# Visiting the 38th BMSS Annual Meeting 5th-7th September 2017 BMSS Introduction to Mass Spectrometry Course 4th & 5th September 2017, Royal Northern College of Music, Manchester, UK

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The 38th British Mass Spectrometry Society (BMSS) Annual Meeting and Introduction to Mass Spectrometry Short Course was held at the Royal Northern College of Music, Manchester, UK from 4th to 7th September 2017. 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 Venue

This year the BMSS Annual Meeting was hosted at The Royal Northern College of Music (RNCM) which is one of the leading conservatoires in the world, located in Manchester, England. It is one of four conservatoires associated with the Associated Board of the Royal Schools of Music. In addition to being a centre of music education, RNCM is one of the UK's busiest and most diverse public performance venues.

The RNCM has a rich history, dating back to the late 19th century and the establishment of the Royal Manchester College of Music (RMCM). In 1858, Sir Charles Hallé founded the Hallé orchestra in Manchester, and by the early 1890s had raised the idea of a music college in the city. Following an appeal for support, a building on Ducie Street was secured. Hallé was appointed Principal and Queen Victoria conferred the Royal title. The RMCM opened its doors to 80 students in 1893, rising to 117 by the end of the first year. Less than four decades later, in 1920, the Northern School of Music (NSM) was established (initially as a branch of the Matthay School of Music), and for many years the two institutions peacefully coexisted. It wasn't until 1955 that NSM Principal, Hilda Collens, in recognising the importance of performance in training students, met with RMCM Principal, Frederic Cox, to raise the question of merging. Discussions continued until September 1967 when a Joint Committee was formed to oversee plans to combine the two colleges. The RNCM was formed by amalgamating the NSM and RMCM in 1972, moving to its purpose-built home on Oxford Road in 1973.

The venue, whilst an ideal geographic location showed by an increased attendance was not conducive for an exhibition, with the utilised space, with around 30 suppliers and sponsors in the exhibition on three levels connected by stairs and with seven exhibitors located in a small room – not easily visible to attendees despite the organisers attempts to alert attendees to this area. Some exhibitors disappointed with the traffic left early. The parallel symposia sessions were held in the Lecture Theatre and the Opera Theatre with the welcome reception, lunches and coffee breaks being held over the three levels.

The posters were positioned in two locations in the Concert Hall and the Brodsky Room, the latter was overcrowded and not in any logical numerical sequence making it difficult to conduct a review easily. This could have been caused by the doubling of communications (around 52 oral presentations and 174 posters) in the programme this year compared to 2016.


*Figure 1. The 38th BMSS Annual Meeting Venue – Royal Northern College of Music, Manchester, UK.*

As usual, academia, industry and government were all well represented among the speakers and around 350 delegates were in attendance, "the largest attendance for over a decade" according to Gavin O'Connor the current chairperson. The events were again accompanied by a one-and-a-half-day short course on 4th and 5th 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 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.

# The BMSS Annual Meeting Conference

Gavin O'Connor opened the meeting with a statement "BMSS is migrating into the next phase of its existence and I encourage all of the British M.S. community to join us on that journey".

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 decided to have all the Special Interest Groups have their own sessions which included keynote speakers.

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 Lars Konermann (Department of Chemistry, The University of Western Ontario, London, ON, Canada). The lecture entitled 'A Journey Through Protein Mass Spectrometry: Enzyme Mechanisms, MD Simulations and Supercharged Proteins' explained, after he quipped about London, Ontario being famous as the birthplace of Justin Bieber and where Johnny Cash proposed to June Carter, 22 February 1968, how native Electrospray ionisation (ESI) permits the formation of desolvated ions from proteins and protein complexes in solution. Further analysis of these gas phase biomolecules by mass spectrometry shows the nature of proteins. He went on to elucidate a journey through protein mass spectrometry showing both gas phase and solution phase options and explaining native ESI with 'supercharging'.

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 social event at the Dog Bowl' a short walk from the conference venue, with the incentive of 'free food and drinks' for the 160 arrivals.

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 'Investigating biodiversity by protein mass spectrometry' and was given by Professor Peter Roepstorff (Department of Biochemistry and Molecular Biology, University of Southern Denmark).

