breath in real time is based on secondary electrospray ionisation coupled to high-resolution mass spectrometry (SESI-HRMS) which provides ppb-ppt limits of detection for compounds with molecular weights up to 1000 Da.

His lecture was followed by the welcome mixer and exhibition, which was held in the Floral Hall.

The welcome mixer, enjoyed by all, consisted of red and white wine, nuts and crisps, a venerable feast for the starving Mass Spectrometrists and exhibitors who had been busy all day. Upon the conclusion those that were of a mind and still hungry left promptly at 20:00 for 'The famous pub quiz' which took place in the Horizon Suite at the View Hotel a short walk from the conference venue, with the incentive of 'free chips' for the first 50 arrivals.

The instrument and supplies exhibition, with a total of 27 vendors (four fewer than last year) covered the floor space available in The Floral Hall and created the ideal forum to assess the state-of-the-art of modern mass spec instrumentation with vendors having the opportunity to go into detail about their new products and developments.

The two-day meeting started in earnest on Wednesday with the Robinson Lecture, a lecture is a to recognise the contribution to Mass Spectrometry of Professor Carol Robinson. The lecture was titled 'Protein Folding & Function: How Far Has Native MS Progressed?' and was given by Professor Alison Ashcroft (University of Leeds).

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

Session 1 - Glycomics	**Session 2 - Protein Complexes and Molecular Conformations**
Chair: **Professor David Harvey (University of Oxford)**	Chair: **Professor Justin Benesch (University of Oxford**)
Professor Anne Dell (ICL) - High Sensitivity Glycomics: Windows to Glycan Function	**Dr Kostas Thalassinos (UCL)** - Combining mass spectrometry approaches for elucidating the structure and function of proteins containing large unstructured regions.
Radoslaw Kozak - Biopharmaceutical erythropoietin characterisation: critical quality attribute (CQA) mapping using LC-ESI-Qtof and automated database searching of glycopeptide and glycan analytes.	**Heidi Gastall** - Regulation of small Heat Shock Protein 27: Insights from Mass Spectrometry
Anna Behrens - Site-specific N-glycan analysis of an HIV-1 Envelope trimer mimic.	**Dr Adam Cryar** - A Systematic Evaluation of the Integration of Ion Mobility into an Online Hydrogen Deuterium Exchange Mass Spectrometry Workflow
Dr Jenny Ho - Full Characterisation of Heterogeneous Antibody Samples Under Denaturing and Native/Native-Like Conditions on a Hybrid Quadrupole-Orbitrap Mass Spectrometer.	**Aimee Paskins** - Promotion and Manipulation of α-Synuclein Aggregation Observed Using ESI-IMS-MS

Two particularly interesting presentations were:

Firstly, **Radoslaw P. Kozak** (Ludger Ltd) discussed how glycosylation greatly influences the clinical performance and safety of recombinant erythropoietin (EPO) drugs and consequently how biopharma companies producing EPO products must carefully optimise, measure and control the glycosylation throughout the production lifetime of their drug. EPO contains 3 native N-link sites and a single O-link site but recombinant variants exist with more N-link sites added so EPO glycopeptide mapping is performed using a combination of an LC-ESI-QTof-MS instrument with a flexible software program for glycopeptide characterisation which is populated with a user defined database of potential glycans. The LC methodology was also discussed using a wide pore nano C18 chromatography column. Another method described was EPO glycan characterisation using an N-glycan release and fluorophore labelling strategy. This method used PNGase-F released procainamide labelled N-glycans which were separated using HILIC chromatography and detected by fluorescence and ESI-MS/MS.

Secondly **Miss Aimee Paskins** discussed how α-Synuclein is an intrinsically disordered, highly heterogeneous protein with no currently determined function and whose aggregation has been implicated in the pathogenesis of Parkinson's disease. The proteins conformation and subsequent aggregation propensity are known to be altered as a response to its environment, and several factors have been identified which increase or decrease the proteins aggregation rate. She utilised Electrospray Ionisation - Ion Mobility Spectrometry - Mass Spectrometry to demonstrate that the aggregation rate of the protein increased in the presence of metals via an increase in the more compact conformational states. This effect is further increased upon mimicking phosphorylation through amino acid substitutions at serine 87 and 129. We have determined the conformational changes

to the three forms of the protein and have observed the subsequent changes in their aggregation rates. The group also identified several novel inhibitors of aggregation, along with a potential mechanism of their action.

