66th ASMS Conference on Mass Spectrometry and Allied Topics held in San Diego from 3rd to 7th June 2018 at the San Diego Convention Center, San Diego, California USA.

Trevor Hopkins, International Labmate Contributing Editor for Chromatography and Spectroscopy.

A very tropical San Diego, California, which provided splendid weather without the normal 'Gloom in June' that is typical for the area, was the venue for the 66th ASMS Conference.

The meeting continued the back to basics concept for the corporate hospitality suites where attendees were encouraged to learn more about Corporate Member products and services while having fun, food, drink and conversation.

Young scientists were featured prominently in the ASMS programme with an Undergraduate Students and First Time (at ASMS) Graduate Students meeting on Sunday from 4:00 - 4:45 pm which covered 'Plan Your Strategy: What to See and Do at ASMS'; and a Special Program for Undergraduate Students with a Sunday, 7:30 - 9:00 pm, Poster competition in the, Exhibit Hall and a Monday, 11:30 am - 1:00 pm, 'Meet the Experts' session with free lunch, where lunch tables were reserved for undergraduate students in the Exhibit Hall.

The conference started early for many enthusiastic attendees; with one-and two-day short courses beginning on Saturday 2nd and Sunday 3rd of June from 9:00 am to 4:30 pm later on Sunday, the four tutorial lectures, started in 2017, were held in two parallel session's starting at 5 pm. In one parallel pathway, M. Arthur Moseley of Duke University School of Medicine presented 'Strategies for Quantitative Proteomics' and Susan D. Richardson from the University of South Carolina presented 'Mass Spectrometry and the Environment'. In the other pathway, Gregory Eiden from the Pacific Northwest National Laboratory discussed, 'Mass Spectrometry and Nuclear Forensics' and Jack Beauchamp of the California Institute of Technology presented 'From the Laboratory to the Stars'.

The brief opening ceremony was followed by a very interesting lecture entitled 'Smart Trials: Moving from Site-centric to Patient-centric Clinical Trials' by Lisa Shipley from the Pharmacokinetics, Pharmacodynamics and Drug Metabolism department of Merck Pharmaceuticals.

Lisa graduated with both a BA in Biology form McDaniel College in 1981 followed by a PhD in Pharmacology and Toxicology in 1985. Her work in the pharmaceutical industry since 1988 as the VP of Drug disposition for Eli Lilly and currently the VP of Pharmacokinetics, Pharmacodynamics & Drug Metabolism, for Merck formed the basis for her lecture. Lisa described the current inefficient system, which has not seen significant change for 70 years, for performing clinical trials which cost the pharma industry $2.6 billion to get a drug approved by the regulators and how for every 10,000 drug candidates produce 1 successful drug over a 12-year period. She then followed by explaining the current 'gold standard', outlined the failings and then proposed a system for 'Smart trials' where smart dosing - using digitally tracked dosing - which Lisa described as 'like taking a selfie when taking the drug' - 8 of 19 major pharma companies are using smart dosing technologies, smart sampling for monitoring pharmacokinetics and biomarkers, smart analysis and finally smart analytics all designed to take the trial from a clinical site to the patient.

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 old friends. Hors d'oeuvres stations scattered through the poster-exhibit hall (enough for dinner!), free 'Stone IPA' and 'Karl Strauss Pilsner' both brewed locally in San Diego and a cash bar for wine were all available. Technical posters were not posted until Monday morning.

Monday saw ASMS start for the early risers with a choice of 11 breakfast seminars, hosted by the corporate members, starting at 7:00 am 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 – 'The Fight Against Doping: From Strychnine to Turinabol' presented by Larry Bower President of LD Bowers, LLC, Larry is renowned for his sports anti-doping efforts during his role as the Chief Science Officer of the US Anti-Doping Agency (USADA) and his professorships at the Universities of Indiana and Minnesota.