Wednesday mornings two parallel sessions followed a one hour coffee break which took place after the Robinson Lecture and included the following oral presentations:

| **Session 1 - Instrumentation** | **Session 2 - MS Solutions for challenging analytes** |
|---|---|
| Chair: **Helen Cooper** | Chair: **Tony Bristow** |
| **Emmanuel Raptakis - Keynote:** Mass spectrometry development in industry: from the Mag-TOF to the Omnitrap. | **Richard Bourne - Keynote:** Self-Optimising Flow Reactors for Rapid Process Development. |
| **Bruno Bellina - Spectroscopy:** Combining Light Activation, Ion mobility and Mass Spectrometry data in a snap #LAIMMS. | **Christopher Gray** - Screening biocatalytic reactions within live bacterial colonies by DESI-(IMS)-MS. |
| **Jason Wildgoose** - Comprehensive DIA on a Q-ToF instrument for discovery and quantitative analysis utilising a scanning quadrupole. | **David Clarke** - A Systematic Evaluation of the Integration of Ion Mobility into an Online Hydrogen Deuterium Exchange Mass Spectrometry Workflow |
| **Ian Sinclair** - Acoustic Mist Ionisation- from Concept to Automated High Throughput Platform. | **Christopher Whitmore** - Quantifying ion suppression in online reaction monitoring by ESI MS. |

Particularly interesting presentations in Session 1 were:

Firstly, **Emmanuel Raptakis – Keynote** lecture which was dedicated to Peter Derrick (1945 – 2017) and his illustrious career as a pioneer in mass spectrometry and how Peter mentored Emmanuel through his PhD at Warwick University. Emmanuel then went on to describe his own career history and pioneering work in developing the Omnitrap platform (FasmaTech), a unique ion processing system designed to provide access to an arsenal of ion activation-dissociation techniques all embedded in the same unit. The Omnitrap platform can be adapted to existing or custom engineered instrumentation. This unique technology is currently available as a retrofit to the Q ExactiveTM instrument series (Thermo Fisher Scientific) and also with Fasmatech's oTOF mass analyser.

Secondly **Bruno Bellina** (Michael Barber Centre for Collaborative Mass Spectrometry, Manchester Institute of Biotechnology, and Photon Science Institute, University of Manchester) discussed how an ion mobility enabled Q-ToF (Waters Synapt G2-S) had been modified to combine 'action spectroscopy IR/UVPD'. The instrument had the trapping and light activation occurring prior to the IMS cell and utilised a newly developed acquisition and analysis software package called ORIGAMI.

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 entitled 'From a spectrum to a speed revolution – 25 years of MALDI mass spectrometry'.

| **Session 3 - Imaging** | **Session 4 – Innovative Separations** |
|---|---|
| Chair: **Malcolm Clench** | Chair: **Julie Herniman** |
| **Josephine Bunch - Keynote:** Developing A Google-Earth View Of Tumour Metabolism Through Multiscale Molecular Imaging. | **John Langley - Keynote:** Supercritical Fluid Chromatography - Mass Spectrometry: The Final Piece in the Hyphenation Jigsaw. |
| **Renata Soares** - Tissue microarrays analysis using DESI-MSI. | **Bob Boughtflower** - The ultimate speed and performance available from Generic Gradient methods – what does this mean for future practice? |
| **Amaia Carrascal Minino** - Imaging oxidative damage in irradiated HCT-116 spheroids using DMPO. | **Lewis Couchman** - Opportunities for ultra-rapid LC-MS/MS in high-throughput bioanalysis. |
| **Cristina Russo** - Method development for quantitative investigation of Terbinafine hydrochloride in a 3D skin model by MALDI-MSI | **Maria A. Van Agthoven** - Two-dimensional mass spectrometry in a linear ion trap. |

The two parallel Wednesday sessions continued after the lunch break with sessions on:

Of interest in these sessions were:

**John Langley** (University of Southampton, Chemistry, Southampton) reported on how SFC now delivers on the chromatographic promises with robust and reliable instrument platforms available from several manufacturers. The solvation power, selectivity and peak capacity of modern Ultrahigh Performance Supercritical Fluid Chromatography (UHPSFC) coupled with mass spectrometry provides the ideal analytical platform to address classes of compounds that were previously a challenge for other chromatographic methods. UHPSFC complements existing liquid chromatography and gas chromatography options (HPLC-MS (ESI/APCI), GC-MS (EI/CI) and provides a comprehensive, modern and fast separation science with the mass spectrometry option to address the wide range of diverse and challenging chemistries. UHPSFC-MS sits between LC-MS and GC-MS affording extended capability and complementarity and delivers unique solutions across a broad range of application areas, e.g. synthetic organics, pharmaceuticals, petrochemistry, lipids, nucleotides and many other areas.

