

## M A R I C A

## D A I - I C H I

23<sup>rd</sup> June 2014

- 10:50-12:10** **Workshop I:** Metabolomics Measurement Technology and Application & Introduction to Worldwide Networks
- 12:30-13:20** **Bruker Luncheon**
- 13:40-16:40** **Workshop II:** Metabolomics data standards, data capture and exchange
- 17:00-17:40** **Opening Ceremony**
- 17:40-18:20** Metabolomics revolutionizes phytochemical genomics and crop improvement.

*Kazuki Saito*

24<sup>th</sup> June 2014

**08:40-09:20** Live feed

- 09:30-10:10** **From mice to man and back again: Applications of metabolomics to understand type 2 diabetes and obesity**

*Julian L Griffin*

## Drug &amp; Medicine

- 10:30-10:45** Ceramide metabolism in the liver and its role in two lysosomal lipidoses - drug-induced phospholipidosis (DIPL) and Sandhoff disease (SD)

*Emmanuelle Lecommandeur*

- 10:45-11:00** In search of metabolic somnogens: A unique signature of sleep restriction from blood in rats

*Arjun Sengupta*

- 11:00-11:15** Activation of fatigue metabolic pathway induces hepatic inflammation in a rat model of fatigue

*Satoshi Kume*

- 11:15-11:30** Metabolomics biomarkers of doxorubicin-induced cardiac injury in B6C3F1 mice

*Laura K Schnackenberg*

- 11:30-11:45** Metabolomics used as a tool to investigate the signature of etanercept treatment response in a psoriasis patient cohort

*Nicholas Rattray*

- 11:45-12:00** Using metabolomics to determine the modes of action of new antibiotics

*Isabel Vincent*

**12:30-13:20** Shimadzu Luncheon

## CVD, Diabetes &amp; Neuroscience

- 13:40-13:55** Longitudinal metabolome en route to type 1 diabetes: potential role of gut microbiota and metabolic vulnerability in the early disease pathogenesis

*Matej Oresic*

- 13:55-14:10** Large scale metabolomics in clinical epidemiology

*Oliver Fiehn*

- 14:10-14:25** Examining the effects of metformin in a large clinical cohort, HepG2 and 3T3-L1 treated cells using untargeted LC-MS metabolomics.

*Emma Boulton*

- 14:25-14:40** Metabolome and lipidome features of human brain development.

*Kasia Bozek*

- 14:40-14:55** Accumulation of metabolic syndrome risk factors and plasma amino acids and their related metabolites: Tsuruoka metabolomic cohort study

*Toru Takebayashi*

**15:00-17:00** Poster Session I

25<sup>th</sup> June 2014

**08:40-09:20** Making metabolomics matter

*David S Wishart*

- 09:30-10:10** **Metabolomics and the measurement of the exposome in epidemiological studies on cancer risk**

*Augustin Scalbert*

## Nutrition, Environment &amp; Model Organism

- 10:30-10:42** Characterization of food products by GCxGC with ToF-MS and GC with high resolution ToF-MS: a food-omics approach

*Jeff Patrick*

- 10:42-10:54** A metabolomics approach shows that green tea extract attenuates UVB-induced skin metabolite alterations in mice

*Eun Sung Jung*

- 10:54-11:06** Non-targeted metabolite profiling discriminates diet-specific biomarkers for consumption of whole grains, fatty fish and bilberries

*Kati Hanhineva*

23<sup>rd</sup> June 2014

- 10:50-12:10** **Workshop I:** Effective metabolomics software: From design to practice
- 12:30-13:20** **LECO Luncheon**
- 13:40-16:40** **Workshop II:** Early-career member network of Metabolomics Society

**17:40-18:20** Live feed

**18:40-19:30** Welcome Reception

24<sup>th</sup> June 2014

**08:40-09:20** Natural variation of a signalling lipid

*Markus Wenk*

- 09:30-10:10** **Use of metabolomics in systems biology: from data to understanding**

*Bas Teusink*

## Flux, Microbiology &amp; Parasitology

- 10:30-10:45** Identification of the metabolic reprogramming underlying metastasis in prostate cancer by combining multi-omic approach and model-driven data analysis