This year there was a whopping 3279 posters (compared to 2889 in 2017, 2982 in 2016 and 3141 in 2015) displayed during the week with a new approach for 2018 which allowed for a one-hour non-overlapping lunch break. All presenters were now scheduled for 3 hours with odd-number posters presented between 10:30 - 11:30 am plus 12:30 - 2:30 pm and even-number posters presented 10:30 am - 12:30 pm plus 1:30 - 2:30 pm with 'Poster Pick-Me-Up Snacks' being served at 1:30 pm. The poster topics covered ranged from instrumentation and imaging to native MS in biology and the fundamentals of Photoionisation and Photodissociation, 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 walked and 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 significantly (13%), compared to the ASMS 2017 conference, at 6338 (see Table 1 for recent history) with attendees from the 49 countries. There were 191 (200 in 2017) exhibit booths. This increase in participation is particularly significant since many West Coast US meetings see a reduced attendance and the XXII International Mass Spectrometry Conference (IMSC) is being held in Florence, Italy later this year.

Table 1. Historical Attendances

Year	Location	Total Attendees	Year	Location	Total Attendees
2012	Vancouver	6,277	2016	San Antonio	6,276
2013	Minneapolis	6,140	2017	Indianapolis	6,338
2014	Baltimore	6,913	2018	San Diego	7,147
2015	St. Louis	6,100			

ASMS Awards

2018 John B. Fenn Award for a Distinguished Contribution in Mass Spectrometry

The ASMS Award for a Distinguished Contribution in Mass Spectrometry was renamed to honour the memory of John B. Fenn, who shared the 2002 Nobel Prize for the development of electrospray Ionisation, and was an active member of ASMS from 1986 until his passing in 2010.

The 2018 John B. Fenn ASMS Award for a Distinguished Contribution in Mass Spectrometry was awarded to **Dr Gert von Helden, Dr Martin F. Jarrold,** and **Dr David E. Clemmer** for their pioneering contributions to the development of ion mobility spectrometry (IMS).

Dr von Helden, Group Leader at the Department of Molecular Physics, Fritz-Haber Institut der Max Planck-Gesellschaft, Berlin, Germany and Professor at the Radboud University, Nijmegen, the Netherlands, applied IMS it to the self-assembly of carbon in plasmas showing that carbon evolved from linear chains - to rings - to fullerenes structurally. To obtain collision cross sections and model structures he used quantum chemical approximation methods and adapted the projection approximation method which produced excellent agreement with his experimentally measured collision cross sections.

Dr Jarrold, Professor and Robert & Marjorie Mann Chair, Department of Chemistry, Indiana University, applied IMS methods to silicon and aluminium assembly, and along with Dr von Helden, showed that fullerenes are formed from the activation of carbon ring systems

and went on to develop the first high-resolution instrument and the trajectory method for obtaining collision cross-sections from complex structures such as biomolecules.

Dr Clemmer, Distinguished Professor, Department of Chemistry, Indiana University, utilised these new IMS methods for analytical applications and developed a new 'nested' IMS-MS technology, which employed ion trapping methods to dramatically increase signal-to-noise ratio and post-IMS dissociation to obtain fragmentation patterns of isomers (or conformers) in a single experiment. These ideas were later incorporated into highly successful commercial instruments.

Biemann Medal

Dr Benjamin A. Garcia the Presidential Professor of Biochemistry and Biophysics at the University of Pennsylvania, Perelman School of Medicine was awarded the 2018 Biemann Medal for his contributions to clarified the set of posttranslational modifications (PTMs) to histone proteins commonly known as the 'histone code'. The Garcia lab has developed a number of methods to detect novel histone PTMs, quantify their relative quantities, monitor in vivo histone PTM dynamics, and identify histone PTMs on specific genome locations.

Dr Garcia pioneering work in chromatin biology and epigenetics research, utilising both high-throughput 'bottom-up' proteomic methods for the detection of histone PTMs and the quantitative comparison of multiple cellular states, and 'middle down' proteomic approaches that facilitate computation of specific combinatorial histone proteoforms.

Ron A. Hites Award Outstanding Research Publication in JASMS

The Ron Hites Award, which includes $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 2018 Award was presented to **Peter B. Armentrout** from the University of Utah and his co-authors for their paper entitled **'How Hot are Your Ions Really? A Threshold Collision-Induced Dissociation Study of Substituted Benzylpyridinium "Thermometer" Ions'**; John E. Carpenter[1], Christopher P. McNary[1], April Furi[1], Andrew F. Sweeney[1], P. B. Armentrout[1]; 1.Department of Chemistry, University of Utah, Salt Lake City, UT; JASMS Vol. 28, Sept 2017, pp. 1876-1888, DOI 10.1007/s13361-017-1693-0

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 2018.