Examples of the wide range of challenging chemistries were shown, together with fast method optimisation and the decision-making process, e.g. if not retained or early eluters by RPUHPLC or a HILIC method (polar compounds) then try SFC.

**Bob Boughtflower (GSK, Medicines Research Centre, Gunnelswood Road, Stevenage)** discussed how reverse phase generic gradient (U)HPLC methods of analysis have been adopted across the analytical measurement industry. However, it is often the case where practitioners do not take advantage of the benefits of separation speed and performance that is available from modern stationary phase materials and instruments. Bob demonstrated that the performance enhancements that are easily accessible and the choices of instrument and column formats. Examples were shown of ultra-fast separations and where these methods can routinely apply.

This session concluded at 15:40 for a tea break and time to peruse the exhibition and posters.

| **Session 5 - New Techniques for Ambient Ionisation** | **Session 6 – Analysis of Big Data** |
|---|---|
| Chair: **Andy Ray** | Chair: **Peter O'Connor** |
| **Stephen Taylor - Keynote:** Desorption Atmospheric Pressure Chemical Ionisation (DAPCI) – development and applications. | **Mark Andre Delsuc – Keynote:** Tackling the Big-Data problem in 2F FT-ICR-MS. |
| **Julia Abda** - Imaging and ex-vivo Tissue Analysis by IR Laser Assisted REIMS – towards an integrated MS-based tissue ID system. | **Remy Gavard** - Themis: batch pre-processing for ultrahigh resolution petroleomics data. |
| **Bryan McCullough** - Results of the Second BMSS Ambient Ionisation SIG Interlaboratory Study. | **Christopher J. Arthur** - Data plotting strategies for the visualisation of complex datasets. |
| **Stephanie Rankin** - Development of a direct surface analysis method for in-situ VOC profiling of biological fluids. | **Catherine Evans** - The SNAP Advantage: Enabling High Resolution Protein Analysis. |

A drinks reception and the conference dinner at the Manchester Museum of Science and Industry rounded off a full first day of the BMSS Annual Meeting and Conference.

Thursday morning started with two parallel sessions.

| Session 7 – Ion Mobility (I) | Session 8 – Clinical & Forensic Analysis using MS |
|---|---|
| Chair: **Perdita Barran** | Chair: **Andrew Davison** |
| **Valerie Gabelica - Keynote:** What nucleic acids studies taught us about ion mobility spectrometry Fundamentals. | **Brian Keevil - Keynote:** LC-MS/MS of steroids in the clinical laboratory. |
| **Nick Tomczy** - Applying the expanding high resolution (Drift)- Time and (CCS)-Space dimensions. | **Danielle Moncrieffe** - Quantification of P-III-NP in humans: meeting the challenge. |
| **Richard Blankley** - Higher Order Structure of Intact Proteins by Capillary Electrophoresis Native Ion Mobility Mass Spectrometry. | **M. Zubair Israr** - Prognostic role of molecular forms of B-type natriuretic peptide in cardiovascular disease. |
| **Shazia Khan** - Sensitive detection and separation of steroid isomers following derivatisation using Ion Mobility. | **Ashley Sage** - Sensitive and Specific Allergen Screening Analysis Using LC-MS/MS. |

