

Mass Spectrometry & Spectroscopy

65th ASMS Conference on Mass Spectrometry and Allied Topics held in Indianapolis from 4th - 8th June 2017 at the Indiana Convention Center, Indianapolis, Indiana USA.

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A very warm and pleasant Indianapolis, Indiana, the home of the Indianapolis 500 and Brickyard 400 automobile races held annually at the Indianapolis Motor Speedway in Indianapolis, was the venue for the 65th ASMS Conference. Returning to Indianapolis after a 10-year hiatus the meeting returned to basics with the hospitality suites, first introduced in Indianapolis, losing the flair and razzmatazz of recent meetings and following the original guiding principles, where attendees could interact and learn more about Corporate Member products and services while enjoying fun, food, drink and conversation.

The conference started early for many enthusiastic attendees; with one-and two-day short courses beginning on Saturday and Sunday 3rd and 4th of June from 9:00am to 4:30pm, and later on Sunday, a new feature for this year's conference were four tutorial lectures held in two parallel sessions starting at 5 pm. In one parallel pathway, Kermit K. Murray of Louisiana State University (Baton Rouge, Louisiana) presented 'MALDI: Past and Future', and Donald F. Hunt of the University of Virginia (Charlottesville, Virginia) presented 'Cancer Immunotherapy and Mass Spectrometry'. In the other pathway, Erin S. Baker of the Pacific Northwest National Laboratory (Richland, Washington) gave a talk titled 'Ion Mobility Spectrometry: Analyzing Molecules as They Tumble through Life', and Norman J. Dovichi of the University of Notre Dame (South Bend, Indiana) presented 'CE/MS—Ready for Prime Time?'

The brief opening ceremony was followed by a very interesting lecture entitled 'Towards a Good Start in Life: Neonatal Screening and Beyond' by David S. Millington from Duke University Medical Center.

David graduated with both a BSc and PhD from Liverpool University, UK in organic chemistry where he became involved in Mass Spectrometry when he answered his own question 'how can I avoid bench chemistry and obtain a PhD'. His work, the basis for his lecture, quickly shifted to newborn screening. Newborn screening has revolutionised the diagnosis of many disorders, notably metabolic disorders such as Phenylketonuria, or PKU as it is more familiarly known. This disease was first recognised in the 1920's with a dietary treatment proposed in the 1930's however it was not until the 1950's that this dietary treatment was actually available. The 'Guthrie Test' a heel prick of newborns became the standard test and David explained how he was instrumental in getting tandem mass spectrometry included in newborn screening. Today the testing is routine by MS/MS with millions of new babies screened in the USA alone annually for a total of 34 core disorders and many secondary disorders.

This was followed by the Opening Reception, located in the poster-exhibit hall, an opportunity to eat, drink and meet up with exhibitors, colleagues and friends. Heavy hors d'oeuvres (enough for dinner!), free 'Hinchtown Hammerdown' Pilsner from Flat 12 Bierwerks and 'Osirus' Pale Ale beers from Sun King Brewery both brewed in Indianapolis and a cash bar for wine were all available. Technical posters were not posted until Monday morning at 10:30.

Monday saw ASMS start for the early risers with breakfast seminars, hosted by the corporate members, starting at 7:00 and the oral presentations, exhibition and posters starting in earnest at 08:30 with a total of 384 oral presentations running in 8 parallel sessions of the scientific programme over the four days (32 sessions daily running concurrently) and culminating in the closing plenary lecture – 'Saving the Great Coral Reefs' presented by Kristen Marhaver from Research Station Carmabi a marine biologist who studies the reproduction of threatened Caribbean corals. Her work combines new and old technologies to help juvenile coral survive their earliest life stages. Marhaver was the first person to successfully rear juveniles of the endangered Caribbean Pillar Coral.

This year there was a much more manageable 2889 posters (compared to 2982 in 2016 and 3141 in 2015) displayed during the week covering topics from ambient ionisation and antibody & antibody drug conjugates (Intact and characterisation) to imaging MS for disease markers 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 talked out by 17:00 then there were 15 Workshops running daily Monday to Wednesday from 17:45 to 19:00 leaving just one hour for dinner before the Corporate Hospitality suites swung into action at 20:00; providing endless finger foods, snacks, refreshments and conversation - all lasting until 22:30.

