

Wednesday, November 7, 2012
LC/MS Symposium
Stravinski Hall

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LC/MS Symposium

09.00-09.05	Jan van der Greef Opening and Welcome <i>Chairman: Jan van der Greef</i>
09.05-09.50	<i>"Roland W Frei lecture"</i> Jan Smeitink OmicsTechnologies and Bioenergetics: Application to Human Disease
09.50-10.20	Coffee break

Parallel session LC-MS Technology and Applications – Stravinski Hall

	<i>Chairman: Rob Vreeken</i>
10.20-10.50	<i>Keynote lecture</i> Robert Mistrik Identification of Unknowns using Mass Spectral Library Cloud
10.50-11.05	Anna Pelander The Role of LC/TOFMS Qualitative Drug Screening in Forensic Toxicology Setting
11.05-11.20	Isabelle Schmitz-Afonso Dereplication of an Annonaceous Acetogenin Extract by LC-MS/MS using Post-column Lithium Infusion
11.20-11.35	Natthida Sriboonvorakul High Throughput LC-MS Method for Quantification of Small Organic Acids in Human Biological Fluids
11.35-11.50	Andrew Marriott Analysis of Carbohydrates and other Polar metabolites in Drought Stressed Plants by Porous Graphitic Carbon (PGC)-HPLC-MS
11.50-12.05	David S Bell Fundamental Investigation of Bio-SPME for the LC-MS Analysis of Small Molecules from Biological Fluids
12.05-12.35	<i>Keynote lecture</i> Jack Henion LC/MS today: From Applications for the Expert to Those for the 'Masses'
12.35-14.00	Lunch break
12.45-14.15	Lunch seminar: Agilent at the 2m2c, foyer level B6
12.45-14.15	Lunch seminar: Waters at the Fairmont Montreux Palace, Salle des Fêtes

Parallel session Clinical Chemistry – Foyer Stravinski B5

	<i>Chairman: Thomas Hankemeier</i>
10.20-10.50	<i>Keynote lecture</i> Brian Fowler Metabolic Networks and Inborn Errors of Metabolism - From Garrod to Metabolomics
10.50-11.20	<i>Keynote lecture</i> Steven Gross Untargeted Metabolite Profiling to Screen for Inborn Errors of Metabolism and Discover Mechanisms of Drug Action
11.20-11.35	Mariette Ackermans Determination of Thyroxin and its Metabolites in Tissue Using SPE UPLC Tandem MS
11.35-11.50	Therese Koal Standardized UHPLC-MS/MS based Steroid Hormone Profile-Analysis
11.50-12.05	Markus Meyer An Automated MS-based Screening Procedure for Clinical and Forensic Toxicology
12.05-12.35	<i>Keynote lecture</i> Karl-Siegfried Boos Current Trends in Clean-up of Biofluids for LC-MS/MS Analysis of Small Molecules
12.35-14.00	Lunch break
12.45-14.15	Lunch seminar: Agilent at the 2m2c, foyer level B6
12.45-14.15	Lunch seminar: Waters at the Fairmont Palace, Salle des Fêtes

**Wednesday, November 7, 2012
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14.00-15.30 **Poster session I - odd numbers**

Chairman: Jack Henion

15.30-16.05 *Plenary lecture*
Renato Zenobi
Novel Applications of Ambient Mass Spectrometry

Parallel session LC-MS Technology and Applications – Stavinski Hall

Chairman: Jack Henion

16.10-16.30 **Michael W Linscheid**
Understanding DNA Repair Mechanisms: New Insights into the Dynamics of Platinum Drug DNA Adduct Formation by means of HPLC/ICP MS

16.30-16.50 **Peter Lindenburg**
Development of Electromigration-driven Techniques for Metabolomics

16.50-17.05 **Josep Gibert**
Multidimensional HPLC+GC-MS vs. LC-MS-MS: Extended Use for Non-volatile and Polar Compounds in Clinical Analysis Using On-line Derivatization

17.05-17.20 **Pekka Keski-Rahkonen**
The Effects of Scan Speed, Mass Resolution, and Continuous Mass Axis Calibration on UHPLC-QTOF Data Quality in Non-Targeted Metabolomics

17.20-17.35 **Jean-Pierre Chervet**
Expanding Role of Electrochemistry/Mass Spectrometry in Life Sciences