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

Session 3 - MS Solutions for Challenging Analytes	**Session 4 - Fundamentals and Instrument Developments**
Chair: **Dr Jackie Mosely (Durham University)**	Chair: **Professor Gareth Brenton (Swansea University)**
Dr Andy Ray (AstraZeneca) - Application of Selected Ion Flow Tube Mass Spectrometry (SIFT-MS) to the analysis of pharmaceutical products.	**Dr Kevin Giles (Waters Corp)** - The (not so) humble ion guide.
Dr Caroline Dessent - Shining Light into Mass Spectrometers: UV Laser-interfaced commercial mass spectrometers as tools for spectroscopic identification of isomeric molecular ions.	**Dr Steve Bajic** - An Aerodynamic Perspective on Impactor API Sources.
Kayleigh Arthur - Targeted and untargeted metabolic profiling by incorporating scanning FAIMS into LC-MS.	**Dr Christopher Wootton** - Supercharging of analytes via a novel modified Ion source.
Edward Wilmot - Analysis of Gasoline using Atmospheric Pressure Ionisation Mass Spectrometry.	**Dr Pavel Ryumin** - Liquid AP-MALDI enables rapid and sensitive analysis with multiply charged ions.

The Wednesday morning two parallel sessions continued after the coffee break - before breaking for lunch at 13:00 with sessions on:

Of interest in these sessions were:

Dr Caroline Dessent (University of York) reported a series of results obtained using custom-adapted laser-interfaced commercial ion-trap mass spectrometers (Bruker Esquire and AmaZon). The results presented were from a UV photodissociation spectroscopy study of the gaseous structure of protonated nicotinamide (NA), produced using electrospray ionisation which demonstrated that by performing low-resolution UV spectroscopy within the commercial mass spectrometer, spectra can be acquired that allow different structural isomers of protonated NA to be distinguished (i.e. isomers associated with protonation at different sites). Photoabsorption and photofragment action spectra were obtained across the full spectral range scanned (215-350 nm), and reveal that gaseous protonated NA existed with either the pyridine or amide group protonated. Analysis of the photofragment action spectra indicated that that the ratio of pyridine/amide protonation is approximately 1.1:1. The results presented demonstrate the broad potential of such measurements as a relatively straightforward analytical tool for identifying geometric isomers that display UV chromophores.

Kevin Giles (Waters Corporation) discussed a brief history of RF ion guide development with an introduction to their operating principles and utilisation in mass spectrometry systems. The use of ion guides operating with radio frequency (RF) confining voltages is commonplace in current mass spectrometry systems and their use has transformed the performance and functionality of modern instruments. A more focussed perspective followed on the role of these guides operating in higher pressure regimes where they provide both efficient ion transportation and additional functionality. Recent developments in ion guide technology were highlighted, including ion mobility separators and advanced ion manipulation approaches.

After lunch, which included an optional Corporate Lunch Seminar sponsored by Thermo Fisher Scientific, the Wednesday afternoon from 15:00 was dedicated to the exhibition and time to peruse and discuss the over seventy posters 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 - New MS Technologies in Proteomics	**Session 6 - Small Molecules**
Chair: **Professor Claire Eyers (University of Liverpool)**	Chair: **Dr Susan Crosland (Syngenta)**
Dr Richard Scheltema (Utrecht University) - Extending the Q Exactive Orbitrap with UVPD; application to peptides, proteins, and protein complexes.	**Professor Perdita Barran (University of Manchester)** - Structural Information to distinguish Small Molecules with Ion Mobility Mass Spectrometry (IM-MS)
Thomas Powell - Subcritical Water Processing of Proteins: Amino acid side-chain modifications.	**Dr Patricia Wright** - Predicting collision-induced dissociation (CID) fragmenation: understanding the role of the mobile proton small molecule fragmentation.
XueXia Huang - Photo-affinity Labelling based Structure-Activity Relationship study of Hsp90 C-terminal Domain.	**Florence Lai** - Detection of DDT in small quantities of mosquito by thermal desorption GCGCMS.
Federico Floris - 2D FT-ICR MS for Top-Down Proteomics.	**Professor James McCullagh** - Targeted and untargeted metabolic profiling of glioma cells expressing IDH1 mutations.

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 at 12:30 with sessions on:

Session 7 - Emerging technologies for Processing MS Data	**Session 8 - Mass Spectrometry in Environmental and Forensic Analysis**
Chair: **Dr Mark Barrow (University of Warwick)**	Chair: **Dr Simona Francese (Sheffield Hallam University)**
Dr Robert Mistrik (HighChem Ltd) - mzCloud: A comprehensively annotated LC/MSn database for the identification of unknowns.	**Dr Melanie Bailey (University of Surrey)** - Ion Beam and Mass Spectrometry Imaging in Forensic Science.
Dan Addison - Lessons from historical data: From data annotation to data mining and beyond, an evolving approach to MS data.	**Professor Rainer Cramer** - Evaluating milk adulteration and animal health using liquid AP-MALDI MS profiling.
Professor Peter O'Connor - The next dimension in proteomics using two-dimensional mass spectrometry.	**Lisa Deininger** - Out Damned Spot! - Bottom Up Proteomics for the Analysis of Bloodied Fingermarks.
Edwin Aponte Angarita - Molecular dynamics simulation protocol for spectra assignment in ion mobility spectrometry.	**Dr David Baker** - Quantitative analysis of 646 pesticides (1,929 MRMs) using high-sensitivity LC-MS/MS with a fast 10.5 gradient.

