The Metabolomics Society is dedicated to promoting the growth, use and understanding of metabolomics in the life sciences. Metabolomics is a newly emerging field of "omics" research concerned with the comprehensive characterization of the small molecule metabolites in biological systems. It can provide an overview of the metabolic status and global biochemical events associated with a cellular physiological state of a cell or organism and of their dynamic responses to genetic, abiotic and biotic environmental modulation.

The Metabolomics Society is an independent, non-profit organization, governed by a Board of Directors composed of dedicated members of the metabolomics community but ultimately responsive to its members. The Metabolomics Society’s vision is to become the premier organization devoted to the development of metabolism-based research. Constituted in 2004, the Metabolomics Society now has more than 500 members in more than 20 countries and publishes its own journal: Metabolomics.

Our Mission
1. To promote the growth and development of the field of metabolomics internationally
2. To provide the opportunity for collaboration and association among the workers in that science and in related sciences and connections between academia, government and industry in the field of metabolomics
3. To provide opportunities for presentation of research achievements and creation of workshops
4. To promote the publication of meritorious research in the field

Society:
www.metabolomicsociety.org

Journal:
www.springer.com/life+sciences/biochemistry+%26+biophysics/journal/11306
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Conference Organisers

Metabolomics 2013 Secretariat
c/o In Conference Ltd, 4-6 Oak Lane, Edinburgh, EH12 6XH, Scotland, UK
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Welcome from the Metabolomics Society

Dear Metabolomics 2013 Participant,

On behalf of the Board of Directors of the Metabolomics Society and all involved in the organisation of this conference it is our very great pleasure to welcome you to the city of Glasgow and to Metabolomics 2013, the 9th Annual Conference of the Metabolomics Society.

The Society’s annual conference has a proven reputation for providing a stimulating array of opportunities to learn about cutting edge metabolomics science, including in both fundamental and applied sciences. Indeed, the objective of the annual meeting is to bring together our metabolomics community to discuss and network. This year we have workshops focussed on analytical chemistry, experimental design, and data standards and exchange. The scientific programme provides a diverse range of sessions from methodology development through to applied research involving microbes, plants and animals, including humans. This reflects the broad interests and describes the highly dynamic environment in which we are all working. Our thanks are expressed in advance to our keynote and session speakers who will discuss their cutting-edge research in metabolomics. Finally, the local organiser’s knowledge of Glasgow has provided a historic and entertaining social programme including a civic reception and a congress dinner at the architecturally stunning Kelvingrove Art Gallery. These social activities along with the poster sessions will allow us all to network and interact.

It is with great pleasure this year to report that 29 travel awards and prizes are available, many to support the attendance and development of our students and young scientists and provide them with an opportunity to network with their peers and present their research. This includes ten travel awards provided by the Metabolomics Society, reflecting our commitment to support the development of our students. This awards scheme will now operate annually, so take note for Metabolomics 2014! We also wish to thank The Metabolic Profiling Forum, Springer, University of Strathclyde, Glasgow Polyomics and SULSA for their financial commitment to support travel awards and prizes.

The Metabolomics Society Board wish to show a huge appreciation to the local organising committee of Metabolomics 2013, with special thanks to the Chair, Dave Watson. Organisation of these conferences requires dedication and a significant amount of time to ensure success. The Board also wish to thank our loyal and committed sponsors; the annual conferences would not be financially feasible without their continued financial support. Societies such as ours depend on you, and we are truly grateful for your contributions throughout the year. Metabolomics is a young science and your support enables us to keep the registration costs – especially for the young scientists we need to support – to a minimum.

Finally, as a Society with ambitions to grow and serve our community, we want to hear from our members about what we are doing well and areas we need to develop further. Please contact our President at President@MetabolomicsSociety.org with your comments and ideas. Indeed, there is the opportunity each year for members of the Society to become more actively involved through election onto the Board of Directors of the Society and to contribute via Task Groups, and we hope that many are encouraged to commit their time and efforts to developing the Society further.

Best wishes to everyone, and we hope you have a great conference!

Mark Viant, President
Dan Bearden, Treasurer
Ute Roessner, Secretary
on behalf of the Board Members of the Metabolomics Society
Discover more metabolites with Agilent’s specific and sensitive LC/MS and GC/MS solutions. Unique metabolome databases and libraries enable confident identification of critical compounds. Visualize these entities in curated pathways to gain biological meaning.

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Sign up at www.agilent.com/chem/metabolomics-sym
It is my pleasure on behalf of the local organisers and all those involved in the organisation of this meeting to welcome you to Metabolomics 2013. I would like to thank the Metabolomics Society for giving Glasgow the opportunity to host the meeting.

Metabolomics as a field is rapidly expanding and this is reflected in the many high quality abstracts submitted to the meeting which has resulted in the first class programme.

We have a record number of invited speakers and the number of abstracts submitted is close to a record number.

Metabolomics has become well established in Scotland with particular emphasis on crop research in Dundee and research on cancer, drug discovery, nutrition, Drosophila and parasitology in Glasgow. These areas of interest are reflected in the programme.

I would like to thank the University of Strathclyde, Glasgow University Polyomics Centre and the Scottish Universities Life Sciences Alliance for their support. Also I would like to thank everyone who has helped with abstract selection and the organisation of the science sessions.

As well as a great science programme we have put together a full social programme with the invaluable help of the team at In Conference who have run a very smooth operation in collating abstracts, obtaining sponsorship and registering participants.

We hope you enjoy your time at the Metabolomics 2013 and also find time to explore Glasgow and the surrounding countryside where there you will find much to interest you.

Dr Dave Watson
University of Strathclyde, Glasgow, UK

On behalf of the Local Organising Committee
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9th Annual Conference of the Metabolomics Society
INDUSTRY SPONSORED SESSIONS

MONDAY 1st JULY

State of the Art Solutions for Metabolomics
12.30 – 13.30
Location: Lomond Auditorium

New Techniques and Approaches in Metabolomics Sciences
12.30 – 13.30
Location: Alsh Room

TUESDAY 2nd JULY

BIOCRATES Targeted Metabolomics Platform!
07.30 – 08.15
Location: Alsh Room

Advances in Instrumentation and Software for Metabolomic Research
12.20 – 13.20
Location: Alsh Room

New Metabolomic Tools and High Resolution Time-of-Flight (HRT) Mass Spectometry
12.20 – 13.20
Location: Lomond Auditorium

WEDNESDAY 3rd JULY

Workflow Strategies for Metabolomics and Lipidomics
12.10 – 13.10
Location: Lomond Auditorium

Solving the “Metabolomics puzzle” by Integrated NMR and MS Solutions
12.10 – 13.10
Location: Boidsdale Room

See the Real Difference in Metabolomics
12.10 – 13.10
Location: Alsh Room
Bruker offers a Metabolic Profiler that combines the structural resolving power of NMR, the unique sensitivity of a mass spectrometer and intuitive software programs, giving you the most complete and highly automated system for metabolomics research today.

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## Scientific Programme

### Monday 1st July

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<td>08.00 – 10.00</td>
<td>NIH Common Funds Metabolomics Initiatives – International Collaborators’ Meeting Glasgow 2013 (Invitation Only)</td>
<td>Boidsdale Room</td>
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<tr>
<td>10.00 – 12.00</td>
<td>Workshop 1A: The Role &amp; Development of Separation Techniques in Metabolomics Chair: Dave Watson, University of Strathclyde, UK</td>
<td>Lomond Auditorium</td>
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<tr>
<td>10.00 – 10.30</td>
<td>Liquid Chromatography Mass Spectrometry</td>
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<td>Dave Watson, Glasgow, UK</td>
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<tr>
<td>10.30 – 11.00</td>
<td>Gas Chromatography Mass Spectrometry</td>
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<td>Oliver Fiehn, Davis, CA, USA</td>
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<tr>
<td>11.00 – 11.30</td>
<td>Capillary Electrophoresis Mass Spectrometry</td>
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<td>Tomoyoshi Soga, Tsuruoka, Japan</td>
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<tr>
<td>11.30 – 12.00</td>
<td>Panel Discussion</td>
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<td>10.00 – 12.00</td>
<td>Workshop 1B: Workshop on Metabolomics Data Dissemination, Standardization and Exchange (COSMOS/MetaboLights/NIH common funds Session)</td>
<td>Alsh Room</td>
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<td>Background General Metabolomics Standards and Data Storage and Data Exchange in Different Standard Formats</td>
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<td>Reza Salek, EMBL-EBI, UK</td>
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<td>Hands on MetaboLights Tools and Data Submission using ISACreator</td>
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<td>Kenneth Haug, EMBL-EBI, UK, Philippe Rocca-Serra, EMBL-EBI, UK &amp; Reza Salek, EMBL-EBI, UK</td>
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<td></td>
<td>Overview COSMOS (COordination Of Standards In MetabolomicS) Initiative on Metabolomics Standards</td>
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<td>Christoph Steinbeck, EMBL-EBI, UK</td>
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<td>Introduction to the NIH Common Funds Metabolomics Consortium, Regional Comprehensive Metabolomics Research Cores” (RCMRC), Data Repository and Coordination Center (DRCC)</td>
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<td>Philip F. Smith, National Institute of Diabetes and Digestive and Kidney Diseases, USA</td>
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<td></td>
<td>Discussion with Users and Participants</td>
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<td>Moderator: Marta Cascante, Universitat de Barcelona, Spain &amp; Christoph Steinbeck, EMBL-EBI, UK</td>
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<td>12.00 – 14.00</td>
<td>Lunch / Exhibition / Posters</td>
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<td>12.30 – 13.30</td>
<td>Lunchtime Symposia</td>
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<td>State of the Art Solutions for Metabolomics</td>
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<td>12.30 – 13.30</td>
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<td>New Techniques and Approaches in Metabolomics Sciences</td>
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<td>14.00 – 16.00</td>
<td>Workshop 2A: Data Processing and Experimental Design Chair: Gavin Blackburn, University of Strathclyde, UK</td>
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<td>14.00 – 14.15</td>
<td>Introduction and Experimental Design - Considerations, Do’s and Don’ts, Who to Include and How to Plan Gavin Blackburn, University of Strathclyde, UK &amp; Karl Burgess, University of Glasgow, UK</td>
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<td>14.35 – 15.00</td>
<td>IDEOM – Demonstration of IDEOM for Metabolite Analysis Darren Creek, University of Melbourne, Australia</td>
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| 15.00 – 15.25 | IMZMine2 – Demonstration of MZMine2  
Tong Zhang, Strathclyde Institute of Pharmacy and Biomedical Sciences, UK | Lomond Auditorium |
| 15.25 – 15.35 | MZMatch-ISO – An R Tool for the High Precision Analysis of Isotope Labelled Mass Spectrometry Data - Discussion of MZMatchISO for Analysis of Labelled Samples  
Unni Chokkathukalam, Glasgow Polyomics, UK | Lomond Auditorium |
| 15.35 – 16.00 | Discussion                                                                                  | Lomond Auditorium |
| 14.00 – 16.00 | Workshop 2B: Mass Spectrometry and NMR in Metabolomics  
Chair: Warwick Dunn, University of Birmingham, UK, & Julian Griffin, Medical Research Council Human Nutrition Research, UK | Alsh Room |
|            | Reporting Standards for Metabolite Annotation and Identification  
Warwick Dunn, University of Birmingham, UK | Alsh Room |
|            | Metabolite Identification and Quantification Applying NMR Spectroscopy  
Tim Ebbels, Imperial College, UK; Julian Griffin, Medical Research Council Human Nutrition Research, UK; David Chong, Chenomx, Canada; Celicia Castro, University of Cambridge, UK | Alsh Room |
|            | Quantitation of Metabolites Applying Liquid Chromatography-triple Quadrupole Mass Spectrometry  
Rob Vreeken, Leiden University and Netherlands Metabolomics Centre, The Netherlands | Alsh Room |
|            | MUSCLE – Software for Automated Optimisation of Targeted LC-MS Methods  
Gregory Genta-Jouve, University of Birmingham, UK | Alsh Room |
| 16.30 – 17.00 | Welcome and Opening  
Chair: Mark Viant, University of Birmingham, UK | Lomond Auditorium |
|            | Welcome by the Local Organising Committee  
Dave Watson, University of Strathclyde, UK | Lomond Auditorium |
|            | Welcome from the President of the Metabolomics Society  
Mark Viant, University of Birmingham, UK | Lomond Auditorium |
|            | Presentation to the Honorary fellows | Lomond Auditorium |
|            | New Metabolomics Journal Prizes | Lomond Auditorium |
| 17.00 – 18.00 | Opening Plenary Lecture  
Chair: Mark Viant, University of Birmingham, UK | Lomond Auditorium |
|            | PL-1  
The Cellular Uptake of Pharmaceutical Drugs: A Problem Not of Biophysics but of Systems Biology  
Douglas Kell, University of Manchester, UK | Lomond Auditorium |
<p>| 18.00 – 19.00 | Welcome Reception hosted by the City of Glasgow | Hall 1 &amp; 2 |</p>
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<td>PL-2 Solving the Biochemical Jacobian – An Equation to Systematically Link the Genotype to the Measured Metabolomic Phenotype</td>
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<td>09.10 – 09.50</td>
<td>PL-3 Comprehensive Metabolomic Analysis for Study of Human Diseases: Integration of Platforms and Tools in the NIH West Coast Metabolomics Center</td>
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<td>10.20 – 11.00</td>
<td>PL-4 Drosophila, Metabolomics and Functional Genomics – A Match Made in Heaven</td>
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<td>11.00 – 11.15</td>
<td>O1A-1 Large-scale Survey of Metabolite Concentrations in Human, Chimpanzee, Macaque and Mouse Tissues suggests Tradeoff between Human Muscle and Brain</td>
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<td>O1A-2 Metabolomics and Systems Biology of Genotype-by-Diet Interactions underlying Metabolic Syndrome in Drosophila</td>
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<td>O1A-3 Metabolomic Analysis of Peanut Allergy in a Mouse Model</td>
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<td>O1A-4 The Combined use of Drosophila and Yeast as Model Organisms for the Identification of Unknown Mitochondrial Protein Function</td>
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<td>Parallel Session 1B: Fluxomics</td>
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<td>10.20 – 11.00</td>
<td>PL-5 Role of Post-Transcriptional Regulation in the Control of Carbon Metabolism</td>
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<td>11.00 – 11.15</td>
<td>O1B-1 Metabolomics and Fluxomics in Mammalian Tissue: Method Optimization and Insights into Metabolite Flux During Exercise</td>
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<td>11.15 – 11.30</td>
<td>O1B-2 A Method to Measure Metabolic Flux with Heavy Isotope Labelling and Mass Spectrometry</td>
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### Scientific Programme

