63rd ASMS Conference on Mass Spectrometry and Allied Topics held in St. Louis from 31st May to 4th June, 2015 at the America's Center, St. Louis, Missouri USA.

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The site of the 63rd ASMS was St. Louis founded in 1764 and named after Louis IX of France. First claimed by the French the region in which the city stands today was ceded to Spain following France's defeat in the Seven Years' War. Its territory east of the Mississippi was ceded to the Kingdom of Great Britain, the victor. After the United States acquired this territory in the Louisiana Purchase the town became the territorial capital and gateway to the western territory and the starting point for the Lewis and Clark expedition, which departed from St. Louis in May 1804 in search of water route to the Pacific Ocean. The city is commonly identified with the 630-foot (192 m) tall Gateway Arch in downtown St. Louis (*Figure 1*).

Figure 1. The Gateway Arch in downtown St. Louis at night.

The conference started early for many attendees; with one-and two-day short courses beginning on Saturday and Sunday 30th and 31st May 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 brief opening ceremony by Vicki Wysocki, ASMS Vice President for Programs, was followed by a lecture entitled The Human Gut Microbiome and Healthy Growth presented by Jeffrey L. Gordon from The Washington University St. Louis School of Medicine who proceeded to describe the work he and his group have undertaken which has focused on childhood under nutrition, which is the single greatest factor in childhood mortality for the under 5 age group in developing countries. The project followed and evaluated 8440 children from different geographical, ethnic and cultural backgrounds and measured weight and height for age and tested faecal samples for pattern in the gut microbiome.

The Opening Reception, located in the poster and exhibition hall, was an opportunity to eat, drink and meet up with colleagues and friends followed this. Heavy hors d'oeuvres (yes, enough for dinner!), free beers from Schlafly brewery in St. Louis, a 21-year-old company which was the first new brewpub to open in Missouri since Prohibition. They provided 2 beers to choose from, and a cash bar for wine lovers was also available. Technical posters did not go up until Monday morning, making this the ideal time to connect with friends, colleagues and exhibitors at their booths.

Monday saw the week start in earnest with a program consisting of 128 parallel oral sessions in the scientific programme and 39 workshops over the four days (32 sessions daily running concurrently with 13 workshops late in the day) and culminating in the plenary lecture - 'The Evolution of Modern Neurosurgery: A History of Trial and Error, Success and Failure' - given by G. Michael Lemole, Jr. from The University of Arizona College of Medicine.

There were also 2764 posters displayed during the week covering topics from new developments in ionisation and sampling, metabolomics, glycan and glycoprotein analysis and quantitative analysis of biomarkers to top-down protein analysis and daily workshops ensuring again 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 the 13 Workshops running 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 all lasting until 23:00.

Attendance was down compared to previous years by 8% compared to the ASMS 2014 conference at 6,100 (see *Table 1* for recent history) with attendees from many of the states in the USA, and 25% of attendees being from overseas with Canada, UK and Germany there en mass. There was an increase in the number of exhibitors, up to 200 from 171 exhibit booths in 2014.

Table 1. Attendance figures for ASMS by year.

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
2015	St. Louis	6100

ASMS Awards

2015 Award for a Distinguished Contribution in Mass Spectrometry

The 2015 ASMS Award for a Distinguished Contribution in Mass Spectrometry was awarded to Dr Brian T. Chait, the Head of the Laboratory of Mass Spectrometry and Gaseous Ion Chemistry and a Camille and Henry Dreyfus Professor at The Rockefeller University, New York, NY.

Dr Chait was recognised for his work on the recognition and demonstration of the link between protein structure and conformation and electrospray ionisation mass spectra. His revelation that a protein's solution phase conformation impacts its electrospray ionisation mass spectrometry (ESI-MS) charge state distribution (CSD) removed prior barriers preventing mass spectrometry from looking at higher order macromolecular structures.

Today as a result of his work, interpreting ESI-MS and MS/MS data for proteins in native solutions many times begins from NMR or crystal structures, based on assumptions that the gas-phase structure will not be too distant. The Chait laboratory opened the world to this possibility, first by demonstrating that electrosprayed cytochrome c molecules assumed about twice as much charge when sprayed from pH 2.6 than from pH 5.2 H2O (*J. Am. Chem. Soc.* 112, 9012 (1990)), by probing conformational changes in proteins via hydrogen/deuterium exchange (*Rapid Commun. Mass Spectrom.* 5, 214 (1991)), and by monitoring solution-phase thermal denaturation processes by ESI-MS (*Anal. Chem*. 65, 1, (1993)).