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 - MS in Translational Medicine	**Session 10 - Mass Spectrometry in Synthetic Biology**
Chair: **Professor Mike Morris (Waters Corp)**	Chair: **Professor Neil Oldham (University of Nottingham)**
Dr Kevin Mills (UCL) - Mass Spectrometry in the Clinic.	**Dr Nik Rattray (University of Manchester)** - The role of Mass Spectrometry in Driving the Design-Build-Test-Learn cycle.
Dr Joanna Denbigh - Exploring the effect of a combined drug therapy on the lipidome of acute myeloid leukaemia cells using mass spectrometry-based lipidomics.	**Lucio Manzi** - Mapping the interactions between the acyl carrier protein and a dehydratase domain installing a cis-double bond using carbene footprinting and mass spectrometry.
Dr Liam Heaney - Exploring the gut microbiome with mass spectrometry.	**Ewa Szula** - Metabolic analysis of small number of mammalian cells - development of mass spectrometry technologies.
Richard Mbasu - Novel Targeted Strategies for Heart Failure Biomarkers.	**Dr Chloe Martens** - Deciphering the molecular mechanisms of sugar transport using a mass-spectrometry based methodology.

The final lecture the Plenary – BMSS Chair's Lecture was given by Professor Jack Henion of Cornell University and Advion, Inc and was titled 'What Will Mass Spectrometry Look Like in The Future?'.

Where he reflected on the last 50 years and gazed into his crystal ball and gave predictions for what the next 50 years will bring in regard to the 'fit and form' as well as the ease-of-use and analytical capabilities.

Late Thursday afternoon saw the presentation of various BMSS awards by the BMSS Chair Dr Christine Eckers as part of the closing ceremony.

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 2016 meeting. This year's awardee was **Lisa Deininger, Centre for Mass Spectrometry Imaging, Biomolecular Sciences Research Centre, Sheffield Hallam University** for her oral presentation titled '**Out Damned Spot! - Bottom Up Proteomics for the Analysis of Bloodied Fingermarks**' which discussed how the currently employed enhancement and detection techniques for blood and blood in fingermarks are not confirmatory due to targeting generic compound classes like proteins, and as such are not sufficiently specific and prone to false positives. She continued to describe how the work presented previously has been developed further to devise a protocol for proteomic in situ analysis of bloodied fingermarks with MALDI-MS imaging, enabling the mapping of blood peptides to fingermark ridges and thus establishing a strong link between the suspect and the cause of bloodshed. In order to achieve this, it was necessary to increase the trypsin concentration significantly compared to on tissue digests.

The Bordoli Prize, sponsored by Waters, is awarded to the best new and upcoming researcher's poster presentation at the 2015 meeting. This year's awardee was **Patrick Knight from the Astbury Centre for Structural Molecular Biology, University of Leeds** for his poster titled '**Characterising the interaction of ataxin-3 and the poly-glutamine aggregation inhibitor QBP1**' which described how given the current growing social and economic burden of amyloid neurodegenerative disorders (Alzheimer's) there is an urgent need to increase the understanding of amyloid diseases in order to develop effective therapies. To this end nESI-ToF-MS was used to directly

Figure 4. Lisa Deininger receiving her Barber prize and Christine Eckers (Photograph courtesy of BMSS)

observe the interactions of QBP1 with with ataxin-3 and species such as monomeric ataxin-3 containing polyQ.

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 **Hannah Britt**, **Durham University** for her poster titled '**Monitoring reactions of small molecules with cell membranes by liquid chromatography-mass spectrometry**' where she discussed how the cell membrane is considered to be an inert structure, how when considering the molecular components there is an indication of potential reactivity with organic drug-like molecules. The use of LC-MS with a high performance mass analyser and then tandem mass spectrometry and ion-mobility was reported to have opened up the field of complex reactions and revealed preferential sites of reactivity within the small molecules.

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.

At the social level, the meeting provided plentiful opportunities to chat and share, over coffee or the inevitable beer – even the Buccaneer next door seemed well stocked and stayed open. Many of the 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, where the continued move away from the use of purpose-built shell structures provided a more open layout in the beautiful Floral Hall.

When asked about the success of the 37th BMSS Annual Meeting BMSS Chair Dr Christine Eckers, summarised the meeting by saying: "The high quality scientific programme has resulted in excellent feedback from a large number of delegates and the opportunities for formal and informal interactions gave rise to some interesting scientific discussions."

The next BMSS annual meeting and conference, its 38th, will held at the Royal Northern College of Music in Manchester, and will take place between 4th and 7th September 2017. Updated details may be found at www.bmss.org.uk

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