**Tuesday 2nd July Continued**

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| 11.30 – 11.45 | **O1B-3** Cross-labeled $^{13}$C -stearate Fate Detection in the [1,2-$^{13}$C$_2$]-D-Glucose Derived Isotopole Improves System Wide Associations when Compared with External [U-$^{13}$C$_{18}$]-stearate Incubation in Rosiglitazone Treated HEPG2 Cells  
László G Boros, Los Angeles Biomedical Research Institute (LABIOMED) at the Harbor-UCLA Medical Center, USA | Alsh Room          |
| 11.45 – 12.00 | **O1B-4** Kinetic Modeling Applied to the Analysis of 13C Tracer Distribution in Metabolites: New Life for the Old Tool  
Vitaly Selivanov, Universitat de Barcelona, Spain |                    |
| 12.00 – 13.30 | **Lunch / Exhibition / Posters**                                        | Hall 1 & 2         |
| 12.20 – 13.20 | **Lunchtime Symposia**  
Advances in Instrumentation and Software for Metabolomics Research  
[LECO](https://www.leco.com) | Alsh Room          |
| 12.20 – 13.20 | **Lunchtime Symposia**  
New Metabolomic Tools and High Resolution Time-of-Flight (HRT) Mass Spectrometry  
[Lomond Auditorium](https://www.lomond.org) | Lomond Auditorium  |
| 13.30 – 15.30 | **Parallel Session 2A: Cancer Research**  
Chair: Eyal Gottlieb, The Beatson Institute for Cancer Research, UK | Lomond Auditorium  |
| 13.30 – 14.10 | **PL-6** Metabolism and Cancer: Why should we Care?  
Eyal Gottlieb, The Beatson Institute for Cancer Research, UK |                    |
| 14.10 – 14.30 | **O2A-1** The Myc/p53-dependent Tumour Suppressor miR-22 Regulates Multiple Metabolic Pathways in Cancer Cells  
Hector Keun, Imperial College London, UK |                    |
| 14.30 – 14.45 | **O2A-2** The Glutamine Metabolism Network in Melanoma  
David Scott, Sanford-Burnham Medical Research Institute, USA |                    |
| 14.45 – 15.00 | **O2A-3** Analysis of the Hypoxia Metabolome  
Alessandro Valli, University of Oxford, UK |                    |
| 15.00 – 15.15 | **O2A-4** Lipidomic Response to Hypoxia Profiled by 2-Dimensional Gas Chromatography/Mass Spectrometry  
Benedikt Kessler, University of Oxford, UK |                    |
| 15.15 – 15.30 | **O2A-5** Use of Liquid Chromatography-mass Spectrometry (LC-MS) Metabolomics to Study Plasma Biomarkers: Case Study using a Potent, Selective Pan-class I Phosphatidylinositol-3-kinase (PI3K) Inhibitor  
Joo Ern Ang, The Institute of Cancer Research, UK |                    |
| 13.30 – 15.30 | **Parallel Session 2B: Crop Improvement**  
Chair: Robert Hall, Centre for Biosystems Genomics, The Netherlands | Alsh Room          |
| 13.30 – 14.10 | **PL-7** Application of Metabolomics to Plant Breeding by Genetic Intervention  
Paul Fraser, Royal Holloway University of London, UK |                    |
| 14.10 – 14.30 | **O2B-1** High Throughput Tree Profiling - A New Dimension in Plant Metabolomics  
Jane Ward, Rothamsted Research, UK |                    |
David Rudell, USDA-ARS, USA |                    |
### Scientific Programme

#### 9th Annual Conference of the Metabolomics Society

**Tuesday 2nd July Continued**

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<th>Time</th>
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<tbody>
<tr>
<td>14.45 – 15.00</td>
<td><strong>O2B-3</strong> Profiling of Spatial Metabolite Distributions in Wheat Leaves under Normal and Nitrate Limiting Conditions</td>
<td>J. William Allwood, University of Birmingham, UK</td>
<td>Aish Room</td>
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<tr>
<td>15.00 – 15.15</td>
<td><strong>O2B-4</strong> Diurnal Compositional Changes of Tomato Fruit and Leaf</td>
<td>Annick Moing, INRA Bordeaux, France</td>
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<tr>
<td>15.15 – 15.30</td>
<td><strong>O2B-5</strong> The Molecular Arms Race between Cladosporium Fulvum and Tomato at the Metabolome Level</td>
<td>Desalegn Etalo, Plant Research International, The Netherlands</td>
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<tr>
<td>15.30 – 16.00</td>
<td>Tea / Coffee / Exhibition / Posters</td>
<td></td>
<td>Hall 1 &amp; 2</td>
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<tr>
<td>16.00 – 17.30</td>
<td>Parallel Session 3A: New Developments in Instrumentation and New Techniques</td>
<td>Chair: Graham Cooks, Purdue University, USA</td>
<td>Lomond Auditorium</td>
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<tr>
<td>16.00 – 16.15</td>
<td><strong>O3A-1</strong> Mass Spectrometry Analysis of Signalling and Metabolic Lipids</td>
<td>Qifeng Zhang, Babraham Institute, UK</td>
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<tr>
<td>16.15 – 16.30</td>
<td><strong>O3A-2</strong> A Prototype Microfluidic MS Platform for Metabolomics</td>
<td>Giuseppe Astarita, Waters Corporation, USA</td>
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<tr>
<td>16.45 – 17.00</td>
<td><strong>O3A-4</strong> Spatially-encoded 2D NMR Strategies for Fast Quantitative Metabolomics</td>
<td>Illa Tea, Université de Nantes, France</td>
<td></td>
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<tr>
<td>17.00 – 17.15</td>
<td><strong>O3A-5</strong> The Use of Standard Reference Materials (SRMs) and Control Materials (CMs) for Metabolomics Quality Control and Stability Assessments</td>
<td>Daniel Bearden, NIST, USA</td>
<td></td>
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<tr>
<td>17.15 – 17.30</td>
<td><strong>O3A-6</strong> Can we Trust Untargeted Metabolomics: Results of the Metabo-ring Initiative, a Large-scale Multi-instruments Inter-laboratory Study</td>
<td>Jean-Charles Martin, INRA, France</td>
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<tr>
<td>16.00 – 17.30</td>
<td>Parallel Session 3B: Plant Physiology</td>
<td>Chair: Lloyd Sumner, The Samuel Roberts Noble Foundation, USA</td>
<td>Aish Room</td>
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<tr>
<td>16.00 – 16.15</td>
<td><strong>O3B-1</strong> Development of Metabolite Profiling Database for Knock-Out Mutants in Arabidopsis (MeKO)</td>
<td>Atsushi Fukushima, RIKEN Center for Sustainable Resource Science, Japan</td>
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<tr>
<td>16.15 – 16.30</td>
<td><strong>O3B-2</strong> Metabolomics as a Tool to Characterize Biochemistry of the Mediator Complex in Plants</td>
<td>Ilka Abreu, Swedish University of Agricultural Sciences, Sweden</td>
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<tr>
<td>16.30 – 16.45</td>
<td><strong>O3B-3</strong> Metabolomics as a Tool to Characterize Genes Involved in the Synthesis of Bioactive Sesquiterpenes</td>
<td>Ric de Vos, Plant Research International, The Netherlands</td>
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<tr>
<td>16.45 – 17.00</td>
<td><strong>O3B-4</strong> Metabolite Profiling of Vaccinium Berry Standard Reference Materials by GC-MS</td>
<td>Karen Phinney, National Institute of Standards and Technology, USA</td>
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### Scientific Programme

#### 9th Annual Conference of the Metabolomics Society

**Tuesday 2nd July Continued**

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<tr>
<th>Time</th>
<th>Session</th>
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</table>
| 17.00 – 17.15 | **O3B-5** Plant Lipidomics Leads to Identification of a Novel Lipid Class Playing an Essential Role in Mitigation of Phosphorus Depletion  
Yozo Okazaki, RIKEN Center for Sustainable Resource Science, Japan | Aish Room       |
| 17.15 – 17.30 | **O3B-6** Identifying Novel Salinity Tolerance Mechanisms by Spatial Analysis of Lipids in Barley Roots  
Ute Roessner, The University of Melbourne, Australia |                |
| 17.30 – 19.00 | **Poster Session I**                                                                        | Hall 1 & 2      |

#### Wednesday 3rd July

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<tr>
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<tr>
<td>07.30 – 18.00</td>
<td><strong>Registration &amp; Speaker Preview</strong></td>
<td>Hall 1 &amp; Etive Room</td>
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</table>
| 08.30 – 09.50 | **Plenary Session 2**  
Chair: Julian Griffin, Medical Research Council Human Nutrition Research, UK | Lomond Auditorium |
| 08.30 – 09.10 | **PL-8** Analytical, Imaging, Miniature and Preparative Mass Spectrometry in Metabolomics  
Graham Cooks, Purdue University, USA |                |
| 09.10 – 09.50 | **PL-9** Stress & Drugs and Rock & Roll: Towards an Understanding of Microbial Adaptation  
Roy Goodacre, University of Manchester, UK |                |
| 09.50 – 10.20 | **Tea / Coffee / Exhibition / Posters**                                                      | Hall 1 & 2      |
| 10.20 – 11.50 | **Parallel Session 4A: University of Strathclyde and Glasgow Polyomics Young Scientist Session**  
Chairs: Mike Barrett, University of Glasgow, UK, & Dave Watson, University of Strathclyde, UK | Lomond Auditorium |
| 10.20 – 10.35 | **O4A-1** Metabolic Phenotyping by 1H-NMR Spectroscopy Detects Lung Cancer via a Simple Blood Sample  
Evelyne Louis, University of Hasselt, Belgium |                |
| 10.35 – 10.50 | **O4A-2** From Metabolic Differences to Genetic Differences via Qualitative Metabolic Network Analysis  
Weiruo Zhang, Stanford University, USA |                |
| 10.50 – 11.05 | **O4A-3** Improving Photosynthesis in *Arabidopsis thaliana*: Fumarate as a Potential Carbon Store  
Beth Dyson, University of Manchester, UK |                |
| 11.05 – 11.20 | **O4A-4** Targeted and Non-targeted LC-MS Metabolic Profiling Identifies Shifts in Amino Acid and Lipid Metabolism in the Inflammatory Skin Disease Psoriasis  
Stuart Snowden, Karolinska Institute, Sweden |                |
| 11.20 – 11.35 | **O4A-5** An Automated Workflow to Reduce LC-MS Data to Biologically Relevant Features Only, with Subsequent Annotation, and its Application to *C.elegans* Longevity Mutant Profiling  
Florian Geier, Imperial College London, UK |                |
| 11.35 – 11.50 | **O4A-6** Discovery of Plant Dual COX and LOX Inhibitors and Models to Prediction through Metabolic Studies and Artificial Intelligence  
Daniela A. Chagas-Paula, University of São Paulo, Brazil |                |
### Parallel Session 4B: Metabolomics Society Student Travel Awards & SULSA Young Scientist Session 1

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<thead>
<tr>
<th>Time</th>
<th>Session Title</th>
<th>Speaker</th>
<th>Institution</th>
<th>Room</th>
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<tbody>
<tr>
<td>10.20</td>
<td>Explorative NMR Metabolomics in the Metabolic Characterisation of TBM in CSF</td>
<td>Shayne Mason</td>
<td>North-West University, South Africa</td>
<td>Alsh Room</td>
</tr>
<tr>
<td>10.35</td>
<td>Metabolomic Analysis of Ovarian Cancer: A Multi-modal GC-MS, LC-MS and NMR Study</td>
<td>Marie Palmnäs</td>
<td>University of Alberta, Canada</td>
<td></td>
</tr>
<tr>
<td>10.50</td>
<td>Urinary Metabolomics of Colorectal Cancer - A Pilot Study Screening for Cross-sectional Markers used in Translational Oncology</td>
<td>David B. Liesenfeld</td>
<td>German Cancer Research Center (DKFZ), Germany</td>
<td></td>
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<tr>
<td>11.05</td>
<td>Metabolic Profiling during Pregnancy and Associations with Maternal Health Parameters and Birth Outcomes</td>
<td>Lea Maitre</td>
<td>Imperial College London, UK</td>
<td></td>
</tr>
<tr>
<td>11.20</td>
<td>Metabolomic Analysis of The Resistance Response in Sunflower Roots to the Parasitic Weed Orobanche Cumana</td>
<td>Anne-Laure Hepp</td>
<td>University of Sheffield, UK</td>
<td></td>
</tr>
<tr>
<td>11.35</td>
<td>Metabolomics and Dereplication Studies of Endophytic Metabolites from Some Egyptian Medicinal Plants in the Search for New Potential Anti-Cancer Drugs</td>
<td>Ahmed Tawfike</td>
<td>University of Strathclyde, UK</td>
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### Parallel Session 4C: Metabolomics Society Student Travel Awards & SULSA Young Scientist Session 2

<table>
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<tr>
<th>Time</th>
<th>Session Title</th>
<th>Speaker</th>
<th>Institution</th>
<th>Room</th>
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<tbody>
<tr>
<td>10.20</td>
<td>Identification of Novel Biomarkers of Dietary Intake</td>
<td>Helena Gibbons</td>
<td>University College Dublin, Ireland</td>
<td>Boidsdale Room</td>
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<tr>
<td>10.35</td>
<td>Antidiabetic Effect of Metformin by Reducing Cortisol Levels via the AMPK/LXRα/POMC Pathway</td>
<td>Kumsun Cho</td>
<td>Seoul National University College of Medicine and Hospital, Republic of Korea</td>
<td></td>
</tr>
<tr>
<td>10.50</td>
<td>Dereplication and Characterization of Novel 17-Hydroxygeranyllinalool Diterpene Glycosides (HGL-DTGs) in 24 Solanaceous Species by U(H)PLC/ESI-TOF-MS and MS/MS</td>
<td>Sven Heiling</td>
<td>Max-Planck Institute for Chemical Ecology, Germany</td>
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<tr>
<td>11.05</td>
<td>Development of Strategies for Integrated Full-scan Profiling and Data Dependent MS/MS and MS/MS Applying CID and HCD on Hybrid Orbitrap Mass Spectrometers</td>
<td>Martin R. Jones</td>
<td>University of Birmingham, UK</td>
<td></td>
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<tr>
<td>11.20</td>
<td>Ovarian Cancer Metabolic Profiles Differ in Ovarian Cancer Initiating Cells</td>
<td>Kathleen Vermeersch</td>
<td>Georgia Institute of Technology, USA</td>
<td></td>
</tr>
<tr>
<td>11.35</td>
<td>Novel Mass Spectrometry Based Lipidomic Methods for the Investigation of Gangliosides in Mouse Models of Guillain-Barré Syndrome</td>
<td>Jo Cappell</td>
<td>University of Glasgow, UK</td>
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<tr>
<td>11.50</td>
<td>(SULSA Young Scientist Award Winner)</td>
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### Scientific Programme

- **11.50 – 13.20** Lunch / Exhibition / Posters  
  **Hall 1 & 2**

- **12.10 – 13.10** Lunchtime Symposia  
  **Workflow Strategies for Metabolomics and Lipidomics**  
  **Lomond Auditorium**

- **12.10 – 13.10** Lunchtime Symposia  
  **Solving the “Metabolomics puzzle” by Intergrated NMR and MS Solutions**  
  **Boidsdale Room**

- **12.10 – 13.10** Lunchtime Symposia  
  **See the Real Difference in Metabolomics**  
  **Aish Room**

- **13.20 – 15.00** Parallel Session 5A: Metabonomic Profiling in Neuroscience  
  Chair: Dan Rujescu, University of Halle, Germany  
  **Aish Room**

- **13.20 – 14.00**  
  **PL-10**  
  **Metabolomics in Schizophrenia**  
  Dan Rujescu, University of Halle, Germany

- **14.00 – 14.15**  
  **OSA-1**  
  Daily Rhythms in the Human Metabolome and the Effect of Sleep and Sleep Deprivation  
  Sarah K. Davies, University of Surrey, UK

- **14.15 – 14.30**  
  **OSA-2**  
  Lipidomic Analysis of Brain Tissues and Plasma in a Mouse Model Expressing Mutated Human Amyloid Precursor Protein/tau for Alzheimer's Disease  
  Keiko Maekawa, National Institute of Health Sciences, Japan

- **14.30 – 14.45**  
  **OSA-3**  
  Metabolomics in Cerebrospinal Fluid of Patients with Amyotrophic Lateral Sclerosis: An Untargeted Approach Using High-resolution Mass Spectrometry  
  Helene Blasco, CHRU BRETONNEAU, France

- **14.45 – 15.00**  
  **OSA-4**  
  Metabolomic Multi-Platform Based on Direct Infusion Mass Spectrometry for Alzheimer’s Disease Diagnosis  
  Jose-Luis Gomez-Ariz, University of Huelva, Huelva

- **13.20 – 15.00** Parallel Session 5B: Environmental  
  Chairs: Mark Viant, University of Birmingham, UK, & Georg Pohnert, Friedrich Schiller University, Germany  
  **Lomond Auditorium**

- **13.20 – 14.00**  
  **PL-11**  
  Deciphering Highly Dynamic Chemically Mediated Interactions of Microalgae Using a Combined Metabolomics / Bioassay Approach  
  Georg Pohnert, Friedrich Schiller University, Germany

