



focus on  
**Mass Spectrometry**  
**Spectroscopy**

## Rocky Mountain High – and Getting Higher by the Day

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### Report on the 59th ASMS Conference, Denver, Colorado, USA, June 5th – 9th

Once again the mighty ASMS Conference flexes its muscles and heads into town, on this occasion Denver, Colorado, even allowing for the fact that it was only a few years ago when the city last hosted the event. For a change this year in the review we invited three, past and current, committee members from the British Mass Spec Society (BMSS), all of whom have visited the event several times before, to give their opinions on what can be a mind (maybe foot as well) numbing week but as ever you get out of it what you put in.

All of the usual stats regarding numbers of attendees, oral and poster numbers, exhibitors (sorry, Corporate members of ASMS) can be found within the reviews but a very salient point was made by Jackie Mosely whose comment that there was room for improvement in some oral presentations reiterated that quantity does not equal quality when it comes to the presentations.

#### Awards

This year's hot topic appeared to be that of Tandem Mass Spectroscopy judged by virtue of the fact that all three ASMS awards went to scientists who had worked in that area. For the uninitiated this is a powerful technique, which can be utilised for structure elucidation and in one case was found to be particularly useful for peptide analysis and study during proteomics studies and various configurational changes undergone during ionisation bombardment.

The award for distinguished contribution in Mass Spectroscopy went to Dr Robert J. Cotter from the John Hopkins School of Medicine for his work in the invention and development of tandem time-of-flight (TOF/TOF) mass spectrometry.

The Biemann medal went to Dr Bela Paizs from The German Cancer Research Center for his work on detailed characterisation studies of peptide ion structures and dissociation mechanisms. The Ron A. Hites award for outstanding research publications in JASMS went to T-Y Huang et al for their paper entitled 'Top Down Tandem Mass Spectrometry of tRNA via Ion Trap Collision- Induced Dissociation'. [1] Professor McLuckey donated the \$2,000 prize towards student travel support.

#### Instrumentation

In view of the fact that 160+ Corporate members attended, unfortunately the overview of new instrumentation has to be restricted to the larger companies. They have been divided into companies who are primarily known for their mass spec technologies and those who have relatively long standing stand alone chromatographic instrumentation technology in the international market place.

**AB SCIEX** followed the theme of tandem MS by unveiling their new 5600 System Triple TOF, claimed by the company 'to offer performance levels not available with other manufacturers instruments due to new-generation technology the company has developed.' The company claims the levels of interest in the instrument has 'exceeded their wildest dreams.' Also launched by AB SCIEX was the SelexION Technology, which delivers unprecedented performance and a new dimension of selectivity in differential ion mobility spectrometry for quantitative and qualitative analysis. This technology is available on the TripleQuad 5500 and QTRAP 5500 series of instruments.

**Bruker**, the pioneer of ultra high-resolution quadrupole time-of-flight mass spectrometry, announced a major extension of the successful maXis™UHR Qq-TOF technology range. In March 2011, Bruker unveiled the revolutionary maXis 4G system, setting entirely new performance heights with record-breaking 60,000 full-sensitivity resolution (FSR) and 600 parts-per-billion (ppb) mass accuracy at UHPLC speed. The maXis 4G has the unique distinction of being the only simultaneous high-speed, ultrahigh resolution and full sensitivity mass spectrometer available today, with the dynamic range and quantitative capabilities needed for many small molecule and proteomics applications. The maXis 4G also excels in top-down and intact protein analysis.

At ASMS 2011, Bruker complemented the performance achievements of the maXis 4G by making uncompromised UHR-QqTOF performance available in an affordable, convenient format. The new maXis impact being introduced is a robust, benchtop instrument with outstanding performance to bring the benefits of the maXis technology within reach of all research, quality control, contract and industrial laboratories.

**Leco Instruments** featured included the Pegasus® 4D GCxGC-MS, the TruTOF® HT GCMS, and the company's new High Resolution Time-of-Flight Mass Spectrometers (HRT). Available in both LC and GC configurations, these HRT systems utilise Leco's exclusive Folded Flight Path™ (FFP™) technology to provide full-range mass spectra

at speeds of up to 200 spectra per second, and resolutions of up to 100,000 with mass accuracies of less than 1 ppm. The Citius LC-HRT represents a substantive innovation in High Performance Mass Spectrometers for the LCMS market. The system utilises Leco's FFP technology to provide full-range mass spectra at speeds of over 200 spectra per second, and resolutions of up to 100,000 with high-performance mass accuracy. The system provides the versatility of ESI, APCI, and DESI (desorption electrospray) ionization sources as options to complement its high-performance MS capabilities and unchallenged dynamic range. The Pegasus GC-HRT represents the next generation of High Performance Mass Spectrometers for the GCMS market. The system also utilises Leco's Folded Flight Path FFP technology to provide full-range mass spectra at speeds of up to 200 spectra per second, and resolutions of up to 50,000 with high-performance mass accuracy.