*Marta Cascante*

- 10:45-11:00** OpenMeubius: An open source software for metabolic flux analysis

*Hiroshi Shimizu*

- 11:00-11:15** Quantitative metabolic modeling for biofuel production at the Joint BioEnergy Institute

*Hector Garcia Martin*

- 11:15-11:30** Stable-isotope labelled metabolomics for network-wide discovery of stage-specific pathways in *Trypanosoma brucei*

*Darren Creek*

- 11:30-11:45** An altered *M. tuberculosis* metabolome induced by katG mutations resulting in drug resistance

*Du Toit Loots*

- 11:45-12:00** LC-HRMS fingerprinting: an innovative strategy to investigate bacterial metabolome during cheese ripening

*Clementine Le Boucher*

**12:30-13:20** Agilent Luncheon

## Cancer

- 13:40-14:00** Oncometabolites: Linking altered metabolism with wancer?

*Patrick Pollard*

- 14:00-14:20** Finding the right path: Constructing a temporal network of RAS activity in cancer

*Emily Armitage*

- 14:20-14:40** Lipidomic profiling reveals a reconfiguration of sphingolipid metabolism that drives glioma angiogenesis and malignancy

*Anthony Don*

- 14:40-15:00** Enhanced pyruvate carboxylation is crucial to non-small cell lung cancer proliferation and anabolism

*Teresa Fan*

**15:00-17:00** Poster Session I

**17:00-18:20** Thermo Scientific Evening Session

25<sup>th</sup> June 2014

**08:40-09:20** Live feed

- 09:30-10:10** **Metabolomics imaging mass spectrometry in clinical research**

*Mitsutoshi Setou*

## Data Analysis, Networks

- 10:30-10:44** Complimentary LC-MS and GC-MS techniques provide broader coverage of the metabolome

*Baljit Ubhi*

- 10:44-10:58** An advanced computational and database framework for the compound identification in untargeted metabolomics

*Robert Mistrik*

- 10:58-11:12** MS DIAL: Untargeted metabolomics software for data independent LC-MS/MS and mass spectral deconvolution: application to algae metabolomics

*Hiroshi Tsugawa*

## M A R I C A

## D A I - I C H I

25<sup>th</sup> June 2014(cont)

- 11:06-11:18** The secret life of the mediterranean lake Medee, the largest deep sea salt saturated formation in the world  
*David Rojo*
- 11:18-11:30** Differential lipid and metabolite levels in response to spawning-induced inappetence in Atlantic salmon *Salmo salar*  
*McKenzie Smith*
- 11:30-11:42** A metabolomic approach to assess neurotoxic effects of imidacloprid on the freshwater snail *Lymnaea stagnalis*  
*Sara Tufi*
- 11:42-11:54** Using omics for identification of the mechanism of the toxic action for perfluorononanoic acid  
*Kasper Skov*
- 11:54-12:06** Metabolome analysis of *Drosophila melanogaster* during embryogenesis  
*Thuy An Phan Nguyen*

## 12:30-13:20 HMT Luncheon

## Young Researchers

- 13:40-13:55** Characterization of the sweat metabolome in screen-positive cystic fibrosis patients  
*Adriana Nori de Macedo*
- 13:55-14:10** Fatty acid profiling in breast cancer biomarker discovery by GC-MS  
*Huai-Hsuan Chiu*
- 14:10-14:25** Metabolome and transcriptome changes in human, macaque and mouse brain development  
*Hindrike Bammann*
- 14:25-14:40** Metabolomics analysis reveals large effects of uremic toxin in heart failure outcome  
*Cheng-Cheng Lin*
- 14:40-14:55** Metabolic changes in stress-tolerant transgenic rice overexpressing calmodulin  
*Surachat Tangpranomkorn*

## 15:00-17:00 Poster Session II

## 17:00-18:20 ABSCIEX Evening Session

26<sup>th</sup> June 2014

- 08:40-09:20** Identifying novel salinity tolerance mechanisms by spatial analysis of lipids in barley roots  
*Ute Roessner*