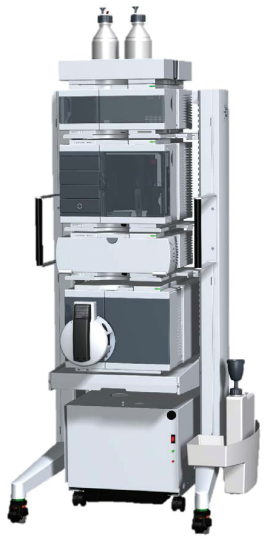

Figure 1. InfinityLab Flex Bench.

Agilent Technologies

After it's bumper year of Mass Spectrometry introductions including 6495B iFunnelLC/TQ, InfinityLabLC/MSD (SQ), 6545XT AdvanceBioLC/Q-TOF, 7250 GC/Q-TOF and the award winning Ultivo LC/TQ announced no new instruments this year at ASMS. Continuing to 'Make the pain points' go away for customers the Agilent theme of 'Innovation with Purpose' was unveiled with new applications for the Ultivo in the food, clinical research and environmental areas. One introduction was the InfinityLab Flex Bench a mobile cart system which permits easy laboratory reconfiguration.

Other areas of innovation highlighted were the 2017 Software introductions and updates which included:

- **MassHunter Quant B.09 Quant-My-Way** with a simplified user interface is easily customised to make workflows more productive
- **MassHunter Walkup C.03.01** with mass-based fraction collection and remote sample submission
- **MassHunter BioConfirm B.09** with intact protein analysis, peptide mapping, released glycan ID, PDF reporting providing bio pharma workflows that require zero MS expertise
- **SureMass** with increased dynamic range for GC/Q-TOF quantitation,
- **OpenLab2.3** with enriched mass information for chromatography -MS base peak m/z labelling and MS peak purity
- **MassHunter Profinder B.08.02** featuring improved data processing with retention time alignment

Bruker

The main introduction of ASMS in 2018 for Bruker was the new **scimaXTM Magnetic Resonance Mass Spectrometer (MRMS)**. The scimaX MRMS is reported to deliver industry-leading mass resolution exceeding twenty million (R > 20,000,000), with a smaller footprint and without the need for any liquid cryogens. Bruker's novel conduction-cooled Maxwell™ magnet technology essentially makes the magnet 'invisible' and allows the use of highest-performance MRMS in standard mass spectrometry laboratories.

This extreme MRMS resolution permits isotopic fine structure (IFS) analysis to easily determine exact elemental formulae in complex mixtures, without any chromatography. Using this unique capability, the scimaX enables the novel workflow of flow injection analysis (FIA-MRMS) for large cohort, high-throughput phenomics studies with up to 200 samples per day.

Figure 2. scimaX™ Magnetic Resonance Mass Spectrometer (MRMS).

Biopharma users can perform advanced native protein and fragment-based drug discovery studies using MRMS, which has recently been called a 'bona-fide' platform for native protein analysis in the scientific literature. With an optional MALDI source, pharma customers have demonstrated the exceptional capabilities of MRMS for label-free MS imaging for PK/PD studies in drug development.

Phenomics and Proteomics Innovations

Bruker's new ***timsTOF™ Pro*** for proteomics uses four dimensions (4D) of separation in this unique nLC-TIMS-MS/MS instrument. It combines proprietary, dual Trapped Ion Mobilitiy Spectrometry (TIMS) using the just published online PASEF method, which has the potential to dramatically improve high-throughput and ultra-high sensitivity proteomics. The ***timsTOF Pro***, has been further enhanced for ASMS, and is now also compatible with ***MaxQuant v1.6.2.0***, and ***PEAKS Studio v8.5*** for protein identification (ID), label-free quantitation (LFQ), and tandem mass tag (TMT) workflows. Rapid development by third-party software collaborators is enabled by Bruker's open file format, and several additional groups are developing timsTOF Pro compatibility into their software suites.

