

focus on

Mass Spectrometry & Spectroscopy

62nd ASMS Conference on Mass Spectrometry and Allied Topics 15-19 June at the Baltimore Convention Center, Baltimore, Maryland USA

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This year the American Society for Mass Spectrometry (ASMS), following on from the centenary celebration of Mass Spectrometry, again provided each conference attendee with a free reproduction of the English Nobel Prize for Physics awardee Sir J.J. Thomson's 1913 edition of Rays of Positive Electricity.

The highlight of the meeting for many was a small exhibit titled 'Spaceflight MASS Spectrometry 1963 – 2018', located in the registration area so available to all attendees, featuring models of spaceflight mass spectrometers used since 1963 in the exploration of the Solar System. The models on display included engineering units, in-flight spares, and reproductions from robotic planetary missions to Venus, Jupiter, Saturn, Titan, and Mars. The display was coordinated by William B. Brinckerhoff, NASA GSFC, Greenbelt, MD.



The conference started early for many attendees; with one-and two-day short courses beginning on Saturday and Sunday 14th and 15th June from 9:00am to 4:30pm, and later on Sunday afternoon with two informative tutorial lectures from 5:00 to 6:30pm.

The brief opening ceremony was followed by a riveting lecture entitled 'The James Web Space Telescope (JWST): From First Light to the Search for Earth 2.0' presented by Jason Kalirai from the Telescope Science Institute who proceeded to describe the US\$8.0 Billion project which will launch, in 2018, an infrared telescope with a 6.5 meter primary mirror into space. The JWST has four main science themes: The End of the Dark Ages: First Light and Reionization, The Assembly of Galaxies, The Birth of Stars and Protoplanetary Systems, and Planetary Systems and the Origins of Life.

This was 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 Heavy Seas Brewery which is brewed in Baltimore and a cash bar for wine were all available. 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 128 parallel oral sessions of the scientific programme over the four days (32 sessions daily running concurrently) and culminating in the plenary lecture, 'How The Genome Folds' by Erez Lieberman Aiden from Baylor College of Medicine and Rice University.

There were also 3141 posters displayed during the week covering topics from advances in instrumentation and isolation, enrichment and derivatisation to top-down protein analysis 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 very sore feet. If you weren't exhausted by 17:00 then there were 13 Workshops run daily from 17:45 to 19:00 leaving one hour for dinner before the corporate hospitality suites swung into action at 20:00; providing endless snacks, refreshments and entertainment ranging from a tribal drummer, world cup soccer, baseball and miniature race car racing to a dancing robot, all lasting until 23:00.

Attendance was up a very healthy 11% compared to the ASMS 2013 conference at 6,913 (see Table 1 for recent history) with attendees from the USA, Canada, UK and Germany there in force. There were 171 exhibit booths.

Table 1. ASMS Attendance from 2009-2014

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
2014	Baltimore	6,913

Table 2. ASMS Attendees by Country

Country	Attendees
USA	5361
CANADA	292
GERMANY	284
UK	264
JAPAN	208
CHINA	183

ASMS Awards

2014 Award for a Distinguished Contribution in Mass Spectrometry

The 2014 ASMS Award for a Distinguished Contribution in Mass Spectrometry was awarded to Dr Richard M. Caprioli, the Stanford Moore Chair in Biochemistry and Director of the Mass Spectrometry Research Center at Vanderbilt University, for the development of Matrix Assisted Laser Desorption Ionization (MALDI) Imaging Mass Spectrometry and the molecular mapping of biological and medial tissue samples.

Professor Caprioli's work led to a rapidly expanding application area of mass spectrometry where molecular measurements are made directly from tissues, enhancing the information that can be obtained from these samples. Application examples are the study of proteins, lipids, metabolites, and pharmaceutical compounds with around 2,500 papers having been published to date on the subject of MALDI imaging mass spectrometry.

From the first publication of Professor Caprioli's 1997 paper (Anal. Chem. 69(23), 4751-4760) where the power of MALDI imaging mass spectrometry for tissue analysis was first shown, he has pioneered advances in sample preparation, instrumentation, and informatics.

The impact of his work is broadly evident in the number of commercial platforms that employ the MALDI technology.

Biemann Medal

Dr Lingjun Li, Professor of Pharmaceutical Sciences and Chemistry at the University of Wisconsin-Madison, was awarded the 2014 Biemann Medal for her work in the field of mass spectrometric study of neuropeptides and functional peptidomics.

Professor Lingjun Li's research program has focused on the development of novel and improved mass spectrometry (MS)-based tools in conjunction with micro separation techniques to study neuropeptides and biomarkers in neurodegenerative diseases.

Dr Li and her team have worked on in-situ peptide mapping, tissue imaging, in vivo micro dialysis and high sensitivity micro-separation discovering more than 300 novel neuropeptides in crustacean model organisms whose genomic sequences are currently unavailable.

