

# Program

Version: 01 June 2012

# MONDAY, June 25

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8:00 A.M. – 10:00 P.M. Registration  
9:45 A.M. – 10:15 A.M. Break

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## Hall B South

10:15 A.M. Workshop: **Software Showcase I**  
*Session Chairs: Steffen Neumann, Sandra Castillo*

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## Lincoln 2-4

10:15 A.M. Workshop: **Practice of Mass Spectrometry-based Metabolomics: Debating Current Hot Issues**  
*Session Chairs: Thomas Hankemeier, Ute Roessner, Oliver Fiehn*

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## Hall B South

12:00 P.M. Vendor Sponsored Lunch Session  
*LECO Corporation – Platinum Sponsor*  
**High Performance Analytical Tools for Lipidomics and Metabolomics**  
*Jeff Patrick – LECO Corporation*

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1:00 P.M. – 1:30 P.M. Break

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## Hall B South

1:30 P.M. Workshop: **Software Showcase II**  
*Session Chairs: Steffen Neumann, Sandra Castillo*

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## Lincoln 2-4

1:30 P.M. Workshop: **Practical NMR For Metabolomics Studies**  
*Session Chairs: Quincy Teng, Jane Ward, Tracey Schock*

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3:00 P.M. – 3:30 P.M. Break

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## Hall B South

3:30 P.M. Workshop: **Statistics and Models**  
*Session Chairs: David Broadhurst, Sudeepa Bhattacharyya*

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## Lincoln 2-4

3:30 P.M. Workshop: **Analytical QC Measures for Interlaboratory Comparability**  
*Session Chairs: Dan Bearden, Mark Viant, Laura Schnackenberg*

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5:00 P.M. – 5:30 P.M. Break

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## Hall B South

5:30 P.M. **Opening Plenary Session**  
**O-001: Metabolomics in Drug Development – Pharmacometabolomics**  
*Frank J. Gonzalez – Laboratory of Metabolism, Center for Cancer Research, National Cancer Institute, National Institutes of Health.*

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7:00 P.M. – 10:00 P.M. **Reception**

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# TUESDAY, June 26

7:00 A.M. – 10:00 P.M. Registration

## Hall B South

7:30 A.M. – 8:30 A.M. Vendor Sponsored Breakfast Session

*Waters Corporation – Silver Sponsor*

### ***A Lipidomic Analysis of White Adipose Tissue from Rats After Dosing with a Peroxisome Receptor (PPAR)-pan Agonist***

*John P. Shockcor, Waters Corporation*

and

### ***Metabolomics in Stress Signal Transduction Studies***

*Albert J. Fornace, Jr., MD, Georgetown University*

## Hall B South

9:00 A.M. – 9:45 A.M. **Plenary Session**

### ***O-002: Environmental Metabolomics: Past, Present and Future***

*Mark R. Viant – Professor of Metabolomics, School of Biosciences, University of Birmingham, UK*

9:45 A.M. – 10:15 A.M. Break

## Hall B South

10:15 A.M. – 11:45 A.M.

### **Medicinal Metabolomics**

*Session Chairs: Rima Kaddurah-Daouk, Don Robertson*

**10:15** O-005: *Global Metabolite Profiling Reveals Thymineless Death as an Unexpected Mechanism of Cytotoxicity by the Colon Cancer*

*Chemopreventive Agent Difluoromethylornithine*  
**Steven Gross**, Weill Cornell Medical College

**10:40** O-006: *Metabolomics: new opportunities for personalized medicine & pharma*

**Thomas Hankemeier**, Leiden University/NMC

**11:05** O-007: *A high-resolution lipid profiling study of Lipodystrophy: a systems medicine approach to understanding the mechanistic causes of Insulin Resistance*

**Michael Eiden**, Medical Research Council - Human Nutrition Research

**11:25** O-008: *Understanding and Targeting Metabolism for Drug Discovery in Multifactorial Diseases*

**Marta Cascante**, University of Barcelona

## Lincoln 2-4

10:15 A.M. – 11:45 A.M.