Dr Chait's achievement must be viewed from the perspective of mass spectrometry in 1990 when spraying 100% aqueous solutions was rare or the need was not obvious. For some an organic sheath solvent (or make-up flow) reduced surface tension enough to complete the analyses; others simply added methanol directly. However, Chowdhury and Chait (*Anal. Chem*. 63, 1660 (1991)) demonstrated that electropolished needles could electrospray water at voltages sufficiently below those inducing dielectric breakdown. That ability to electrospray 100% H_2O was key to observing the charge state distribution differences associated with natively folded proteins. Equally important was Dr Chait's ability to rationalise and prove that the source of the observed CSD difference had to be solution-phase structure.

Little is known about electrospray ionisation today; and even less was known 25 years ago, yet the ideas that Dr Chait precisely articulated about the electrospray CSD/conformation relationship were a major turning point for biological mass spectrometry.

Biemann Medal

Dr Michael J. MacCoss a professor in the Department of Genome Sciences, University of Washington, Seattle has made numerous high impact contributions to the field of proteomics. Primarily his software development, which he makes freely available and continually supports, has greatly benefitted the proteomic sciences.

Other Bioinformatics tools developed by the MacCoss laboratory in Seattle has included tools for liquid chromatography mass spectrometry (LC- MS) feature finding, spectrum library searching, peak detection, post-processors for peptide database searching, and more. The Percolator algorithm developed by his lab, improved peptide identification from proteomic analyses through machine learning (Käll et al. 'Semi-supervised learning for peptide identification from shotgun proteomics datasets', *Nature Methods*, 2007). Open source libraries and licenses for Percolator resulted in widespread adoption Percolator became widely adopted and encouraged its incorporation into multiple commercial packages (e.g. Mascot and Proteome Discoverer). Skyline, another project from the MacCoss laboratory, is an integrated set of software tools (MacLean et al. 'Skyline: an open source document editor for creating and analysing targeted proteomics experiments', *Bioinformatics*, 2010; available from http://skyline.maccosslab.org). Most importantly Skyline is a manufacturer-neutral set of tools enabling methods to be transferred easily, tested and validated across labs, even those utilising different instrument platforms.

Dr MacCoss's most recent project 'The Chorus Project' (http://chorusproject.org) is a not-for-profit and cost effective mechanism enabling laboratories to visualise, share, analyse and backup data to the cloud.

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 2015.

Agilent Technologies announced the launch of the **6545 LC/Q-TOF System**, designed to provide added sensitivity for routine analyses.

The new midrange system includes advances in hardware and software that make it both more reliable and easier to use for trace-level analysis of small-molecule compounds in applications such as food safety, environmental testing, forensic toxicology and pharmaceuticals.

The 6545 is engineered to be Agilent's most reliable Q-TOF ever, building on a legacy for LC/MS reliability and adding hardware advances such as ion shaping optics, high-voltage power supplies, and longer-life parts to increase robustness.

The system's new autotune software leverages particle swarm technology to optimise the instrument for small-molecule analyses with the click of a button. In just about 15 minutes, it optimises the instrument to get up to five times more sensitivity for small molecule compounds, including low-intensity compounds.

Figure 2. The Agilent 6470 LC/MS Triple Quadrupole system.

Agilent also introduced a new triple quadrupole mass spectrometer for LC/MS applications requiring the highest sensitivity and robustness. The **Agilent 6470 LC/MS Triple Quadrupole** system (*Figure 2*), featuring a lower LDL of <4fg, a smaller footprint and the system is upgradeable to the 6495 and is designed for Food Testing, Environmental Analysis, Drug Development and Clinical Research.

The latest addition to Agilent's industry-leading ICP-MS portfolio, the **7800 ICP-MS** provides a wide dynamic range, exceptional matrix-tolerance, and superior interference removal, together with optimisation tools and documentation to simplify method development and operation.

The new features and automation tools enables fast implementation, easy method setup, and simpler routine operation for many common sample types and applications, with Agilent offering industry-specific application packages to help users fast-track routine analyses.

Packages available now include those for drinking water, environmental waste and pharmaceutical applications. Packages for food testing and other applications will be available soon. The packages include standard operating procedures, method-specific batch templates and predefined report layouts.

