

Wednesday October 6 - Workshops & Short Courses, Plenary Session

Registration Opens						
Poster Viewing & Exhibition - Atrium						
Room	Cambridge 30	Boston 9	Boston 17	Boston 19	Boston 13	Boston 12
08:30						
10:00 - 18:30						
10:30 - 13:15*	<p>Workshop/Short Course 1</p> <p>Markus Mickel¹, Loic Beyet² AB SCIEX (¹Darmstadt, Germany, ²Paris, France)</p> <p>Advanced QTRAP® functionalities for simultaneous quantitative and qualitative LC/MS/MS analysis</p>	<p>Workshop/Short Course 2</p> <p>Jens Trafkowski¹, Iain Gibb², Julie Moriceau³ AB SCIEX (¹Darmstadt, Germany, ²Warrington, UK, ³Paris, France)</p> <p>Method development & troubleshooting for LC/MS/MS and U-HPLC/MS/MS systems</p>	<p>Workshop/Short Course 3</p> <p>Kristin von Czapiewski¹, Dan Blake², Bertram Nieland³, AB SCIEX (¹Darmstadt, Germany, ²Warrington, UK, ³Nieuwerkerk a/d IJssel, The Netherlands)</p> <p>Workflow enabling tools to simplify access to mass spectrometry: Cliquid® software, iMethods™ tests, MultiQuant™ software & mass spectral libraries</p>	<p>Workshop/Short Course 4</p> <p>Jan Lembcke¹, Steve Lock², Dan Leigh³, AB SCIEX (¹Darmstadt, Germany, ²Warrington, UK)</p> <p>Multi-targeted and general unknown screening and identification in LC/MS/MS</p>	<p>Workshop/Short Course 5</p> <p>Dietrich Merkle¹, Jörg Dojahn¹, Antonio Serna², AB SCIEX (¹Darmstadt, Germany, ²Madrid, Spain)</p> <p>Proteomics workflows; What's up and what's new?</p>	<p>Workshop/Short Course 6</p> <p>Axel Besa, Mathias Glückmann AB SCIEX (Darmstadt, Germany)</p> <p>What significance has a lipidomics approach? Tools for "omics" studies including metabolomics</p>
13:15-14:30	Lunch, Exhibition & Poster Viewing - Atrium					
14:30- 17:15	<p>Plenary Session – Room Sorbonne 2 Chair: Gisbert Schäfer, AB SCIEX (Darmstadt, Germany)</p>					
14:30-14:45	Andy Boorn, AB SCIEX (Toronto, Canada) & Gisbert Schäfer, AB SCIEX (Darmstadt, Germany) Welcome and Introduction					
14:45-15:15	Tom Covey, AB SCIEX (Toronto, Canada) Title to be confirmed					
15:15-15:45	Gerard Hopfgartner, Laboratory of Pharmaceutical Analytical Chemistry, Life Sciences Mass Spectrometry, University of Geneva (Geneva, Switzerland) The impact of combining fast chromatography and fast accurate mass spectrometry for simultaneous quantitative and qualitative analysis in complex matrices					
15:45-16:15	Coffee Break – Atrium					
16:15-16:45	Ruedi Aebersold, ETH, Swiss Federal Institute of Technology (Zurich, Switzerland) Mapping and measuring proteomes					
16:45-17:15	Jana Hajslova, Department of Food Chemistry and Analysis, Institute of Chemical Technology (Prague, Czech Republic) Leveraging cutting-edge mass spectrometric equipment to overcome challenges in trace analysis of organic food contaminants with special focus on perfluorinated compounds					
17:15-17:45	Detlef Thieme, Institute of Doping Analysis and Sports Biochemistry (Kreischka, Germany) Influence of liquid chromatography-tandem mass spectrometry on doping analysis					
17:45-18:45	Poster Viewing & Exhibition - Atrium					
19:00-20:00	Reception, Mingle & Meet, Poster Viewing & Exhibition- Atrium					
20:00-22:00	Conference Dinner – NH Conference centre restaurant Samuel					
22:00	End of day 1 ECMSMS 2010					

*: includes a 30 minute coffee break in the Atrium

Wednesday October 6 - Detailed descriptions of Workshops & Short Courses

Advanced QTRAP® functionalities for simultaneous quantitative and qualitative LC/MS/MS analysis