### **Environment & Ecology**

*Session Chairs: Dan Bearden, Karen Machin*

**10:15** O-009: *The importance of genotype in environmental monitoring by metabolomics: applications with the soil super-sentinel organism *Lumbricus rubellus**

**Jake Bundy**, Imperial College London

**10:40** O-010: *Metabolomics for Biomonitoring in Waterways Exposed to Wastewater Treatment Plant Effluents*

**David Skelton**, United States Environmental Protection Agency

**11:05** O-011: *Metabolomics reveals key metabolites that convert drosophilid larvae to a freeze tolerant organism*

**Petr Simek**, Biology Centre, Czech Academy of Sciences

**11:25** O-012: *The Investigation into Cheetah (*Acinonyx Jubatus*) Mortalities at a Captive Breeding Facility In South Africa: Preliminary Findings using a Metabolomic Approach*

**Adrian Tordiffe**, National Zoological Gardens of South Africa

## Hall B South

12:00 P.M. Vendor Sponsored Lunch Session

*Agilent Technologies – Platinum Sponsor*

### **Advances in Instrumentation and Software for Metabolomics Research**

*Jennifer Gushue, Ph.D., Theodore Sana, Ph.D. and Norton Kitagawa, Ph.D. – Agilent Technologies*

## Lincoln 2-4

12:00 P.M. Vendor Sponsored Lunch Session

*Metabolon – Platinum Sponsor*

### **Application of Global Metabolomics in Drug Discovery**

*Dr. John Ryals, CEO, Metabolon, Inc.*

1:00 P.M. – 1:30 P.M. Break

## Hall B South

1:30 P.M. – 3:00 P.M.

### **Human Disease and Health Biomarkers I - Metabolomics in Women's and Children's Health**

*Session Chairs: Rick Beger, Rick Dunn*

**1:30** O-013: *Metabolomics in infant nutrition: metabolic implications of different feeding practices*  
**Aifric O'Sullivan**, UC Davis

**1:55** O-014: *An Integrated Study of Biofluids: Metabolic Profiling for Prenatal Health Monitoring*  
**Ana Maria Gil**, University of Aveiro

**2:20** O-015: *Profiling Precursor-Product Ratio In Newborn Screening Of Congenital Adrenal Hyperplasia*  
**Paul Lee**, LA Biomedical Research Institute, Harbor-UCLA Medical Center

**2:40** O-016: *Progression to celiac disease is associated with systemic lowering of serum molecular lipids*  
**Marko Sysi-Aho**, VTT Technical Research Centre of Finland

## Lincoln 2-4

1:30 P.M. – 3:00 P.M.

### **Plant I – Developments in Plant Metabolomics**

*Session Chairs: Robert Hall, Lloyd Sumner*

**1:30** O-017: *In Vivo Flux Probing of Interactions between Leaf Development and Environmental Stresses*

**Alexander Erban**, Max Planck Institute of Molecular Plant Physiology

**1:55** O-018: *Plant metabolomics – PARAFAC2 resolution of bioactive triterpenoid saponins in LC-MS profiles from *Barbarea vulgaris* and implications for plant-insect interactions*  
**Bekzod Khakimov**, University of Copenhagen

**2:20** O-019: *Developing qualitative LC-MS methods for characterizing plant metabolites in NIST Standard Reference Materials (SRMs)*  
**Mark Lowenthal**, National Institute of Standards and Technology

**2:40** O-020: *Enhancing glycolysis in rice plants under deep water conditions*  
**Miyako Kusano**, RIKEN, PSC

3:00 P.M. – 3:30 P.M. Break

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**Hall B South**

3:30 P.M. – 5:00 P.M.