Bruker Introductions at ASMS 2015:

A Comprehensive Mycobacteria Library 3.0 for High-Performance MALDI Biotyper Mycobacteria Identification. The new *Mycobacteria Library 3.0* now includes 149 different species for comprehensive species coverage, enabling significantly improved rapid and accurate identification of almost all described mycobacteria species. Intra-species diversity is covered by hundreds of analysed strains. Twenty-four laboratories from nine countries from all over the world provided well-characterised clinical mycobacteria strains, completing an already comprehensive set of isolates from strain collections. A recently published research study has shown that out of 1,045 mycobacteria samples, 94% could be identified on the species level with high confidence, and another 4.5% could be identified with lower confidence [1], using *Mycobacteria* Library 3.0.

The genus *Mycobacterium* includes, as major groups, the important pathogens of the *Mycobacterium tuberculosis* complex (MTC) and the non-tuberculous mycobacteria (NTM). Members of the latter group are increasingly the cause of opportunistic infections among immuno-compromised patients. This trend and the rise of antibiotic resistance in this genus require improved differentiation of mycobacteria species.

MALDI Tissuetyper™ Solution with new high speed rapifleX™ MALDI-TOF MS System for Anatomical Pathology Research

The introduction of the revolutionary rapifleX as the new instrument platform for MALDI imaging anatomical pathology eliminates many previous bottlenecks in mass spectrometry imaging (MSI), with much improved speed, throughput, ease-of-use, robustness and spatial resolution. At the same time, MSI maintenance efforts are reduced to a minimum by a streamlined design of the ion source for maximum uptime and optimised accessibility.

The MALDI Tissuetyper solution works up to 20 times faster than traditional MALDI-TOF systems, using Bruker's proprietary smartbeam™ 3D laser. The new scanning smartbeam 3D laser provides a fast moving laser-beam that is synchronised with the movement of the MALDI target stage. In combination with the laser repetition rate of 10 kHz, this architecture allows for real high throughput where MALDI imaging researchers have dramatically increased flexibility in pixel size or target tissue size. Depending on the sample size, typical tissue sections can now be imaged in approximately 30 minutes. Mass spectrometry images from small tissue biopsies are available within a few minutes.

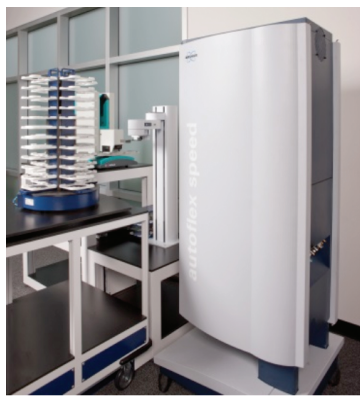

Figure 3. MALDI PharmaPulse.

Tissue typing of protein signature distributions continues to be one of the most powerful techniques available in areas such as anatomical pathology or biomarker research. Current research results indicate potential future clinical pathology applications in tumour staging, supporting therapy decisions or disease prognosis. The ***MALDI Tissuetyper*** offers exclusive statistical analysis software and bioinformatics tools for data mining, as well as visualisation of two-dimensional and even three-dimensional imaging datasets from multiple tissue sections.

The new ***MALDI PharmaPulse*** solution (*Figure 3*) is the latest addition to Bruker's portfolio of products designed to assist pharmaceutical, biotech and CRO customers accelerate drug discovery and development.

The features of the MALDI PharmaPulse solution include: less than 1 second per sample analysis time, comparable to the pulse of the human heart; autoflex speed MALDI TOF equipped with proprietary 2 kHz smartbeam™-II laser; integrated automation solution from HighRes Biosolutions seamlessly prepares and feeds MALDI plates from 96, 384 or 1536 assay plates; MALDI-detection removes the need for SPE cartridges or LC columns and uses 100x less solvent per sample than conventional LC-MS methods; does not require derivatisation in comparison to fluorescence workflows; development times for new assays and complexity is dramatically reduced without the need for chromatographic method development, SPE or MRM setup, or derivatisation protocols; the extremely low sample volumes required for detection (typically ~1 L) enables 'Single Well Kinetic Readout' by sampling multiple time points per assay; the full automation, coupled with speed of MALDI TOF, enables the screening of over 50.000 compounds per day.

Sciex

Figure 4. Sciex BioBA Solution.

