

focus on Mass Spectrometry & Spectroscopy

61st ASMS Conference on Mass Spectrometry and Allied Topics 9-13th June, Minneapolis Convention Center, Minneapolis, Minnesota USA.

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This year ASMS was celebrating 100 years of Mass Spectrometry and provided each conference attendee with a free reproduction of the English Nobel Prize for Physics awardee Sir J.J Thomson's (pictured) 1913 edition of Rays of Positive Electricity. The conference started early for some attendees; with one-and two-day short courses beginning on Saturday and Sunday 8th and 9th June from 9:00 am to 4:30 pm, and later on Sunday afternoon with two informative tutorial lectures from 5:00 to 6:30 pm. The opening ceremony and lecture were followed by the Opening Reception - located in the poster-exhibit hall - which was an opportunity to eat, drink and meet up with colleagues and friends. Heavy hors d'oeuvres (yes, enough for dinner!), free beer from Summit Brewing which is brewed just across the river in St. Paul and a cash bar for wine. Technical posters did not go up until Monday morning - making this the ideal time to connect with exhibitors at their booths or corporate posters.



Monday saw the week start in earnest with 124 oral sessions of the scientific programme over the four days (27 sessions daily running concurrently) and culminating in the plenary lecture discovery of the elusive Higgs Boson by Peter Onyisi from the University of Texas at Austin.

There were also in excess of 3000 posters displayed during the week and daily workshops ensuring that if you did not utilise a prior selection process of some sort you would miss out on many interesting topics, and have sore feet.

Attendance was down slightly compared to recent ASMS conferences at 6,140 (see Table 1 for recent history) with attendees from the USA, Canada, UK and Germany there in force (see Table 2). There were 168 exhibit booths.

Table 1. Recent attendance history.

Year	Location	Total Attendees
2009	Philadelphia	6,530
2010	Salt Lake City	6,096
2011	Denver	6,477
2012	Vancouver	6,277
2013	Minneapolis	6,140

Table 2. Attendees by country.

USA	4159	Switzerland	88
Canada	314	France	87
UK	252	Netherlands	76
Germany	242	South Korea	68
Japan	194	Australia	54
China	118	Other	488

ASMS Awards

Award for a Distinguished Contribution in Mass Spectrometry

The increasing role of mass spectrometry (MS) in the physical and biological sciences can be attributed in a large part to the versatility afforded by the growing number of ionisation methods and to mass spectrometry's increasing sensitivity.

The development of the electrodynamic ion funnel in the laboratory of Dr. Richard Smith - Battelle Fellow and Chief Scientist in the Biological Sciences Division and Director of Proteomics Research at Pacific Northwest National Laboratory (PNNL) - has been an important factor in the latter increase. The ion funnel was originally created in the Smith lab in 1997 to replace ion transmission-limited skimmers and to efficiently capture ions in the expanding gas jet while radially focusing them. It has been adapted for a variety of uses and has proven to be a broadly applicable tool for ion focusing and manipulation at elevated pressures that challenged conventional approaches.

Although it has undergone several iterations in the last 15 years, the defining features of the ion funnel have not changed. The ion funnel concept continues to be adapted in a growing number of applications such as ion trapping, ion cooling, low pressure electrospray, and ion mobility spectrometry; however, its original use, decreasing ion losses in the interface of high pressure sources, has remained its most prevalent.

Currently, the funnel is employed by Bruker Daltonics' and Agilent Technologies and similarities can be seen in Thermo-Fisher's recent S-lens design found on the newer generations of Orbitrap instruments.

In the ion funnel, Dr Smith's obsession with sensitivity has provided a basis to greatly improve mass spectrometers, today allowing routine detection of low concentration species that would have been undetectable 15 years ago.

Biemann Medal

Dr Yinsheng Wang - Professor of Chemistry at the University of California-Riverside - has focused his research on discovering the biological consequences of DNA damage and on unravelling mechanisms of action for anti-tumour drugs and environmental toxicants.

His laboratory's use and development of mass spectrometry, synthetic organic chemistry, biochemistry and molecular biology enables us to understand and quantify, at the molecular level, how various DNA damage products are repaired, and how they perturb the efficient flow and fidelity of genetic information during DNA replication and transcription.