**Systems Biology and Pathways***Session Chairs: Alistair Fernie, Silas Villas-Bôas*

**3:30** O-021: *Generating and Curating High-Quality Metabolic Models using Chemical Structure*  
**John May**, EMBL-EBI

**3:55** O-022: *Generalized and exact <sup>13</sup>C metabolic flux ratio analysis for complex systems*  
**Manuel Hörl**, Institute of Molecular Systems Biology, ETH Zurich

**4:20** O-023: *Mining the unknown: A systems approach to metabolite identification combining genetic and metabolic information*  
**Jan Krumsiek**, Helmholtz Zentrum München

**4:40** O-024: *Super model of the world – Enterococcus faecalis*  
**Carla Portela**, University of Auckland

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**Lincoln 2-4**

3:30 P.M. – 5:00 P.M.

**Understanding Microbial Metabolism with Metabolomics***Session Chairs: Per Bruheim, Masaru Tomita*

**3:30** O-025: *In vitro metabolic pathway reveals the action of enzyme effectors*

**Natsumi Saito**, Institute for Advanced Biosciences, Keio University

**3:55** O-026: *A novel degradation mechanism, not feedback to CarAB or PyrBI, maintains pyrimidine end-product levels in Escherichia coli*  
**Marshall Louis Reaves**, Princeton University

**4:20** O-027: *Metabolome analysis of Enterococcus faecalis during oxidative stress reveals the role of menaquinone biosynthesis in the oxidative stress management of this bacterium*  
**Silas Villas-Boas**, The University of Auckland

**4:40** O-028: *Rapid detection and quantification of food spoilage*  
**Roy Goodacre**, University of Manchester

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5:00 P.M. – 5:30 P.M.      Break

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5:30 P.M. – 7:00 P.M.      **Posters and Social (Even Numbered Posters)**

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**Hall B South**

7:00 P.M. – 10:00 P.M.

**Special Interest Session  
Bottlenecks in Metabolomics  
Research**

*Rima Kaddurah-Daouk, Chair*  
*Panel of experts: David Wishart,*  
*Thomas Hankemeier, Jules*  
*Griffin, Christoph Steinbeck,*  
*Shankar Subramaniam, Oliver*  
*Fiehn and Daniel Raftery*

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**Lincoln 2-4**

7:00 P.M. – 8:30 P.M.

**Special Interest Session  
Biomarkers**

*Richard Beger, Chair*  
*Panel of experts: Chris Leptak,*  
*Chris Beecher, and John*  
*Thomas*

# WEDNESDAY, June 27

7:00 A.M. – 10:00 P.M. Registration

## Hall B South

8:00 A.M. – 8:45 A.M. Vendor Sponsored Breakfast Session  
*Biocrates Life Sciences – Bronze Sponsor*

## Hall B South

9:00 A.M. – 9:45 A.M. **Plenary Session**  
**O-003: Metabolomics as a Tool for Plant Breeding**  
*Alisdair Fernie – Central Metabolism, Max-Planck-Institute for Molecular Plant Physiology*

9:45 A.M. – 10:15 A.M. Break

## Hall B South

10:15 A.M. – 11:45 A.M.  
**New Technology & Measurements I – Applications**

*Session Chairs: Dan Bearden, Quincy Teng*  
**10:15** O-029: *Integration of carbon, nitrogen, and oxygen metabolism in Escherichia coli*  
**Daniel Amador-Noguez**, Princeton University

**10:40** O-030: *Direct Analysis in Real Time (DART) for Fast Untargeted Metabolomic Profiling of Human Serum*  
**Facundo Fernandez**, Georgia Institute of Technology

**11:05** O-031: *New Experimental Approaches in Metabolomics with the Nematode C. elegans*  
**Arthur Edison**, University of Florida

**11:25** O-032: *The Application of Hyphenated Thermal Desorption Electrospray Ionisation-Ion Mobility-Mass Spectrometry to the Targeted Analysis of Volatile Biomarkers from Human Skin and Breath*  
**Helen Martin**, Loughborough University

## Lincoln 2-4

10:15 A.M. – 11:45 A.M.  
**Plant II – Plant Physiology and Metabolism**

*Session Chairs: Ute Roessner, Kazuki Saito*  
**10:15** O-033: *<sup>1</sup>H-NMR-MS Metabolomic Analysis of Arabidopsis Uncovers a Novel, Nitrate-Gated, Carbon Flux Safety Valve*  
**Jane L Ward**, Rothamsted Research