Attendance was up slightly (1%), compared to the ASMS 2016 conference, at 6338 (see Table 1 for recent history) with attendees from the USA, Canada and 28% from overseas visitors where UK, Australia and Asia were there in force. There were 200 (188 in 2016) exhibit booths.

Table 1. ASMS attendance by year.

Year	Location	Total Attendees
2012	Vancouver	6,277
2013	Minneapolis	6,140
2014	Baltimore	6,913
2015	St. Louis	6,100
2016	San Antonio	6,276
2017	Indianapolis	6,338

ASMS Awards

2016 Award for a Distinguished Contribution in Mass Spectrometry

The 2017 ASMS Award for a Distinguished Contribution in Mass Spectrometry was awarded to **Dr Catherine E. Costello** a William Fairfield Warren Distinguished Professor from the Department of Biochemistry, Cell Biology & Genomics, Department of Physiology & Biophysics, and Department of Chemistry, Boston University, Boston, MA, for her contributions to the development of tandem mass spectrometry of glycans and glyco-conjugates.

Glycans differ from proteins in that their biosynthesis is from a series of enzymatic not from a template-driven process. Glycans, depending on class, may be branched, meaning that their structural determination requires determination of linkage positions and stereochemistry. The function of a glycan depends on the target to which it binds. A difference in a single monosaccharide linkage in a glycan alters the partners to which a glycan or glycol-conjugate binds. The complexity of glycan and glycol-conjugate structures in glycomics results in a serious analytical challenge.

Professor Costello's research has revolutionised glycomics by enabling comprehensive structural characterisation of free glycans and glycoconjugates quickly and at high sensitivity.

Biemann Medal

Dr Ryan Julian, a professor in the Department of Chemistry at the University of California, Riverside, was awarded the 2017 Biemann Medal for his contributions in developing and examining photo-initiated gas phase radical ion chemistry to elucidate peptide and protein structures. Several applications employing this chemistry have been developed by Ryan's lab e.g. (a) examining 3D protein structure in the gas phase, (b) identification of Cys residues and disulphide pairs, (c) identification of peptide epimers, (d) characterisation of oligosaccharide, and (e) monitoring energy transfer with UV action spectra.

Professor Julian has developed bond selective chemistry for initiating controllable radical directed dissociation (RDD) which is performed by photoexcitation with UV photons, leading to homolytic dissociation of specific bonds and the generation of a radical species. Ryan's lab has demonstrated that this chemistry can be used to create radicals in various types of biomolecules via dissociation of carbon-iodine, carbon-sulphur, and sulphur-sulphur bonds associated with numerous chromophores, regardless of molecular size, charge state, charge polarity, or sequence.

Ron A. Hites Award Outstanding Research Publication in JASMS

The Ron Hites Award, which included \$2,000 and a certificate for each author, is awarded to a scientist for an original outstanding research publication, based on its novelty, technical and presentation quality, potential stimulation of future research and the impact on other future applications.

The 2017 Award was presented to **Thomas Rizzo** from the École Polytechnique Fédérale de Lausanne and his co-authors for their paper entitled 'Infrared Spectroscopy of Mobility-Selected H⁺-Gly-Pro-Gly-Gly (GPGG)' by Antoine Masson¹, Michael Z. Kamrath¹, Marta A. S. Perez¹, Matthew S. Glover², U. Röthlisberger¹, David E. Clemmer² and Thomas R. Rizzo¹;

¹École Polytechnique Fédérale de Lausanne, ²Indiana University; JASMS Vol. 26, Sept 2015, pp. 1444-1454

New Product Roundup

In the interests of impartiality companies introducing new instruments and products are again listed in alphabetical order, we have attempted to feature the majority of new product introductions for 2017.

Agilent Technologies

Announced the results of a recently commissioned global survey which "will help the company continue to focus more intently on the needs of its customers around the world". The Frost & Sullivan independent survey - Understanding Key Challenges and Pain Points in the Global Laboratory Market was conducted on Agilent's behalf. The primary objective of the survey, which included 700 laboratory employees covering five market segments in four countries, was to understand key customer concerns.

Lab managers were asked to rank their top five challenges which included instrument maintenance and downtime (73%), instrument testing requirements (63%), sample preparation (60%), changing regulations (52%) and better data management (50%). 45% of lab managers reported that they face increasing pressure to process more samples per week.

The survey also showed that one in five of lab managers (18%) consider lab size to be affecting their lab's performance with 75% of them reporting that space-saving designs of instruments could help.

