

Mass Spectroscopy Focus

Evolution not revolution but interesting all the same

Report on the 57th ASMS Conference, Philadelphia, Pa, USA May 31st - June 4th and the 18th IMSC, Bremen, Germany, September 1st - 4th 2009.

Once every 3 years both of the major meetings aimed at the mass spectrometry community are held. Not necessarily a bad situation but in days of reduced funds available both for practising scientists and commercial activists it could lead to a choice of which to attend, however both organising committees have taken a pragmatic view on this and focussed on making the meetings affordable since without the end-users the commercial side of the proceedings will not contribute to the same degree. Members of the American Society for Mass Spectrometry (ASMS) were charged only \$150 and this no doubt helped the attendance of conferees to be almost similar in number, ca 6,500, to the 2008 number.

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The number of exhibitors was slightly down but the corporate hospitality suite numbers reduced from 25 to 18 reflected some cost saving by the manufacturers and service providers. The International Mass Spectrometry (IMSC) had a slightly higher tariff for attendees but early bird discounting no doubt helped the record breaking attendance to reach excess of 2,600 and a very healthy exhibition to be presented. The meeting was held in the city which houses the manufacturing bases of two of the major players in the Mass Spectrometry world, Thermo Fisher Scientific and Bruker Daltonik GmbH so the meeting was never going to suffer from a lack of 'gravitas'.

The high proportion of students present at both meetings was a healthy sign that the thirst for knowledge continues and, particularly within the life sciences application areas, there is growing need for techniques that can help the – omics scientists. Another application field which has risen from the pack is that of the use within Clinical applications and as a diagnostic tool. It will be some time before the technique of LC/MS/MS becomes a regular tool within the armoury of the clinicians on a regular basis but the creation of dedicated products and supporting software options by most of the major manufactures recognises that here lies potential for the technique of Mass Spectrometry.

The sheer number of different oral presentations, workshops tutorials, vendor presentations, exhibitor offerings and, at ASMS almost 3000 posters (almost 1200 at IMSC) means that attendees really do have to engage in some selective and well thought out time management in advance.

THE SCIENCE

Application areas where Mass Spectrometers are used have mushroomed over the last 10-15 years inversely as the price for Instruments in some sections has decreased. From the original community of high end magnetic sector devotees firstly the rise of environmental scientists using MS variants hooked to GC systems, quickly followed by life scientists using mainly LC at the front end, originating from proteomic backgrounds are now avid users and fuel the demand for manufactures to come up with new and innovative ionisation techniques, instrument designs and software to improve sensitivity and accuracy of the data. As ever much of this advancement comes with better understanding of the multi-disciplinary fundamentals essential to the basics of smashing samples with electronic beams and measuring to varying degrees of accuracy the fragments. Physics, Laser technology, material scientists are all involved at the ground level.

At the IMSC a breakdown of the top level headings of the oral sessions showed that over 40% of all presentations were on topics concerning Life Science applications, followed by almost equal proportions of the other five headings. This vividly illustrates the market segment that attracts the most attention and where manufacturers apply their resources. However for those not working in this area then it could be considered too focussed and much of the presented work was viewed as being fairly obvious and not particularly cutting edge.

Two oral presentations which did merit positive comment were those by Professor David Clemmer, Indiana University, USA on the topic of advances in ion mobility mass spectrometry and Michael O. Glocker, University Rostock, Rostock, Germany 'Mass Spectrometric Epitope Analysis of Autoantigens and Applications to Autoimmune Disease Diagnostics'. Professor Clemmer had already given the plenary lecture that morning on 'Developing High-Resolution Ion Mobility-MS techniques for the Analysis of Complex Mixtures' and clearly struck a chord with some delegates.

One particular hot-topic which continued to cause discussion amongst delegates was the constant chase for even more accurate mass measurement and the manufacturers were particularly interested in receiving feedback on this. All manufacturers have a particular instrument which is aimed at those working on that particular aspect of mass spectrometry and it yet has several orders of magnitude to run.

AWARDS

Recognition of one's contribution for the advancement of science in general should be the aim of all scientists. In this case the topic is Mass Spectrometry. Awards from the ASMS committee for Distinguished Contribution in Mass Spectrometry were made jointly to Professor Simon J. Gaskell from the University of Manchester, U and Professor Vicki H. Wysocki from the University of Arizona for their work on the 'Mobile Proton Model'. The Biemann Medal was presented to Professor Neil L. Kelleher from the University of Illinois (Urbane-Champaign) for his work in the field of top-down proteomics. Finally the inaugural Ron Hites award for an outstanding research publication in the society's journal (JAMAS) went to Professor Alison E. Ashcroft from Leeds University, UK.