The new Sciex BioBA Solution provides a comprehensive collection of components that are necessary for generating robust, reproducible and sensitive bioanalytical data, and is designed to turn the complexities of biologics bioanalysis into a simple process for expert and non-expert bioanalytical scientists. The BioBA solution is comprised of sample preparation kits for biologics quantification, a fully automated Biomek® liquid handler from Beckman Coulter, a robust LC (ExionLC™) with outstanding resolution and a sensitive Sciex triple quadrupole MS, and a set of iMethod™ applications that make implementation simple.

Lipidizer™ Platform is a new lipidomics solution that enables scientists to rapidly identify and quantify over one thousand lipid molecular species and is expected to play a role in researching diseases including cardiovascular disease, diabetes and neurodegenerative disorders. Built on Sciex technology, and powered by Metabolon know-how, the Lipidyzer Platform includes newly developed sample preparation kits, Sciex separations technologies and mass spectrometry, software, and data analysis services powered by one of the global leaders in metabolomics, Metabolon®.

OneOmics™ Project – Announced as a beta program by Sciex last year, brings together SWATH®-based proteomics (NGP) and the Illumina next-generation sequencing (NGS) tools in a cloud computing environment. A commercial version of the Sciex applications for BaseSpace® is also now available. At ASMS 2015, Illumina and Sciex officially launched the project and hosted a workshop on "Next- Generation Omics in the Cloud: the OneOmics™ Project in BaseSpace".

Shimadzu Scientific Instruments introduced the following products at ASMS 2015:

The **LCMS-8060** includes a stronger vacuum system and a redesigned UF-Qarray ion optical system, for high levels of sensitivity in both MRM and scan modes. The instrument's redesigned UF-Qarray features highly effective ion focusing capabilities. This technology helps reduce electrode contamination that can lead to poor instrument performance. Because the instrument stays clean and free of contaminants, the LCMS-8060 can provide highly reliable data even for long, continuous analysis of potentially contaminated items like biological and food samples.

As part of the UFMS series, the LCMS-8060 incorporates a number of Ultra Fast Technologies to enable high levels of analytical throughput. These technologies provide for a scan speed of 30,000 u/sec while maintaining mass accuracy and multiple reaction monitoring (MRM) speeds of 555 ch/sec. A polarity switching speed of 5 msec. ensures highly reproducible data and provides sufficient data points for the narrowest peaks. These features allow high-speed acquisition of both quantitative and qualitative data in a single run.

The new **ATHAP MALDI Matrix Kits** are designed to improve the detection of hydrophobic proteins or peptides containing transmembrane domains. Membrane proteins containing hydrophobic regions have been traditionally difficult to analyse by LC-MS/MS or MALDI-TOF MS. Alkylated trihydroxyacetophenone (ATHAP) has demonstrated superior detection capabilities over conventional MALDI matrices for such proteins/peptides.

They also expanded the range of Noviplex™ cards with the introduction of **Noviplex™ Duo Plasma Prep Card** for preparing two plasma samples from a single application of blood. Like the original Noviplex Card, the Duo prepares a blood sample anytime and anywhere without the need for a power source. The technology is ideal for use with LC-MS/MS analysis.

Thermo Fisher Scientific

Thermo celebrated 10 years of scientific research and discoveries based on its Orbitrap mass spectrometry technology. Orbitrap technology continues to spawn new product innovations, enabling customers in research and applied markets to advance scientific discovery and improve laboratory productivity.

The Orbitrap celebration and innovative new technologies were among the product launches at this year's ASMS that included:

The new **Thermo Scientific Orbitrap Fusion Lumos Tribrid Mass Spectrometer** (*Figure 5*), the newest addition to the line of Orbitrap Tribrid mass spectrometers. Designed to expand researchers' capabilities in advanced proteomics and metabolomics applications, including targeted, data-independent acquisition (DIA) and top-down analyses, the Orbitrap Fusion Lumos Tribrid has high sensitivity, delivers complete protein sequence coverage and allows scientists to perform more inclusive analyses.

Also making its appearance at ASMS was the **Thermo Scientific Q Exactive GC-MS/MS**, the industry's first instrument to integrate high-resolution gas chromatography (GC) and high-resolution accurate-mass (HRAM) Orbitrap mass spectrometry (MS). This new-generation system provides pharmaceutical, metabolomics, anti-doping and food safety laboratories with improved levels of productivity by combining the highest level of targeted and non-targeted detection and identification capabilities to GC-MS applications.

Figure 5. Thermo Scientific Orbitrap Fusion Lumos Tribrid Mass Spectrometer.

Thermo Fisher also introduced the **Thermo Scientific Pesticides Explorer** Collection, a set of LC-MS solutions specifically tailored to fit the needs of laboratories performing routine quantitation, targeted screening and non-targeted analysis of pesticide residues in food matrices.