Agilent announced the launch of the **Agilent Ultivo Triple Quadrupole LC/MS system** a new triple quadrupole liquid chromatography mass spectrometers (triple quad LC/MS). The Ultivo is optimised for the food and environmental routine testing segments that employ triple quad LC/MS systems for quantitative analyses featuring robust performance, intelligent diagnostics for superior uptime, and a new VacShield vacuum provides vent-less ion injector exchange resulting in easier serviceability, in a 70% smaller footprint.

Also introduced was the **Agilent 7250 GC/Q-TOF** system which combines gas chromatography and quadrupole time-of-flight mass spectrometry with a Low Energy Electron Ionization source that enables greater exploration of unknown chemical samples. The new system combines a high-resolution, accurate-mass GC/MS with a low-energy ionisation source, permitting analyses that were not previously practical or possible.

In addition, Agilent introduced updates to several software tools:

A full workflow solution for biopharma featuring the recently released AdvanceBio 6545XT LC/Q-TOF LC/MS with BioConfirm B.09, the AdvanceBio Peptide Plus LC column for peptide separations, and new applications in AssayMAP automated sample prep.

- **MassHunter BioConfirm B.09 Software** now available as a reportedly "no MS expertise required" version.
- **Quant-my-way** where the administrator now tailors the feature set to each method and all operators - **even novices** - experience faster, easier and error-free analysis, review and reporting

Bruker

The main focus of ASMS in 2017 for Bruker was software and solutions however some hardware was introduced.

Software for MALDI Imaging

The new **SCiLS Cloud software** offers web-based tools to facilitate distributed workflows, where data and analysis results can be shared, viewed and manipulated with a web browser through secure access. **SCiLS Lab** provides advanced and user-friendly solutions for data handling, visualisation and computational analysis for both Bruker MALDI imaging and other non-Bruker mass spectrometers.

Software for Metabolomics and Proteoform Profiling

Bruker introduced **MetaboScape® 3.0**, for discovery metabolomics, with support for direct-injection (DI) or MALDI Magnetic Resonance Mass Spectrometry (MRMS) a new algorithm called Time-aligned-Region-complete-eXtraction (**T-ReX**), which automatically extracts all relevant information in a "region complete" manner. Included in **MetaboScape 3.0** are workflows for chromatography-free DI-MRMS or MALDI-MRMS data.



Figure 1. Agilent Ultivo Triple Quadrupole LC/MS system.

Proteoform Profiling™ 1.0 solution enables the systematic, large-scale, label-free study of all expressed proteoforms.

Bruker also released the new **nanoElute®** nano-flow UHPLC system, together with the new **Proteoform Profiling™ 1.0** solution.

Both innovations take advantage of the impact II and ETD-enabled **maXis II** UHR-QTOF's. The **Proteoform Profiling 1.0** workflow automates the use of **Dissect™** and **SNAP™** algorithms.

Applied Toxicology and Forensics

Bruker announced the release of **TargetScreener 3.0HR** (high-resolution), which includes **TASQ™ 1.4** (Target Analysis for Screening and Quantitation) software for automated **screening** and **quantitative** applications in forensic, food and environmental safety markets. Bruker also launched **ToxTyper 2.0E** for routine, high-throughput forensic toxicology and integrates the new Elute UHPLC systems.

The new **timsTOF** is a flexible, research-grade instrument for the separation and analysis of unresolved compounds and conformations. The Ion Mobility Expansion (imeXTM) TIMS technology can be adjusted for research or analytical needs and has an Open Data Format that supports user-created software tools tailored to specific research questions.

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

The New Bruker **rapifleX™**, claimed to be the highest performance MALDI-TOF/TOF mass spectrometer, is an advanced TOF/TOF system, and was re-designed from the ground up to meet the demands for in-depth intact and top-down protein characterisation, and high-performance, high-throughput mass spectrometry imaging (MSI).

Bruker also announced the launch of the **rapifleX™ MALDI PharmaPulse™ (MPP)** designed to assist pharmaceutical, biotech and CRO customers to accelerate drug discovery.

The new **Bruker HDX Solution** provides a complete workflow combining the LEAP H/D-X PAL autosampler with pre-defined labelling experiments, a UHPLC system, the maXis II ETD UHR-QTOF mass spectrometer, plus the Sierra Analytics HDEaminer HDX-MS interpretation software.

Software updates were also released, and included:

PesticideScreener™ 2.1 a database of over 800 pesticides and a pre-defined UHPLC methods and workflow.

