

focus on Mass Spectrometry & Spectroscopy

60th Anniversary of ASMS Celebrated in Canada

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Who would have believed it that the American Society For Mass Spectroscopy and Allied Topics would hold its 60th Annual meeting not in one of the 50 states available to it but in another country. Well they did and with only the weather putting a damper on things a successful meeting it was. Admittedly the attendance was down a little from the 6,500 in 2011 but never the less the meeting reached the accomplished high standard we have become used to and even the Hospitality Suites failed to notice the smaller numbers. Nothing to do with that leaving more sustenance for everyone else.

Awards

Award for a Distinguished Contribution in Mass Spectrometry

Efforts to detect, characterise, and differentiate microorganisms are driven by the needs of homeland security, counterterrorism and counter-proliferation programs, medical providers, food safety labs and microbiologists.

Professor Catherine Fenselau (University Of Maryland, College Park) was honoured for her pioneering work in this arena. The current paradigm for rapid MS characterisation of intact microorganisms relies on the detection and identification of unique biomarker molecules from experimental mass spectra, a paradigm that can be traced back to Anhalt and Fenselau. In 1975, they were the first to report that biomolecules from different pathogenic bacteria, introduced intact in a mass spectrometer a) could be vaporised and directly ionised, b) could be structurally identified; c) and, most importantly, that the compositions and abundances of these chemical biomarkers, revealed in the mass spectra, permitted taxonomic distinctions.

Fenselau's pioneering philosophy to employ intact molecular biomarkers for rapid microorganism characterisation by mass spectrometry was in stark contrast to concurrent research elsewhere advocating vigorous pyrolysis prior to MS analysis.

Biemann Medal

ETD, the ion-ion analogue of ECD, has become an essential method for protein sequencing because it allows for the dissociation, and consequently the sequence and analysis of large peptide cations, peptide cations bearing post-translational modifications, and even intact proteins. By allowing chemists and biologists to probe previously inaccessible regions of the proteome, ETD offers a unique lens through which to study proteins. Besides being a critical participant in the development of electron transfer dissociation (ETD), **Joshua Coon (University of Wisconsin –Madison)** was honoured for coupling this fragmentation technique with the high-resolution Orbitrap analyser. Coon was instrumental in demonstrating the greatly enhanced analytical capabilities of the ETD/Orbitrap configuration in large-scale proteomics applications, and in developing related mass spectrometric techniques, such as Supplemental activation for ETD and real-time decision making to blend dissociation methods. In a seminal study, Coon's team discovered that the fundamental difference between radicals and even-electron species stretches into the molecular mass domain, and that these species can always be separated given sufficient mass accuracy.

Instrumentation

Limited space dictates that a certain number of companies miss out on the review but in the interests of balance we have tried to at least feature the more interesting products from the community and maybe next year some of the smaller companies offerings will be of interest.

AB Sciex announced the launch of the second generation of the **TripleTOF® 5600 System**. The new TripleTOF® 5600+ System delivers new innovation for biomolecule research with MS/MSALL with SWATH™ Acquisition and supports a higher level of selectivity when coupled with **SelexION™ Technology**. The new system also comes with software that is capable of supporting 21 CFR Part 11 compliance, making TripleTOF® technology more accessible for regulated labs in the pharmaceutical industry

Claimed to represent an advancement in accurate mass technology that combines high resolution with high sensitivity and high speed, this new system builds on the proven innovation of the TripleTOF® 5600, which was launched at ASMS in 2010. The new TripleTOF® 5600+ system is now the industry's fastest, high sensitivity and high-resolution mass spectrometer for



Remote view of Stanley Park with the mountains in the background

simultaneous high-performance qualitative and quantitative analysis. A built-in capability to support SelexION™ Technology also adds versatility and breakthrough levels of selectivity.