**10:40** O-034: *Exploiting Chemical Diversity for Triterpene Saponin Gene Discovery in Medicago truncatula*  
**Lloyd W. Sumner**, The Samuel Roberts Noble Foundation

**11:05** O-035: *The Role of Hydroxycinnamic Acid Amides for Pathogen Defense of Potato*  
**Melanie Dobritsch**, Leibniz Institute of Plant Biochemistry

**11:25** O-036: *Prediction of freezing tolerance of natural Arabidopsis accessions using metabolomics from field trials and controlled chamber experiments*  
**Ellen Zuther**, Max-Planck-Institute of Molecular Plant Physiology

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**Hall B South**

12:00 P.M. Vendor Sponsored Lunch Session

*Bruker – Platinum Sponsor*

**Strategies for Fast De-replication and Unknown Identification in LC-MS-based Metabolomics**

*Dr. Friederike Teichert - Bruker Daltonik GmbH, Bremen, Germany and*

**NMR-based Screening of Neonate Urines**

*Dr. Manfred Spraul, Claire Canet, David Krings - Bruker Biospin GmbH, Silberstreifen, Rheinstetten, Germany*

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**Lincoln 2-4**

12:00 P.M. Vendor Sponsored Lunch Session

*Thermo Scientific – Platinum Sponsor*

**Finding the REAL Difference Metabolomics with Q Exactive MS and the New SIEVE Software**

*and m/z Cloud™ - Novel Spectral Library for Metabolite Identification*

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1:00 P.M. – 2:00 P.M. **Poster Viewing (Odd Numbered Posters)**

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**Hall B South**

2:00 P.M. – 3:30 P.M.

**Human Disease and Health Biomarkers II - Understanding Complex Diseases through Metabolomics**

*Session Chairs: Dan Raftery, Mikhail Bogdanov*

**2:00** O-037: *Fumarate hydratase deficient cancer cells exhibit reversed urea cycle activity and excrete the biomarker argininosuccinate*  
**Leon Zheng**, Cancer Research UK, Beatson Institute

**2:25** O-038: *Targeted Metabolic Profiling of Hepatocellular Carcinoma and Hepatitis C using LC-MS/MS*  
**Hamid Baniasadi**, Purdue University

**2:50** O-039: *Translational Metabolomics and Genomics for Chronic Obstructive Pulmonary Disease (COPD): Discovering a Promising Role for Sphingolipids*  
**Nichole Reisdorph**, National Jewish Health

**3:10** O-040: *Early detection of Alzheimer's disease in blood and cerebrospinal fluid using metabolomics*  
**Matej Oresic**, VTT Technical Research Centre of Finland

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**Lincoln 2-4**

2:00 P.M. – 3:30 P.M.

**Plant III – Applied Genetical Metabolomics**

*Session Chairs: Mike Beale, Robert Hall*

**2:00** O-041: *Drought in Wheat: Combining Genetics and Metabolomics to Identify Novel Traits Related to Drought Tolerance*  
**Ute Roessner**, The University of Melbourne

**2:25** O-042: *Metabolome quantitative trait loci analysis for investigation of genotype–phenotype associations in rice*  
**Kazuki Saito**, RIKEN Plant Science Center

**2:50** O-043: *Identification of metabolites associated with quality traits in barley (*Hordeum vulgare*) using a non-targeted indiscriminate MS/MS metabolomics approach*  
**Adam Heuberger**, Colorado State University

**3:10** O-044: *Metabolomics-assisted breeding based on metabolite profiling and discovery of key genes of secondary metabolism*  
**Takayuki Tohge**, Max-Planck-Institut für Molekulare Pflanzenphysiologie

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3:30 P.M. – 4:00 P.M. Break

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## Hall B South

4:00 P.M. – 5:30 P.M.