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 2014.

AB Sciex released five new mass spectrometry solutions in launching their theme of 'Answers for Science. Knowledge for life' that will allow scientists globally to find answers to improve scientific understanding and safeguard health.

The new solutions include the following:

The **TripleTOF® 6600 system** with **SWATH™ Acquisition 2.0** designed for quantitative proteomics and biologics. This high-resolution, accurate-mass system, combined with the new SWATH™ Acquisition 2.0, is ideal for studying changes in biotherapeutics when combined with **BioPharmaView** software, this solution helps the researcher gain a rapid, accurate, and confident understanding of compounds in the area of drug development.



The AB Sciex Triple Quad™ 3500 System

BioPharmaView™ Software is a powerful new product for automating workflows and can efficiently analyse and compare batches while monitoring critical quality attributes according to the FDA's well-characterised biotherapeutic product (WCBP) model.

StatusScope™ Remote Monitoring service is a configurable, real-time service that supports most AB Sciex mass spectrometers and Eksigent Micro and Nano LC products. With three user levels – lab manager, lab director and technician – StatusScope service permits viewing instrument performance and workflow status remotely, capturing errors quickly minimising downtime.

Triple Quad™ 3500 System is a new enhanced basic mass spectrometry system that is designed to meet the demands of food and environmental testing laboratories by enabling laboratories to detect more compounds in each injection, with a three-fold increase in sensitivity over its predecessor, the API 3200 system.

Agilent Technologies announced the launch of the **7010 Triple Quadrupole GC/MS System** featuring a totally redesigned ion source that is a radical departure from the conventional ion sources currently on the market. The new high-efficiency electron ionisation (EI) source creates more than 20 times as many ions as current EI sources. This high ionisation efficiency translates directly to greater efficiency in the laboratory, as it will now be possible to:

- Inject smaller volumes of sample for decreased load on GC liners and columns, thereby increasing the number of samples run between maintenance operations;
- Scale down sample prep volumes to save on expensive reagents and standards, and decrease waste;
- Eliminate time-consuming and error-prone pre-concentration steps; and
- Add more compounds to target lists easily by lowering the dwell times of existing targets.

Also introduced was the **Agilent 6120VL**, an entry-level mass detector based on the proven 6120SQ Agilent single quadrupole LC/MS technology. This new affordable single quadrupole MS system is fully integrated with Agilent's UHPLC systems and will allow academic, industrial and pharmaceutical laboratories to benefit from the analytical advantages of mass detection.

Agilent also introduced a new flagship triple quadrupole mass spectrometer for LC/MS applications requiring the highest sensitivity and robustness. The **Agilent 6495 LC/MS Triple Quadrupole** system, featuring a 2 year warranty, is fully integrated with Agilent's 1200 series UHPLC systems to deliver turnkey performance and is designed for both routine laboratory analysis and for the most challenging quantitation in life sciences, food and environmental applications.

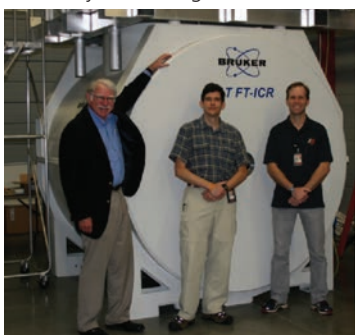
Bruker announced the successful installation of the world's first 21 Tesla (T) magnet for Fourier Transform Ion Cyclotron Resonance (FT-ICR). FT-ICR is by far the highest resolution mass spectrometry technique available, and is useful in the analysis of extremely complex mixtures, including applications in petroleomics, dissolved organic matter (DOM), metabolomics, top-down proteomics, and MALDI imaging. The 21T magnet was designed and built by Bruker in collaboration with NHMFL scientists, and will be used in the NHMFL FT-ICR program in a project funded by the National Science Foundation.

Bruker introductions at ASMS 2014:

Bruker also announced several mass spectrometry-based product introductions including:

The **New impact II™** ultra-high resolution QTOF mass spectrometer now with >50,000 Full-Sensitivity Resolution (FSR) and broad mass-transfer ion optics and fast 50 Gbit/sec sampling technology produces a dynamic range of 5 orders of magnitude at UHPLC speeds, with up to 50 Hz spectrum acquisition enabling fast, intact protein profiling of over 1,000 proteoforms in a single, less than 30 minute UHPLC-UHR-QTOF run.

A New **multi-OMICS** platform to increase productivity, versatility, and provide deeper biological insights, which includes the **MaxQuant** software which is designed for analysing large mass-spectrometric data sets. It is specifically aimed at high-resolution MS data. Several labelling techniques as well as label-free data processing workflows are supported and in addition MaxQuant enables researchers to utilise the full potential of mass spectrometry driven proteomics in multi-OMICS approaches.