Also new for 2018 is full integration with the Evosep One (www.evosep.com) separation device with Bruker's Hystar LC/MS control for high-throughput clinical proteomics of up to 200 samples per day. This novel combination delivers superb sensitivity (50 ng HeLa) and high throughput for LFQ of ~1,200 proteins in only ~5 minutes.

Bruker also introduced at ASMS 2018 the ***spotON LC-MALDI*** spotter for automated, wizard-based workflows that include post-column matrix addition, supporting both nano and capillary HPLCs. The ***spotON LC-MALDI*** facilitates the use of the complementary MALDI technique in biopharma applications, such as for sequencing by non-conventional proteolytic enzymes, for the determination of disulphide bonds, for glycopeptide identification, for top-down sequencing of membrane proteins, and for the identification of protein clips through N-and C-terminal sequencing. The ***spotON*** has superior carry-over performance and includes an optional nitrogen mask for spotting in an inert environment.

Life Sciences and Translational Mass Spectrometry Imaging

Bruker also introduced ***SCiLS Lab***, version 2019, with the addition of a quantitation module for mass spectrometry imaging (MSI) workflows. MSI has the advantage of being both label-free and spatially resolving, in contrast to other established quantitative methods. In drug development and toxicology studies, ***SCiLS Lab***'s new user-friendly software workflows for MSI quantitation should enable researchers to easily quantify target molecules directly from tissue.

Software for Metabolomics and Proteoform Profiling

Bruker introduced **MetaboScape®** 4.0, powered by MRMS ***aXelerate™***, which incorporates a 3-tier confidence engine to allow confident assignment of molecular formulae. This new version supports handling large studies of > 1000 samples in phenomics research. Based on the unbeatable, across-the-mass range, ultrahigh resolution of the scimaX MRMS, the aXelerate workflow goes beyond LC throughput, complexity and robustness limitations to analyse approximately 200 samples a day.

The ***T-ReX 4D*** algorithm supports ***timsTOF*** by enabling processing of 4D TIMS-separated LC-MS/MS data and gives access to exact Collisional Cross Section (CCS) values. The extended Annotation Quality Scoring includes these values for higher confidence in compound ID, including a sophisticated machine learning algorithm, which calculates theoretical CCS of lipids and compares these to measured values for increased confidence in lipid identification.

Bruker also introduced a solution for non-targeted metabolomics profiling, called ***T-ReX LC-QTOF***. This total solution comprises the 'phenomics workhorse' impact II UHR-QTOF, an Elute UHPLC, T-ReX Metabolomics column kit (RP), software (MetaboScape 4.0 with TASQ 2.0) and high-quality content (standard operating procedures for sample prep and method setup, as well as updated Bruker HMDB Metabolite Library 2.0, including retention time).

Applied Toxicology and Forensics

Bruker announced the release of **TargetScreener 3.1HR** (high-resolution), encompassing an additional 600 compounds in the field of veterinary drugs, new psychoactive substances and pesticides, resulting in a database exceeding 2,800 compounds. All versions of TargetScreener contain ***TASQ™*** (Target Analysis for Screening and Quantitation) software to provide a unified platform for automated screening and quantitative applications in forensic, food and environmental safety markets. TASQ uses a unique method for providing positive identifications from the highly curated database, which results in minimal false positives and false negatives, while simultaneously performing seamless quantitation.

Sciex released its latest Innovations for Improving Healthcare and Well-being at ASMS.

They highlighted additions to the Sciex biopharma portfolio:

- OptiFlow™ Quant Solution, which delivers highly sensitive micro flow quantitation for peptides. This solution includes the OptiFlow™ Turbo V Source with M5 MicroLC to deliver micro flow sensitivity at analytical flow usability, with flexible and user-friendly sample handling.
- Multiple Attribute Methodology (MAM) Workflow for simple yet in-depth LC-MS characterisation and development of biologics, supported through the newly released Sciex BioPharmaView™ 3.0 software. The MAM Workflow provides more complete analysis of the product quality profile while minimising the burden of product quality attribute (PQA) monitoring and product purity testing.

New OS software:

- Sciex launched its Sciex OS 1.4 software at ASMS, bringing the full package for quantitative and qualitative analysis to the majority of Sciex instruments. The new operating system also offers complete 21 CFR Part 11 compliance for labs in regulated fields.