By incorporating support for **MS/MSALL with SWATH™ Acquisition** on the TripleTOF® 5600+ platform, researchers will be able to obtain more information about proteins, peptides and other biomolecules from a sample than ever before. SWATH™ Acquisition is a groundbreaking mass spectrometry-based technique that quantifies nearly all peptides and proteins in a sample from a single analysis. The TripleTOF® 5600+ is the only platform in the industry that has the speed, sensitivity and dynamic range to enable SWATH™ Acquisition, which was developed through a collaboration with Ruedi Aebersold, PhD, a leading proteomics researcher who is based at ETH Zurich.

AB Sciex is also extending the utility of TripleTOF® technology for use in pharmaceutical laboratories, addressing a need for compliance to 21 CFR Part 11 for electronic records and signatures. With software that is capable of supporting 21 CFR Part 11 compliance, the new TripleTOF solution opens up new possibilities for drug discovery labs to meet this regulatory requirement.

Compatibility with SelexION™ Technology is another new feature of the TripleTOF® 5600+ system developed in response to customer feedback garnered ever since AB Sciex launched it at ASMS in 2011. SelexION™ Technology delivers a new dimension of selectivity by adding differential ion mobility to conventional mass spectrometry for both quantitative and qualitative analysis. It significantly improves selectivity and performance for any application requiring the separation of isobaric species, isolation of challenging co-eluting contaminants and elimination of high background noise. This advancement reduces sample preparation requirements and improves overall data quality.

Bruker announced the launch of the new **ultrafleXtreme™ MALDI TOF/TOF** system. Bruker's market leading, top of the range product has been significantly enhanced to offer both increased analytical power and entirely new functionality, extending the applications envelope of MALDI TOF/TOF far beyond the conventional concepts of what's possible in molecular histology, glycoprotein and biopharmaceuticals analysis.

Already the acknowledged leader in Mass Spectrometry Imaging (MSI), the next-generation

ultrafleXtreme system incorporates the Bruker patented *smartbeam*[™] laser, now with up to 2 kHz repetition rate with true-pixel image resolution at 20µm for proteins. This development marks a new milestone in the pioneering *smartbeam* laser technology, designed and manufactured exclusively by Bruker for unmatched performance in MALDI mass spectrometry.

The second product launch involved the introduction of its new *nano-Advance* UHPLC system for capillary and nano-flow LC-MS applications. Combining the novel *nano-Advance* UHPLC with mass spectrometry platforms, including the *amaZon* Ion Trap series and *maxis* UHR-TOF series, enhances Bruker's integrated solutions for proteomics.

The new *nano-Advance* UHPLC delivers reproducible retention times with accurate gradients down to 50nL/min. With run-to-run sample carryover typically less than 0.005%, the *nano-Advance* UHPLC delivers industry-leading separation performance critical to the success of many proteomics workflows. The *nano-Advance* UHPLC was specifically designed to eliminate dead volume and gradient delay wherever possible. When combined with Bruker's unique *CaptiveSpray Ion* source, the combination can deliver up to twice the MS utilisation rate of typical nano-LC systems coupled to nanospray MS sources. The increased mass spectrometry utilisation rate enables more proteins and peptides to be identified and quantified in a single LC-MS run. This is especially significant for detection of low abundance proteins in complex samples, which are easily missed due to the inability of the mass spectrometer to keep up with significant numbers of co-eluting peptides.

Shimadzu Corporation introduced the GCMS-TQ8030 ultra fast triple quadrupole gas chromatograph mass spectrometer, achieving the next step forward in Shimadzu's GC-MS history of innovation. Shimadzu also released the LCMS-8040 and LCMS-8080 to expand its LC-MS/MS product portfolio.

"The newly-developed GCMS-TQ8030 features powerful capability in terms of both high sensitivity and ultrafast performance, enabling trace analysis at the ppt (parts per trillion) level," said Hiroto Itoi, General Manager of Mass Spectrometry Business Unit, Life Science Business Department of Analytical & Measuring Instruments Division. In such areas as food and water safety, regulatory bodies typically set the concentration level of residual pesticides at below 10ppb unless there is any toxicology result. These analyses must be done in complex matrices and the number of target components has been increasing year by year. "The GCMS-TQ8030 is designed to fulfil these needs," said Hiroto Itoi.