## Plant Physiology

- 09:30-09:45** Integrated metabolomics, gene expression, and GWAS identify new saponin biosynthetic genes in *Medicago truncatula*  
*Lloyd Sumner*
- 09:45-10:00** Metabolomic exploration toward understanding of key cellular events leading to wax ester fermentation in *Euglena gracilis*  
*Takumi Ogawa*
- 10:00-10:15** Monitoring primary carbon metabolism in mature *Arabidopsis thaliana* leaves  
*Pernilla Linden*
- 10:15-10:30** Untargeted metabolomics of Habanero pepper (*Capsicum chinense* Jacq. var. Orange) fruits subject to nitrogen and phosphorus deficiency  
*Carlos Rodriguez-Lopez*

## Crops

- 10:50-11:06** Composition and metabolite differences between near-isogenic gm and conventional maize are associated more with back-crossing than with the gm traits  
*Mark Leibman*
- 11:06-11:22** The application of metabolomics to the biochemical phenotyping of staple crops from developing countries  
*Elisabete Carvalho*
- 11:22-11:38** GC-MS based metabolite profiling of barley kernels-impact of induced drought-stress  
*Alexandra Wenzel*
- 11:38-12:54** Combining metabolomic profiling and sensory evaluation to understand consumer perception of rice flavor  
*Venea Dara Daygon*
- 11:54-12:10** Allelopathy in canola  
*Md Asaduzzman*

## 12:30-13:20 Waters Luncheon

- 13:40-14:20** GoogleMap-type view of specialized molecules from microbes, their communities and hosts including people  
*Pieter C Dorrestein*

## 14:20-14:50 Closing Ceremony

25<sup>th</sup> June 2014(cont)

- 11:12-11:26** MASTR-MS: A web-based collaborative Laboratory Information Management System (LIMS) for metabolomics  
*Saravanan Dayalan*
- 11:26-11:40** Data-driven sample size determination for human metabolic phenotyping studies  
*Benjamin Blaise*
- 11:40-11:54** Searching PubChem with tandem mass spectrometry data: Teaming molecular fingerprint prediction and fragmentation trees  
*Sebastian Boecker*
- 11:54-12:08** Systematic approaches for identification and removal of non-biological sources of variation in metabolomics data  
*Rohan Benjamin Hugh Williams*

## 12:30-13:20 ABSCIEX Luncheon

## Young Researchers

- 13:40-13:55** Construction of a metabolome library for transcription factor-related single gene mutants of *Saccharomyces cerevisiae*  
*Zanariah Hashim*
- 13:55-14:10** Metabolomics-based semi-rational identification of gene targets conferring 1-butanol tolerance in *Saccharomyces cerevisiae*  
*Shao Thing Teoh*
- 14:10-14:25** Quantitative analysis of stressed *Caenorhabditis elegans* using isotopic ratio outlier analysis  
*Gregory S Stupp*
- 14:25-14:40** Global metabolomic analysis of <sup>13</sup>C-enriched mixtures using INADEQUATE  
*Chaevien S Clendinen*
- 14:40-14:55** Classification of reliable MetFrag candidate identifications for tandem mass spectra from selected lipid samples.  
*Christoph Ruttkies*

## 15:00-17:00 Poster Session II

## 19:00-21:00 The Metabolomics Society Banquet

26<sup>th</sup> June 2014

- 08:40-09:20** Googling biology using gene networks  
*Insuk Lee*

## New Technology

- 09:30-09:50** A novel multi-platform software tool (MUSCLE) for the robust, objective and automated optimisation of targeted LC-MS/MS analyses  
*Mark Viant*
- 09:50-10:10** CSPP networks aid the detection of *in vivo* substrates and products of enzymes  
*Kris Morreel*
- 10:10-10:30** Comprehensive two-dimensional liquid chromatography: a new technique for high-resolution metabolomics?  
*Oliver Jones*

## Omics Integration

- 10:50-11:06** A unique brain lipidome and metabolome biosignature in alzheimer disease  
*Giuseppe Astarita*
- 11:06-11:22** <sup>13</sup>C-based Metabolomics: Integrating LC-MS IROA with NMR  
*Arthur Edison*
- 11:22-11:38** MetaboLights: Open access metabolomics repository and reference data  
*Reza Salek*
- 11:38-11:54** Reconstruction of global signal flow of insulin from phosphoproteome and metabolome data  
*Katsuyuki Yugi*
- 11:54-12:10** A catalog of human metabolic individuality  
*Gabi Kastenmuller*

## 12:30-13:20 Thermo Scientific Luncheon

- 13:40-14:20** Live feed