# PROGRAM Metabolomics 2005

## Monday June - 20th

**Afternoon Session:**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Speaker</th>
<th>Title</th>
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<tbody>
<tr>
<td>15:00</td>
<td>Plenary</td>
<td>Masaru Tomita</td>
<td>Welcoming Remarks</td>
</tr>
<tr>
<td>15:10</td>
<td>Plenary</td>
<td>Rima Kaddurah-Daouk</td>
<td>Introductions and award presentation</td>
</tr>
<tr>
<td>15:25</td>
<td>01</td>
<td>Jeremy Nicholson</td>
<td>Modelling Metabolic Dysfunction and Disease Processes in hypercomplex systems</td>
</tr>
<tr>
<td>16:10</td>
<td>02</td>
<td>Age K. Smilde</td>
<td>Dynamic Metabolomics for Biosystems Identification</td>
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<tr>
<td>16:40</td>
<td></td>
<td></td>
<td>Coffee break</td>
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<tr>
<td>17:00</td>
<td>03</td>
<td>Edward Dennis</td>
<td>Overview of the LIPID MAPS Initiative and Lipidomics</td>
</tr>
<tr>
<td>17:30</td>
<td>04</td>
<td>Masaru Tomita</td>
<td>Metabolomics, Biosimulation and Systems Biology</td>
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<tr>
<td>18:15</td>
<td></td>
<td>Bio-Lab Tour</td>
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<tr>
<td>19:30</td>
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<td>Reception at Grand el Sun</td>
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## Tuesday June – 21st

**Morning Session:**

<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Speaker</th>
<th>Title</th>
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<tbody>
<tr>
<td>9:00</td>
<td>Metabolomics Technologies</td>
<td>Roy Goodacre, Chair</td>
<td>Introduction</td>
</tr>
<tr>
<td>9:10</td>
<td>05</td>
<td>Tomoyoshi Soga</td>
<td>Comprehensive and High Throughput Metabolomics by CE-MS and its Application</td>
</tr>
<tr>
<td>9:35</td>
<td>06</td>
<td>John Lindon</td>
<td>Investigating Metabonomics in Intact Tissues using High Resolution Magic Angle Spinning NMR Spectroscopy</td>
</tr>
<tr>
<td>10:00</td>
<td>07</td>
<td>Roy Goodacre</td>
<td>Direct Laser Desorption Mass Spectrometry for High-Throughput Metabolomics</td>
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<tr>
<td>10:25</td>
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<td></td>
<td>Coffee break</td>
</tr>
<tr>
<td>10:40</td>
<td>08</td>
<td>Istvan Pelcer</td>
<td>Saliva as an Alternative Biofluid and Implications to Animal and Human Diagnostics. An NMR-Based Case Study on Young Horses</td>
</tr>
<tr>
<td>11:05</td>
<td>09</td>
<td>Henri Brunengraber</td>
<td>Pathway Discovery via the Association of Metabolomics and Mass Isotopomer Analysis</td>
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<tr>
<td>11:30</td>
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<tr>
<td>11:55</td>
<td>10</td>
<td>Armin Graber</td>
<td>Difference in Technology and Performance of Qualitative and</td>
</tr>
</tbody>
</table>
Tuesday June – 21st

**Afternoon Session:** Policy Makers, Databases, Structures and Informatics

13:30 - 13:40  
**Douglas Kell**, Chair  
Introduction

13:40 - 14:05  
11 **Douglas Kell**  
Optimization of Metabolome Analyses through Evolutionary Computation

14:05 - 14:30  
12 **Oliver Fiehn**  
Databases and Structures

14:30 - 14:55  
13 **Pedro Mendes**  
Databases and Visualization

14:55 - 15:20  
14 **W. Paul Lee**  
The Nature of Metabolome Data

15:20 - 15:55  
Break

15:55 - 16:20  
15 **Eberhard Voit**  
Modelling Sphingolipid Metabolism in S. cerevisiae

16:20 - 16:55  
16 **Bernhard Palsson**  
The Plasticity of the E. coli Metabolome during Adaptive Evolution

16:55 - 17:10  
Break

Tuesday June – 21st

**Evening Session:** Selected Poster Presentations

17:10 - 19:10

Wednesday June – 22nd

**Morning Session:** Plant Metabolomics

8:30 - 8:35  
**Lloyd W. Sumner**, Chair  
Introduction

8:35 - 9:00  
17 **Kazuki Saito**  
Integrated Analysis of Metabolome and Transcriptome towards Identification of Novel Gene Function and Networks in *Arabidopsis thaliana*