For over a decade triple quadrupole LC/MS/MS instruments have been widely accepted as the gold standard for targeted quantitative analysis. However, scientists often desire to quantify and identify compounds within a single LC/MS/MS run. The AB SCIEX QTRAP® hybrid linear ion trap instrument achieves this goal by combining triple quadrupole and linear ion trap modes of operation within a single experiment. In this session we discuss the theoretical aspects of the QTRAP® LC/MS/MS system, that allow the combination of triple quadrupole and linear ion trap experiments within one acquisition using "Information Dependant Acquisition" (IDA) workflows. We also discuss how the QTRAP® system is used to facilitate in-depth structural elucidation using MS3 experiments. Finally we describe how the unique MRM3 scan function of the QTRAP® system provides highly selective, quantitative analysis in complex matrices by eliminating spectral interferences that may be observed in classical triple quadrupole MRM experiments.

Method development & troubleshooting for LC/MS/MS and U-HPLC/MS/MS systems

In recent years there has been considerable interest in exploiting the high throughput and efficient separation capabilities of ultra-high pressure HPLC technology (U-HPLC) with mass spectrometric detection. However, the narrow peak widths afforded by modern U-HPLC systems means that there is less time for a mass spectrometer to collect a sufficient number of data points across the chromatographic peak. This can lead to a compromise in the chromatographic fidelity leading to incorrect peak integration and poor quantitative data. The problem only worsens as the chromatographic peak widths shorten and / or the number of analytes within a run increases. The first part of this workshop will provide an overview of the differences of LC/MS/MS and U-HPLC/MS/MS and describe the benefit of the AB SCIEX Scheduled MRM™ algorithm in developing the U-HPLC methods that are suitable for both quantitative and qualitative workflows. The second part of the session will take a deeper look into troubleshooting both LC/MS/MS and U-HPLC/MS/MS applications.

Workflow enabling tools to simplify access to mass spectrometry: Cliquid® software, iMethods™ tests, MultiQuant™ software & mass spectral libraries

Cliquid® 3.0 software from AB SCIEX simplifies the use of LC/MS/MS for routine testing in both quantitation and screening experiments. Designed with an intuitive point-and-click and four-step workflow, Cliquid® software simplifies the process from injecting samples to the generation of a report. Furthermore the open access architecture of Cliquid® enables even novice users to predefine tests for deployment of turnkey quantitation and compound identification / verification assays.

'Ready to go' iMethod™ tests can be downloaded from the AB SCIEX homepage and methods that have previously been established in-house can easily be shared amongst different laboratories under the Cliquid® interface. Mass spectral libraries (e.g. pesticides, forensics and veterinary drugs) help to identify or verify the presence of compounds of interest with a higher degree of confidence than classical MRM ratios. Additionally tests can be created using the built-in MRM catalogue to further customize the required workflow. We will also describe MultiQuant™ software as the next generation of data processing software for quantitative multicomponent analysis.

Multi-targeted and general unknown screening with identification in LC/MS/MS

Multiple reaction monitoring (MRM) lends itself to sensitive, quantitative analysis of known or suspected target components in LC/MS/MS. However MRM is unsuitable for the General Unknown Screening (GUS) investigations because there cannot be any prior knowledge as to the identity of the compound(s) present. GUS is therefore a very challenging task and can be seen as a search for the "needle in the haystack". GUS therefore requires a non-selective 'universal survey' scan in conjunction with sophisticated software for data mining and interpretation purposes to detect and identify unexpected compounds. Full scan data acquisitions offer the best possibility for the GUS workflow and high sensitivity full scan data can be acquired using a QTRAP® system in both MS and MS/MS modes. When used in conjunction with Cliquid™ software, MS/MS library databases and MarkerView™ a principle component analysis software tool, the possibility of finding the needle in the haystack increases significantly. The use of high resolution, accurate mass instruments can also be used to guide the analyst through their investigations.

Proteomics workflows: What's up and what's new?

High resolution MS instruments with accurate mass capability are crucial functionalities for the investigation of unknown species in the proteomics domain. In the first part of the session we give an overview of the latest MS innovation from AB SCIEX.