- **14.00 – 14.15**  
  **OSB-1**  
  Comprehensive Metabolomics Analysis of a Yellowstone National Park Hot Spring Phototrophic Microbial Mat Over a Diel Cycle Reveals a High Potential for Metabolic Coupling Among Community Members  
  Thomas Metz, Pacific Northwest National Laboratory, USA

- **14.15 – 14.30**  
  **OSB-2**  
  Metabolomic and Transcriptomic Analysis Reveals Endocrine Disruption in Skeena River (British Columbia) Sockeye Salmon during the 2008 Spawning Migration  
  John Cosgrove, AXYS Analytical Services Ltd, Canada

- **14.30 – 14.45**  
  **OSB-3**  
  Application of both Targeted and Untargeted Metabolomics Approaches to Assess Potential Biological Effects of Simulated Sonar Signals on Bottlenose Dolphins  
  Gregory Genta-Jouve, University of Birmingham, UK

- **14.45 – 15.00**  
  **OSB-4**  
  Metabolomic Profiling of Cancer and Child-mother Cohorts to Identify Biomarkers of Exposure and Disease: Results from the EnviroGenoMarkers Study  
  Alexandros Siskos, Imperial College London, UK

- **15.00 – 15.30** Tea / Coffee / Exhibition / Posters  
  **Hall 1 & 2**

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**Wednesday 3rd July Continued**
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<th>Session</th>
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<th>Chair(s)</th>
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<tr>
<td>15.30 – 17.00</td>
<td>Parallel Session 6A: Drug Discovery</td>
<td>Utility... SCQs isolated from Marine Sponges</td>
<td>Lynsey MacIntyre, University of Strathclyde, UK</td>
</tr>
<tr>
<td>15.30 – 16.00</td>
<td>Parallel Session 6B: Data Extraction and Interpretation</td>
<td>Towards a Generative Model of LC/MS Data to Improve Metabolite Identification</td>
<td>Ronan Daly, University of Glasgow, UK</td>
</tr>
<tr>
<td>15.30 – 17.00</td>
<td>Parallel Session 6B: Data Extraction and Interpretation</td>
<td>Global Metabolomics of Stressed Caenorhabditis elegans using Isotopic Ratio Outlier Analysis</td>
<td>Gregory S. Stupp, University of Florida, USA</td>
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<td>17.00 – 18.30</td>
<td>Poster Session II</td>
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<td>20.00 – 23.30</td>
<td>Conference Dinner/Ceilidh</td>
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<tr>
<td>Time</td>
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<td>08.00 – 17.00</td>
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<tr>
<td>09.00 – 10.25</td>
<td><strong>Parallel Session 7A: Fermentation</strong></td>
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<td></td>
<td>Chair: Roy Goodacre, University of Manchester, UK</td>
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<tr>
<td>09.00 – 09.40</td>
<td><strong>PL-12</strong> High Throughput Metabolomics of the Entire E. coli Deletion Library</td>
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<tr>
<td>09.40 – 09.55</td>
<td><strong>O7A-1</strong> Interpreting Mechanism from Metabolic Footprinting Data of Single-gene <em>Pseudomonas aeruginosa</em> Knockouts</td>
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<tr>
<td>09.55 – 10.10</td>
<td><strong>O7A-2</strong> Improved Bioprocess by Metabolite Profiling and Modelling on the Cellular Level</td>
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<tr>
<td>10.10 – 10.25</td>
<td><strong>O7A-3</strong> Searching for the New Zealand Sauvignon Blanc Juice and Wine <em>Terroir</em> through Metabolomics</td>
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<td>Farhana Pinu, New Zealand Institute of Plant and Food Research, New Zealand</td>
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<tr>
<td>09.00 – 10.25</td>
<td><strong>Parallel Session 7B: Metabolomic Profiling in Diabetes and Heart Disease</strong></td>
<td>Lomond</td>
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<td>Chairs: Ruth Andrew, University of Edinburgh, UK, &amp; Christopher Newgard, Duke University Medical Center, USA</td>
<td>Auditorium</td>
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<tr>
<td>09.00 – 09.40</td>
<td><strong>PL-13</strong> Metabolomics Profiling in Diabetes and Heart Disease</td>
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<tr>
<td>09.40 – 09.55</td>
<td><strong>O7B-1</strong> Differential Fatty Acid Profiles in LPS-treated Mice Liver using Stable Isotope Labelling and Gas Chromatography-mass Spectrometry with Single Sample Analysis</td>
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<tr>
<td>09.55 – 10.10</td>
<td><strong>O7B-2</strong> A Novel Lipidomic Strategy to Investigate the Dynamics of Intracellular Lipid Pattern in Skeletal Muscle Cells under Lipotoxic Conditions</td>
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<tr>
<td>10.10 – 10.25</td>
<td><strong>O7B-3</strong> From Blind Fingerprinting to Functional Profiling: Ceramide and Related Compounds in Experimental Models of Oxygen Sensing</td>
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<td>Francisco J. Rupérez, Universidad CEU-San Pablo, Spain</td>
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<td>10.25 – 10.50</td>
<td>Tea / Coffee / Exhibition / Posters</td>
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<tr>
<td>10.50 – 11.50</td>
<td><strong>Parallel Session 8A: Human Metabolic Responses to Food and Drink</strong></td>
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<td>Chair: Roy Goodacre, University of Manchester, UK</td>
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<tr>
<td>10.50 – 11.05</td>
<td><strong>O8A-1</strong> Different Metabolic Responses of Caffeinated and Decaffeinated Green Tea Extract during Rest and Moderate Intensity Exercise</td>
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<tr>
<td>11.05 – 11.20</td>
<td><strong>O8A-2</strong> Metabotyping in Cardiovascular Risk Subjects Reveals Differences in their Urinary Profiles after Wine Intake</td>
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<tr>
<td>11.20 – 11.35</td>
<td><strong>O8A-3</strong> New Biomarkers of Coffee Consumption Identified by Non-Targeted Metabolomic Profiling in Cohort Study Subjects</td>
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<td>Yoann Fillâtre, INRA, France</td>
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<tr>
<td>11.35 – 11.50</td>
<td>O8A-4</td>
<td><strong>Discovery Biomarkers of Bread Intake in Cardiovascular High-risk Participants. A Mass Spectrometry-based Metabolomics Approach</strong>&lt;br&gt; Cristina Andres-Lacueva, University of Barcelona, Spain</td>
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<td>Aish Room</td>
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<tr>
<td>10.50 – 11.50</td>
<td>Parallel Session 8B: Metabolomic Profiling in Diabetes and Heart Disease (Continued)</td>
<td><strong>O8B-1</strong>&lt;br&gt; From Metabolite Profiling to Biomarkers, Glyoxylate and Type 2 Diabetes&lt;br&gt; Dietrich Rein, Metanomics Health GmbH, Germany</td>
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<td>Lomond Room</td>
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<tr>
<td>10.50 – 11.05</td>
<td></td>
<td><strong>O8B-2</strong>&lt;br&gt; A Metabolomic Evaluation of Short and Long Term Effects of Different Macronutrient Intake in Overweight and Obese Postmenopausal Women&lt;br&gt; Elin Chorell, Public Health and Clinical Medicine, Sweden</td>
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<tr>
<td>11.05 – 11.20</td>
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<td><strong>O8B-3</strong>&lt;br&gt; Discovery of Novel Biomarkers for Fabry disease Using a Mass Spectrometry Metabolomic Approach&lt;br&gt; Christiane Auray-Blais, Université de Sherbrooke, Canada</td>
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<tr>
<td>11.20 – 11.35</td>
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<td><strong>O8B-4</strong>&lt;br&gt; Examining Response to Aspirin Therapy using a Pharmacometabolomics-Informed-Pharmacogenomics Approach&lt;br&gt; Anastasia Georgiades, Duke University School of Medicine, USA</td>
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<tr>
<td>11.50 – 13.10</td>
<td>Lunch / Exhibition / Posters (Exhibition &amp; Posters close at 13.10)</td>
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<td>Hall 1 &amp; 2</td>
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<tr>
<td>13.10 – 15.10</td>
<td>Parallel Session 9A: Personalised Medicine, Nutrition and General Human Health</td>
<td>Chair: Guowang Xu, Metabolomics Research Centre, China</td>
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<td>Lomond Auditorium</td>
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<tr>
<td>13.10 – 13.50</td>
<td></td>
<td><strong>PL-14</strong>&lt;br&gt; Towards Personalised Medicine of Cancer based on MS-based Metabolomics&lt;br&gt; Guowang Xu, CAS Key Laboratory of Separation Science for Analytical Chemistry, China</td>
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<tr>
<td>13.50 – 14.05</td>
<td></td>
<td><strong>O9A-1</strong>&lt;br&gt; Vitamin B-6 Restriction in Healthy Men and Women Affects Metabolite Profiles Reflecting Altered One-carbon Metabolism and Tryptophan Catabolism&lt;br&gt; Jesse Gregory, University of Florida, USA</td>
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<td>14.05 – 14.20</td>
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<td><strong>O9A-2</strong>&lt;br&gt; An Exploration of the Urinary Metabolome in the European Prospective Investigation on Cancer and Nutrition (EPIC) Cohort to Identify Novel Dietary Biomarkers&lt;br&gt; William Edmands, International Agency for Research on Cancer, France</td>
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<td>14.20 – 14.35</td>
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<td><strong>O9A-3</strong>&lt;br&gt; Analytical Strategies to Identify Low Abundant Metabolites in Complex Sample Matrices: Bioavailability of Polyphenols as Showcase&lt;br&gt; Justin van der Hooff, University of Glasgow, UK</td>
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<td>14.35 – 14.50</td>
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<td><strong>O9A-4</strong>&lt;br&gt; Using Lipidomics to Study the Metabolism of Dietary Lipids and the Effect on Candidate Markers for Cardio Metabolic Diseases&lt;br&gt; Albert Koulman, MRC HNR, UK</td>
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<td>14.50 – 15.05</td>
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<td><strong>O9A-5</strong>&lt;br&gt; Effects of Marginal Selenium Deficiency in Mice on Liver Metabolism&lt;br&gt; Kerstin Geillinger, Technical University of Munich, TUM, Germany</td>
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<tr>
<td>15.05 – 15.10</td>
<td></td>
<td><strong>Discussion</strong></td>
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### Parallel Session 9B: Parasitology and Infectious Diseases

**Chairs:** Graham Coombs, University of Strathclyde, UK & Michael Barrett, University of Glasgow, UK

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<th>Speaker &amp; Institution</th>
<th>Room</th>
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<td>13.10</td>
<td>PL-15 Metabolomic Analysis of Parasitic Protozoa</td>
<td>Michael Barrett, University of Glasgow, UK</td>
<td>Hall 1 &amp; 2</td>
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<tr>
<td>13.28</td>
<td>O9B-1 Development of a General Method for the HPLC/MS-based Analysis of Coenzyme A Derivatives and Cofactors from Cell Extracts</td>
<td>Katrin Müller, Technische Universität Braunschweig, Germany</td>
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<tr>
<td>13.40</td>
<td>O9B-2 Dissection of the Carbon and Energy Metabolism of Apicomplexan Parasites Important for Virulence using 13C-stable Isotope Resolved Metabolomics</td>
<td>Malcolm McConville, University of Melbourne, Australia</td>
<td>Aish Room</td>
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<tr>
<td>13.58</td>
<td>O9B-3 <em>Plasmodium Falciparum</em> Phosphoenolpyruvate Carboxylase Identified as a Key Enzyme in Redox Maintenance and Energy Generation</td>
<td>Sonal Sethia, University of Glasgow, UK</td>
<td>Aish Room</td>
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<td>14.10</td>
<td>O9B-4 Absolute Quantification of Metabolites for Flux Analysis in Trypanosomes using Orbitrap-based LC-MS</td>
<td>Dong-Hyun Kim, University of Glasgow, UK</td>
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<td>14.22</td>
<td>O9B-5 Metabolomics-guided Advances in Cell Culture and Drug Discovery for Trypanosomiasis and Malaria</td>
<td>Darren Creek, University of Melbourne, Australia</td>
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<td>14.34</td>
<td>O9B-6 <em>Trichomonas Vaginalis</em> Produces S-methyl-L-cysteine using Cysteine Synthase</td>
<td>Gareth Westrop, University of Strathclyde, UK</td>
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<td>14.46</td>
<td>O9B-7 New Metabolite Markers Implicating Adaptations of the Human Host to <em>Mycobacterium Tuberculosis</em> and <em>Vasa Versa</em></td>
<td>Du Toit Loots, North-West University, South Africa</td>
<td>Aish Room</td>
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<td>14.58</td>
<td>O9B-8 Metabolic Response of <em>Candida Albicans</em> to Phenylethyl Alcohol under Hyphae-inducing Conditions and its Role on Morphogenesis</td>
<td>Silas Villas-Boas, The University of Auckland, New Zealand</td>
<td>Aish Room</td>
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<td>15.10</td>
<td>Tea / Coffee</td>
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<td>15.30</td>
<td>The Complementary Roles of Metabolomics and Proteomics in Systems Biology</td>
<td>Chair: Warwick Dunn, University of Birmingham, UK</td>
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<td>Thomas Hankemeier, Leiden University, The Netherlands</td>
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<td>Harald Mischak, University of Glasgow, UK</td>
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<tr>
<td>16.30</td>
<td>Closing Remarks and Conference Prizes</td>
<td>Chair: Mark Viant, University of Birmingham, UK</td>
<td>Lomond Auditorium</td>
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<td>Conference Prize Ceremony</td>
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<td>Presentation on 2014 Metabolomics Society Conference</td>
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SPONSORED LUNCHEON SYMPOSIA

Monday 1st July 12.30 – 13.30
Location: Lomond Auditorium

State of the Art Solutions for Metabolomics
Chair: Stéphane Moreau, Shimadzu Europe, Germany

When Unmatched Speed Meets Sensitivity and Accuracy
Stéphane Moreau, Shimadzu Europe, Germany

Metabolomics Analysis for Medical Research
Masaru Yoshisa, Kobe University Graduate School of Medicine, Japan

Lipidomic Response to Hypoxia Profiled by 2-Dimensional Gas Chromatography/Mass Spectrometry
Alessandro Valli, University of Oxford, UK

Monday 1st July 12.30 – 13.30
Location: Alsh Room

New Techniques and Approaches in Metabonomics Sciences
Chair: Robert Tonge, Business Development Manager, Discovery and Life Sciences, Europe and ME

Innovative Solutions for Mass Spectrometry in Metabolomics
Giuseppe Astarita, Principal Scientist Lipidomics and Metabolomics, Waters Corporation, Milford, USA

The New Scale of Metabolic Profiling: Towards Comprehensive Coverage in Human Population Screening
Matthew R. Lewis, Mass Spectrometry Manager, MRC-NIHR Phenome Center, Department of Surgery and Cancer, Imperial College, London, UK
Tuesday 2nd July 12.20 – 13.20
Location: Alsh Room

Advances in Instrumentation and Software for Metabolomics Research
Chair: Theodore Sana, Agilent Technologies, USA

Untargeted Metabolite Profiling of Pleuripotent Stem Cells to Uncover the Molecular Bases for Huntington’s Disease and Function of the Huntington Gene
Steven Gross, Weill Cornell Medical College, New York, USA

Metabolomics of Opiate-induced Changes in Murine Brain by GC/Q-TOF
Jennifer Gushue, Agilent Technologies, USA

NMR Metabolomics using CRAFT – From spectra to spreadsheet and Pathway driven analysis
Patrik Jarvoll, Agilent Technologies, UK

Tuesday 2nd July 12.20 – 13.20
Location: Lomond

New Metabolomic Tools and High Resolution Time-of-Flight (HRT) Mass Spectrometry
Welcome introduction and Chair: Alec Kettle, LECO UK, UK

New Metabolomic Tools and Applications: A review of the latest developments and news on the HRT technology from LECO Corporation
Lorne Fell, LECO Product Manager, Separation Science, USA

Comprehensive Metabolite Analysis Using Rapid CE-MS Separations Combined with Ultrafast, High Resolution Time-of-flight Mass Spectrometry
Juergen Wendt, LECO European HRT Specialist, Germany