9:00 - 9:25  
18 **Robert Hall**  
GCMS Metabolomics and Multivariate Correlative Analysis of Complex Quality Traits in Tomato

9:25 - 9:50  
19 **R. George Ratcliffe**  
Measuring Multiple Fluxes in Plant Metabolic Networks

9:50 - 10:05  
Break

10:05 - 10:15  
**Oliver Fiehn**, Chair
Introduction

10:15 - 10:40  20 Richard Trethewey
Plant Metabolomics: Innovation in Gene Function Analysis and
Diagnostics with Wide Application

10:40 - 11:05  21 Will Allwood
Dual Metabolome Profiling of Host and Pathogen in Arabidopsis
Suspension Cultures Inoculated with Pseudomonas syringae

11:05 - 11:30  22 Lloyd W. Sumner
Metabolomics: A Tool for Gene Validation, Gene Discovery,
Hypothesis Building, and Mechanistic Understanding

11:30 - 11:55  23 Mike H. Beale
Application of [1H]-NMR Screening to Plant Functional
Genomics

11:55 - 12:00  Mike Beale
Plant Metabolomics 2006, UK
Lunch
Metabolomics Journal, Editorial Board

**Wednesday June – 22nd**

**Afternoon Session:** Models and Pre-Clinical Studies in Metabolomics

13:00 - 13:10  George Harrigan, Chair
Introduction

13:10 - 13:35  24 John Ryals
Biomarkers and Drug Discovery

13:35 - 14:00  25 Ryo Taguchi
An Analytical System for Phospholipids from Mass Data for
Lipidomics

14:00 - 14:25  26 Matej Orešić
Lipidomic Characterization of Animal models in Studies of
Metabolic Diseases

14:25 - 14:50  27 Takaaki Nishioka
Applications of Metabolome Analysis to Metabolic
Regulation

14:50 - 15:15  28 Bruce Kristal
A Metabolic Serotype for Caloric Intake

**Wednesday June – 22nd**

**Excursion:** Tsuruoka Sightseeing
15:30 - 19:00

**Thursday June – 23rd**

**Morning Session:** Metabolomics in Health Care

8:30 -  8:40  Rima Kaddurah-Daouk, Chair
Introduction
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<tr>
<th>Time</th>
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<tbody>
<tr>
<td>8:40 - 9:05</td>
<td>Elaine Holmes</td>
<td>Metabolite Profiling Strategies for Clinical and Epidemiological</td>
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<td></td>
<td></td>
<td>Metabolomics</td>
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<tr>
<td>9:05 - 9:30</td>
<td>James Bain</td>
<td>Application of Metabolomics for Creation of New Diabetes Therapies</td>
</tr>
<tr>
<td>9:30 - 9:55</td>
<td>Wayne R. Matson</td>
<td>Metabolic Sub-Classification of CNS Disorders</td>
</tr>
<tr>
<td>10:20 - 10:45</td>
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<td>Coffee Break</td>
</tr>
<tr>
<td>10:45 - 11:10</td>
<td>Laszlo Boros</td>
<td>Stable Isotope Based Metabolic Profiling (SIDMAP) and its Applications</td>
</tr>
<tr>
<td>11:10 - 11:35</td>
<td>Don Morris</td>
<td>Advantages of Targeted Profiling Platforms: Examples from Lipids</td>
</tr>
<tr>
<td>11:35 - 12:00</td>
<td>George Harrigan</td>
<td>Metabolomics in Discovery Pharma</td>
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Thursday June – 23rd

**Afternoon Session:** Policy, Terms Used in the Field and Standards in Metabolomics

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<tr>
<td>13:30 - 14:00</td>
<td>Art Castle</td>
<td>New Metabolomics Technologies Developed under Roadmap</td>
</tr>
<tr>
<td>14:00 - 14:30</td>
<td>Rick Beger</td>
<td>Metabolomics within NCTR at FDA</td>
</tr>
<tr>
<td>14:30 - 15:00</td>
<td>Pedro Mende, Oliver Fiehn, John Lindon, Art Castle</td>
<td>Update on the metabolomics Standards workshop and open discussion on terms used in the metabolomics field and suggestions</td>
</tr>
<tr>
<td>15:00 - 15:05</td>
<td>Rima Kaddurah-Daouk</td>
<td>Closing Comments, Metabolomics 2006 Boston, USA</td>
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