ToxScreener™ 2.1 designed to allow forensic toxicology labs to easily screen, identify and quantify hundreds of low level drugs of abuse or poisons in various complex samples.

Sciex

Sciex released new mass spectrometry solutions in launching their theme of 'It's Time to see the future differently'.

They highlighted the first and **only FDA-cleared (via the de novo pathway) LC-MS based Vitamin D assay kit, the Vitamin D 200M Assay, exclusively for the Sciex Topaz™ System. The Topaz System** is a fully integrated LC-MS platform driven by ClearCore™ MD, a new software designed specifically for use in clinical labs.

Other solutions featured by Sciex were:

5 Years of SWATH with expanded applications

SWATH® Acquisition launched 5 years ago, now includes the ability to optimise acquisition with variable sized Q1 windows and microflow for sample throughput increasing in the number of proteins and peptides quantified. SWATH is now reportedly used in metabolomics, forensics, food testing, environmental analysis, and biologics characterisation.

Biotransformation solutions

The Routine Biotransform Solution and the Advanced Biotransformation Solution are powered by the new Sciex MetabolitePilot™ Software 2.0, with an easy to use interface that shows processing, interpretation and reporting all in one place.

Shimadzu Corporation

Shimadzu Corporation Introduced the following new products at ASMS 2017.

A preview the **MALDI-8020** Shimadzu's return to benchtop matrix assisted laser desorption ionisation time of flight mass spectrometry (MALDI-TOF MS). The MALDI-8020 reportedly achieves performance specifications similar to those of larger, more expensive MALDI-TOF models but in a significantly smaller footprint. The MALDI-8020 is designed to improve laboratory efficiency and analysis via a new designed 'load-lock system' for fast sample introduction and a solid-state laser for faster data acquisition speeds. Linear time of flight enables low-level detection of proteins, peptides and polymers. It also has an integrated barcode scanner for a seamless and TrueClean™ automated UV laser source cleaning and a new ion optic design for improved robustness and better up-time.



Figure 2. Bruker nanoElute® nano-flow UHPLC system



Figure 3. Shimadzu MALDI 8020

Shimadzu also featured the **nSMOL (nano-surface and molecular orientation limited proteolysis)** Antibody Bio-Analysis Kit a ready-to-use reagent kit for collecting monoclonal antibodies from blood or other biological samples using immunoglobulin collection resin, and then performing selective proteolysis of the Fab region of these antibodies via trypsin-immobilised nanoparticles and subsequent quantification via MRM measurements. The simplified workflow eliminates the steps of denaturing, reduction, and alkylation normally associated with protein digestion.

Shimadzu and Phytronix, announced an agreement at ASMS to offer the industry's first Triple Ion Source. Ideal for both screening and confirmation work, this new high-speed platform will significantly improve productivity in high-throughput laboratories performing toxicology, drug discovery and food safety applications.

Shimadzu announced they have recently celebrated three anniversaries:

Shimadzu Celebrates 20+ Years Manufacturing in the USA.

Shimadzu Celebrates 60th Anniversary of Manufacturing GC Instruments

Shimadzu Celebrates 60th IR Anniversary GCMS-TQ8050 triple quadrupole gas chromatograph mass spectrometer.

Thermo Fisher Scientific

Celebrating '50 years of MS Innovation' Thermo Fisher Scientific headlined with the new **TSQ Altis** Triple Stage Quadrupole mass spectrometer and **TSQ Quantis** Triple Stage Quadrupole mass spectrometers designed to deliver reproducible, reliable results, even by less experienced users.

- TSQ Altis offers sensitivity, selectivity and speed while providing the analytical flexibility and reproducibility for demanding applications.
- TSQ Quantis mass spectrometer is designed to be a quantitative workhorse.

Accelerating Proteomics Research

Also launched was the Thermo Scientific **Q Exactive HF-X** Quadrupole Orbitrap mass spectrometer designed for sensitivity and reproducibility in the analysis of complex biological samples.

The Q Exactive HF-X is available with new consumables and software that enable researchers to customise workflows and identify thousands of proteins of interest in a single run.



Figure 4. Thermo Scientific Q Exactive HF-X

Breaking New Ground in Tribrid Mass Spectrometry

New options for the Orbitrap Fusion Lumos mass spectrometer include a new, integrated Ultraviolet Photodissociation (UVPD) feature that is designed to improve productivity and provide accurate structural information and is standard on new systems and available as an upgrade to existing Fusion Lumos instruments.