Pictured with the 21 T FT-ICR magnet at the NHMFL lab are (from left to right): Professor Alan Marshall, the Robert O. Lawton Professor of Chemistry and Biochemistry at Florida State University and Director of the High Field FT-ICR program at the NHMFL; John Quinn, 21 T FT-ICR engineering lead at NHMFL; Dr Chris Hendrickson, 21 T FT-ICR Project Advisor at the NHMFL.

Also included in the multi-OMICS platform is the new **Compass™ PathwayScreener™** software which is designed to provide a new layer of insight into metabolomics samples so users can get twice the results, performing pathway-driven, targeted metabolomics analysis on the same dataset used for non-targeted data mining.

ToxScreener™ a new accurate mass, high dynamic range forensic toxicology solution for Bruker QTOF systems, incorporating broadband CID (bbCID) acquisition to provide a rapid and reliable way for scientists to confidently screen for hundreds or even thousands of known or previously unknown compounds of forensic relevance, delivering the highest degree of confidence, and data that is defensible in court. At the heart of the ToxScreener, is an accurate mass database covering drugs of forensic relevance allowing users to attain enhanced levels of confirmation for conclusive identification compared to alternative screening techniques.

The European launch of **Toxytper™ 1.1**, was also announced. Toxytper 1.1 is a robust and easy to use forensic and clinical research solution for routine, fast, push-button toxicology on approximately 900 compounds. The new Toxytper 1.1 includes novel library identification algorithms and reporting with a library update to over 900 target compounds. Toxytper 1.1 now also comes with a targeted drugs-of-abuse sub-library and the new Toxytper 1.1 search algorithms are fully compatible with the recently published 'Maurer/Wissenbach/Weber LC-MSn library of Drugs, Poisons and their Metabolites', an ion trap library which holds over 1,000 parent compounds and 2,700 metabolites.

New **autoflex™ speed** MALDI TOF(TOF) system with Bruker 2 kHz smartbeam™-II laser to enhance productivity in protein analysis, MALDI imaging and MALDI Biotyper incorporates numerous advances to further enhance data quality, acquisition speed, mass and dynamic range, all with robust and efficient performance. It further extends the applications of MALDI TOF(TOF) in protein sequencing, biomarker discovery, polymer analysis, lipid and glycan analysis, molecular imaging, as well as in high-throughput MALDI Biotyper microbiological identification.

Shimadzu Corporation introduced the following products at ASMS 2014:

GCMS-TQ8040 Mass Spectrometer with Smart MRM - featuring Smart Productivity which enables the analysis of 400+ compounds in a single MRM run for high-efficiency sample throughput, Smart Operation for quick and easy method development, and Smart Performance for low detection limits and Scan/MRM.



The Shimadzu GCMS-TQ8040 Mass Spectrometer

They also introduced several mass spectrometry-based applications of **Noviplex™ cards**. Noviplex Cards allow for the rapid collection of a volumetric sample of plasma from an unmeasured amount of whole blood within minutes. Demonstrated applications included peptides, proteins and small molecules.

Open Solution QuantAnalytics™, a software package and LC/MS/MS data tool for the pain management and clinical markets which increases the speed and efficiency of data processing and review by allowing users to highlight and review results that are of specific importance to clinicians. The software can automatically flag data that is outside acceptable criteria, which allows the analyst to accept, reject, or rerun a sample.

Shimadzu and **Indigo BioSystems** announced a partnership to develop and market mass spectrometry solutions that simplify and accelerate clinical data acquisition and data review for applications in clinical research, forensic toxicology and new drug development. Shimadzu will combine its ultra-fast mass spectrometry platforms with Indigo BioSystems' expert system software. ASCENT™ clinical analysis software is a comprehensive and powerful data analysis suite that interprets visual data results from instruments and automatically reviews the data for problematic results.

Shimadzu Corporation announced the mutual support between the **Skyline** quantitative proteomics software and Shimadzu's high-sensitivity triple quadrupole LC/MS/MS platform. As mass spectrometry-based proteomics technologies play an ever-increasing role in biomarker discovery, validation and translation for biological and clinical applications, advances in throughput and multiplexing are necessary this emerging field referred to as quantitative Clinical Chemistry Proteomics (qCCP). Shimadzu has integrated its ultra-fast LC/MS/MS platforms with the Skyline quantitative proteomics software to bring qCCP applications closer to clinical laboratories.

Thermo Fisher Scientific's product launches at this year's ASMS include:

Headlining the new Thermo Scientific launches is the **Q Exactive HF** (high field) liquid chromatography-mass spectrometry (LC-MS) system, which significantly increases the performance of the highly successful Q Exactive Plus platform by combining it with an ultra-high field Orbitrap mass analyser. The Q Exactive HF system is engineered for faster characterisation; quantification and confirmation to help life sciences researchers dramatically increase analytical speed and sensitivity in applications such as protein identification.