Professor Wang has identified and characterised new DNA lesions, including bulky lesions induced by reactive oxygen species. His laboratory developed LC-MS/MS combined with a plasmid-based shuttle vector to quantitatively assess how structurally defined DNA lesions alter the frequency and efficiency of DNA replication and transcription in cells, and to measure the types and frequencies of mutations induced by lesions.

They also discovered that N-2-(1-carboxyethyl)-2'-deoxyguanosine (N-2-CedG) is the major stable DNA adduct derived from methylglyoxal, and demonstrated that it is the previously unknown endogenous substrate for DinB (polymerase IV). Dr Wang's new methods have provided some long-sought biomarkers for oxidative stress: cyclopurine lesions including 8,5'-cyclo-2'-deoxyadenosine and 8,5'-cyclo-2'-deoxyguanosine.

New Product Roundup

In the interests of impartiality companies introducing new instruments and products are listed in alphabetical order, we have tried to feature the majority of new products introductions for 2013.

AB Sciex announced three new solutions for biological researchers to improve identification and quantitation of proteins, peptides, metabolites and lipids. They extended the applicability of SelexION™ Technology, SWATH™ Acquisition and ProteinPilot™ Software for academic research in the field of systems biology.

The launch of SelexION Technology on the TripleTOF® 5600+ System provides more confident identification and quantitation of molecules by delivering an additional level of separation between the liquid chromatography (LC) system and the mass spectrometer. This separation can be applied at the molecular level, the biological sub-class level or for the general removal of background interferences.

AB Sciex also introduced new enhancements to two critical tools in proteomics workflows, including SWATH Acquisition, a technique that enables researchers to reproducibly quantify all detectable components in a single injection. Next-generation SWATH Acquisition improves data scoring, filtering and support for variable window acquisition, up to 5x speed and scale improvement and enhanced tools for visualisation and transfer of complex data sets. Also introduced was a new version of ProteinPilot Software, which improves identification and quantitative results faster on larger data sets.

AB Sciex also highlighted several new solutions, workflows and services geared specifically for routine analysis.

New tools include: Doubling throughput and improving data quality to identify more compounds with a new MPX™ solution. Significantly improving the ability to identify known and unknown contaminants with a new software package called MasterView™ Software, featuring automatic compound ID, new comprehensive accurate mass spectral libraries and efficient data review and reporting. Expansion to the Eksigent LC product portfolio with the new Eksigent® ultraLC 110 system.

New services include: Targeted support for labs on a tight budget with the new 'AB Sciex Connect' service which will provide immediate phone and online support, backed by guaranteed onsite response times, software maintenance support with the new service called 'AB Sciex Software Maintenance' which allows labs to easily choose the software portfolio that best covers their applications, and access to a range of self-support tools, including a comprehensive and expanding range of training modules, with the new service called 'AB Sciex Online'.

Agilent Technologies announced the launch of the RapidFire 365 High-throughput Mass Spectrometry System. The system offers increased plate capacity, full integration with Agilent's BenchBot Robot automation technology and improved productivity for researchers working on drug discovery, clinical research and forensic toxicology.

Fully compatible with Agilent's entire line of mass spectrometers, the RapidFire 365 high-throughput mass spectrometry system offers numerous advancements:

- The system runs unattended for up to 60 hours, facilitating more than 20,000 injections and enabling over-the-weekend runs.
- It analyses multiple assays in a single, unattended run.
- It automates method development for novel analytes.
- It provides intuitive data review and visualisation, using RapidFire Integrator 2.0 software.

The RapidFire 365 can also identify active compounds against challenging targets, confirm the activity of those compounds, and assess absorption, distribution, metabolism, elimination and physiochemical properties of those compounds.

Agilent also announced three enhancements for its LC and LC/MS products. They have increased mass scan speeds on the LC/MS single quadrupole instruments, launched the StreamSelect LC/MS system, and released new MassHunter walk-up software.

Faster Analyses with Higher Scan Speeds

Agilent has doubled the mass scan speed on its single quad LC/MS instruments by using exclusive signal-processing algorithms. The increased speed supports faster separations so that labs can run more samples per day. Also, the ultra-fast scan speeds are compatible with the sub-second peak widths resulting from high-speed, UHPLC separations on the Agilent 1290 Infinity LC system.

StreamSelect LC/MS System

The StreamSelect LC/MS system consists of two Agilent 1200 Series LCs (with optional online sample cleanup) coupled to a single 6400 Series Agilent Triple Quadrupole LC/MS. Easy-to-use Agilent MassHunter StreamSelect software controls the timing of staggered injections and analysis windows for higher throughput.