**Agilent Technologies**, as ever a major event for Agilent and this year was no exception. Highlights were the new Agilent 6550 iFunnel quadrupole time-of-flight liquid chromatography /mass spectrometry (Q-TOF LC/MS). This instrument is designed to offer low femtogram sensitivity, fast acquisition up to 50 spectra/sec, up to 5 orders of intra-scan dynamic range with robust performance and operation, it is aimed at the metabolomics, food safety screening, early stage drug development and protein study markets.

Also launched was the 7200 Q-TOF GC/MS, the company's first GC time-of-flight instrument. Designed to deliver improved chromatographic and spectral resolution from increasingly complex samples it is aimed at the environmental, sports doping and natural products research markets.

The company also launched 6420 Triple Quad LC/MS, 6100B Series Single Quad LC/MS and new MassHunter Software in addition to a proprietary sample preparation card for dried-blood spotting bioanalysis.

**PerkinElmer** announced the launch of its AxION™ Mass Spectrometry platform. The AxION hardware and software platform is specifically designed to deliver rapid and accurate mass identification and quantification to monitor water quality to ensure its safety as well as safer pharmaceutical and food products. The combination of the state of art AxION hardware and software suite, brings highly specific, fast and accurate quantification to quality control and research-based organisations. The AxION platform is intended to help companies deliver better quality products and services to consumers across the environmental, food and pharmaceutical sectors.

**Thermo Fisher Scientific** focussed its new lines mainly on its proprietary Orbitrap technology with three main product introductions. The Thermo Scientific Velos Pro is an ion trap with 'unsurpassed speed for MSn molecular structure elucidation and an ideal front end for Orbitrap hybrid instruments.' The Orbitrap Elite is a new high-field Orbitrap instrument aimed at revolutionising proteomics research by increasing the speed and resolution of current Orbitrap technology four fold. Thirdly the Q Exactive Orbitrap aka the 'Quantification instrument' which offers the ability to quantify and confirm from a single experiment across a growing range of applications including drug metabolism and pesticide analysis.

**Waters** two main instruments flag shipped the Waters offering this year, the new Xevo TQD tandem quadrupole mass detector and the SYNAP G2-S mass spectrometer. The Xevo TDQ features the same universal ion source (Z-Spray™) architecture present on advanced mass spectrometers such as the Xevo TQ-S and the SYNAP G2-S. It is designed for routine analysis to give maximum productivity with minimum effort. The SYNAP G2-S is a new high definition mass spectrometer aimed at maximising sensitivity and selectivity. It incorporates both high-sensitivity Waters StepWave ion transfer optics and Triwave ion mobility technologies along with a suite of new informatics tools to improve quantitative and qualitative high-resolution performance.

ASMS 2011 was an excellent choice of show for the launch of PerkinElmer's AxION MS platform to a broad customer audience covering the environmental, pharmaceutical and food industries. The AxION MS portfolio of hardware and software solutions was very well received by customers as it offers integrated solutions across multiple applications. There was a great deal of interest in the new AxION eDoor™ for open access environments.

This offers remote access for inexperienced users, from adding samples to a queue using a bar code reader, to receiving results by email. New accessories, such as the innovative AxION Separation Probe which minimises the dead volume so important in UHPLC separation and the Direct Sample Analysis (DSA) APCI ion source, which enables rapid analysis of solid, liquid or gas pharmaceuticals with little or no sample preparation, proved particularly popular with those looking to optimise workflow analysis in academic, food, pharmaceutical and environmental laboratories.

On arrival at the Denver Convention Centre, and once again seeing the big blue bear staring through the window, there was a feeling of déjà vu. After all, it was only a couple of years ago since the annual ASMS conference had visited Mile High City – would mass spectrometry have changed much during this relatively short time, or would it all seem strangely familiar, like Denver itself?