Using High Resolution Time-of-flight Mass Spectrometry for Analysis of Small Molecules
Oliver Fiehn, Director, West Coast Metabolomics Center, UC Davis Genome Center, USA
Wednesday 3rd July 12.10 – 13.10
Location: Lomond Auditorium

**Workflow Strategies for Metabolomics and Lipidomics**
Chair: Baljit Ubhi, AB SCIEX, UK

**Discovery Metabolomics Using TripleTOF® 5600+ System Technology**
Baljit Ubhi, AB SCIEX, UK

**Metabolomics of Non genotoxic carcinogens - reaching the PPARts other omes to not reach**
Jules Griffin, University of Cambridge, UK

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Wednesday 3rd July 12.10 – 13.10
Location: Boidsdale Room

**Solving the “Metabolomics puzzle” by Integrated NMR and MS Solutions**
Chair: Aiko Barsch, Market Manager Metabolomics, Bruker Daltonics, Bremen, Germany

**From Structure to Function - Locating Metabolites with High Resolution Mass Spectral Imaging Approaches**
Manuel Liebeke, Faculty of Medicine, Imperial College London, UK

**Combining Non-targeted and Metabolic Pathway Driven Targeted Metabolomics based on the Same LC-QTOF Data Set – Exemplified on Coffee Metabolomics**
Heiko Neuweger, Bruker Daltonics, Bremen, Germany

**NMR Applications and its Potential in the Study of Body Fluids**
Claire Cannet, Bruker Biospin GmbH, Rheinstetten, Germany

---

Wednesday 3rd July 12.10 – 13.10
Location: Alsh Room

**See the Real Difference in Metabolomics**
Chair: Ken Miller, VP of Marketing, Life Sciences Mass Spectrometry, Thermo Fisher Scientific, USA

**Transforming Metabolomics Research with New Tools from Thermo Scientific**
Ken Miller, VP of Marketing, Life Sciences Mass Spectrometry, Thermo Fisher Scientific, USA

**New Metabolomics Software Portfolio Overview**
Mark Sanders, Director, Software Product Marketing, Life Sciences Mass Spectrometry, Thermo Fisher Scientific, USA

**Instrumentation and Computational Innovations to Advance Metabolite Identification Capabilities**
Warwick Dunn, School of Biosciences, University of Birmingham, UK
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6. MicroSolv Technology Corporation
7. Bruker Corporation
8. Sigma-Aldrich
9. SULSA
10. Glasgow Polyomics and University of Strathclyde
11. West Coast Metabolomics Center
12. Euriso-top
13. BIOCRATES Life Science AG
14. Labman Automation Ltd
15. Spectral Works
16. Agilent Technologies
17. AB SCIEX UK Limited
18. Nonlinear Dynamics
19. Metabolomic Discoveries GmbH
20. Peak Scientific Instruments

[Image of the exhibition and venue floor plan with numbered spaces labeled for each exhibitor and areas marked for catering, registration, access to meeting rooms, posters, and speaker preview.]

Speaker Preview

Exhibition & Floor Plan
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Tel: +44 (0) 1442 233555
Email: Sara.gagliardi@thermofisher.com
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Waters Corporation creates business advantages for pharmaceutical discovery and life science organizations by delivering innovations that enable customers to make significant advancements. Waters delivers a connected portfolio of separations, analytical science, mass spectrometry and chemistries along with dedicated informatics specifically designed for proteomics, metabolomics, and lipidomics applications.

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Attend our vendor seminar
“See the Real Difference in Metabolomics”
Wednesday July 3rd
12:10 pm - 1:10 pm, Alsh Room

Transforming Metabolomics Research with New Tools from Thermo Scientific
Ian Jardine, PhD, VP and CTO, Life Sciences Mass Spectrometry, Thermo Fisher Scientific

New Metabolomics Software Portfolio Overview
Mark Sanders, PhD, Director, Software Product Marketing, Life Sciences Mass Spectrometry, Thermo Fisher Scientific

Instrumentation and computational innovations to advance metabolite identification capabilities
Warwick Dunn, PhD, School of Biosciences, University of Birmingham

Pre-registration online or on site at Booth #1 is required to confirm your seat for the workshop.

Don’t miss our poster presentations:
• Untargeted metabolomics workflow using UHPLC/Q Exactive benchtop Orbitrap mass spectrometer and SIEVE
• A strategy to identify endogenous metabolites using a novel high performance Orbitrap and the m/zCloud library
• Addressing the bottlenecks in Metabolomics: making an expedient transition from global profiling to targeted quantitation
• Untargeted metabolomics: From statistical objects to the efficient identification of “known unknowns”
• A new lipid software workflow for processing Orbitrap-based global lipidomics data in translational and systems biology research
• Using Capillary Ion Chromatography Mass Spectrometry for Metabolic Application

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GENERAL INFORMATION

Certificate of Attendance
A certificate of attendance will be emailed to all participants at the end of the conference.

Conference Etiquette
Delegates are advised that they are not allowed to take photographs of any posters or presentations without the author’s/ presenter’s consent. Delegates should also obtain consent from an author before citing any of their work that was presented at the conference.

If you intend to ‘blog’ or ‘tweet’ results from this congress you must inform the conference organisers in advance and get the permission of the author or presenter.

Mobile phones should be switched off or placed on ‘silent’ during sessions. Thank you for your co-operation.

Exhibition
In order to keep registration fees to a minimum, it is important that we have the support of commercial organisations at the conference. Please take time to visit the Exhibition which is located in Hall 2.

The exhibition will be open during the following times:
Monday 1st July 11.00 - 19.00
Tuesday 2nd July 09.30 - 19.00
Wednesday 3rd July 09.30 - 18.30
Thursday 4th July 09.30 – 13.10

Insurance
The Conference Organisers cannot accept any liability for personal injuries or for loss or damage to property belonging to delegates, either during, or as a result of the meeting. Please check the validity of your own personal insurance before travelling.

Message Board
There will be a notice board next to the registration desk for those wishing to leave messages or notifications during the conference.

Registration/Information Desks
All delegates will receive their name badge, conference documents, ordered tickets and all relevant conference information upon arrival at the SECC.

The Registration and Information Desks will be open at the following times:
Monday 1st July 08.00 – 18.00
Tuesday 2nd July 07.00 – 18.00
Wednesday 3rd July 07.30 – 18.00
Thursday 4th July 08.00 – 17.00

Security
Your name badge must be worn at all times otherwise you will not be allowed entry to the conference centre.

Please leave any luggage or poster tubes with the staff at the cloakroom. This will be manned during the normal opening hours of the conference. There will be a £1 charge per item.

Speaker Preview Room
This is located in the Etive Room. All presenters are required to check in their presentation a minimum of 4 hours prior to their talk.

The Speaker Preview Room will be open at the following times:
Monday 1st July 08.00 – 18.00
Tuesday 2nd July 07.00 – 18.00
Wednesday 3rd July 07.30 – 18.00
Thursday 4th July 08.00 – 17.00

Tea/Coffee Breaks and Lunch Arrangements
Catering points will be located in Hall 1 & 2. If attending a lunchtime symposia, lunches will be provided outside the session room or alternatively delegates can collect a lunch from Hall 1 or 2 and take it into the session. Please follow the directions of the staff at the Conference Centre.

If you have requested a special diet at the time of registering this will be shown on the reverse of your badge. Please show this to a member of the catering team.

WiFi Access
The conference is providing free WiFi access to delegates. Please see the registration notice board for password and log in details.
SOCIAL PROGRAMME

MONDAY 1st JULY
Welcome Reception - 18.00 – 19.00
Hall 1 & 2, SECC

The Welcome Reception will take place at the conference venue (SECC). This is an informal evening hosted by the City of Glasgow and refreshments and canapés will be served.

WEDNESDAY 3rd JULY
Conference Dinner – 20.00 – 23.30
Kelvingrove Art Gallery and Museum, Argyle St Glasgow G3 8AG, UK

This will be an informal and fun evening open to all delegates who have pre-registered to attend. A buffet supper and 2 drinks vouchers per delegate will be provided. Cash bar facilities will also be provided.
There will be traditional Scottish dancing and entertainment where everyone is invited to join in!
Please note that seating is limited.

POSTER INFORMATION

There will be two poster sessions taking place during the conference which are as follows:

Poster Session I
Posters can be put up from 12.00 on Monday 1st July and must be taken down by 19.00 on Tuesday 2nd July.

Themes in session:
- Model Organisms
- Fluxomics
- Cancer Research
- Plant Physiology and Crop Improvement
- New Developments in Instrumentation and New Techniques
- Metabolomic Profiling in Neuroscience
- Environmental

Poster Session II
Posters can be put up from 08.00 on Wednesday 3rd July and must be taken down by 13.10 on Thursday 4th July

Themes in session:
- Drug Discovery
- Data Extraction and Interpretation
- Fermentation
- Metabolomic Profiling in Diabetes and Heart Disease
- Personalised Medicine, Nutrition and General Human Health
- Parasitology and Infectious Diseases

There are two dedicated poster sessions taking place at the following times during each of the above poster sessions. Authors have been asked to stand by their boards during this time to discuss their work with delegates.

Posters in Session I
Tuesday 2nd July: 17.30 – 19.00

Posters in Session II
Wednesday 3rd July: 17.00 – 18.30

The posters will be displayed in Halls 1 & 2 in order of the themes in which they were submitted.

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Douglas Kell
University of Manchester, UK

Douglas Kell is Professor of Bioanalytical Science at the University of Manchester and is on secondment as Chief Executive of the Biotechnology and Biological Sciences Research Council. He coauthored the paper that coined the term ‘metabolomics’, and has published more than 400 papers, with an H-index of 67.

Session: Opening Plenary Lecture, Monday 1st July: 17.00 – 18.00

PL-1
THE CELLULAR UPTAKE OF PHARMACEUTICAL DRUGS: A PROBLEM NOT OF BIOPHYSICS BUT OF SYSTEMS BIOLOGY

Douglas B. Kell
School of Chemistry and the Manchester Institute of Biotechnology, The University of Manchester, 131 Princess St, Manchester, Lancs, M1 7DN, UK

A fundamental question remains as to whether xenobiotic drugs cross cellular membranes mainly (or exclusively) by ‘passive’ (transporter-independent) diffusion across cellular membranes, or whether they normally (or exclusively) ‘hitchhike’ rides using the carriers normally involved in the metabolism of natural metabolites. The former would involve a biophysical mechanism, based mainly on lipophilicity, while the latter requires a mechanistic understanding of which carriers are involved, and is thus a problem of network or systems biology. In other words [1], is carrier-mediated transport of pharmaceutical drugs the exception or the rule?

A huge amount of literature [1-5, and references therein], that I shall summarise, indicates that there is no serious evidence for transbilayer-mediated transfer of pharmaceutical drugs across biological membranes, while there is abundant and increasing evidence for the carrier-mediated route. A recent approach in yeast illustrates this experimentally [6], while the digital availability of principled metabolic network models [7,8] allows one to determine [9], consistent with this, that successful pharmaceutical drugs are much more like metabolites than are the ‘Lipinski-compliant’ molecules typically available in drug discovery libraries. This suggests that cellular drug uptake is more or less exclusively transporter-mediated, and that knowledge of both the metabolome and of the transporters used by individual xenobiotics will be of much value in designing better drugs [10].

References:
Wolfram Werkwerth
University of Vienna, Austria

In 2008 Wolfram Werkwerth moved as a full professor to the University of Vienna and founded the Department of Molecular Systems Biology (MOSYS). The Werkwerth lab develops genome-wide metabolomics and proteomics/phosphoproteomics technologies as elementary systems biology techniques. Further research comprises data integration strategies by combining experimental approaches with multivariate statistics, pattern recognition and modeling of metabolism.

Session: Plenary Session 1, Tuesday 2nd July: 08.30 -09.50

PL-2
SOLVING THE BIOCHEMICAL JACOBIAN – AN EQUATION TO SYSTEMATICALLY LINK THE GENOTYPE TO THE MEASURED METABOLIC PHENOTYPE

Wolfram Werkwerth
Department for Molecular Systems Biology, University of Vienna, Althanstr.14, 1090 Vienna, Austria

Systems biology is the approach to combine molecular data, genetic evolution, environment and species-interaction with the computer-assisted understanding, modeling and prediction of active biochemical networks. The idea relies strongly on the existence of complete genome sequences and the development of new technologies for the analysis of molecular data. Here, projection of metabolomics data into genome-wide metabolic networks combined with metabolic modeling emerge as important technologies for improving gene annotation processes (Werkwerth, 2011b). Using quantitative proteomics and metabolomics we begin to investigate the genome-scale molecular phenotype and the interrelation of the metabolome, the proteome and its environment (Werkwerth, 2011a). Metabolomics and proteomics data integration strategies and modeling approaches will be discussed for model systems as well as ecosystems. For these approaches an extended metabolomics platform comprising GC-MS and LC-MS is presented (Scherling et al., 2010; Doerfler et al., 2012; Mari et al., 2012). However, before data reveal their interrelation, extended statistical and mathematical concepts are required for the integrative analysis of multifactorial phenomena (Werkwerth, 2003). The detection of significant correlations between the different components based on principal components analysis or related techniques is the basis for biological interpretation (Morgenthal et al., 2005; Werkwerth and Morgenthal, 2005; Werkwerth, 2008; Wienkoop et al., 2008). We have extended this idea and developed an approach which connects systematically the predicted genotype with the statistical features of metabolomics data (Sun and Werkwerth, 2012). By using this approach, recently, we were able to calculate the differential biochemical Jacobian from perturbed metabolomics data for the first time (Doerfler et al., 2012). Results and implications of this approach will be discussed.

References:
Werkwerth W (2011a) Green systems biology - From single genomes, proteomes and metabolomes to ecosystems research and biotechnology. J Proteomics 75: 284-305
Oliver Fiehn  
NIH West Coast Metabolomics Center, USA

Dr. Fiehn is Full Professor at the UC Davis Genome Center, teaching biochemistry at the graduate and undergraduate level. Since September 2012, he heads the NIH West Coast Metabolomics Center, directing his research laboratory and overseeing the service core laboratory with a total of 13 mass spectrometers and 25 staff members.

Session: Plenary Session 1, Tuesday 2nd July: 08.30 -09.50

PL-3  
COMPREHENSIVE METABOLOMICS FOR STUDY OF HUMAN DISEASES: INTEGRATION OF PLATFORMS AND TOOLS IN THE NIH WEST COAST METABOLICOMICS CENTER

Oliver Fiehn  
NIH West Coast Metabolomics Center, Davis CA, USA

The NIH Common Fund has created three regional resource cores to increase the capacity for metabolomic research for NIH-funded projects. At UC Davis, the West Coast Metabolomics Center integrates more than 30 mass spectrometers and 5 NMR instruments in eight laboratories, focusing on glycomics, complex lipids, eicosanoids and lipid mediators, imaging, primary metabolism and identification of unknowns. In addition, integration with genomic data including pathway mapping and statistics is part of research advancements and fee-based services. In its first year, the West Coast Metabolomics Center has hosted three symposia on cancer metabolism, microbial metabolism and a hands-on workshop for training the next generation of scientists. The yearly pilot project funding competition for external clinical and biomedical scientists has been decided, and the projects will be highlighted briefly.

Platforms and example studies conducted by the West Coast Metabolomics Center are presented to give insights into the approach taken by our Center. We will elaborate how metabolomic data could formulate hypotheses that are subsequently validated by genomic data in pharmametabolomic studies, we will show how discoveries in glycomics led to different treatments of newborns in the neonatal care unit at the UC Davis hospitals, and we demonstrate how novel biomarkers in lung cancer enable diagnosis of the disease up to one year before patients present to the clinic, giving more time for treatment for these patients.

Julian Dow  
University of Glasgow, UK

Julian Dow is M.A. Ph.D. Sc.D. in Zoology from Cambridge University. He is Professor of Molecular and Integrative Physiology at Glasgow. He studies Earth’s dominant life-forms, the insects, using the technologies of functional genomics to find how different tissues integrate to make a working organism. He runs FlyAtlas.org.