### Safety Monitoring and Biomarkers

Session Chairs: Richard Beger, Mike Reily

**4:00** O-045: *Metabolomic Screening for Toxicological and Efficacy Markers in Drug Discovery*

**Nelly Aranibar**, Bristol-Myers Squibb

**4:25** O-046: *Detection of Idiosyncratic Hepatotoxicity Potential with Metabolite Profiling*

**Hennicke Kamp**, BASF SE

**4:50** O-047: *Metabolomics Revealed the Impact of Isonazid on the Endobiotics in Mouse Liver*

**Feng Li**, Kansas University Medical Center

**5:10** O-048: *Identification of Urinary Biomarkers of Ionizing Radiation Exposure in Non-Human Primates by MS-based Metabolomics*

**Caroline Johnson**, NCI/NIH

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## Lincoln 2-4

4:00 P.M. – 5:30 P.M.

### Student Presentations (15 minutes each)

Session Chairs: Jules Griffin, Jake Bundy

**4:00** O-049: *Metabolite Profiling of *Deinococcus radiodurans* to Discover the Basis for Radioresistance Conferred by Endogenous Nitric Oxide*

**Alex Hansler**, Weill Cornell Graduate School of Medical Sciences

**4:15** O-050: *Metabolomics approach for characterizing fatty acid synthesis pathway – a target for brain tumour therapies*

**Ngoc Ha Dang**, University of Calgary

**4:30** O-051: *Chemometric-assisted tool on plant metabolomics: Chemotypes distribution from *Solanum* species using PARAFAC-HCA method*

**Alan Pilon**, Institute of Chemistry-UNESP

**4:45** O-052: *Fast and sensitive metabolic profiling of very polar metabolites using HILIC chromatography and capillary-flow UPLC-MS*

**David Jonathan Fischer**, Functional Genomics Center Zurich

**5:00** O-053: *Metabolomic profile of colorectal cancer patients shows reproducibility in pre-operative and intra-operative conditions*

**Farshad Farshidfar**, University of Calgary

**5:15** O-054: *Maternal urine metabolic profiling: a means to follow the metabolic adaptations throughout pregnancy and predict prenatal disorders*

**Silvia Oliveira Diaz**, University of Aveiro

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5:30 P.M. – 6:00 P.M.

Break

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6:00 P.M. – 9:00 P.M.

## Conference Banquet

Join us at the National Zoo (Walking Distance)

3001 Connecticut Ave., NW

Washington, DC 20008

*BBQ Dinner Reception at the Great Cats Exhibit*

- All-American BBQ Dinner with both meat and meatless options
  - Reception and Dinner also includes All-U-Can-Drink Beverages
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# THURSDAY, June 28

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7:00 A.M. – 10:00 P.M. Registration

## Hall B South

8:00 A.M. – 8:45 A.M. Vendor Sponsored Breakfast Session  
*Metanomics Health – A BASF Group Company – Bronze Sponsor*

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## Hall B South

9:00 A.M. – 9:45 A.M. **Plenary Session**  
**O-004: How to Cheat with Chemometrics**  
*Rasmus Bro – Professor, Copenhagen University, Faculty of Life Sciences*

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9:45 A.M. – 10:15 A.M. Break

## Hall B South

10:15 A.M. – 11:45 A.M.

### Databases and Data Analysis

*Session Chairs: Christoph Steinbeck, Eldon Ulrich*

**10:15** O-055: *MetaboLights: a Database for Metabolomics Experiments and Derived Information*  
**Kenneth Haug**, European Bioinformatics Institute

**10:40** O-056: *MzMatch/mzMatch.R: an Open Source Software for the Sequential Processing and Analysis of Mass Spectrometry Data*  
**Andris Jankevics**, University of Groningen

**11:05** O-057: *Metabolomics Using an Automated Metabolite Identification Pipeline*  
**Julio Peironcely**, TNO Research Group Quality & Safety

**11:25** O-058: *Differential Correlation Networks as Complex Phenotypes in Metabolomics*  
**Timothy Ebbels**, Imperial College London

## Lincoln 2-4

10:15 A.M. – 11:45 A.M.