17.35-19.00 Welcome reception

**Wednesday, November 7, 2012
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Parallel session Clinical Chemistry – Foyer Stravinski B5

Chairman: Steven Gross

16.10-16.30 **Pierluigi Mauri**
MudPIT Proteomics Analysis for Clinical Diagnosis

16.30-16.50 **Bertrand Rochat**
Exactive Plus High Resolution MS for Quan/Qual Analysis. A Focus on Quantification in Clinical Research Labs

16.50-17.05 **John Shockcor**
A UPLC/QToF Based Lipidomic Analysis of White Adipose Tissue from Rats after Dosing with a Peroxisome Proliferator Activated Receptor (PPAR)-pan Agonist

17.05-17.35 *Keynote lecture*
Piero Rinaldo
Information Management of Complex Metabolic Profiles in Population Screening and Individualized Medicine

17.35-19.00 Welcome reception

**Thursday, November 8, 2012
LC/MS Symposium**

Stravinski Hall

Chairman: Karl-Siegfried Boos

09.00-09.35

Plenary lecture

Thomas Hankemeier

Metabolomics: Opportunities for Personalized Medicine & Pharma

VENDOR NEWS SESSION

09.35-09.45

Benedicte Duret, ThermoFisher Scientific

Evaluation of Exactive Ultra High Resolution Mass Spectrometer in Targeted Screening Method for Urine Analysis in Comparison to Immunoassay and GC-MS Techniques

09.45-09.55

Theodore Sana, Agilent Technologies

Advances in LC/MS Instrumentation and Multi-Omics Data Interpretation Software Facilitates Targeted Pathway Survey of Antibiotic Challenged Mycobacterium Tuberculosis

09.55-10.05

James Murphy, Waters Corporation

The Development and Evaluation of a High Pressure Microfluidic Device for High-throughput Applications

10.05-10.15

Michael Becker, Bruker Daltonik GmbH

Parallel LC-MALDI and MALDI Imaging Workflow for Direct Identification of Biomarkers from Tissue

10.15-10.25

Marcus Mreyen, Shimadzu Europa GmbH

Latest Ultrafast Mass Spectrometry (UFMS) for Better Data Quality and Flexibility in the Throughput

10.25-10.55

Coffee break

10.55

Start of parallel sessions

**LC-MS Technology and Applications & Clinical Chemistry
and Metabolomics**

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Parallel session LC-MS Technology and Applications – Stravinski Hall

Chairman: Robert D. Voyksner

- 10.55-11.15 **Sebastiaan Eeltink**
Polymer Monolithic Columns for High-Resolution LC-MS Separations of Peptides and Protein Isoforms
- 11.15-11.35 **Patrick Arpino**
Identification of Methoxyisoflavone Metabolites in Human Urine by Ultra-Performance Liquid Chromatography Quadrupole Time-of-Flight Mass Spectrometry (UPLC-Q-TOF)
- 11.35-11.50 **Ralf Kellman**
Unified Mass Spectroscopy Control Database and its Application in Steroid Profiling
- 11.50-12.05 **Michael McGinley**
Developing New Paradigms for LC/MS Analysis of Intact Protein and Peptide Mixtures Using Core-Shell Columns
- 12.05-12.20 **Virginie Domalain**
Diastereomers Analysis by Ion Mobility – Mass Spectrometry: Influence of Cationisation
- 12.20-12.35 Open slot for last minute presentation
- 12.35-14.00 Lunch break
- 12.45-14.15 Lunch seminar: Thermo at the 2m2c, foyer level B6
12.45-14.15 Lunch seminar: Waters at the Fairmont Montreux Palace, Salle des Fêtes

Parallel session Metabolomics – Foyer Stravinski B5

Chairman: Brian Fowler

- 10.55-11.15 **Laurent Debrauwer**
Metabolomics for Food and Environmental Toxicology: from Targeted to Global Integrative Approaches
- 11.15-11.35 **James Cox**
The Use of Model Organisms in Metabolomics to Determine the Function of Genes in the Human Genome
- 11.35-11.50 **Hubert Chassaigne**
The Role of Untargeted Metabolomic Profiling Methods in In-vitro Systems Toxicology – Towards an Integrated Approach
- 11.50-12.05 **Yoshiaki Ohashi**
Combinatorial Approach of LC and CE/MS for Biomarker Finding, Biochemical Research, and Clinical Test Development
- 12.05-12.35 *Keynote lecture*
Nicola Zamboni
Deep Phenotyping of Cellular Metabolism by High Throughput, Accurate Mass Metabolomics
- 12.35-14.00 Lunch break
- 12.45-14.15 Lunch seminar: Thermo at the 2m2c, foyer level B6
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**Thursday, November 8, 2012
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14.00-15.30 **Poster session II - even numbers**