This launch follows the MPX™ 2.0 software, which was recently developed for multiplexing LC separations within a single MS system, saving valuable laboratory time while improving flexibility.

Shimadzu Corporation introduced the following new products at ASMS 2018:

The Shimadzu LCMS-9030 a quadrupole time-of-flight (Q-TOF) research grade mass spectrometer designed to deliver high-resolution, accurate-mass detection with incredibly fast data acquisition rates, allowing scientists to identify and quantify more compounds with greater confidence. It utilises the same engineering DNA from our proven, rugged, high-performance triple quadrupole (LC-MS/MS) platform and integrates that with powerful TOF architecture to transform high mass accuracy workflows by achieving high-sensitivity, high-speed, and high-resolution detection.

Figure 3. Shimadzu LCMS-9030 Q-TOF with UHPLC

Shimadzu also announced the release of the **Cell Culture Media Analysis Platform, C2MAPTM-2000**, a fully automated and integrated sample preparation workstation for the analysis of cell culture media. The C2MAP system measures changes of 95 components in a culture supernatant - including amino acids, sugars, vitamins and other critical components - as culturing progresses using LC-MS/MS to improve antibody production and accelerate process optimisation.

This system can be used for a wide range of applications, from basic research of cell cultures including pluripotent stem cells (iPS cells and ES cells), mesenchymal stem cells, and antibody-producing cells (such as CHO cells), to optimising the scale-up process of culture volumes and process development.

Shimadzu also released the **Nexera Mikros Microflow Liquid Chromatography Mass Spectrometry System**. Covering the complete range from microflow to semi-microflow, this system allows operators to realise high sensitivity, yet with the reliability and ruggedness of HPLC.

Shimadzu announced they have recently celebrated another anniversary:

Shimadzu Celebrates 30th Anniversary in Matrix-Assisted Laser Desorption Ionization Time-of-Flight Mass Spectrometry

Thermo Fisher Scientific

Thermo Fisher Scientific headlined with the new **Orbitrap ID-X Tribrid** Mass Spectrometer which claims to combine the best of their leading quadrupole, Orbitrap and linear ion trap mass analyser technologies, enabling users to acquire data with less experimental setup and interpretation expertise. The instrument supports intelligent data acquisition, enhancing scientists' interpretation of an unknown compound's mass spectra.

Thermo Scientific also released the **Q Exactive UHMR Quadrupole Mass Spectrometer** as the first platform to combine high-resolution, high-sensitivity MS2 and pseudo-MS3 capabilities in a seamless workflow. This gives structural biologists and biopharmaceutical scientists access to an ultra-high mass range (UHMR) system for high-quality native mass spectrometry and top-down analysis.

The new **ChromaCare** line of flush solutions and ultra-high-performance LC-MS (UHPLC-MS) solvents, ensure laboratories can now consistently access interference-free separations and maximise instrument uptime.

The **TSQ Fortis Triple Quadrupole** mass spectrometer, the third member of the TSQ family is positioned as a mid-range MS and is ideal for routine applications.

The TriPlus AutoSampler and Liquid Handling System with Robotic Tool Change claims to deliver greater productivity and efficiency for laboratories by reducing time-consuming steps and increasing sample throughput. Fully customisable to accommodate a wide range of sample processing needs in pharmaceutical, contract research, food safety, environmental, clinical research and forensics applications.

Improving small molecule characterisation

The new **Thermo Scientific Compound Discoverer 3.0** software is ideal for detecting pharmaceutical and food impurities, environmental contaminants, novel metabolites that could improve disease diagnosis and for screening of controlled substances and related designer drugs. It includes a comprehensive, integrated set of libraries, databases and statistical analysis tools that enable the complete characterisation of small molecules using mass spectrometry.

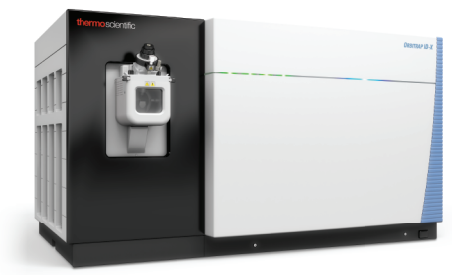

Figure 4. Thermo Scientific Orbitrap ID-X Tribrid

Waters Corporation

Waters previewed the new **Xevo TQ-GC mass spectrometer, GC-MS/MS system** for food safety and quality laboratories. The system, to be officially launched later in the year, allows laboratories to consistently meet and exceed limits of detection when quantifying pesticides residues and other contaminants in food using GC-MS/MS methods set forth by worldwide regulatory agencies/authorities.