MassHunter Walkup Software

MassHunter walkup software for LC/MS and LC systems gives many users the ability to submit and analyse their samples using multiple LC and LC/MS systems, with little specialised knowledge of mass spectrometry or chromatography. The new software also enables users to administer these systems remotely.

They also introduced the GC/MS/MS Pesticide Residue Analysis Guide, a comprehensive reference developed by Dr Katerina Mastovska, the head of Excellcon International, LLC, in collaboration with scientists from the California Department of Food and Agriculture, the Florida Department of Agriculture and Consumer Services, and Agilent.

Bruker announced two important collaborations, firstly the Strategic Collaboration between Bruker Daltonics and CovalX in High Mass MALDI detection and secondly an exclusive patent license agreement with 3M Company, which allows Bruker to include 3M patented innovations relating to MALDI imaging. They also announced the launch of several powerful new Mass Spectrometry Systems and Solutions for Life-Science Research, Clinical Research, Pharma and Applied Markets

Major Bruker Innovations at ASMS 2013 included;

The 'Game-changing >10 million' eXtreme Resolution on new solariX™ XR System with the scientifically acclaimed ParaCell™ as its core technology, enables the solariX XR to provide resolving powers of greater than 650,000 in a 1 second acquisition (at m/z 400) for routine LC/MS or MALDI imaging experiments, and ultimately over 10 million resolving power for the most challenging complex mixture applications, from top-down proteomics, to petroleomics and dissolved-organic matter (DOM) analysis, to eXtreme Resolution MALDI imaging.

The 'Industry-leading 50 Gbit/sec sampling'; The new Impact HD is the latest innovation in Bruker's unique UHR-QqTOF (Ultra-High Resolution Qq-Time-Of-Flight) mass spectrometry product line with industry-leading >40,000 Full-Sensitivity Resolution (FSR), broad mass-transfer ion optics and the fastest 50 Gbit/sec sampling technology, a dynamic range of 5 orders of magnitude is achieved at UHPLC speeds, and with up to 50 Hz MS/MS capabilities. These features open up enhanced analytical performance levels for all applications where trace analysis from complex, high-background matrices is a challenge – such as biomarker research, identification of impurities or residue screening.

The Novel CaptiveSpray NanoBooster™, for new performance levels in proteomics and glycoanalysis, enables over 8,400 unique protein IDs in proteomics on impact™ HD UHR-QTOF System. This newest version of Bruker's highly regarded CaptiveSpray ion source with proprietary dopant-enriched ionisation boosts nano-flow sensitivity, and drives up protein and peptide ID rates significantly.

The new EVOQ™ Elite ER LC-triple quad mass spectrometer, for undistorted peptide quantification with proprietary VIP™ (vacuum-insulated probe) HESI source, is the latest addition to the EVOQ family of LC-TQ systems, with an extended mass range to 2,000 m/z, for peptide quantitation or other high m/z applications.

All EVOQ LC-TQ systems incorporate Bruker's new Advance™ Ultra-High Pressure Liquid

Chromatography (UHPLC) systems. The Advance HPLC, UHPLC, and the UHPLC-OLE (on-line extraction) products offer ultra-low dead volume, which enables excellent reproducibility at analytical flow-rates, an integrated column-oven, and bench-space savings.

Shimadzu Corporation, introduced the new MALDI-7090™ MALDI TOF-TOF mass spectrometer which combines high throughput, high resolution and high-energy for the ultimate in tandem MS capabilities targeted for proteomics and tissue imaging research. The combination of Shimadzu's extensive MALDI-TOF-TOF expertise with novel patented technology provides the MALDI-7090 with ultimate capabilities for identification and structural characterisation of biomolecules.

Innovative technology incorporated into the MALDI-7090, such as ASDF™- Axial Spatial Distribution Focusing, delivers market-leading high-resolution MALDI MS/MS for accurate compound characterisation. This, in combination with proprietary solid-state laser technology, true 2 kHz acquisition speed in all modes (MS and MS/MS), an integrated 10-plate loader and newly designed MALDI Solutions™ software, sets a new benchmark in MALDI TOF-TOF design.