Other options announced include Advanced Peak Determination (APD) and 1M resolution.



Figure 5. Thermo Scientific Orbitrap Fusion Lumos

Custom Kits and New Software

Thermo Fisher also announced an agreement with Biocrates Life Sciences AG, to offer the Biocrates AbsoluteIDQ p400 Kit enabling researchers to reduce the complexity of metabolomics by enabling the rapid and reliable characterisation of small molecules.

The new, ready-to-use Thermo Scientific InsuQuant Mass Spectrometric Kit designed to simplify sample preparation during insulin bioanalysis.

In addition to previewing new versions of software, including ProteinCenter 4.0, TraceFinder 5.0 and Biopharma Finder 3.0, Thermo Fisher also introduced updated versions of its Proteome Discoverer 2.1 and Compound Discoverer 2.1 software.

In addition to the new products above being released at ASMS, ThermoFisher also reviewed their new software releases and cloud based applications.

Waters Corporation

Waters introduced the new **LiveID™ Software** for near-instantaneous, direct-from-sample measurement and classification of food products including meat and crops by Waters' quadrupole, time-of-flight (QToF) mass spectrometers. The new software enables Waters® Xevo® G2-XS QToF or SYNAPT® G2-Si Mass Spectrometers equipped with an iKnife™ Sampling device, Rapid Evaporative Ionization Mass Spectrometry (REIMS™) ion source and MassLynx® Mass Spectrometry Software to help laboratories detect food fraud. Waters LiveID Software is available now on a worldwide basis.

Also introduced were 'next generation columns for nano- and microflow UPLC/MS applications'. The **Waters® nanoEase™ M/Z columns** are packed with sub-2-particles and are specifically tested for protein and peptide analysis and are available in several pore sizes and with several bonded phases including BEH C18, CSH C18, HSS T3 or Symmetry C18 (trap column only). The columns are simple to install, reduce connection variability and deliver high efficiency and selectivity utilising ZenFit™ Connection Technology.

Also unveiled were further upgrades and options for the **Progenesis® QI for proteomics software**. This latest version is designed with support for all common vendor data formats and a guided workflow to keep Progenesis QI for proteomics compatible with current MS approaches, while also increasing flexibility and usability.

- **Spectral library searching** - interfacing with 14 different search engines now with the functionality of spectral library searching.
- **SONAR Support** - a recently introduced data independent acquisition (DIA) mode for Waters High Resolution Mass Spectrometry (HRMS) instruments. Data from SONAR can now be analysed in Progenesis QI for proteomics. "Stop looking and start seeing"
- **Automatic thresholding** for data independent acquisition: It is now possible to utilise automatic peak detection thresholding for MSe, HDMSe and SONAR data.
- Progenesis QI for proteomics now supports mzIdentML export for Mascot and Ion Accounting searches, as developed by the Proteome Xchange Consortium for public sharing of data sets.
- Progenesis QI for proteomics now seamlessly integrates with the Proteolabels software, developed by Omic Analytics.
- **Symphony connectivity** - Users can now initiate a Progenesis QI for proteomics experiment within the Symphony™ data pipeline.

Waters Corporation and Andrew Alliance have reportedly signed an agreement that will bring drug development scientists an easy-to-use, semi-automated sample preparation approach for released N-glycan profiling and analysis by LC and LC-MS. Under the co-marketing agreement, Waters will combine its existing Glycoworks® RapiFluor-MS® N-Glycan Kit with an Andrew pipetting robot permitting laboratories expanded glycan profiling capacity with improved accuracy and precision of LC and LC-MS results.

Also announced was a collaborative engagement with **IonSense** (Saugus, Mass.) to interface

the compact Waters® ACQUITY® QDa® Mass Detector with the **IonSense® DART®** ionisation source. The combination will enable the rapid generation of mass data directly from liquid or solid samples with little or no sample preparation.

ASMS Closing

Thursday's closing event was held at the Indiana State Museum a short walk from the convention center and included a buffet dinner, an IMAX show on the coral reefs that followed on well from the closing plenary session by Kristen Marhaver from the Research Station Carmabi entitled 'Saving the great coral reefs'.

Future ASMS Dates

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

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

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

68th ASMS Conference, June 14 - 18, 2020, Denver, CO

69th ASMS Conference, June 6 - 10, 2021, Philadelphia, PA



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