



Bruker Daltonics Mass Spectrometry



MassSpectator

September 2016, Issue 72

Upcoming Events

September 7-9 – JASIS, Makuhari

September 9-12 – The 34th China Mass Spec Annual conference, Qinghai

September 11-14 – DGHM, Ulm

September 18-22, HUPO Taipei, Taipei

September 20-23 – ILMAC, Basel

October 4-7 – World of Technology and Science, Utrecht

October 10-12 – analytica China, Shanghai

October 16-21 – SOFT Annual Conference, San Antonio

December 10-14 – 6th BrMass-1st IbMS, Rio de Janeiro

In this issue

Welcome to another inspiring issue of Bruker's **MassSpectator**! Our highlights this month are the launch of the next-generation solariX™ 2XR Fourier Transform Mass Spectrometer (FTMS) and the new MetaboScape® 2.0 Software at the IMSC 2016 as well as our upcoming webinars with Prof. Dr. Matthias Mayer and Prof. Pim Leonards.

As a note, we consistently seek to improve our engagement with you, so please [contact us](#), and follow us on [twitter](#), [LinkedIn](#), [YouTube](#) and [facebook](#).

Kind regards,
Your Bruker Daltonics Sales & Marketing Team

Bruker Accelerates Extreme Resolution Isotope Fine Structure (IFS) Mass Spectrometry with launch of new solariX™ 2XR FTMS System



At the IMSC 2016, Bruker introduced the **next-generation solariX™ 2XR Fourier Transform Mass Spectrometer (FTMS)** to accelerate 'extreme resolution' mass spectrometry with mass resolving powers in the range of 1-10 million, which are not achievable with any other mass spectrometry technologies. Faster and easier IFS analysis with mass resolving power of 1.2 million in one second can now routinely determine the molecular sum formulae of unknown small molecules with an affordable 7 Tesla magnet.

[Learn more.](#)

New MetaboScape® 2.0 Software launched, enabling seamless annotation of unknown compounds and confident annotation of known compounds!



At the IMSC 2016, Bruker announced a new version of **MetaboScape** software. This integrated solution for non-targeted metabolomics links LC-QTOF-MS/MS data to the underlying biology based on metabolic pathway mapping. Version 2.0 enables the **annotation of unknown compounds** and provides scientists with a higher degree of confidence in the identification of known metabolites through the **use of high resolution accurate mass MS/MS fragment information**.

Learn more in the new [MetaboScape brochure](#) and the [Application Note "What are we eating?"](#)

Webinar with Prof. Dr. Matthias Mayer on “Hydrogen Exchange Mass Spectrometry automation for the maXis Ultrahigh Resolution QTOF”



Hydrogen exchange mass spectrometry (HX-MS) is a highly suitable method to analyze the conformational state of proteins and changes caused by folding and unfolding, protein-protein-interactions, ligand binding and allostery. It can thus be used to assess the quality of protein preparations, to identify stable and flexible regions within proteins and how they change over time or under different conditions and for epitope-mapping. This webinar will cover **principles of HX-MS and some of the basic considerations when setting up HX-MS experiments**, and then discuss a fully automated system consisting of a LEAP robot and a Bruker maXis mass spectrometer.

[Click here](#) to register for the webinar on September 6, 4 pm CEST.

Can metabolomics research help to discover developmental disorders in children related to environmental contaminants? Webinar on September 22



Worldwide, serious concern has arisen about the increased incidence of learning and developmental disorders in children. Various recent epidemiological studies have indicated that exposure to low doses of environmental biologically active contaminants, such as biocides, during human development can have deleterious effects on cognitive development in childhood.

In this webinar **Prof. Pim Leonards, Institute for Environmental Studies, VU University of Amsterdam, Netherlands**, discusses the workflow to perform target and non-target metabolomics, and provides some examples to understand the underlying molecular mechanisms of observed effects of biocide exposure in rats in relation to behavior and cognitive changes.

[Click here](#) to register for the webinar on September 22, 4 pm CEST.

Register now for our Luncheon Seminars at HUPO 2016 in Taipei



We are pleased to invite you to join us in Taipei for the HUPO 15th Annual World Congress (HUPO 2016). This event is a highlight for the scientific community interested in proteomics research, development of new technologies, applications and training. We look forward to meet you at our **booth #18 + 24**.

The registrations for our **lunch seminars** are now open:

- Lunch seminar 1, September 19: “Uncompromised performance: Exploiting the potential of UHR-Q-TOF for discovery proteomics”
- Lunch seminar 2, September 20: “Answering the proteoforms challenge: alternative approaches for Biomarker Discovery”

[Click here](#) for complete details and to register.