Awards from the International Mass Spectrometry Foundation were made firstly to Professors Cathy Costello (Boston University School of Medicine, USA), Catherine Fenselau (University of Maryland) and Peter Roepstorff (University of Southern Denmark) with the Thomson Medal for their contributions to the development to Mass Spectrometry. Secondly for his contribution to Mass Spectrometry the Curt Brunnée award was made to Dr Alexander Makarov (Thermo Fisher Scientific).

Naturally with such a diversity of topics being discussed, it is difficult to obtain a consensus of opinion as to the most informative, interesting and ground breaking presentations during the week. Opinions ranged from wanting more discussion on accurate mass measurement to those thinking that the poster sessions contained more ground breaking innovative work than many of the oral presentations. Proteomics and metabonomics were judged to have been allocated the correct amount of time for discussion.

EXHIBITION

The annual ASMS meeting in early June is the focal point for many of the large manufacturers to make new product introductions and re-state their positioning in the market place to their customers.

The two events do have differing degrees of involvement when it comes to the role that the trade exhibition plays in the 5 days of knowledge dissemination. For the ASMS tradition has long dictated that in order to be offering a level playing field to corporate members only one booth of 10 x 10 feet is allowed per member in the official area and printed literature only is allowed to be distributed from that point. However the concept of hospitality suites where working demo units and plentiful supplies of solid and liquid refreshments go hand in hand is an integral part of the proceedings. Major manufacturers vie for the attention and attendance of conferees. The ASMS show is always held around the end of May/early June thus a fair proportion of the year remains, allowing manufacturers time to recoup some of their hospitality budget in the way of sales.

Consequently there was little new in the way of major new product introductions at IMSC for the global players but those whose main market is Europe took the opportunity

to at least introduce products which may not necessarily be new to the market but would be to many customers.

The exhibition area was spread over two floors with all the big manufactures being housed in the main area as no restrictions were placed on booth size although hospitality suites were encouraged for the first time at this event. Certain booths decided to offer happy hour events to boost traffic and since Bremen is the home to the famous Becks brewery this generally went down well.

Space constraints prevent reviewing of all the booths offerings so I have tried to summarise some of the more interesting offerings on show. For more information on many products readers should refer to the pages following this article and also visit the websites www.Labmate-online.com and www.imsc-bremen-2009.de where more information may be found.

One of the major talking points around the IMSC exhibition was the news that the Applied Biosystems / MDS Analytical Technologies joint venture had been purchased by Danaher Corporation, a name not associated at all with Mass Spectrometry yet a cash rich company. The ABI/MDS product line ranging from triple quadrupole mass spectrometers to innovative hybrid triple quadrupole-linear ion trap systems is amongst the market leaders so interesting times lie ahead.

INSTRUMENTATION

Most manufacturers have their product offering designed to appeal to scientists who have specific requirements from their systems be it resolution, sensitivity, high mass accuracy, speed, quantification, qualification, ionisation mode, type of measurement or any combination of these, the permutations are almost endless. Where there is room for differentiation from company to company is in systems combining focus on more than one criterion from the preceding list possibly aimed at specific markets, eg. metabolomics, clinical, proteomics.

Some of the major 'names' in the Mass Spectrometry Instrument business are now offering a potentially new

exciting series of 'hybrid' mass spectrometers. New improved versions featuring the latest technologies were on offer from most of the major manufacturers with **Waters** heavily promoting their SYNAPT™ G2 series along with no less than eight enhancements to their Mass Lynx software suite, **Thermo Scientific** launched their LTQ Velos and LTQ Orbitrap Velos™ instruments aimed at producing faster analysis speeds and ultra-high resolution and accurate mass data than had previously been attainable. **Agilent Technologies** launched the model 6540 QTOF instrument as part of an LC/MS/MS product line alongside their model 1290 LC System which was heavily promoted at IMSC along with its ability to interface with the increasing range of mass specs that the company offers. **AB SCIEX** have the **AB SCIEX QTRAP 5500 LC/MS/MS** combined with Linear Ion Trap technology, **Bruker Daltonics** have the solarix Qq-FTMS and. **Shimadzu** offer the LC/MS-IT-TOF combining ion trap and TOF capabilities and the features and benefits associated with both.

SOFTWARE

Complex and copious amounts of data is often produced with MS systems and although all Instrument manufacturers have their own suite offerings, some scientists prefer to use dedicated software for their particular situation and several were on show. Medicwave for example offer a suite dedicated to finding protein biomarkers and detecting protein deviations. ACD /Labs were demonstrating their IntelliTarget software for determining the presence of known compounds in LC and GC/MS analyses.

COMPONENT 'ADD-ONS'

Parker and Peak Scientific Instrument exhibited a range of gas generators and a company named MS NOISE offered a range of noise reduction boxes for use with vacuum pumps which naturally no MS system can run without.

DEDICATED APPLICATIONS SYSTEMS

An interesting approach was taken by PerkinElmer

who at IMSC launched a dedicated system aimed at the clinical market with their steroid profiling system based on an LC-MS/MS platform. Consumables and software were included as part of the system. Possibly more dedicated systems could be the future route into the clinical market for manufacturers.