Session: Parallel Session 1A: Model Organisms, Tuesday 2nd July: 10.20 -12.00

PL-4  
DROSOPHILA, METABOLOMICS AND FUNCTIONAL GENOMICS – A MATCH MADE IN HEAVEN

Julian A.T. Dow, Dominika Korzekwa, Elizabeth Cannell, Shadi Al Johani, Daniel Erben, Venkateswara R. Chintapalli, Shireen A. Davies, Rainer Breitling¹, David G. Watson²  
Institute of Molecular, Cell & Systems Biology, College of Medical, Veterinary and Life Sciences, University of Glasgow, Glasgow G12 8QQ, UK; ¹Computational & Evolutionary Biology, Faculty of Life Sciences, University of Manchester M13 9PL, UK; and ²Strathclyde Institute Of Pharmacy And Biomedical Sciences, Strathclyde University, Glasgow G4 0NR, UK

Compared to classic models like yeast, multicellular organisms present the challenge of complexity but also the opportunity to understand function of the whole organism in the context of its constituent parts. Drosophila is an ideal "bridge" organism, with a compact, sequenced genome, and powerful genetic resources and reverse genetic technologies that allow gene function to be elucidated in the context of the whole organism. Previously, we published a tissue and life-stage specific transcriptional atlas for Drosophila (FlyAtlas.org), providing insights into what individual tissues contribute to overall function. We have also shown that Drosophila is amenable to global metabolomic analysis, using the Orbitrap mass spectrometer to identify around 500 compounds in each run. This approach has been particularly useful in studying fly models for human inborn errors of metabolism, such as xanthinuria. We have also shown that, just like mRNA levels in FlyAtlas.org, baseline metabolomes differ between tissues in larval and adult fly, providing useful insights into pathways of particular importance in specific tissues. To take our analysis to a further level, we have developed a model of core metabolism in MATLAB/COBRA, and used flux balance analysis to identify gaps. Presently, we are engaged in filling these gaps experimentally by reverse genetics, and extending the model.
Jean-Charles Portais
University of Toulouse, France

Jean Charles Portais is Professor of Biochemistry at the University of Toulouse (France) and he is heading the Research Group MetaSys (Metabolic Systems), which aims at the comprehensive, system-level understanding of metabolism and its role in cellular behaviour, with applications in biotechnology and human health. Prof. JC Portais is also heading MetaToul, the Metabolomics & Fluxomics Centre of Toulouse.

Session: Parallel Session 1B: Fluxomics, Tuesday 2nd July: 10.20 -12.00

PL-5
ROLE OF POST-TRANSCRIPTIONAL REGULATION IN THE CONTROL OF CARBON METABOLISM

Olga Revelles1,2,3, Pierre Millard1,2,3, Jean-Philippe Nougayrède4,5,6,7, Ulrich Dobrindt8, Eric Oswald4,5,6,7, Fabien Létisse1,2,3 and Jean-Charles Portais1,2,3,9.

1Université de Toulouse; INSA, UPS, INP, LISBP, 135 Avenue de Rangueil, F-31077 Toulouse, 2INRA, UMR792 Ingénierie des Systèmes Biologiques et des Procédés, F-31400 Toulouse, 3CNRS, UMR5504, F-31400 Toulouse, France; 4INRA USC1360, 5Inserm U1043, 6CNRS UMR5282, 7Université de Toulouse, UPS, Centre de Physiopathologie de Toulouse Purpan (CPTP), F-31400 Toulouse, France, 8Institute for Hygiene, University of Münster, 48149 Münster, Germany.

Metabolism is a basic cellular function that sustains survival, growth and adaptation of living organisms. As such metabolism is submitted to intense regulation by highly sophisticated global regulatory networks coordinating the physiological and metabolic responses. If metabolic and transcriptional regulations of metabolism have been studied in details, the role of post-transcriptional regulation in the control of carbon metabolism has been poorly investigated. The Carbon Storage Regulator (Csr) system is a post-transcriptional regulation system that controls a broad range of physiological mechanisms (including formation of biofilm, motility and virulence) and is a global regulator of central metabolism in the bacterium *Escherichia coli*. To get comprehensive understanding of the role of Csr in metabolic adaptation, we have investigated mutants altered for the various components of the Csr system. The results show that mutants altered for CsrA, the main component of this system have decreased growth efficiencies on a broad range of physiologically relevant carbon sources. Detailed investigations of the metabolomes and fluxomes of mutants and wild-type cells grown on various carbon sources revealed significant and nutrient-dependent re-adjusting of central carbon metabolism, indicating a significant role of CsrA in the control of carbon metabolism.

Eyal Gottlieb
The Beatson Institute for Cancer Research, UK

Professor Eyal Gottlieb runs the Apoptosis and Tumour Metabolism lab at the Beatson Institute for Cancer Research in Glasgow. His laboratory combines analytical chemistry (metabolomics), cell biology, and biochemical approaches to study metabolic transformation.

Session: Parallel Session 2A: Cancer Research, Tuesday 2nd July: 13.30 -15.30

PL-6
METABOLISM AND CANCER: WHY SHOULD WE CARE?

Eyal Gottlieb
The Beatson Institute for Cancer Research, Glasgow, UK

As a result of increased bioenergetic demands and the need to grow and proliferate, cancer cells have unique metabolic traits compared to normal cells. At the same time, cancer cells are exposed to more extreme conditions of metabolic stress due to the uncontrolled growth of the tumour away from the vascular system that provides oxygen and nutrients to its cells. Therefore, cancer cells have developed defence mechanisms that are selected under conditions of stress and cells that survive this strongly selective environment have a more aggressive phenotype. Targeting these survival mechanisms may help eliminate cancer growth and specifically induce cancer cell death. Our work utilizes analytical chemistry and system biology approaches to study metabolic transformation. We investigated cells deficient in the mitochondrial tumour suppressor fumarate hydratase (FH). FH is a tricarboxylic acid (TCA) cycle enzyme and a tumour suppressor which is lost in some severe cases of renal cell cancer. Using genetically-modified primary mouse renal cells we collected metabolomics data and applied a computational model, generated to study their unique metabolome. We identified several important metabolic pathways which are specific and crucial for the survival of cells deficient in FH. These include the heme biosynthesis and degradation pathway.
as well as mechanisms of alleviating TCA cycle carbon stress. These technologies are not only important for understanding the basic biochemistry of cancer cells but they can inform us on future clinical management of cancer and may lead to new therapeutic approaches to target cancer-specific metabolic pathways.

**Paul Fraser**  
Royal Holloway University of London, UK

Dr. Paul D. Fraser is a permanent member of staff at Royal Holloway University of London. Dr. Fraser has worked on the analysis, biosynthesis, regulation and metabolic engineering of carotenoids and other isoprenoids, both in plant and microbial systems, publishing over 100 peer reviewed articles in the field. Dr. Fraser is also the coordinator of the FP7 METAPRO project (www.isoprenoid.com) the Vice-chair of FA1006 High value products from plants (www.plantengine.eu) and EU Chair for the US/EU Taskforce on Plant Bioethchnology-added value plant products working group.

**Session: Parallel Session 2B: Crop Improvement, Tuesday 2nd July: 13.30 -15.30**

**PL-7 APPLICATION OF METABOLOMICS TO PLANT BREEDING BY GENETIC INTERVENTION**

Paul, D. Fraser  
Centre for Systems and Synthetic Biology, Biological Sciences, Royal Holloway University of London, Egham Hill, Egham, Surrey, TW20 OEX. UK

Tomato fruit and its products are one of the most widely consumed fruits and vegetables in the world. They are important components of the human diet supplying essential micronutrients. In addition to being an important economic crop, tomato is also a model for all crop plants. Excellent genetic resources exist in tomato culminating in the recent release of the tomato genome sequence (www.solgenomics.net). The depth and breath of chemical diversity found in tomato has also contributed to the development of metabolomics/metabolite profiling expertise in tomato and other Solanaceae. In this presentation the role of metabolomics in:

(i) The large-scale multi-platform metabolite analysis of natural variation in tomato that exists in the form of the *Solanum pennellii* near isogenic introgression (II) will be described. Collectively this data generated has provided, a valuable metabolite resource, a rapid means of associating trait to metabolite and in some cases effector gene and revealed valuable insights into the organisation of metabolism in tomato fruit and other plant systems.

(ii) The metabolomic characterisation of genetic engineering approaches for high value isoprenoids in *Solanaceae* illustrating the perturbations that arise across metabolism and how changes in the composition of metabolites can impact on the plastids generated and their internal ultrastructure.

Acknowledgements. Financial support from the EU, BBSRC, Royal Society and Syngenta Ltd (formally Zeneca) is gratefully acknowledged

**Graham Cooks**  
Purdue University, USA

Graham Cooks is Henry Bohn Hass Distinguished Professor of Chemistry at Purdue University and Director of the Center for Analytical Instrumentation Development. He is a pioneer in the conception and implementation of MS/MS and of desorption ionization. These interests led to the construction of miniature ion trap mass spectrometers and their application to problems of trace chemical detection. Cooks is a past President of the American Society for Mass Spectrometry and the International Mass Spectrometry Society and a Life Member of the British Mass Spectrometry Society. He is the recipient of the ACS awards in Mass Spectrometry and in Analytical Chemistry, the Robert Boyle and Centennial Medals of the Royal Society of Chemistry.

**Session: Plenary Session 2**  
Wednesday 3rd July: 08.30 -09.50

**PL-8 ANALYTICAL, IMAGING, MINIATURE AND PREPARATIVE MASS SPECTROMETRY IN METABOLOMICS**

R. Graham Cooks  
Department of Chemistry and Center for Analytical Instrumentation Development, Purdue University

A minor revolution is occurring in mass spectrometry with the growing recognition that it is possible to simplify sample preparation and still obtain high quality chemical information on complex real-world samples. At the core of this
development is a set of ambient ionization experiments in which ionization is performed in air, outside the mass spectrometry, on samples in their native form. Starting with the use of a charged spray (desorption electrospray ionization, DESI) in 2004, implementation included plasmas, lasers and thermal agents. The fundamentals of DESI and the paper spray method are reviewed and their applications to metabolomics are illustrated. These include DESI imaging applied to disease diagnosis and paper spray for the quantitative analysis of therapeutics and metabolites in whole blood. Comparisons with traditional LC/MS/MS methods of trace quantitative analysis are made to validate these rapid methods. Remarkable reaction rate enhancements are observed in the spray based ambient ionization methods that allow increased sensitivity and specificity in metabolite determination in biofluids. An overview of mass spectrometry instrumentation is followed by a discussion of the current state of development of miniature mass spectrometers, especially their use as portable instruments for in-situ applications.

Roy Goodacre
University of Manchester, UK

Roy Goodacre is Professor of Biological Chemistry at the University of Manchester and works in the Manchester Institute of Biotechnology. His research focuses on developing MS-based metabolomics along with new chemometric approaches that he applies to help understand how organisms respond to external perturbations. His group also develops Raman spectroscopy for chemical imaging and surface enhanced Raman scattering for trace detection of (bio)chemicals.

Session: Plenary Session 2
Wednesday 3rd July: 08.30 -09.50

PL-9
STRESS & DRUGS AND ROCK & ROLL: TOWARDS AN UNDERSTANDING OF MICROBIAL ADAPTATION

Felicity Currie, Emma Wharfe, Soyab Patel, Warwick Dunn, David Broadhurst, Yun Xu, Catherine Winder, and Roy Goodacre
Manchester Institute of Biotechnology (MIB) & School of Chemistry, University of Manchester, UK

Human pharmaceuticals are readily detected in wastewater treatment plants, rivers and estuaries. Whilst levels are not yet high enough to cause immediate harm to aquatic life, it is widely acknowledged that there is insufficient information available to determine whether exposure to low levels of these substances over long periods of time is having an impact on the microbial ecology of these environments. In order to investigate the effect on the metabolic potential of the microbial community we have been adopting a metabolomics approach using various analytical platforms including vibrational spectroscopic approaches for generating metabolic fingerprints, gas chromatography-mass spectrometry (GC-MS) for metabolic profiling and direct infusion (DIMS) and liquid chromatography mass spectrometry (LCMS) for lipid profiling. Analysis of environmentally relevant microbes and algae will be presented. We shall show that Propranolol had significant effects on the lipid components of Pseudomonas putida cells, and in particular we detected changes in the acyl chains of cardiolipins (the degree of saturation) which may have changed in order to maintain correct membrane fluidity (so called homeoviscous adaptation). Propanolol is a chiral pharmaceutical and we shall also show that some bacteria respond differently to the two enantiomers and this results in different effects on cellular phenotype. Finally, we turn our attention to exploiting metabolomics for probing real complex environmental systems and investigate phenol-degrading bioreactors containing yet to be defined microbial communities.

Dan Rujescu
University of Halle, Germany

Dan Rujescu is head of the Department of Psychiatry of the University of Halle with wards for 100 in-patients. He is involved in the research of genetics of psychiatric diseases including national and international genome and post-genome projects. His group has recruited a large sample of patients and controls (n=4,500).

Session: Parallel Session 5A: Metabolomic Profiling in Neuroscience,
Wednesday 3rd July: 13.20 -15.00
PL-10
METABOLICIN SCHIZOPHRENNIA

Dan Rujescu
Department of Psychiatry, University of Halle, Germany

A major challenge in medicine is to understand genetic, molecular and cellular mechanisms underlying common mental disorders including schizophrenia, which involve complicated genetic and environmental determinants. Schizophrenia is a common mental disorder, affecting 0.5-1% of the population. It mostly presents with several episodes and tends to become chronic. The underlying molecular mechanism of schizophrenia is poorly understood. Metabolomics can provide valuable information about disease pathogenesis and result in metabolic signatures that could be developed as biomarkers for disease and progression. Comparative studies in plasma could help map peripheral changes in metabolism in schizophrenia and enable a more accessible way for biomarker development. Using targeted metabolomics we quantified and compared 103 metabolites in plasma samples from 216 healthy controls and 265 schizophrenic patients, including 52 cases without antipsychotic medication. Compared with healthy controls, levels of five metabolites were found significantly altered in schizophrenic patients (p-values ranged from 2.9×10-8 to 2.5×10-4) and in neuroleptics-free probands. These metabolites include four amino acids (arginine, glutamine, histidine and ornithine) and one lipid (PC ae C38:6) and are suggested as candidate biomarkers for schizophrenia. Furthermore we constructed a molecular network connecting these five aberrant metabolites with 13 schizophrenia risk genes. Our result implicated aberrations in biosynthetic pathways linked to glutamine and arginine metabolism and associated signaling pathways as genetic risk factors, which may contribute to patho-mechanisms and memory deficits associated with schizophrenia. This study illustrated that the metabolic deviations detected in plasma may serve as potential biomarkers to aid diagnosis of schizophrenia.

Georg Pohnert
Friedrich Schiller University, Germany

Georg Pohnert studied Chemistry Karlsruhe and pursued his doctoral studies on algal pheromones in the Group of Prof. W. Boland in Bonn. In 1997 he joined the Ganem-group at the Cornell University as a postdoc working on the biochemical and biophysical characterisation of E. coli receptors. As group leader at the Max-Planck-Institute for Chemical Ecology he addressed algal defence reactions. In 2005, he was appointed as assistant professor at the EPFL, Lausanne and moved in 2007 to the Friedrich-Schiller-University in Jena where he holds a chair in Instrumental Analytics.