The new AB SCIEX hybrid mass spectrometer is the first high-resolution, accurate mass, instrument specifically designed from the ground up, to deliver the speed, sensitivity and quantitative accuracy only previously obtainable on high end triple quadrupole instruments. The new instrument simultaneously facilitates advanced accurate mass workflows that allow conclusive identification and precise quantitation of low abundance compounds in complex samples, all in one run and without compromising any of its qualitative or quantitative performance characteristics.

The second part will elucidate the workflow of a top-down sequencing strategy. Here we describe molecular imaging experiments and tips and tricks to maximize your productivity using the AB SCIEX TOF/TOF™ 5800 instrument.

What significance has a lipidomics approach? Tools for "omics" studies including metabolomics

The first part of this session will cover a typical lipidomics workflow with commonly used technologies from discovery through to routine lipid quantitation. Lipidomics workflows using state-of-the-art technology on the latest AB SCIEX MS instrumentation as well as the newly developed LipidView™ software fulfill the requirements for lipid analysis. Routine lipid analysis is supported by new software tools from AB SCIEX based upon lipid profiling, lipid identification and lipid quantitation.

The second part will cover the analysis of potential metabolic biomarkers in a variety of matrices. In metabolomics experiments researchers typically work through four different stages in order to find and identify biomarkers:

- I Separate diseased and non-diseased samples
- II Find potential biomarkers
- III Determine the elemental formula for the potential biomarkers
- IV Confirm the identification

We will show how AB SCIEX MarkerView™ software helps researchers to find and identify potential biomarkers with statistical tools such as "PCA-analysis" and "t-tests".

08:00-Close						Registration, Posters and Exhibition in Atrium					
8:45-12:00						Morning Sessions					
Room	Cambridge 30		Boston 17		Boston 19		Boston 9		Boston 12/14		
	Food, Beverages & Feeds		Pharmaceutical Sciences Emerging Quantitative Workflows		Biomarker Discovery & Validation Protein Analysis and Protein Quantitation		Clinical Research & Toxicology		Advances in MS/MS Technology		
8:45-9:50	Chair: Rudolf Krška, Department for Agrobiotechnology, IFA Tulln (Tulln, Austria)		Chair: TBD		Chair: Friedrich Lottspeich, Max-Planck-Institute of Biochemistry (Munich, Germany)		Chair: Charles Turner, Kings College London, Evelina Childrens Hospital (London, UK)		Chair: Susanna Baque, AB SCIEX (Barcelona, Spain)		
8:50-9:10	Steve Lock, AB SCIEX (Warrington, UK)		Introduction AB SCIEX		Christie Hunter, AB SCIEX (Foster City, USA)		Bruno Casetta, AB SCIEX (Monza, Italy) Evolution of a state-of-the-art strategy for the routine quantitation of amino acids by LC-tandem mass spectrometry		Introduction AB SCIEX		