With the LCMS-8040 and LCMS-8080 release Shimadzu's LC-MS/MS product portfolio now includes middle-range and high-end models. With novel technologies designed for trace quantitative works in complex matrices, the LCMS-8080 provides best-in-class sensitivity. This high-end model achieves a thirty-fold increase in sensitivity over the LCMS-8030 (released September 2010). Furthermore, the LCMS-8040 boosts the sensitivity five times higher than the LCMS-8030 while maintaining its ultrafast performance. With this combination of speed and sensitivity, the LCMS-8040 will help scientists to conduct 'Qual/Quan' analysis and cover a wide range of applications such as food safety, environmental, pharmaceutical, forensic and clinical.

Agilent Technologies, a major move was announced two days before the show and became the biggest talking point for the show was the acquisition of the Danish Cancer Diagnostics Company, Dako, for \$2.2 billion. This is the biggest acquisition ever made by Agilent and just what ramifications it will have for the future of the Agilent MS product portfolio remains to be seen. For this show however Agilent had two main launches, one being the Agilent 8800 triple quadrupole ICP-MS (ICP-QQQ), the first and only instrument of its kind. The new ICP-QQQ system offers improved performance compared to single quadrupole ICP-MS, and provides MS/MS operation for controlled and consistent interference removal in reaction mode. ICP-QQQ also addresses high-end application requirements, with flexible analysis capabilities unavailable on single quadrupole machines.

The second product was the Agilent Automated Card Extraction LC/MS system, a fully integrated instrument for the analysis of dried blood spots and other dried media. Aimed at pharmaceutical and clinical research laboratories, the AACE LC/MS provides an integrated, automated workflow solution to improve productivity and streamline sample processing.

Dried blood-spot analysis can be used in pharmaceutical as well as other settings to obtain detailed quantitative data about the compounds in animals and human subjects, using small volumes of blood (typically 10 to 20µl). The stability of blood spots is often superior to frozen plasma or serum samples. Agilent already supports dried blood-spot analysis for hole-punch methodologies, and this new product provides an automated online system for direct LC/MS analysis.

Thermo Fisher Scientific's analytical power of their highly successful LTQ Orbitrap[®] hybrid platform was enhanced by a new suite of software designed to further advance the performance of its recently introduced Elite[™] and Q Exactive[™] mass spectrometers. Next-generation **SIEVE[™] 2.0 software** increases is designed to improve throughput during complex metabolite and protein biomarker discovery experiments, while new **ExactFinder[™] 2.0 software** dramatically improves analysis time in the rapidly changing field of food safety testing. Also introduced was a **Protein Deconvolution** software to fully leverage the high-resolution/accurate mass (HR/AM) data produced by the Q Exactive system during complex protein analysis. These three new offerings were among eight software packages introduced at the show.

For laboratory customers who need to perform quantitative and qualitative analysis, but currently have limited capital budgets, the new Thermo Scientific Exactive Plus liquid chromatography/mass spectrometry (LC/MS) system was launched. The Exactive Plus system is designed specifically to address the need for high-throughput screening of compounds in a range of applications, including drug metabolism/pharmacokinetics (DMPK), metabolomics, forensic toxicology, environmental analysis and food safety testing. The new Exactive Plus LC/MS can be readily upgraded to match the higher performance of the premier Q Exactive mass spectrometer.

The Company's commitment to advancing triple quadrupole technology was evident in its new TSQ 8000 high-performance gas chromatography-mass spectrometry system (GC-MS/MS), also launched at ASMS. The TSQ 8000 system allows users to view targeted compounds at lower

concentrations, making even more complex analyses possible. Compatible with the company's leading TraceFinder[™] 2.1 software, the TSQ 8000 GC-MS/MS is designed for routine applications, including the identification of food and environmental contaminants.