The new **Thermo Scientific Xcalibur 4.0** software is a unified platform for acquisition and analysis of MS data. The easy-to-use software creates a convenient and organised launch platform for new or previously installed Thermo Scientific software. It also provides direct access to the **Xcalibur Apps Store**, easy software updates and links to the mzCloud™, **Thermo Fisher Cloud** and **Planet Orbitrap** to access spectral libraries and new MS data.

Rounding out Thermo Fishers' ASMS highlights were:

Thermo Fisher announced that New Objective's **PicoChip**™ technology is now available on select Thermo Fisher mass spectrometry platforms, broadening the low-flow separation options available to proteomics, pharmaceutical and other researchers.

Thermo Scientific SMART Digest kit, a new tool for protein digestion substantially reducing preparation times and associated errors for biopharmaceutical and protein research applications;

Thermo Scientific Vanquish UHPLC, offering improved performance in sample separation, throughput and ease-of-use for applications ranging from pharmaceutical QA/QC to food safety testing; and

Fisher Chemical UHPLC-MS Optima solvents designed to address the trace analysis needs of chromatographers performing state-of-the-art UHPLC.

Waters Corporation unveiled:

The new Waters® Vion IMS QTof Mass Spectrometer, a new bench-top tandem mass spectrometer featuring ion mobility and REIMS Research System with iKnife Sampling, combining direct-from-sample ionisation with high-performance time-of-flight (ToF) mass spectrometry.

Waters also expanded its family of solid phase extraction products with the first-of-its-kind Oasis PRiME HLB and added to its portfolio of protein separation columns with the ACQUITY UPLC® Glycoprotein BEH Amide Column for glycan analysis.

Vion IMS QTof Mass Spectrometer

Combining the benefits of high-resolution tandem mass spectrometry and ion mobility separation in a bench top instrument, the Waters® Vion IMS QTof Mass Spectrometer (*Figure 6*) brings clarity and confidence to routine analyses. Ion mobility removes spectral interferences and generates collision cross-section (CCS) values for every ion, giving scientists more information than they can get from traditional LC-MS experiments. Waters intends to commence shipments of the Vion IMS QTof Mass Spectrometer in the second half of this year.

Figure 6. Waters® Vion IMS QTof Mass Spectrometer.

The **UNIFI® Scientific Information System, Version 1.8**, is a new release of the software with features intended to enhance laboratory productivity. Today's announcement coincides with the introduction of the Vion™ IMS QTof Mass Spectrometer that is the first Waters mass spectrometer to be fully supported on UNIFI. New features of this release of UNIFI software include support of the Vion IMS QTof MS System; native atmospheric pressure gas chromatography (APGC) control, time-of-flight (Tof) multiple reaction monitoring (MRM) support, support of collision cross section (CCS) data, and Tof quantitative and qualitative workflows providing a comprehensive, single software solution.

Combining direct-from-sample ionisation with high performance time-of-flight mass spectrometry and powerful, intuitive analytics, the **Rapid Evaporative Ionisation Mass Spectrometry™ (REIMS™) Research System with iKnife™** Sampling System eliminates the need for sample preparation and chromatographic separation, providing food, microbiology and tissue researchers with near-instantaneous data acquisition.

In REIMS, direct, rapid heating of the samples leads to the formation of vapour that is rich in sample-specific chemical information. The vapour is taken directly into the mass spectrometer (Xevo® G2-XS QTof or SYNAPT® G2-Si HDMS) where the molecules are analysed by time-of-flight mass spectrometry. Using this technology researchers can quickly and easily differentiate samples from one another and confidently identify the differentiating features, allowing greater insight into the chemical and biological systems under investigation.

Waters also announced the new **ACQUITY UPLC® Glycoprotein BEH Amide 300Å 1.7-µm Column** that enables biopharmaceutical companies to better understand where glycan molecules are located within the therapeutic proteins they are developing. Identifying the precise location of glycans within a protein structure is essential to delivering safe and effective biotherapeutic proteins.

Future ASMS Dates:

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

64th ASMS Conference, 5 – 9 June, 2016, San Antonio, TX

65th ASMS Conference, 4 – 8 June, 2017, Indianapolis, IN

66th ASMS Conference, 3 – 7 June, 2018, San Diego, CA

67th ASMS Conference, 2 – 6 June, 2019, Atlanta, GA