Session: Parallel Session 5B: Environmental, Wednesday 3rd July: 13.20 -15.00

PL-11
Deciphering Highly Dynamic Chemically Mediated Interactions of Microalgae Using a Combined Metabolomics / Bioassay Approach

Georg Pohnert
Institute for Inorganic and Analytical Chemistry Bioorganic Analytics, Friedrich Schiller University, Germany

It is well established that unicellular algae in biofilms and in the plankton have established means to interact with other organisms using chemical signals. Algal exudates and metabolites stored in the cells can e.g. mediate feeding activity of herbivores and interactions with conspecific algae via pheromones. But also the surrounding microbial community can be influenced by released metabolites. We introduce an approach to address such chemically mediated interactions based on a comparative metabolomics approach. Metabolomic surveys indicate that diatoms exhibit a high plasticity of metabolic activity in response to environmental factors and biotic interactions. Metabolite concentration changes dramatically in response to limiting nutrients or osmotic stress and a pronounced circadian variability can be observed as well. But our results also indicate that the regulation of biosynthetic pathways in microalgae is highly dependent on the ecological context of the cells. We used bioassays to demonstrate how the variable chemical profiles of the algae are causing pronounced variability of the chemical interaction with the environment. Such comparative metabolomics approaches enabled the identification of the first diatom pheromone, novel diatom defense metabolites and of compounds influencing diatom-diatom interactions. Consequences for future investigations of diatom chemical interactions and ocean functioning are discussed.
Uwe Sauer  
ETH Zurich, Switzerland

With a Ph.D. in Microbiology (1992, Univ. Göttingen), Uwe Sauer is Professor of Systems Biology at the ETH Zurich. His research focuses on quantitative understanding of the complex regulation processes that control cellular metabolism. His lab has pioneered development of high-throughput metabolomics and flux analysis methods.

Session: Parallel Session 7A: Fermentation, Thursday 4th July: 09.00 -10.25

PL-12  
HIGH THROUGHPUT METABOLOMICS OF THE ENTIRE \textit{E. coli} DELETION LIBRARY

Uwe Sauer  
Institute of Molecular Systems Biology, ETH Zurich

Given that we know the structure of metabolic networks relatively well, our focus is on understanding how metabolic fluxes emerge from the interactions of thousands of genes, proteins and metabolites (1). In particular we ask how these network-wide fluxes are managed and which of the multiple overlapping regulatory mechanisms and the metabolic feedback into these regulatory networks actually control flux under a given condition (2, 3). Since the throughput of $^{13}$C-based flux experiments for systematic large-scale studies remains still limited, we developed a novel method for high-throughput intracellular metabolomics (4). Here I will discuss the application of this method to all 8600 clones of the \textit{E. coli} genome-deletion (KEIO) library (5), and how those results can be exploited for functional assignment of novel enzymatic functions and in learning from metabolomics data about active regulation mechanisms.

References:

Christopher Newgard  
Duke University Medical Center, USA

Christopher B. Newgard, Ph.D. is Director, Sarah W. Stedman Nutrition and Metabolism Center and the W. David and Sarah W. Stedman Distinguished Professor at the Duke University Medical Center. His laboratory applies an interdisciplinary approach for understanding of diabetes, obesity, and cardiovascular disease mechanisms.

Session: Parallel Session 7B: Metabolomic Profiling in Diabetes and Heart Disease, Thursday 4th July: 09.00 -10.25

PL-13  
METABOLOMICS PROFILING IN DIABETES AND HEART DISEASE

Christopher B. Newgard, PhD  
Sarah W. Stedman Nutrition and Metabolism Center, Duke University Medical Center, Durham, NC USA

We seek to apply metabolomics for understanding of mechanisms underlying the pandemic metabolic diseases of our era--diabetes, obesity, and cardiovascular disease. We have used these tools to define mechanisms underlying development of peripheral insulin resistance and glucose intolerance in animals and humans. For example, we have recently identified perturbations of branched chain amino acid (BCAA) catabolism in multiple cohorts of insulin resistant humans compared to normally insulin sensitive controls. Our studies and those of others have demonstrated the prognostic power of this signature to predict incident diabetes and intervention outcomes. These metabolites are also uniquely sensitive to the most efficacious interventions for obesity and diabetes. We have translated these findings to rodent models to demonstrate a contribution of BCAA to abnormalities in mitochondrial metabolism that contribute to the insulin resistant state, as well as to behavioral abnormalities associated with obesity. We have also identified novel metabolic signatures of imminent cardiovascular events, including BCAA and a cluster of short-chain dicarboxylated acylcarnitines, and are integrating genomic and metabolomics analyses in large cohorts of human subjects to identify pathways involved in the production of these metabolites and their relationship to risk of cardiovascular disease. These examples will serve to illustrate the potential of comprehensive metabolic profiling methods for providing insights into metabolic disease mechanisms.
Guowang Xu
CAS Key Laboratory of Separation Science for Analytical Chemistry, China

Prof. Dr. Guowang Xu is Director of Metabonomics Research Center in Dalian institute of chemical physics, Chinese Academy of Sciences. He has published more than 300 peer-reviewed papers and holds 20 China patents, co-written 4 books. His main research field is in chromatography, MS and the metabolomics applications in disease biomarker discovery, traditional Chinese medicines and food safety.

Session: Parallel Session 9A: Personalised Medicine, Nutrition and General Human Health, Thursday 4th July: 13.10 – 15.10

PL-14
TOWARDS PERSONALISED MEDICINE OF CANCER BASED ON MS-BASED METABOLOMICS

Guozhu Ye, Peiyuan Yin, Lina Zhou, Xin Lu, Guowang Xu
CAS Key Laboratory of Separation Science for Analytical Chemistry, National Chromatographic R&A Center, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, China

In the 21st medicine a growing interest is to develop an individually tailored therapeutic approach by using the disease information characterized at the molecular level to improve diagnoses and produce better medical outcomes. Biomarkers are the foundation for personalised medicine. Metabolomics is a tool to study all endogenetic small molecules in a biological system, it can provide the metabolic state (phenotype) of an individual and find the potential biomarkers.

In our lab a comprehensive metabolomics platform has been established by using chromatography-mass spectrometry and capillary electrophoresis-mass spectrometry techniques. More than 10 analytical methods have been developed. With these methods, great attention has been paid to the early diagnosis and personalized treatment of hepatocellular carcinoma and oral squamous cell carcinoma. Several metabolites have been identified as combinational biomarkers for cancer diagnosis, evaluation of the operation and chemotherapy efficacy, and prediction of tumor recurrence after surgery. We also found that serum metabolites were sensitively responsive to TPF induction chemotherapy, and the metabolites were beneficial to the evaluation and prechemotherapy prediction of induction chemotherapy outcomes, illustrating the metabolomics potentials for personalised induction chemotherapy.

References:

Michael Barrett
University of Glasgow, UK

Mike Barrett is Professor of Biochemical Parasitology at the University of Glasgow. He is particularly interested in applying metabolomics to learn about parasite biology, how drugs work, mechanisms of drug resistance and metabolite biomarkers to diagnose disease. He is founding director of the Scottish Metabolomics Facility and “Glasgow Polyomics”.

Session: Parallel Session 9B: Parasitology and Infectious Diseases, Thursday 4th July: 13.10 – 15.10

PL-15
METABOLOMIC ANALYSIS OF PARASITIC PROTOZOA

Mike Barrett
Wellcome Trust Centre for Molecular Parasitology and Glasgow Polyomics, University of Glasgow

Metabolomics allows the simultaneous identification of many hundreds of metabolites within a given system. We have applied untargeted LC-MS based metabolomics approaches (based on Orbitrap technology) to numerous systems including trypanosomes and leishmania. In studying modes of action of trypanocidal drugs we show how metabolomics can point to drug targets e.g. ornithine decarboxylase in treatment with eflornithine and also drug resistance mechanisms (loss of drug uptake associated with eflornithine resistance). In differentiation of slender bloodstream form to short stumpy form trypanosomes we note increases in carnitine levels as slender forms
transform to stumpy forms and both the pentose phosphate pathway and cellular thiol levels increase. In Leishmania we have identified mechanisms for resistance to amphotericin B by taking a polyomic based approach comparing wild-type and resistant cells at the level of genome, proteome and metabolome, with changes to sterol metabolism shown to underlie resistance related to alterations to the parasite’s CYP51 enzyme. Novel unexpected pathways of metabolism have also been identified by studying the distribution of heavy atom isotopes of various substrates. In addition to identifying many aspects of parasite biochemistry we have also investigated how host’s respond to parasite infection and reveal important markers of infection.
O1A-1
LARGE-SCALE SURVEY OF METABOLITE CONCENTRATIONS IN HUMAN, CHIMPANZEE, MACAQUE AND MOUSE TISSUES SUGGESTS TRADEOFF BETWEEN HUMAN MUSCLE AND BRAIN
Kasia Bozek
Partner Institute for Computational Biology CAS-MPG, Shanghai, China
We performed a large-scale comparative study of metabolite concentrations in three brain regions and two non-neural tissues (muscle and kidney) of humans, chimpanzees, macaques and mice. We found a large excess of human-specific metabolic divergence in prefrontal cortex part of brain (PFC) and muscle of 4- and 7-fold respectively. We hypothesize that the rapid metabolic evolution of human PFC and muscle shaped unique human cognitive functions and physical features such as muscle strength.

O1A-2
METABOLOMICS AND SYSTEMS BIOLOGY OF GENOTYPE-BY-DIET INTERACTIONS UNDERLYING METABOLIC SYNDROME IN DROSOPHILA.
Laura Reed
University of Alabama, Tuscaloosa, AL, USA
Metabolic Syndrome affects more than 30% of adults living in Westernized societies and is the result of both genetic and environmental effects. We use Drosophila as a model system to elucidate the relative contributions of genotype and diet to Metabolic Syndrome as mediated through metabolomic and transcriptomic profiles. We demonstrate that both familiar and novel mechanisms contributing to Metabolic Syndrome can be identified using this systems biology approach in a naturally variable population.

O1A-3
METABOLOMIC ANALYSIS OF PEANUT ALLERGY IN A MOUSE MODEL
Brian McCarry
McMaster University, Hamilton, Ontario, Canada
A tandem column LC-ESI-TOF-MS method was used for a time-series analysis of both polar and non-polar metabolites in sera of control mice and mice that had been sensitized to peanuts following an intraperitoneal injection of peanut extract. Statistical analyses of 3500 metabolic features revealed significant changes in the purine catabolism pathway. Subsequent experiments in two mouse models of peanut allergy showed that uric acid is a mediator of both peanut sensitization and peanut anaphylaxis.

O1A-4
THE COMBINED USE OF DROSOPHILA AND YEAST AS MODEL ORGANISMS FOR THE IDENTIFICATION OF UNKNOWN MITOCHONDRIAL PROTEIN FUNCTION.
James Cox
University of Utah, Salt Lake City, UT, USA
To determine the function of unknown mitochondrial proteins we have developed a GC/LC-MS based metabolomics platform using the model organisms S. cerevisiae and Drosophila. Yeast offer two advantages, rapid mutant generation and large scale mitochondria isolation. The fly also offers two advantages complimentary to yeast, a segmented life cycle and distinct tissues. Using this platform we identified the function of Mpc1 and Mpc2, essential mitochondrial pyruvate carrier proteins also found in humans.
O1B-1
METABOLOMICS AND FLUXOMICS IN MAMMALIAN TISSUE: METHOD OPTIMIZATION AND INSIGHTS INTO METABOLITE FLUX DURING EXERCISE
Charles Evans
University of Michigan, Ann Arbor, MI, USA
We present results from LC-MS and GC-MS analysis of rodent tissue collected under various modes of anesthesia. Different modes of anesthesia resulted in significant alterations in central carbon metabolism including changes in hexose phosphates, lactate, TCA cycle intermediates, and nucleotide phosphates. We applied optimized methods to study metabolic flux by administering carbon-13 enriched stable-isotope tracers to rodents prior to treadmill exercise. Mass isotopomer analysis enabled assessment of relative metabolite flux under different exercise conditions.

O1B-2
A METHOD TO MEASURE METABOLIC FLUX WITH HEAVY ISOTOPE LABELLING AND MASS SPECTROMETRY
Pernilla Lindén1,2
1Swedish University of Agricultural Sciences, Umeå, Sweden, 2Umeå Plant Science Centre, Umeå, Sweden
We present a method measuring metabolic flux in plants. By combining heavy isotope labelling and GC- and LC-MS techniques the 13C- incorporation can be followed. For validation we used a mutant, lacking the most highly expressed isoform of mitochondrial malate dehydrogenase (mMDH1). Labelling was done for two hours in mid-photoperiod under three different CO₂ conditions. The results support previous findings regarding the role of mMDH1 in photorespiratory metabolism and the strength of this method.

O1B-3
CROSS-LABELED 13C-STEARATE FATE DETECTION IN THE [1,2-13C2]-D-GLUCOSE DERIVED ISOTOPOLOME IMPROVES SYSTEM WIDE ASSOCIATIONS WHEN COMPARED WITH EXTERNAL [U-13C18]-STEARATE INCUBATION IN ROSIGLITAZONE TREATED HEPG2 CELLS
László G Boros
Los Angeles Biomedical Research Institute (LABIOMED) at the Harbor-UCLA Medical Center, Department of Pediatrics, Torrance, Los Angeles, CA, USA
[1,2-13C2]-D-glucose derived cross-labeled 13C-stearic acid improves system wide associations between ribonucleic and fatty acids in rosiglitazone treated HepG2 cells, in comparison with associations obtained when external [U-13C18]stearate was used. Internally cross-labeled 13C-stearate from the single [1,2-13C2]-D-glucose tracer readily serves as the precursor of other fatty acids and RNA ribose, while external [U-13C18]stearate pends transport and substrate availability constraints. Targeted [1,2-13C2]-D-glucose assisted metabolomics recognizes important substrate-product relationships on a system wide scale in the same experiment.

O1B-4
KINETIC MODELING APPLIED TO THE ANALYSIS OF 13C TRACER DISTRIBUTION IN METABOLITES: NEW LIFE FOR THE OLD TOOL.
Vitaly Selivanov
Universitat de Barcelona, Barcelona, Spain
The adaptation of kinetic modeling for the analysis of time course of isotopic isomer distributions is presented. The advantages of the kinetic approach: i) extraction the most complete information from the dynamics of labeling, ii) evaluation of the characteristics of metabolism more profound than just flux distribution, such as metabolism compartmentation, parameters of enzymatic reactions, regulatory mechanisms. Several examples of the application of kinetic modeling for 13C tracer data analysis are considered.
**O2A-1**
THE Myc/p53-DEPENDENT TUMOUR SUPPRESSOR miR-22 REGULATES MULTIPLE METABOLIC PATHWAYS IN CANCER CELLS
Hector Keun
Imperial College London, London, UK
MicroRNAs play a key role in producing common tumour metabolic phenotypes such as the Warburg effect and glutaminolysis. From an integrative analysis of molecular profiles from the NCI-60 cancer cell panel we identified the MYC/p53-dependent gene, miR-22, as having a profound association to metabolic phenotype. miR-22 overexpression suppressed glycolysis, promoted de novo fatty acid synthesis and glycogen storage, and targeted one-carbon metabolism - roles that could contribute to its proposed function as a tumour suppressor.

**O2A-2**
THE GLUTAMINE METABOLISM NETWORK IN MELANOMA
David Scott
Sanford-Burnham Medical Research Institute, La Jolla, California, USA
Glutamine is an important nutrient for cancer metabolism. Many cancer cells, including melanoma, die in culture without added glutamine. Using 13C-metabolite tracing and quantification of metabolites by GC-MS, together with selective gene knockdowns, we are mapping the use of glutamine as a carbon source in melanoma cells, particularly fluxes in and out of the TCA cycle. Thereby, we aim to identify vulnerabilities in the melanoma glutamine metabolic network that are amenable for therapeutic targeting.

**O2A-3**
ANALYSIS OF THE HYPOXIA METABOLOME
Alessandro Valli
1 Weatherall Institute of Molecular Medicine, University of Oxford, Oxford, UK, 2 Target Discovery Institute, Nuffield Department of Medicine, University of Oxford, Oxford, UK
Cancer cell metabolism strongly differs from normal cells; the low oxygen tension of the intra-tumoral mass induces the activation of hypoxia inducible factors HIF-1α. Colorectal cancer cells wild-type and hif-1alpha knockout were cultivated in normoxia or hypoxia and used for metabolomics analysis. We established a metabolomics platform based on nanoflow LC-MS reversed- and in-phase chromatography. Metabolomics microarray analysis shows that many metabolites are regulated independently of HIFs including glycolytic intermediates.