The result of the ongoing collaboration announced at ASMS 2017 between Waters and IonSense™, Inc (Saugus, Mass.) the **Waters™ DART™ QDa™ with LiveID™ System** was announced. The system uses direct analysis for rapid molecular fingerprinting of food commodities, ingredients and processed products. Featuring the LiveID software platform, which trains and validates multivariate statistical models using the chemical profile obtained from the DART QDa analysis, the models can be used to identify unknown samples, generating easy-to-interpret results in near real time and a simple yes/no answer in seconds.

Figure 5. Waters™ DART™ QDa™ with LiveID™ System

The **ACQUITY™ QDa Practical MS Education Package**, developed jointly with the National Mass Spectrometry Facility at Swansea University in the UK, was also released at ASMS 2018 The system was created to give university chemistry departments an affordable means to enable undergraduates to access mass spectrometry equipment during their degree programmes and educate them in the fundamentals of mass spectrometry.

Waters and Elucidata Corporation (Cambridge, Mass. and New Delhi, India) have entered into a co-marketing agreement that combines the **Waters Symphony Data Pipeline™ Software** with Elucidata's **Polly™ Workflows** and cloud applications to enable efficient automated processing and interpretation of metabolic flux analysis studies from Waters mass spectrometry data.

Waters and Biognosys AG (Schlieren, Switzerland) have expanded their marketing agreement to include **Biognosys® Spectronaut Pulsar® X software and the PQ500 Reference peptide kit** for the Waters Xevo G2-XS QTOF quadrupole time-of-flight mass spectrometer running SONAR™ Software, a novel Data Independent Acquisition (DIA) technology. The combined platform quantitates reproducibly a large number of proteins (<500) in 15 minutes with single digit CVs. The platform is well-suited for enabling biomedical research laboratories to rapidly characterise and quantitate the protein profile of large sets of samples in a systematic and standardised way for clinical proteomics research.

Also introduced were the release of the **Targeted Omics Library**, including the new **MetaboQuan-R™** Method Packages. Each Method Package includes a **Quanpedia™** file containing all chromatographic and mass spectrometric settings for 'load and go' use on the Waters ACQUITY UPLC™ I Class Plus System and Xevo TQ-S micro triple quadrupole mass spectrometer and comes with an application note for the associated method.

The latest version of **Progenesis™ QI** software for proteomics, which creates and queries spectral libraries, is now capable of handling data dependent analysis (DDA) data, supporting identifications from all the DDA search engines supported by Progenesis QI for proteomics. It also incorporates a mass spectrometry/mass spectrometry (MS/MS) spectral clean-up tool for cleaner library matching.

ASMS Closing

Thursday's closing event was held aboard the USS Midway, a retired aircraft carrier of the United States Navy, the lead ship of her class. Commissioned just after the end of World War II, the USS Midway was the largest ship in the world until 1955, as well as the first U.S. aircraft carrier too big to transit the Panama Canal. The ship operated for 47 years, during which time she saw action in the Vietnam War and served as the Persian Gulf flagship in 1991's Operation Desert Storm. Decommissioned in 1992, the USS Midway is now a museum ship at the USS Midway Museum, in San Diego, California. In addition to a buffet dinner on the flight deck there were docents and exhibits to share the Midway's history, plus a variety of flight simulation games available.

Future ASMS Dates:

Dates and venues for the forthcoming ASMS meetings have been announced as follows:
67th ASMS Conference, 2 – 6 June 2019, Atlanta, GA
68th ASMS Conference, 14 – 18 June 2020, Denver, CO
69th ASMS Conference, 6 – 10 June 2021, Philadelphia, PA

Read, Share and Comment on this Article, visit: www.labmate-online.com/article

Interested in publishing a Technical Article?

Contact Gwyneth on +44 (0)1727 855574
or email: **gwyneth@intlabmate.com**