To compliment the new software and Instrumentation a new Chromatography and Consumables catalogue was launched featuring new HPLC column chemistries and sample preparation products.

Waters introduced two new additions to its popular line of Xevo mass spectrometers – the Xevo[®] G2-S QToF and Xevo G2-S ToF – for the first time bringing Waters proprietary StepWave[™] ion optics technology to Waters[®] benchtop time-of-flight mass spectrometers. Equipped with StepWave's unique, off-axis ion source technology, Xevo G2-S QToF and Xevo G2-S ToF mass spectrometers are up to 20x more sensitive than earlier generation instruments.

Waters' StepWave ion optics technology transfers ions from the ion source with the highest possible efficiency while actively filtering out undesirable neutral contaminants. As a result, MS signals are dramatically increased and, because critical components in the device stay clean for longer periods of time, quantitative results are more reproducible and laboratories experience less downtime due to routine cleaning and maintenance.

Previously available on only the **Waters benchtop Xevo TQ-S** tandem quadrupole and research-grade **Synapt G2-S mass spectrometers**, StepWave brings a new level of sensitivity performance - to the Xevo quadrupole time-of-flight and time-of-flight instruments. It combines with proven QuanTof[™] technology to also deliver UPLC[®]-compatible mass resolution, matrix-tolerant dynamic range, quantitative performance, mass accuracy and speed of analysis – simultaneously.

The new Xevo G2-S mass spectrometers bring the following benefits to the analytical laboratory:

- Durable sensitivity - StepWave allows Xevo G2-S systems to achieve – and maintain – sensitivity over time, enabling them to resist sensitivity-diminishing contamination. That means that the need for routine maintenance is reduced, increasing uptime for busy laboratories.
- UPLC-compatible mass resolution - the new Xevo systems are expressly designed to work in combination with **Waters ACQUITY UPLC systems** and provide mass resolution at a speed compatible with UPLC.
- Matrix-tolerant dynamic range - StepWave and Waters' proven QuanTof technology give scientists the ability to analyse the most complex of samples with no compromise in mass resolution or data quality.

Since their introduction in 2008, ' **Xevo mass spectrometers** have distinguished themselves on the basis of their trademark simplicity and universal ion source architecture, giving scientists a wide selection of interchangeable ion sources best suited for the analysis at hand. All Xevo mass spectrometers also feature IntelliStart[™] Technology, which automates MS resolution and calibration checks and monitors system performance during a run.



Local Transport

Thoughts from an Attendee

Dr Jackie Mosely, University of Durham.

"Vancouver. It certainly made us Brits feel at home weather-wise, but the rain did not manage to dampen this great scientific event."

The meeting was opened with a lecture by Dr Chris Reddy from Woods Hole Oceanographic Institution who talked about the Deepwater Horizon Oil Spill: from the pipe to the plume. This fascinating lecture highlighted the problems of collecting samples under very hostile conditions, deep water, pressure and temperature etc. and that was below the surface! On the surface there were numerous vessels in close proximity, many of which were trying to control the fire. Regardless, Dr Reddy was successful in sampling at sufficient locations to accurately map the underwater plume, providing direction, size and chemical content of the plume.

From 8 parallel sessions, a number of which co-hosted by Mass Spectrometry Societies from the Pacific Rim, and the order of 750 posters each day meant that there was plenty of science to choose from. Proteomics and life-science featured heavily, as always, however this year there was a better balance of non-biological applications such as petroleomics and polymers and for those of us less interested in applied MS, this year saw a strong return to the fundamentals of mass spectrometry. As to the questions 'what's new?' well instrumentation development has been all about new time-of-flight detectors plus teasers of what we can expect in the future in terms of extremely high resolving power FT ICRs. So the take home message from this years ASMS? Watch this space...

Future Dates

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

June 9-13th 2013 Minneapolis, MN

June 15-19th, 2014, Baltimore, MD