9:10-9:40	Bert Poepping & Julia Heick, Eurofins (UK & Hamburg, Germany) Detection of food allergens: past, present and future in the legal context		Martina Nibbio, Siena Biotech S.p.A. (Siena, Italy) From a discovery-oriented bioanalytical and data analysis approach, to a robust quantitative method, PK and TK analysis		Rune Linding, The Institute of Cancer Research, Chester Beatty Laboratories (London, UK) Integrative network biology and proteomics		Thomas Grobosh, Institute of Clinical Toxicology – Clinical Toxicology and Poison Control Centre, BBGes (Berlin, Germany) Development of a systematic toxicological screening method using an automated on-line SPE/LC/QqTOF System - First experiences		Detlev Schleuder, AB SCIEX (Darmstadt, Germany) Advances in QTRAP® technology		
9:40-10:10	Amadeo R. Fernandez-Alba, European Reference Laboratory for Pesticides in Fruit and Vegetables, University Almeria (Almeria, Spain) Multi-class residue analysis in challenging food matrices - New approaches to overcome matrix effects		Fabio Garofolo, Algorithme Pharma (Quebec, Canada) Limitations of quantitative LC/MS/MS and their resolution with MRM3; The Macrolide immunosuppressant drugs case study		Henning Urlaub, Max-Planck-Institute for Biophysical Chemistry (Goettingen, Germany) Absolute quantification for determination of protein stoichiometries within protein complexes – challenges and pitfalls		Michael Oellerich, Department of Clinical Chemistry, George August University (Goettingen, Germany) Applications of tandem mass spectrometry and biomarkers in therapeutic drug monitoring		Stephen Tate, AB SCIEX (Toronto, Canada) Use of alternate scan methods with the TripleTOF™ 5600 system to provide qualitative and quantitative data		
10:10- 10:40						Coffee Break in Atrium					
10:40 - 10:50	Kristin von Czapiewski, AB SCIEX (Darmstadt, Germany)		Introduction AB SCIEX		Christie Hunter, AB SCIEX (Foster City, USA)		Introduction AB SCIEX		Introduction AB SCIEX		
10:50 - 11:20	Hans Mol, RIKILT, Institute of Food Safety (Wageningen, The Netherlands) Combined screening of toxicants in food and feed using LC full scan high resolution accurate mass spectrometry		Paul Abu-Rabie, GlaxoSmithKline (Stevenage, UK) Direct quantitative bioanalysis of drugs in dried blood spot samples		Keith Ashman, Spanish National Cancer Research Center (Madrid, Spain) If biology is blind, it cannot hit the mark		Sandra Feyel, Labor Becker, Olgemöller und Kollegen (Munich, Germany) Metanephrines and normetanephrines in urine and plasma by LC/MS/MS		Almeida Reinaldo, Advion (Norwich, UK) Liquid extraction surface analysis (LESA) combined with nESI-MS for direct sampling of planar tissues		
11:20-11:50	Eric Verdon, ANSES, French agency of Food, Environmental and Occupational Health Safety (Fougeres, France) Validating methods for veterinary drug residue control – To an international recognized format? A review with particular consideration to LC/MS/MS		Ronald de Vries, Janssen Pharmaceutica (Beerse, Belgium) Challenges in the absolute quantification of peptides using state-of-the-art mass spectrometry		Edwin Romijn, Philips Research Labs (Eindhoven, The Netherlands) Biomarker discovery and verification using mass spectrometry		Jaak Billen, Department of Laboratory Medicine, Catholic University of Leuven (Leuven, Belgium) Quantification of 1 α ,25(OH) $_2$ -vitamin D3 in serum by LC/MS/MS: a robust and performing method.		Tom Covey, AB SCIEX (Toronto, Canada) The future of MS at AB SCIEX		
11:50-12:00	Q&A		Q&A		Q&A		Q&A		Q&A		
12:00 - 13:30						Lunch, exhibition and poster viewing in Atrium					