There was no need to worry, we would not be disappointed. As someone working with proteins and biomolecular complexes, the range of topics and quality of presentations in these areas were impressive. The emphasis this year, in this field, was focussed on the use of mass spectrometry coupled to an arsenal of chemical techniques including cross-linking, hydrogen-deuterium exchange, and oxidative labelling to pin-point the key regions of a wide range of proteins which are responsible for that particular protein's structure and function. Macromolecular protein complexes, protein-ligand interactions, and recent developments in hardware and software were all covered in depth. Ion mobility spectrometry-mass spectrometry also featured highly, having grown from having a small group of followers a few years ago to now having an army of users. This year the subject warranted two full sessions of oral presentations plus a dedicated workshop, which together covered data interpretation, instrumentation and, in particular, structural biology applications.

The weather in Denver was hot, in excess of 30 oC, or so we were told. Spending almost a good 12 hours per day inside the Convention Centre left little opportunity for sun and sight-seeing, but was a strong testimonial to the quality of oral and poster presentations, the corporate exhibitions and the lively workshops. The latter were scarcely over before the hospitality suites opened to finish off the day. To summarise ASMS 2011 in numerical form, there were: 6437 delegates, 340 oral presentations, 2783 posters, 15 courses, 167 corporate exhibitors and 9 hospitality suites. Roll on ASMS 2012 and Vancouver.

**Alison E Ashcroft, University of Leeds**

A welcome return to Denver and the behemoth that is ASMS was preceded by a day trip into Rocky Mountain National Park. This amazing place was the perfect remedy for travel weariness and ensured my brain was on the same continent as my body for the start of ASMS. This began with the usual array of Users' meetings and then the conference for real kicked off with two splendid Tutorial lectures, Jim Jorgenson (Uni. North Carolina) lectured on 'LC and MS: A match made in Heaven' with focus on UHPLC and Mark Duncan (Uni. Colorado) gave an outstanding presentation on 'Good Mass Spectrometry and its Place in Good Science: Sometimes Close Enough is Really not Good Enough'. This presentation should be compulsory reading for all practitioners, highlighting the need for analytical rigour at all stages of experiment and reporting thereof. The opening Plenary Lecture 'Our Stellar Origins Revealed by Stardust Grains', by Larry Nittler explained how all elements came from the stars. This was evinced throughout the conference oral and poster presentations where the contents mimicked the periodic table. There were a number of precious metal presentations but also many of Tin and Lead; as ever ASMS was a true Curate's egg.

From a personal viewpoint this was one of the best ASMS conferences I can recall. I am not sure if this is because I attended with a focussed list of objectives, all of which were met or whether it was truly a better event. No doubt the familiarity with Denver and the friendly nature of the city helped, a stark comparison with Philadelphia two years previous (Gold and Lead again). There was a reasonable balance between small molecule MS, biomolecular MS and 'omics, the lipidomics sessions being particularly well attended and in general very good quality presentations, Bob Murphy giving his usual high quality presentation. There were a number of interesting developments from the manufacturers often improved sensitivity, mass resolving power and enhanced capability. These developments made the hospitality suites very busy, along with the deceptive lure of peculiar flashing objects and other associated freebies.

Networking is always a challenge at a meeting with ~6500 delegates and 700 posters daily, the latter taxing the brain and feet. As ever it was easy and great to catch up with distant friends and colleagues, others were more of a challenge. Nevertheless I managed to meet up with nearly everyone I needed to, often initiated by use of mobile phone other times relying on the tried and trusted mass spectrometry networking tool of going to a bar.

The meeting finished on a high spot with a trip to Coors Field to see the Rockies play the Dodgers – it is a shame ASMS had not block booked a section of the ground for an end of conference event, this would have been the perfect end to a very enjoyable ASMS. Now it is time to plan the trip to the 60th ASMS 2012 in Vancouver; there is a special irony that ASMS will be celebrating their diamond jubilee in Canada.

**Dr John Langley, Chemistry, University of Southampton**

## Future dates

Dates and venues for the forthcoming ASMS meetings have been announced as follows:

**May 20-24th 2012 Vancouver, BC, Canada**

**June 9-13th 2013 Minneapolis, MN**

**June 15 - 19, 2014, Baltimore, MD**

## References

[1] Huang T-Y, Liu. J, & McLuckey S.A.; JASMS, 2010, Vol. (21)6, 890-898

## Final thought

There continues to be acquisitions across the industry with the large players picking up technology and expertise, sometimes as a part of other technologies, which may lead to some interesting mass spec hybrids in the future.

What price Thermo Fisher Scientific utilising some technology from the Dionex ion chromatography product line, Danaher (owners of AB SCIEX) and possibly the Beckman Coulter capillary electrophoresis line with Agilent incorporating some Varian technology in the future maybe?

Solutions looking for problems or a hit on a new exciting applications area? Watch this space.