**O2A-4**
LIPIDOMIC RESPONSE TO HYPOXIA PROFILED BY 2-DIMENSIONAL GAS CHROMATOGRAPHY/MASS SPECTROMETRY
Benedikt Kessler
Target Discovery Institute, Nuffield Department of Medicine, University of Oxford, Oxford, UK
Cellular transformation from healthy to cancerous states includes reprogramming of metabolic pathways. Altered metabolism might support the unrestrained proliferation of cancer cells, leading to the formation of a tumor mass characterized by a low tissue oxygen tension (hypoxia).

Analysis of lipophilic cellular extracts of normal and hypoxic cancer cells by GCxGC-MS revealed enhanced de novo lipid biosynthesis and a more general lipogenic phenotype representing an important component of the metabolic reprogramming in cancer cells.

**O2A-5**
USE OF LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY (LC-MS) METABOLOMICS TO STUDY PLASMA BIOMARKERS: CASE STUDY USING A POTENT, SELECTIVE PAN-CLASS I PHOSPHATIDYL-INOSONITOL-3-KINASE (PI3K) INHIBITOR.
Joo Ern Ang
Cancer Research UK Cancer Therapeutics Unit, The Institute of Cancer Research, Sutton, Surrey, UK
Selective and potent PI3K inhibitors, such as GDC-0941, show promise in clinical trials; their development could potentially be accelerated by the use of minimally-invasive biomarkers. In this study, we identified plasma metabolites consistently modulated with the application of GDC-0941 in murine models and patients with time-dependent dose-response relationships. The impact of time-of-day and timed meals as potential confounders of these results were additionally studied in a separate group of volunteers maintained under stringently-controlled laboratory conditions.
O2B-1
HIGH THROUGHPUT TREE PROFILING - A NEW DIMENSION IN PLANT METABOLOMICS
Jane Ward
Rothamsted Research, Harpenden, Herts, UK
Research into woody bioenergy crops is looking towards metabolomics to aid selection of genotypes with improved biomass yield and quality for a number of industrial applications. Long established methods from our HTP screen using NMR-MS required complete revision to deliver robust analyses of tissues from biomass willows. The talk will explore primary and secondary C-flow under diurnal and abiotic stress conditions and detail approaches towards mapping mQTLs and delivery of new industrial products.

O2B-2
INTEGRATED METABOLOMATIC AND TRANSCRIPTOMIC PROFILING ILLUSTRATES SUCCESSIVE PHASES OF INCREASING GENE EXPRESSION ASSOCIATED WITH CHILLING-RELATED APPLE PEEL CELL DEATH
David Rudell
USDA-ARS, Wenatchee, WA, USA
Cold storage provoked cell death of apple peel (superficial scald) significantly impacts annual profits from susceptible apple cultivars. We used integrated transcriptomic/metabolomic analysis to identify metabolic processes associated with the period preceding and during symptom development to aid in understanding targets for crop improvement and diagnostic tools. Identified processes included associations among changes in volatile metabolite levels and specific genes that may be involved in providing precursor for this cell death associated pathway.

O2B-3
PROFILING OF SPATIAL METABOLITE DISTRIBUTIONS IN WHEAT LEAVES UNDER NORMAL AND NITRATE LIMITING CONDITIONS
J. William Allwood1,2
1School of Chemistry, Manchester Institute for Biotechnology, 131 Princess Street,, Manchester, M1 7DN, UK, 2School of Bioscience, University of Birmingham, Edgbaston, Birmingham, West Midlands, B15 2TT, UK
Nitrogen and carbon assimilation are co-ordinated in plant non-photosynthetic/photosynthetic tissues. In developing Wheat leaves, physiological measurements confirmed changes from heterotrophy to autotrophy. FT-IR and GC-TOF/MS profiling revealed metabolic responses as the leaf develops photosynthetic capacity in the presence or absence of nitrate. GC-TOF/MS profiles were assessed with multi- and uni-variate statistics and a novel approach, Bayesian Network analyses. The approach revealed altered metabolite distributions with respect to leaf position, nitrate supplementation, and photosynthetic development.

O2B-4
DIURNAL COMPOSITIONAL CHANGES OF TOMATO FRUIT AND LEAF
Annick Moing1,2
1INRA Bordeaux, Villenave d’Omon, France, 2Metabolome Facility of Bordeaux Functional Genomics Center, Villenave d’Ornon, France
The Fruit Integrative Modelling Eranet EraSysBio+ project aims at describing and modelling the influence of environmental factors on tomato (Solanum lycopersicum cv Moneymaker) fruit central metabolism. For this purpose, high-throughput biochemical phenotyping, GC-MS, LC-MS and NMR spectrometry have been used to estimate the metabolite content of expanding fruit and mature leaf for tomato plants cultivated in a greenhouse throughout a day and night cycle. Significant diurnal compositional changes have been detected for each tissue.

O2B-5
THE MOLECULAR ARMS RACE BETWEEN CLADOSPORIUM FULVUM AND TOMATO AT THE METABOLOME LEVEL
Desalegn Etalo1,2
1Centre for BioSystems Genomics, Wageningen, The Netherlands, 2Netherlands Metabolomics Centre, Leiden, The Netherlands
The molecular arms race between plants and pathogen involves an array of tools, from defence-related proteins to small molecules, like secondary metabolites. Using untargeted metabolomics technologies, in resistant tomato plants, we identified important classes of small molecules like hydroxycinnamic acid amides (HCAAs) and benzenoids that are induced during C. fulvum infection. Moreover, in susceptible plants, we showed how the pathogen manipulates the host defence system and metabolism, to access the plant carbon reserve.
**PARALLEL SESSION 3A: 16.00 – 17.30: LOMOND AUDITORIUM**

**NEW DEVELOPMENTS IN INSTRUMENTATION AND NEW TECHNIQUES**

**O3A-1**

**MASS SPECTROMETRY ANALYSIS OF SIGNALLING AND METABOLIC LIPIDS**

Qifeng Zhang

*Babraham Institute, Cambridge, UK*

A unique normal phase HPLC separation hyphenated with high resolution and accurate mass (HR/AM) tandem mass spectrometry approach has been developed, validated and adapted to routine analysis of almost all known lipids including 27 classes of neutral lipids, phospholipids and sphingolipids from a single Folch extraction of any cellular or tissue samples. This method is especially powerful in analysis of trace but biologically-important signalling lipids from complex matrixes.

**O3A-2**

**A PROTOTYPE MICROFLUIDIC MS PLATFORM FOR METABOLOMICS**

Giuseppe Astarita

*Waters Corporation, Milford, MA, USA*

Prototype microfluidic devices were optimized for MS analysis of metabolites in complex biological extracts. The devices are fabricated from resistant ceramic materials that permit operation at high pressure with sub 2 micron particles, leading to highly efficient LC separations of small molecules. Such microfluidic-based metabolomics analyses lead to equivalent results to using analytical-scale columns, with an overall reduction in solvent consumption of > 200 x.

**O3A-3**

**MULTI-SEGMENT INJECTION-CAPILLARY ELECTROPHORESIS-MASS SPECTROMETRY FOR METABOLOMICS: HIGH SAMPLE THROUGHPUT MEETS HIGH DATA QUALITY?**

Philip Britz-McKibbin

*McMaster University, Hamilton, ON, Canada*

Separation science plays a key role for enhancing the performance of mass spectrometry (MS)-based metabolomic studies. However, sample throughput is limited when using conventional separation platforms. We have developed a new approach for multiplexed analysis based on multi-segment injection (MSI)-capillary electrophoresis (CE)-MS that enhances sample throughput while improving data quality. We demonstrate that up to seven distinct sample plugs can be analyzed simultaneously within a “single capillary” while maintaining isomeric resolution without deleterious ion suppression.

**O3A-4**

**SPATIALLY-ENCODED 2D NMR STRATEGIES FOR FAST QUANTITATIVE METABOLOMICS**

Illa Tea

*Université de Nantes, CNRS, CEISAM UMR 6230, Nantes, France*

The development of precise and accurate quantitative 2D is highly important in the field of metabolomics. The combination of structural identification and quantification forms a unique combination for the metabolomics community. In this context, the work demonstrates for the first time the interest of an “ultrafast 2D metabolomics” approach, showing an unequalled precision compared to conventional approaches, moreover in a relatively short duration.

**O3A-5**

**THE USE OF STANDARD REFERENCE MATERIALS (SRM) AND CONTROL MATERIALS (CMS) FOR METABOLICS QUALITY CONTROL AND STABILITY ASSESSMENTS**

Daniel Bearden

*National Institute of Standards and Technology, Charleston, SC, USA*

For studies which may cover extended time frames or which include numerous individuals in sample processing, the issue of data consistency should be addressed in the experiment design so that the results are interpreted in the proper context. Here, we report on the systematic use in NMR-based metabolomics of matrix matched control materials (CM) and standard reference materials (SRM).

**O3A-6**

**CAN WE TRUST UNTARGETED METABOLOMICS: RESULTS OF THE METABO-RING INITIATIVE, A LARGE-SCALE MULTI-INSTRUMENTS INTER-LABORATORY STUDY**

Jean-Charles Martin

*INRA, Marseille, France, ²INRA, Clermont-Ferrand, France*

Our study was designed to evaluate the reliability of the untargeted metabolomics approach to produce convergent results when performed on the same set of samples by instruments of various technologies and located in different laboratories while using non-standardized procedures. This is thus far the largest inter-laboratory test implemented for metabolomics. Our main finding is that there is a high convergence in the spectral information produced from various instruments irrespective of the technology or standardization.
O3B-1
DEVELOPMENT OF METABOLITE PROFILING DATABASE FOR KNOCK-OUT MUTANTS IN ARABIDOPSIS (MEKO)
Atsushi Fukushima
RIKEN Center for Sustainable Resource Science, Yokohama, Kanagawa, Japan
To make the dataset available as an efficient public functional genomics tool for hypothesis generation, we developed the MeKO database (http://prime.psc.riken.jp/meko/), which allows evaluation of whether a mutation affects metabolism during normal growth in Arabidopsis. This database includes images of mutants, statistical data analyses, and data on differential metabolite accumulation. Non-processed data, including chromatograms, mass spectra, and experimental meta-data, follow the guidelines of the Metabolomics Standards Initiative (MSI) and are freely downloadable.

O3B-2
METABOLOMICS AS A TOOL TO CHARACTERIZE BIOCHEMISTRY OF THE MEDIATOR COMPLEX IN PLANTS
Ilka Abreu1,2
1Swedish University of Agricultural Sciences, Umeå, Sweden, 2Umeå Plant Science Centre, Umeå, Sweden, 3Umeå University, Umeå, Sweden
The metabolic profile of Mediator complex subunits have not been studied in plants. Arabidopsis mutant lines for 13 different subunits were analysed by LC-TOFMS and Orbitrap-MS. The OPLS-DA of each mutant showed differences from wild type and the predictive loading vectors were subjected to hierarchical cluster analysis and heat-map visualization. The metabolomic approach revealed novel metabolite-phenotype and provided a solid base for further studies on Mediator subunit function in integration of signals from different environments.

O3B-3
METABOLOMICS AS A TOOL TO CHARACTERIZE GENES INVOLVED IN THE SYNTHESIS OF BIOACTIVE SESQUITERPENES
Ric de Vos1,2
1Plant Research International, Wageningen University & Research Centre, Wageningen, The Netherlands, 2Netherlands Metabolomics Centre, Leiden, The Netherlands
Sesquiterpene lactones comprise a diverse group of plant terpenoid compounds with proven pharmaceutical activities. We aim to identify, isolate and characterize genes involved in the biosynthesis of these bioactive compounds by combining metabolomics with gene expression analyses and gene cloning strategies. Novel biosynthetic genes have been isolated and functionally characterized using metabolomics approaches. Simultaneous heterologous expression of sequential pathway genes in planta resulted in the accumulation of novel sesquiterpene-thiol conjugates.

O3B-4
METABOLITE PROFILING OF VACCINIUM BERRY STANDARD REFERENCE MATERIALS BY GC-MS
Karen Phinney
National Institute of Standards and Technology, Gaithersburg, MD, USA
Vaccinium berries such as cranberries are believed to have many health benefits, and therefore their metabolite profiles are of significant interest. In previous work, nontargeted analysis of six Vaccinium berry Standard Reference Materials was performed by LC-MS, and approximately 70 metabolites were identified. In the current work, a similar analysis has been performed by GC-MS with derivatization. Comparison of the resulting spectra with mass spectral libraries and retention indices resulted in identification of nearly 100 metabolites.

O3B-5
PLANT LIPIDOMICS LEADS TO IDENTIFICATION OF A NOVEL LIPID CLASS PLAYING AN ESSENTIAL ROLE IN MITIGATION OF PHOSPHORUS DEPLETION
Yozo Okazaki
RIKEN Center for Sustainable Resource Science, Yokohama, Japan
Phosphorus supply is one of the major factors responsible for reduced crop yields. Untargeted lipidomics successfully led to the discovery and elucidation of the biosynthetic pathway of a novel plant lipid, glucuronosyl-diacylglycerol, which is essential for the protection of plants against phosphorus depletion.

O3B-6
IDENTIFYING NOVEL SALINITY TOLERANCE MECHANISMS BY SPATIAL ANALYSIS OF LIPIDS IN BARLEY ROOTS
Ute Roessner
The University of Melbourne, Melbourne, Victoria, Australia
Lipidomics is used to compare the plasma membrane (PM) compositions of barley genotypes with contrasting salinity tolerance. Our aim is to link PM composition and functionality in salinity response by examining whether lipids are involved in the alteration of fluidity or lipid-based downstream signalling. We also use MALDI-FT-MS to monitor spatial distributions of lipids across root sections of salt treated barley. This will increase our understanding of the role of lipids in salt tolerance.
O4A-1
METABOLIC PHENOTYPING BY 1H-NMR SPECTROSCOPY DETECTS LUNG CANCER VIA A SIMPLE BLOOD SAMPLE
Evelyne Louis

To determine the metabolic phenotype of lung cancer, fasting venous blood samples of 78 lung cancer patients and 78 controls are collected and analyzed by 1H-NMR spectroscopy. Orthogonal partial least squares discriminant analyses are performed to investigate whether the metabolic composition of blood plasma discriminates between lung cancer patients and controls. This analysis shows that lung cancer can be detected with a sensitivity of 86% and a specificity of 95%.

O4A-2
FROM METABOLIC DIFFERENCES TO GENETIC DIFFERENCES VIA QUALITATIVE METABOLIC NETWORK ANALYSIS
Weiruo Zhang

We have developed a computational method to identify candidate genes that may be responsible for a measured difference in metabolites. The method uses a curated metabolic network (YeastCyc) and mass spectrometry data of measured metabolite differences to identify genes that may cause the metabolic differences. We validated the algorithm on S. cerevisiae using single-gene deletion mutants and drugs targeting the arginine and ergosterol pathways, and it identified the relevant genes with high accuracy.

O4A-3
IMPROVING PHOTOSYNTHEIS IN ARABIDOPSIS THALIANA: FUMARATE AS A POTENTIAL CARBON STORE.
Beth Dyson

Increases in photosynthesis have the potential to increase the growth of crop plants, however, the rate at which carbon is assimilated into traditional plant storage compounds is limited, and accumulation of metabolic intermediates can down-regulate photosynthesis. We have used FTIR, GCMS-EI-TOF and enzymatic analyses to identify conditions where the organic acid fumarate is used as a significant carbon store during increases in photosynthesis in Arabidopsis thaliana, potentially avoiding these carbon storage issues.

O4A-4
TARGETED AND NON-TARGETED LC-MS METABOLIC PROFILING IDENTIFIES SHIFTS IN AMINO ACID AND LIPID METABOLISM IN THE INFLAMMATORY SKIN DISEASE PSORIASIS.
Stuart Snowden

Psoriasis is a chronic immune-mediated skin disease for which there is no cure. A combination of targeted and non-targeted LC-MS metabolic profiling identified amino acid, sphingolipid and 12-LOX pathways as being modulated by disease pathogenesis and treatment. Modulation of nitric oxide via the urea cycle and of the pro-inflammatory ceramides provides insights into the mechanisms of the systemic inflammatory component of the disease, and how treatment acts to resolve this inflammation.