Stravinski Hall

Chairman: Renato Zenobi

15.30-16.05 *Plenary lecture*
Patrick Diel
Biomarker profiling and bioactivity assays - novel strategies in the fight against human doping

LC-MS Technology and Applications – Stavinski Hall

Chairman: Renato Zenobi

16.10-16.30 **Katrien Maes**
In Vivo Monitoring of Neuromedin N during Epileptic Seizures using Nano Liquid Chromatography-Electrospray Ionization-Tandem Mass Spectrometry

16.30-16.50 **Robert D Voyksner**
Identifying Peptide Markers to Peanut and Tree Nut Allergens using LC/Q-TOF-MS

16.50-17.05 **Marion Martignac**
Removal of Pharmaceutical Compounds by Advanced Oxidation Processes

Keynote lecture
17.05-17.35 **Holly D Cox**
Quantitation of Biomarkers for Growth Hormone Abuse in Dried Blood Spots

19.30-22.30 Conference dinner with aperitif at Fairmont Montreux Palace

Parallel session Metabolomics – Foyer Stravinski B5

Chairman: Rawi Ramautar

16.10-16.30 **Christoph Borchers**
Pathway-specific Metabolomics: Comprehensive Analysis of Central Carbon Metabolism Using LC-MS

16.30-16.50 **Sandra C Gouveia**
Targeted Metabolomics using LC-ESI/MS-MS to Study Adverse Health Effects of Air Pollutants on Asthma

16.50-17.05 **Nyasha Munjoma**
Synthesis of stable isotope labelled lipid standard using *Saccharomyces cerevisiae*

17.05-17.35 *Keynote lecture*
Gabi Kastenmüller
Genetics meets Metabolomics: Inborn Variations in Human Metabolism

19.30-22.30 Conference dinner with aperitif at Fairmont Montreux Palace

Friday, November 9, 2012
LC/MS Technology and Applications
Stravinski Hall

Chairman: Patrick Arpino

- 09.00-09.20 **Gaud Dervilly-Pinel**
The Potential of LC-HRMS Metabolomics Fingerprinting in Food Analysis:
Application to the Control of Forbidden Anabolic Practices in Breeding
Animals
- 09.20-09.40 **Tiina Kauppila**
Desorption Atmospheric Pressure Photoionization-Mass Spectrometry
- 09.40-09.55 **Yee-Soon Ling**
Developmental of NP-RP 2D-LC MS/MS in Enhancing Phosphatidylcholine
and Ceramide Species Profiling for Mice Liver Post-Naphthalene Exposure
- 09.55-10.10 **Kevin McCann**
Low pg/ml Detection of 17 β -Estradiol in Serum through Increased Ion
Sampling Efficiency Using Dual Ion Funnel LC/MS/MS Technology
- 10.10-10.25 **Subodh B. Nimkar**
What does High Resolution Accurate Mass (HR/AM) Analysis buy you in
the Quantitative Analysis of Anabolic Steroids
- 10.25-10.55 Coffee break
- Chairman: Ruud Berger*
- 10.55-11.25 *Key-note lecture*
Katharina Rentsch
The role of LC-MS in the Automated Clinical Laboratoy
- 11.25-11.45 **Kati Hanhineva**
Non Targeted LC-MS Metabolite Profiling Highlights the Between- Tissue
Differences caused by High-fat Diet in a Pig Model
- 11.45-12.05 **Augustin Scalbert**
Characterization of the Polyphenol Metabolome by High Resolution Mass
Spectrometry in Urine Samples from the EPIC Cohort
- 12.05-12.10 Announcement next Montreux meeting
- 12.10-12.20 "Roland W. Frei "- Poster Award
presented by the President of the IAEAC
- 12.20-12.25 **Thomas Hankemeier**
Closure of the meeting