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 - before breaking for lunch at 12:30 with sessions on:

| Session 9 – Ion Mobility (II) | Session 10 - Mass Spectrometry in Medicine |
|---|---|
| Chair: **Frank Sobot** | Chair: **Zoltan Takas** |
| **Kostas Thalassinos - Keynote:** Ion mobility Mass Spectrometry Studies of Alpha1-Antitrypsin Variants. | **Isabelle Fournier - Keynote:** Amazing Spidermass: Tracing the Future of Intraoperative Diagnosis. |
| **Vincen Wu** - The exclusion of contaminants from tissue samples using DESI Ion Mobility imaging. | **James S. O. McCullagh** - Biomarker discovery using ion chromatography - mass spectrometry (IC-MS): Significantly elevated 2-hydroxyglutarate in the plasma of IDH+ patients with intrahepatic cholangiocarcinoma (ICC). |
| **Lucy Woods** - The Next Generation Ion Mobility Separation (IMS) Adds A New Dimension to Substance Characterization and Identification. | **Menelaos Tzafetas** - iKnife – REIMS and its use as an intraoperative technique for real time tissue identification of cervical disease. |
| **Rian L. Griffiths** - Native LESA mass spectrometry for direct analysis of proteins and their complexes: Imaging, ion mobility and protein-ligand binding. | **Boakye Gyimah** - Mass Spectrometry analysis of omega-3 polyunsaturated fatty acids in biological samples after dietary supplementation. |

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.

| Session 11 – (Bio)Pharma | Session 12 – MS in Environmental & Food Analysis |
|---|---|
| Chair: **Rachel Garlish** | Chair: **Gavin O'Connor** |
| **Vojtech Franc - Keynote:** All-inclusive proteoform profiling of human serum glycoproteins by hybrid mass spectrometry approaches. | **Nathalie Gillard - Keynote:** Food allergens analysis: contribution of mass spectrometry. |
| **Tony Bristow** - The development of MALDI-TOF-MS techniques for the characterisation of dendrimer drug conjugates. | **Joanne Connoly** - Discrimination of honey of different botanical origins using an untargeted highdefinition metabolomic workflow. |
| **Will Burkitt** - Challenges in peptide mapping mass spectrometry of biopharmaceuticals. | **Juergen Wendt** - Development of a GC-MS method for the simultaneous screening of target and nontarget contaminants in river water. |
| **Martic Bachman** - Sample-per-second metabolome and lipidome profiling for accelerated drug discovery. | **Will Kew** - Chemical Complexity and Diversity of Scotch Whisky by FTICR MS |

The final lecture - the Plenary – BMSS Chair's Lecture was given by Professor R. Graham Cooks on 'Accelerated Organic Reactions in Microdroplets and Thin Films: Mechanisms and Scale up of Organic Synthesis by Mass Spectrometry'.

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 Agilent, was awarded to the best new and upcoming researcher's oral presentation at the 2017 meeting in honour of Mickey Barber who had a dislike of giving oral presentations. This year's awardee was **Danielle Moncrieffe of the Analytical and Environmental Sciences Division, King's Forensics, King's College London** for her Thursday morning oral presentation titled **'Quantification of P-III-NP in humans: meeting the challenge'** which discussed how Procollagen III amino terminal propeptide (P-III-NP) a circulating bone marker present in human blood at low concentrations is used clinically to help diagnose liver damage and as a biomarker in anti-doping.

**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 2017 meeting. This year's awardee was **Rani Moons from the Biomolecular and Analytical Mass Spectrometry group, University of Antwerp for her poster titled 'Bridging the gap between molecular properties and aggregate morphology of IDPs in the presence of small molecules'** which described how using ion mobility-mass spectrometry the group followed the gas phase structural changes of human α-synuclein (AS) under different solution phase conditions. They also developed new methodologies for linking the molecular studies of AS individual subunits properties with the AS aggregate morphology produced under different conditions.

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 Sciex, 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 David Romero Perez from the Department of Electrical Engineering & Electronics, University of Liverpool** for his poster titled **'Comparison of Paper Cutting Methods for Paper Spray Mass Spectrometry'** where he discussed the use of paper spray (PS) ionisation in mass spectrometry and how this typically requires a small paper triangle to be cut, which can lead to human error in the size. Alternative cutting methods laser and automatic blade cutting, were compared to manual cutting and dual wax-printed paper triangles. Automated blade cutting was favoured since consistent geometry was achieved in line with the laser method but without the capital equipment cost.

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 for vendors and delegates alike.

**The next BMSS annual meeting and conference, its 39th, will held at the Churchill College, Cambridge, Storey's Way, Cambridge, CB3 0DS and will take place between 10th and 13th September 2018.**

**Updated details may be found at www.bmss.org.uk**

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