### Nutritional Metabolomics

*Session Chairs: Isabel Bondia-Pons, Vijayalakshmi Varma*

**10:15** O-059: *Regulated, Non-Stochastic Modulation of the Fatty Acyl Composition of Rat Liver Mitochondrial Cardiolipins in Response to Diet*  
**Bruce Kristal**, Brigham and Women's Hospital

**10:40** O-060: *Discovery of Metabolomics Biomarkers of Nuts Consumption to Decipher the Role in the Improvement of the Metabolic Syndrome Status*  
**Cristina Andres-Lacueva**, University of Barcelona

**11:05** O-061: *A data driven strategy to discover dietary biomarkers and validate new diet recording tools suitable for epidemiological studies*  
**John Draper**, IBERS

**11:25** O-062: *Metabolomics Analysis of Cultured HepG2 Liver Cell Line Reveals Fructose Structure and Hexose Concentration Dependent Changes in Metabolite Profiles*  
**John Meissen**, UC Davis

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11:45 A.M. Lunch break

1:00 P.M. – 2:00 P.M. **Poster Viewing (Odd Numbered Posters)**

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**Hall B South**

2:00 P.M. – 3:30 P.M.

**Human Disease and Health  
Biomarkers III - Pathophysiology and  
Metabolic Pathways***Session Chairs: Ana Maria Gil, Matej Oresic***2:00** O-063: *Liver fat changes the metabolic flexibility of the liver in non-alcoholic fatty liver disease***Tuulia Hyotylainen**, VTT Technical Research Centre of Finland**2:25** O-064: *Quantitation of Intracellular Metabolic Fluxes in Cancer Cell Lines***Jing Fan**, Princeton University**2:50** O-065: *ATP-related 1H/13C NMR Metabolomic Analysis in a Neonatal Rat Brain Slice Model of Oxygen-Glucose Deprivation Followed by Mild Hypothermia Treatments***Jia Liu**, University of California, San Francisco**3:10** O-066: *NMR Metabolomics of Blood Plasma and Urine: Potential in Lung Cancer Screening and Diagnosis***Iola Duarte**, University of Aveiro**Lincoln 2-4**

2:00 P.M. – 3:30 P.M.

**New Technology and Measurements  
II - Technology***Session Chairs: Thomas Hankemeier, Du Toit Loots***2:00** O-067: *High-Resolution Metabolomics to Operationalize the Exposome***Dean Jones**, Emory University**2:25** O-068: *Characterization of couarray identified plasma metabolite biomarkers using LC-UV fractionation and MS and NMR-based detection***Susan Bird**, Brigham and Women's Hospital**2:50** O-069: *Push-through Direction Injection NMR Automation***Quincy Teng**, US Environmental Protection Agency**3:10** O-070: *microRNAs act in parallel to insulin/IGF-1 signalling to control healthspan and ageing in Caenorhabditis elegans***Cecilia Castro**, Department of Biochemistry, Cambridge

3:30 P.M. – 4:00 P.M. Break

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**Hall B South**

4:00 P.M. – 5:30 P.M.

**Funding Opportunities and  
International Initiatives***Session Chairs: Young Kim, Christoph Steinbeck***4:00** O-071: *National Institutes of Health-Common Funds Metabolomics Research Opportunities***Philip Smith**, National Institute of Diabetes, Digestive and Kidney Diseases**4:25** O-072: *Funding Opportunities at the National Science Foundation***Jane Silverthorne**, National Science Foundation**4:50** O-073: *Bioplatforms Australia – an initiative to translate 'omics technologies to systems biology***Ute Roessner**, The University of Melbourne**5:10** O-074: *Canadian Initiatives and Innovations in Metabolomics***David Wishart**, University of Alberta

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**Lincoln 2-4**

4:00 P.M. – 5:30 P.M.

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**Hall B South**

5:30 P.M. – 6:00 P.M.

**Award Ceremony – Conference Ends**