CONSUMABLES AND 3RD PARTY SALES/SERVICE

Economic issues within many companies has meant good times for 3rd party service organisations many of which also offer refurbished equipment with upgrades and much of it is fairly recent issue. Many pharmaceutical companies are down sizing and relocating their R+D efforts meaning top end spec machines are available at interesting prices. **Kinesis RSS**, along with an increasing number are amongst the companies who offer nearly new and refurbished Instruments

Many members of long standing in the Mass Spec community at both the end user and commercial orientation will have been occasional visitors to the annual ASMS event over the years. They will no doubt have noted that this ISMC was starting to incorporate some of that meetings organisational feature such as on-site hospitality suites and a closer working relationship with the sponsors who hopefully will allow the costs of attendance and appeal of the meeting to continue to grow if deemed a success on this occasion.

FOLLOW THAT

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

May 23-27th	2010	Salt Lake City, Utah
June 5-9th	2011	Denver, Colorado
May 20-24th	2012	Vancouver, BC, Canada

The next meeting, the 19th, of the IMSC will be held for the first time outside of Europe in 2012 in Kyoto, Japan (September 15-21) under the organisation of the Mass Spectrometry Society of Japan, MSSJ. For further information please go to www.imsc2012.jp

Discovering Undetected Peptide Modifications

Shimadzu Scientific Instruments introduced PTM Finder™ software, which uses data mining to investigate post-translational modifications in complex protein samples, including data for hypothetical, novel modifications. The software is designed to integrate with Shimadzu's AXIMA™ line of MALDI mass spectrometers.

With PTM Finder software, users can identify peptide sequences carrying one or more modifications using MS/MS data. The software facilitates consecutive Mascot searches using all the functionality of MS/MS Ion Search.

Peptides that do not match any proteins during the searches are directed toward a 'PTM Define' module where users define their own hypothetical modifications and screen the remaining MS/MS data for specific shifts in fragment masses, neutral losses and/or diagnostic ions. Such searches are quick and thorough, as they are performed based on a reduced database of protein sequences.

Users can easily import amino acid sequences with a simple copy/paste function or use the proteins derived from the initial Mascot search results, giving more flexibility to search for PTMs whether or not they know the protein they are using.

Circle no. 42

Conquering Mass Spectrometry Application Challenges

Waters Corporation introduced eight new MassLynx™ workflow enhancements at the 57th American Society of Mass Spectrometry (ASMS) Conference on Mass Spectrometry and Allied Topics, all designed to enhance laboratory productivity and expand mass spectrometry applications.

Brian Smith, Vice President, Mass Spectrometry Business Operations for the Waters Division, said: "These software innovations realise the full potential of mass spectrometry across our entire portfolio of LC/MS and GC/MS systems. MassLynx software continuously addresses new analytical challenges, and streamlines existing ones, through advanced data interrogation capabilities and simplified workflow processes."

The POSITIVE system™ is for high throughput screening of complex food safety, water quality and environmental samples by combining qualitative and quantitative processes into one. POSITIVE takes Waters system solution paradigm to the next level by uniquely integrating chromatography, exact mass MS and informatics for screening applications. The BiopharmaLynx™ 1.2 increases confidence in peptide characterisation leveraging comprehensive exact mass UPLC/MSE data in biopharmaceutical applications. Quanpedia, QCMonitor and TrendPlot, critical components of the Xevo™ TQ MS quantitative workflow solution software, are now available for a broader range of Waters mass spectrometers. Laboratories will cut sample analysis times and optimise resource utilisation to increase productivity with the latest version of OpenLynx™ Open Access. Clinical pathology laboratories will benefit from automated workflows for UPLC/MS/MS that include seamless HL7 LIMS integration. MetaboLynx™ XS and MarkerLynx™ XS for accelerated metabolite identification and profiling are now available on all Waters MS Systems. Management of large proteomic data sets is accelerated with ProteinLynx Global SERVER™ (PLGS) 2.4 for nanoACQUITY 2D UPLC/MSE while data are now also interchangeable with PRIDE, Scaffold and mzML. DriftScope™ 2.1 features ion mobility spectrometry (IMS) peak detection, visualisation & comparison, together with collision cross section (CCS) determinations, for the original SYNAPT High Definition MS™ system and the new SYNAPT G2 HDMS system.

Circle no. 43

TLC-MS Interface

Rapid and convenient extraction directly into your MS



Not all samples may be processed by HPLC-MS. As an alternative the CAMAG TLC-MS Interface extracts compounds from a TLC/HPTLC plate. Samples are fed into a MS for substance identification:

- No scraping off from the TLC/HPTLC plate
- Semi-automatic operation
- Online transfer into all common HPLC-MS systems

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