Afternoon Sessions					
Room	Cambridge 30	Boston 17	Boston 19	Boston 9	Boston 12/14
13:30-16:30	Food, non-Food & Agrochemical Analysis	Pharmaceutical Sciences Discovery & Development	Biomarker Discovery & Validation Metabolomics & Lipidomics	Clinical Research & Toxicology	Water, Marine Biota and Environmental Analysis
	Chair: Hans Mol, RIKILT, Institute of Food Safety (Wageningen, The Netherlands)	Chair: Mauro Aiello, AB SCIEX (Toronto, Canada)	Chair: Henk Blom, VU Free Univ. Medical Centre Amsterdam (Amsterdam, The Netherlands)	Chair: Bruno Casetta, AB SCIEX (Monza, Italy)	Chair: Amadeo R. Fernandez-Alba, European Reference Laboratory for Pesticides in Fruit and Vegetables, University Almeria (Almeria, Spain)
13:30-13:40	Harald Moeller-Santner AB SCIEX (Germany)	Introduction AB SCIEX	Christie Hunter, AB SCIEX (Foster City, USA)	Introduction AB SCIEX	Detlev Schleuder, AB SCIEX (Germany)
13:40-14:10	Rudolf Krska, Department for Agrobiotechnology, IFA Tulln (Tulln, Austria) Modern LC/MS Methods for the determination of fungal and bacterial metabolites in plants, foods and indoor environment	Theo Noij, Notox BV ('s Hertogenbosch, The Netherlands) Achieving better science with less animal testing in pharmacokinetics using high resolution LC and high sensitivity MS/MS techniques	Klaus Weinberger, Biocrates life sciences AG (Innsbruck, Austria) Targeted metabolomics: the AbsoluteIDQ kit and new developments	Neil Dalton, Kings College London, Evelina Childrens Hospital (London, UK) The potential of dried blood and urine spots in clinical diagnosis and patient monitoring	Rakesh Kanda, STL Labs (Reading, UK) Development, validation and application of analytical methodology to determine haloacetic acids (HAAs) and other anions by ion chromatography tandem mass spectrometry
14:10-14:40	Oliver Schmidt, LAVES, Lower Saxony State Office for Consumer Protection and Food Safety (Lueneburg, Germany) LC/MS/MS based analysis of hazardous substances in non-food consumer products - advances and pitfalls	Michelle Gleave Pfizer Inc, Pharmacokinetics, Dynamics and Metabolism, Global Research and Development (Sandwich, UK) 'Pick 'n' Mix: MS approaches to detect and identify drugs and metabolites	Andreas Dunkel, Technical University Munich (Munich, Germany) Multiparametric analysis of the nonvolatile sensometabolome of food	Uta Ceglarek, Institute of Laboratory Medicine, Clinical Chemistry and Molecular Diagnostics, University Hospital Leipzig (Leipzig, Germany) Rapid quantification of steroid patterns in human serum by on-line SPE combined with LC/MS/MS	Damià Barceló, Institute of Environmental Assessment and Water Research (IDAEA)- CSIC (Barcelona, Spain) Trends in the analysis and fate of pharmaceuticals and their degradation products in water and sludge by LC-hybrid MS systems (QqLIT and QqTOF)
14:40-15:10	Coffee Break in Atrium				
15:10-15:20	Introduction by Tomas Korba AB SCIEX (Prague, Czech Republic)	Introduction AB SCIEX	Introduction by Christie Hunter, AB SCIEX (Foster City, USA)	Introduction AB SCIEX	15:10- 15:30 Philipp Hess, IFREMER, French Research Institute for Exploitation of the Sea (Nantes, France) LC-MS-MS analysis of lipophilic marine biotoxins - challenges and recent progress in development and validation of methods
15:20-15:50	Reinhard Dötzer, BASF Agricultural Center (Limburgerhof, Germany) The potential of high resolution MS in agrochemical analytics	Gerard Hopfgartner, Laboratory of Pharmaceutical Analytical Chemistry, Life Sciences Mass Spectrometry, University of Geneva (Geneva, Switzerland) Simultaneous qual/quant approaches for drug metabolism and metabolomic studies using the TripleTOF™ 5600 system	Jerzy Adamski, Helmholtz Institute (Munich, Germany) Impact of genetic variation on human metabolism	Simon Elliott, ROAR Forensics (Malvern, UK) Cat and Mouse: The applied use of QTRAP® LC/MS/MS technology in finding designer drugs	15:30-15:50 Giuseppe Mascolo, CNR -IRSA, National Research Council, Water Research Institute (Bari, Italy) Breakthrough in the determination of polybrominated diphenyl ethers and other flame retardants in sewage sludge by UPLC/MS/MS using both APCI and APPI
15:50-16:20	Speaker to be announced Title to be confirmed	Filippos Michopoulos, AstraZeneca (Alderley Park, UK) Watch out for turbulence - plasma metabolomics using LC/MS	Kim Ekroos, Zora Biosciences (Espoo, Finland) Title to be confirmed	Wolfgang Weinmann, Institute for Legal Medicine, University of Bern (Bern, Switzerland) Multi-target screening in forensic and clinical toxicology with mass spectral library for drug identification	15:50-16:10 Wolfram Seitz, Zweckverband Landeswasserversorgung, Laboratory for Operation Control and Research (Langenau, Germany) Prospects and challenges of direct LC/MS/MS analysis of organic contaminants in water
16:20-16:30	Harald Moeller-Santner AB SCIEX (Darmstadt, Germany) Closing Talk & Farewell	Closing Talk & Farewell	Closing Talk & Farewell	Closing Talk & Farewell	16:10-16:20 Discussion and Q&A 16:20-16:30 Detlev Schleuder, AB SCIEX (Germany) Closing Talk & Farewell
16:30	End of ECMSMS 2010				