New application-specific Thermo Scientific software helps researchers turn mass spectral data into answers to the most challenging scientific questions. **PepFinder 1.0** peptide mapping software increases the quality and accuracy of biotherapeutic protein characterisation critical in drug development and production quality control. As mass spectrometry becomes the primary method of identifying proteins in complex biological samples, **Proteome Discoverer 2.0** software provides outstanding sensitivity and a wide array of bio-software tools and customisable workflows.

New reagents for sample preparation were introduced designed to enrich target proteins, peptides and therapeutic antibodies for analysis. **Mass Spectrometric Immunoassay** pipette tips feature proprietary micro column technology to provide enhanced, reproducible target purification in biological samples prior to LC-MS analyses.

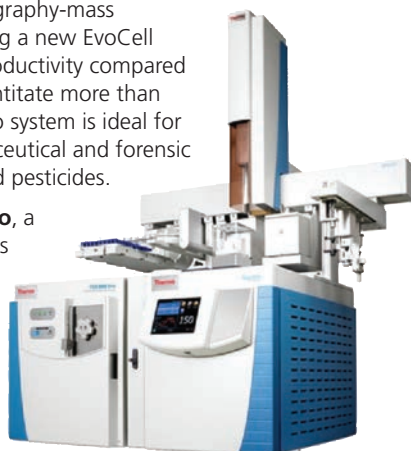
In addition, the **Tandem Mass Tag Reagent** family is specially designed to enable a rapid transition from method development to high-throughput protein quantitation.

The **TSQ 8000 Evo** triple quadrupole gas chromatography-mass spectrometry system was also launched incorporating a new EvoCell technology which delivers a threefold increase in productivity compared to its predecessor, allowing users to screen and quantitate more than 1,000 compounds in a single run. The TSQ 8000 Evo system is ideal for laboratories analysing food, environmental, pharmaceutical and forensic samples for complex compounds such as dioxins and pesticides.

Waters Corporation unveiled the **Xevo® TQ-S micro**, a new and compact benchtop tandem quadrupole mass spectrometer which is designed to acquire sensitive, robust and dependable data at accelerated rates of acquisition for numerous analytes at varying concentrations.

Also introduced was the **Xevo® G2-XS** mass spectrometer, a new high performance benchtop quadrupole time-of-flight (QToF) mass spectrometer featuring the new XS Collision Cell. The Xevo G2-XS QToF offers sensitivity and selectivity in a benchtop QToF mass spectrometer.

The expansion of the **ionKey/MS™** System to the SYNAPT G2-S, SYNAPT G2-Si, Xevo G2-S QToF and the newly introduced Xevo G2-XS QToF micro mass spectrometer was also announced and also includes new iKey chemistries, specifically HSS T3 (high strength silica) and BEH C4 (Bridged Ethyl Hybrid) 1.7 µm UPLC grade particles in 5 and 10 cm pathlengths. When first introduced, the iKey featured C18, BEH 300, Å CSH (Charged Surface Hybrid) and C18 BEH 130 Å only.



The Thermo Scientific TSQ Evo triple quadrupole GC-MS system

Waters also unveiled **Progenesis® QI for proteomics Version 2.0**, which enables more rapid and reliable quantification and identification of differentially changing proteins in laboratory samples. The new features of Progenesis QI include Pathway Analysis, QC Metrics and Process Automation.

Waters also announced two new partnership agreements:

The first with Prosoia, Inc for the exclusive rights to **DESI** (Desorption Electrospray Ionization) technology for clinical research applications for use with Waters® time-of-flight mass spectrometers, including its SYNAPT® G2 Si and Xevo® G2-XS QToF mass spectrometers.

When used for clinical research studies, DESI is a non-destructive means by which researchers using mass spectrometry can determine, with specificity and speed, the molecular distributions of drugs, lipids and metabolites from human tissue samples.

The second that Omics LLC's **PetroOrg** Petroleomics Software is now available for Waters® SYNAPT® G2-Si. The combined solution delivers time saving performance, enhanced results and comprehensive data for chemical composition characterisation of petroleum.



The Waters Xevo® TQ-S micro

Future ASMS Dates

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

- 63rd ASMS Conference, May 31 - June 4, 2015, St. Louis, MO
- 64th ASMS Conference, June 5 - 9, 2016, San Antonio, TX
- 65th ASMS Conference, June 4 - 8, 2017, Indianapolis, IN
- 66th ASMS Conference, June 3 - 7, 2018, San Diego, CA
- 67th ASMS Conference, June 2 - 6, 2019, Atlanta, GA



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