"The 2 kHz laser speed and high MS/MS resolution in the MALDI-7090 has accelerated our research in proteomics analysis for protein complex and histone modification using LC-MALDI," said Takeshi Kawamura, Assistant Professor from RCAST, University of Tokyo.

The 20 keV high-energy CID capability of the MALDI-7090 efficiently produces additional fragment ions to further enhance characterisation.

Thermo Fisher Scientific's innovation making headlines at this year's ASMS include:

The Thermo Scientific Orbitrap Fusion 'Tribrid' mass spectrometer; a new top-of-the-line research instrument that uniquely combines three Thermo Fisher mass analysers – the industry-leading Orbitrap, quadrupole and linear ion trap – for unprecedented analytical capabilities in proteomics, lipidomics, glycoproteomics and other life sciences research, offering a greater depth of analysis of complex biological samples to provide new levels of knowledge. It offers up to 450,000 resolution, which allows life sciences researchers, for example, to measure extremely low-concentration drug metabolites that could not previously be identified. In addition, the Orbitrap Fusion can enable scientists to conduct a wide range of existing experiments faster and more effectively to accelerate the discovery process.

Scientists performing quantitation experiments – from proteomics and toxicology to food and environmental testing may now use the new Quantiva triple-stage quadrupole mass spectrometer; a triple quadrupole mass spectrometer that was built from the ground up to deliver ultimate sensitivity at the attogram (10⁻¹⁸ gram) level, speed and dynamic range for challenging quantitation experiments, such as detecting ultra-low levels of peptides for cancer research.

To optimise around-the-clock analyses, such as forensics, pharmaceutical QA/QC, and food and environmental testing, the new TSQ Endura triple stage quadrupole mass spectrometer was designed to minimise maintenance requirements for exceptional uptime. Ultimate Performance and Usability.

Thermo Fisher also introduced a new suite of software designed to make the power of these new-generation mass spectrometers accessible to a wider customer set by improving usability and increasing the speed of analysis.

Thermo Fisher also introduced several new reagents:

- The iodoTMT reagents and labelling kit for the measurement of protein and peptide cysteine modifications by multiplex quantitative mass spectrometry.
- Thermo Scientific Pierce Trypsin Protease, MS Grade for protein digestion.
- Thermo Scientific Pierce Mass Spec Sample Prep Kit for Cultured Cells, an easy-to-use comprehensive kit for preparing clean peptide mixtures.
- Thermo Scientific Pierce Abundant Protein Depletion Products, spin columns for removing albumen and antibody components from human plasma for mass spec or electrophoresis analysis.
- Thermo Scientific Pierce Reserpine Standard for LC-MS.

Waters Corporation unveiled the new Waters® SYNAPT® G2-Si Mass Spectrometer and also previewed its UNIFI® CCS Research Edition and the new TransOmics Version 2.0 informatics products for the new SYNAPT G2-Si mass spectrometer.

The SYNAPT G2-Si System integrates a third dimension of resolution and separation power into a new suite of untargeted and targeted LC/MS/MS workflows and now combines the unique power of Travelling Wave (T-Wave) Ion Mobility Separations with new data acquisition and informatics technologies, and collision cross section (CCS) measurements to bring to the toughest analytical applications, unparalleled information and confidence at a level not possible by mass and chromatographic separation alone.

The SYNAPT G2-Si mass spectrometer is the first MS system to elevate CCS alongside retention time and mass to charge ratio (m/z) as a robust, reliable identification parameter in library-based screening.

Waters also previewed an enhanced range of Omics Research Platform Solutions, powered by TransOmics™ 2.0 Informatics. The new TransOmics 2.0 informatics packages for proteomics and metabolomics/lipidomics, created exclusively for Waters by its strategic business partner Nonlinear Dynamics, are based on extended versions of the Nonlinear Dynamics Progenesis™ LC-MS and CoMet products. The TransOmics 2.0 informatics packages are specifically designed to process and visualise SYNAPT High Definition Mass Spectrometry (HDMS) Omics data, denominated with Collision Cross Section (CCS), from the new Waters SYNAPT G2-Si HDMS mass spectrometer.

Future ASMS Dates

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

- 62nd ASMS Conference, 15 – 19 June, 2014, Baltimore, MD
- 63rd ASMS Conference, 31 May - 4 June, 2015, St. Louis, MO
- 64th ASMS Conference, 5 – 9 June, 2016, San Antonio, TX