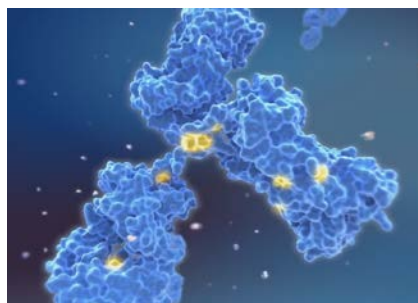
Join Bruker at the MipTec 2016 Exhibition



We invite you to join our Bruker team at this year's MipTec exhibition in Basel. Meike Hamester, Bruker Daltonics, will present her talk on “**Maldi mass spectrometry: a label-free solution for ultra-high-throughput screening**” during the “Best Abstracts Oral Session” on September 20. Jens Fuchser, Bruker Daltonics, will also be presenting the poster on “**Ultra-high mass resolution imaging reveals secondary metabolites produced during interaction of micro-organisms with higher organisms**”. We are looking forward to interesting discussions with you.

For more information about the MipTec, please [click here](#).

New Software Upgrade: DisulfideDetect 1.2



Bruker's DisulfideDetect software is a quantum leap in ease-of-use for detecting and evaluating disulfide bonds within therapeutic proteins, such as monoclonal antibodies. It provides an easy to understand, visually-based, workspace for disulfide bond analysis for both native and non-native bonds as well as inter- and intra-chain disulfide bonds within the protein/antibody.

We are pleased to announce **version 1.2 of DisulfideDetect software**. With this release several outstanding bugs are fixed and results visualization is much improved. After registration you can download the software for free ([click here](#)). If you would like to learn more about the software and the DisulfideDetection workflow, please go to our website on bruker.com.

New Application Note: Automated Quality Control of Active Pharmaceutical Ingredients (API) by LC-UV-ion trap MS using Compass Open Access



This Application Note shows a **case study on gamma-irradiated oxybutynin** clearly illustrating the additional value and complementary character of ion trap mass spectrometry in addition to UV detection for drug substance quality control (QC). Impurities were identified by Bruker software such as MetaboliteTools and FragmentationExplorer during the QC process. A completely automated workflow for a comprehensive QC of oxybutynin samples was established by the Bruker Compass OpenAccess QC software package.

[Click here to read the AppNote.](#)

New blog article: New tools in the box - meeting challenges in Biotherapeutics

**MASS
per SPECtive**

Protein pharmaceuticals are the fastest growing class of novel therapeutic and diagnostic agents, and a major focus in biopharmaceutical product development. Compared to small molecule drugs, their structure is immensely more complex. Mass spectrometry (MS) is mostly used in a "bottom-up" approach, which is limited because biotherapeutics are fragmented before analysis and the overall context within the protein sequence or between isoforms is lost. However, novelIMS methods that start with the intact protein have emerged. This **fast-growing toolbox of so-called "top-down" approaches** holds enormous potential in addressing challenges in biotherapeutics characterization.

[Click here](#) to read the full article.

Want to learn more?



On our [Webinar Portal](#) you can stream all of our webinars live and on-demand:

- July 26th: [Applications of GC-MS-MS and LC-Ion Trap MS-MS in Postmortem Forensic Toxicology](#)
- June 28th: [Streamlining Drug Development: Native LC-MS for Rapid Screening and Drug Product QC Release Testing of Antibody Drug Conjugates](#)
- June 28th: [Structure Elucidation with Trapped Ion Mobility Spectrometry](#)
- June 16th: [Uncovering Metabolic Pathways in Disease to Support Drug Discovery Using High Resolution MALDI Imaging Mass spectrometry](#)

Latest Literature

- Brochure: [MetaboScape® 2.0](#)
- Brochure: [solariX XR](#)
- Brochure: [Poster Hall Metabolomics Ed. III](#)
- Brochure: [timsTOF™](#)
- Brochure: [rapifleX™](#)
- Brochure: [PesticideScreener](#)
- Brochure: [ToxScreener](#)
- Brochure: [MetaboScape](#)
- Brochure: [Training Courses 1.0](#)
- Brochure: [MALDI Biotyper Poster Hall 2016](#)
- Flyer: [HDX Solution](#)
- Poster Note: [PN-35 A trial of TLC-MALDI for analysis of industrial materials](#)
- Poster Note: [PN-34 2ω-FT-ICR Mass Spectrometry](#)
- App-Note: [LCMS-116 What are we eating? MetaboScape® Software; Enabling the De-replication and Identification of Unknowns in Food Metabolomics](#)
- App-Note: [LCMS-115 Automated Quality Control of Active Pharmaceutical Ingredients \(API\) by LC-UV-ion trap MS using Compass Open Access](#)
- App-Note: [LCMS 114 Rapid Analysis of Low Level Testosterone in Serum with the Bruker EVOQ Elite LC-TQ](#)
- App-Note: [LCMS-113 Rapid Analysis of Low Level Estrogens in Serum with the Bruker EVOQ Elite LC-TQ](#)

with Quadrupolar Detection

Find more scientific contributions [here](#).

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