O4A-5
AN AUTOMATED WORKFLOW TO REDUCE LC-MS DATA TO BIOLOGICALLY RELEVANT FEATURES ONLY, WITH SUBSEQUENT ANNOTATION, AND ITS APPLICATION TO C. ELEGANS LONGEVITY MUTANT PROFILING
Florian Geier

We present a stable isotope based workflow, that allowed us to reduce LC-MS data by 99.9 %, leaving non-redundant and biologically relevant features only, which are also annotated with a molecular formula. This workflow was tested with triply labelled E.coli and C.elegans samples. The genuine, annotated biological molecules where then used in a C.elegans longevity mutant screen (30 mutants), to build models of the relationships between longevity and metabolism.

O4A-6
DISCOVERY OF PLANT DUAL COX AND LOX INHIBITORS AND MODELS TO PREDICTION THROUGH METABOLIC STUDIES AND ARTIFICIAL INTELLIGENCE
Daniela A. Chagas-Paula

Screening of Asteraceae plants against an interesting mechanism of action: dual inhibition of cyclooxygenase-1 and 5-lipoxygenase. Anti-inflammatory (AI) medicines with this mechanism of action should be with high efficacy and low side effects. We found extracts from food, known and cerrado(bioregion faced in risk of extinction) species that displayed this mechanism of action. Then through the metabolomic studies we determide and derreplicated the biomarkers and built robust models to prediction of new AI.
O4B-1
EXPLORATIVE NMR METABOLOMICS IN THE METABOLIC CHARACTERISATION OF TBM IN CSF
Shayne Mason
Centre for Human Metabonomics, North-West University, Potchefstroom, South Africa,
The application of 

\[ ^1 \text{H} \] Nuclear Magnetic Resonance (NMR) spectroscopy as an untargeted global metabolomics explorative approach was used to characterise the metabolic profile of tuberculous meningitis (TBM) in infants and children and considered the first step to defining a possible TBM bio-signature in cerebrospinal fluid (CSF) for improved early diagnostic purposes. The highly specific nature of NMR yielded spectra whereby metabolites of significance were identified both qualitatively and quantitatively from these highly complex biological samples.

O4B-2
METABOLOMICS ANALYSIS OF OVARIAN CANCER: A MULTI-MODAL GC-MS, LC-MS AND NMR STUDY.
Marie Palmnäs
1Faculty of Science, Department of Biological Sciences, Calgary, Alberta, Canada, 2Faculty of Medicine, Department of Biochemistry and Molecular Biology, Calgary, Alberta, Canada
Ovarian cancer is the deadliest gynecological cancer. Using a multimodal metabolomics approach including NMR spectroscopy, GC-MS and LC-MS, we investigated the serum metabolome of ovarian cancer patients (N=31) and matched healthy controls (N=31). A distinct metabolic profile could be identified for ovarian cancer. Currently we are studying the correlation between the ovarian cancer metabolome and tumor stage and subtype. Unraveling the biological mechanisms underlying ovarian cancer may improve how such tumors are detected and treated.

O4B-3
URINARY METABOLOMICS OF COLORECTAL CANCER - A PILOT STUDY SCREENING FOR CROSS-SECTIONAL MARKERS USED IN TRANSLATIONAL ONCOLOGY
David B. Liesenfeld
1Division of Preventive Oncology, National Center for Tumor Diseases (NCT), Heidelberg, Germany, 2German Cancer Research Center (DKFZ), Heidelberg, Germany
We investigated the metabolome of fasting spot urine from 115 Colorectal Cancer (CRC) patients (stages I-IV) from a prospective patient cohort as well as spot urine from 20 control subjects using an oximation/silylation GC-MS approach. Additionally, spot urine of patients was analyzed post-surgery. We were able to identify potential metabolite markers for CRC, which will be validated within the multicentric ColoCare study (>500 CRC patients) and assessed for their clinical use as prognostic or predictive markers.

O4B-4
METABOLIC PROFILING DURING PREGNANCY AND ASSOCIATIONS WITH MATERNAL HEALTH PARAMETERS AND BIRTH OUTCOMES
Lea Maitre
Imperial College London, London, UK, 2CREAL, Barcelona, Spain
Maternal metabolic factors affect the intrauterine environment and fetal growth. Our aim was to identify dynamic metabolic changes during pregnancy and their relationship with maternal health and birth outcomes. 1,700 urine samples from pregnant women were profiled using 

\[ ^1 \text{H} \] NMR spectroscopy. Consistent findings across two cohorts and the 1st and 3rd trimesters underpinned complex relationships between maternal BMI, weight gain during pregnancy and lipid metabolism. This study demonstrates the role of metabolomics in pregnancy research.

O4B-5
METABOLOMICS ANALYSIS OF THE RESISTANCE RESPONSE IN SUNFLOWER ROOTS TO THE PARASITIC WEED OROBNANCHE CUMANA
Anne-Laure Hepp
University of Sheffield, Department of Animal and Plant Sciences, Sheffield, UK
Orobanche cumana is a root parasitic angiosperm of sunflower that causes devastating losses in yield in Europe and Asia. We performed a non-targeted metabolomic analysis of the roots of susceptible and resistant sunflower cultivars challenged with O. cumana using Ultra-high Performance Liquid Chromatography-high resolution Mass Spectrometry. We identified defence pathways (e.g. flavonoid, isoflavonoid and alkaloid biosynthetic pathways) and metabolites (e.g. chlorogenic acid, ferulic acid and the phytoalexin scopoletin) that were upregulated during the resistance reaction.

O4B-6
METABOLOMICS AND DEREPLICATION STUDIES OF ENDOPHYTIC METABOLITES FROM SOME EGYPTIAN MEDICINAL PLANTS IN THE SEARCH FOR NEW POTENTIAL ANTI-CANCER DRUGS
Ahmed Tawfike
1Strathclyde institute of pharmacy and biomedical science, Glasgow, UK, 2Faculty of Pharmacy, Helwan University, Cairo, Egypt
This study involved isolation of five endophytic fungal strains from four different Egyptian medicinal plants. Identification of the strain has been achieved through molecular biological methods. Metabolomic profiling, using 2D-NMR and HR-ESIFTMS were done at different stages of the growth phase for both solid and liquid culture media. This led to the identification of compounds (1-12) from Aspegillus flocculosus and compounds (13-24) from A. aculeatus. Compounds 1a, 1b and 2 are novel anti-cancers.
O4C-1
IDENTIFICATION OF NOVEL BIOMARKERS OF DIETARY INTAKE
Helena Gibbons
Institute of Food and Health, University College Dublin, Dublin, Ireland
The identification of novel biomarkers of dietary intake, through the application of metabolomics, offers the potential of a more objective measure of dietary intake compared to traditional dietary assessment methods. Heat map analysis, performed to identify correlations between $^1$H NMR spectra and food group intakes, found that high energy beverages were associated with formate, citrulline, taurine and isocitrate. Future work will ascertain how to translate these markers for use in nutrition epidemiology.

O4C-2
ANTIDIABETIC EFFECT OF METFORMIN BY REDUCING CORTISOL LEVELS VIA THE AMPK/LXRα/POMC PATHWAY
Kumsun Cho
Department of Clinical Pharmacology and Therapeutics, Seoul National University College of Medicine and Hospital, Seoul, Republic of Korea
The aim of this study is to identify the changes of urinary endogenous metabolites by metformin treatment and the molecular mechanism showing antidiabetic effect of metformin.
We identified metabolites affected by metformin treatment in healthy subjects through LC/Q-TOF MS analysis. Of importance, this study also demonstrated that metformin suppressed the cortisol levels via the AMPK/LXRα/POMC pathway.

O4C-3
DEREPILATION AND CHARACTERIZATION OF NOVEL 17-HYDROXYGERANYLLINALOOL DITERPENE GLYCOSIDES (HGL-DTGs) IN 24 SOLANACEOUS SPECIES BY U(H)PLC/ESI-TOF-MS AND MS/MS
Sven Heiling
Max Planck Institute for Chemical Ecology / Department for Molecular Ecology, Jena, Thüringen, Germany
In this study, we established a mass-spectrometry based workflow to rapidly dereplicate and identify novel 17-hydroxygeranyllinalool diterpene glycosides (HGL-DTGs) from new biological matrices. Furthermore we showed that the biosynthetic step of malonylation of HGL-DTGs is highly conserved in various solanaceous species. We also identified tissue-specific variations in the response of these metabolites to methyl jasmonate, a phytohormone that activates induced defensive responses in plants. This workflow is readily applicable to many additional compound classes.

O4C-4
DEVELOPMENT OF STRATEGIES FOR INTEGRATED FULL-SCAN PROFILING AND DATA DEPENDENT MS/MS AND MS^n APPLYING CID AND HCD ON HYBRID ORBITRAP MASS SPECTROMETERS.
Martin R. Jones
$^1$School of Biosciences, University of Birmingham, Birmingham, UK, $^2$Institute of Human Development, The University of Manchester, Manchester, UK
Comprehensive metabolite annotation remains an eminent challenge facing metabolomics researchers. Here we address this challenge, demonstrating, for a chemically diverse subset of metabolites, the complementarity of CID and HCD ion-activation mechanisms in chemical search-space reduction and metabolite annotation and identification. We highlight the importance of Data Dependent Analysis parameters (for example, collision energy) in maximising the number of informative MS/MS or MS^n mass spectra acquired.

O4C-5
OVARIAN CANCER METABOLIC PROFILES DIFFER IN OVARIAN CANCER INITIATING CELLS
Kathleen Vermeersch
Georgia Institute of Technology, Atlanta, GA, USA
A key emerging area in cancer research is the study of stem-like “cancer initiating cells” (CICs). Here we present the results of an in vitro glucose deprivation experiment to model in vivo tumor conditions in ovarian cancer cells and ovarian CICs. Distinct metabolic profiles were found for the two cell types and between the control and glucose-deprived cells. A systems-level understanding of the metabolome of CICs could profoundly affect our understanding of cancer.

O4C-6
A LIPIDOMIC INVESTIGATION OF GANGLIOSIDES IN GUILLAIN-BARRE SYNDROME
Jo Cappell
University of Glasgow, Glasgow, UK
Gangliosides have long been implicated in autoimmune diseases such as Guillain-Barré Syndrome (GBS) and Multifocal Motor Neuropathy. Mouse models have been developed in which essential enzymes in ganglioside biosynthesis are knocked out and rescued in different tissues in order to investigate. We have developed two novel Lipidomic methods to profile gangliosides from murine brain and nerve tissue that benefit from sensitive label-free detection and identification by mass and chromatographic position.
O5A-1
DAILY RHYTHMS IN THE HUMAN METABOLOME AND THE EFFECT OF SLEEP AND SLEEP DEPRIVATION
Sarah K. Davies
University of Surrey, Guildford, Surrey, UK
Determining the effect of time of day and exogenous factors such as sleep on metabolite levels may impact greatly on the interpretation of metabolomic data. We used liquid chromatography-mass spectrometry to analyse plasma taken from healthy males under highly controlled laboratory conditions to examine the effects of time of day and sleep on the human metabolome. Multivariate data analysis indicates that time of day has a greater effect on the metabolome than does sleep.

O5A-2
LIPIDOMIC ANALYSIS OF BRAIN TISSUES AND PLASMA IN A MOUSE MODEL EXPRESSING MUTATED HUMAN AMYLOID PRECURSOR PROTEIN/TAU FOR ALZHEIMER’S DISEASE
Keiko Maekawa
National Institute of Health Sciences, Setagaya-ku, Tokyo, Japan
This study aimed to evaluate alterations in lipids in brain and plasma from mice model for Alzheimer disease (AD) at various disease stages. The species of cholesterol ester, ethanolamine plasmalogens, sphingomyelins showed different levels between brains from AD and control mice at various stages of AD. Several oxidative fatty acids were concomitantly changed in both brain and plasma at presymptomatic phase. Present results provide fundamental information on lipid dysregulation during various stages of human AD.

O5A-3
METABOLOMICS IN CEREBROSPINAL FLUID OF PATIENTS WITH AMYOTROPHIC LATERAL SCLEROSIS: AN UNTARGETED APPROACH USING HIGH-RESOLUTION MASS SPECTROMETRY
Helene Blasco1,2
1U930, Universite Francois Rabelais, Tours, France, 2CHRU Bretonneau, laboratoire de biochimie et biologie moléculaire, Tours, France
Amyotrophic lateral sclerosis (ALS) presents a diagnostic challenge. To our knowledge, we present the first study that utilizes LC-HRMS spectroscopy to explore metabolic markers in CSF from patients with ALS. Multivariate analysis yielded distinct metabolic profiles for ALS and controls, with about 80% of correct diagnosis prediction. Univariate analysis identified 6 discriminating compounds, including glutamate and ascorbate. This study provides evidence that metabolomics using LC-HRMS may help to diagnose ALS and could identify novel biomarkers.

O5A-4
METABOLOMICS BASED ON DIRECT INFUSION MASS SPECTROMETRY FOR ALZHEIMER’S DISEASE DIAGNOSIS
Jose-Luis Gomez-Ariza1,2
1Department of Chemistry; University of Huelva, Huelva, Spain, 2Research Center of Health and Environment (CYSMA). University of Huelva, Huelva, Spain
The complementary use of electrospray and atmospheric pressure photoionization in a metabolomic approach based on direct infusion mass spectrometry, combining a two-step serum extraction of polar and lipophilic metabolites with analysis by positive and negative ionization modes, allowed obtaining comprehensive fingerprints from serum samples for the study of Alzheimer’s disease. This multi-platform provided numerous potential biomarkers, which may help to understand the biochemical processes and pathology associated with disease.
O5B-1
COMPREHENSIVE METABOLOMICS ANALYSIS OF A YELLOWSTONE NATIONAL PARK HOT SPRING PHOTOTROPHIC MICROBIAL MAT OVER A DIEL CYCLE REVEALS A HIGH POTENTIAL FOR METABOLIC COUPLING AMONG COMMUNITY MEMBERS

Thomas Metz
Pacific Northwest National Laboratory, Richland, Washington, USA

We performed targeted and untargeted metabolomics analyses of microbial mat cores collected during a diel cycle. Metabolites were segregated into four different chemical classes - volatile organic acids, polar metabolites, wax esters, and polyhydroxyalkanoates (PHAs) - and analyzed using separate GC-MS methods, resulting in a total of 104 metabolites and molecules identified, with 72 quantified. The cycling of metabolite abundances was consistent in part with previous transcriptomics studies of the same microbial mat.

O5B-2
METABOLOMIC AND TRANSCRIPTOMIC ANALYSIS REVEALS ENDOCRINE DISRUPTION IN SKEENA RIVER (BRITISH COLUMBIA) SOCKEYE SALMON DURING THE 2008 SPAWNING MIGRATION

John Cosgrove
AXYS Analytical Services Ltd., Sidney, BC, Canada

A 2008 study examining the health of 2 major BC Sockeye salmon spawning migrations (Fraser and Skeena Rivers) revealed abnormal sex-specific hepatic gene transcript profiles in salmon collected at the Skeena River spawning grounds. To characterize alterations in biochemical pathways and elucidate potential sources of exposure, we re-examined the 2008 Skeena Stock for changes in the hepatic metabolome using targeted metabolomics. Unique metabolomic profiles were associated with gender, migration, and alterations in hepatic mRNA expression.

O5B-3
APPLICATION OF BOTH TARGETED AND UNTARGETED METABOLOMICS APPROACHES TO ASSESS POTENTIAL BIOLOGICAL EFFECTS OF SIMULATED SONAR SIGNALS ON BOTTLENOSE DOLPHINS.

Gregory Genta-Jouve
Environmental Metabolomics Research Laboratory, School of Biosciences, University of Birmingham, Birmingham, UK

This paper presents the results of both targeted and untargeted approach to assess potential biological effects of simulated sonar signals on bottlenose dolphins. The first part of the study was focused on steroids quantification, as this family of compounds is known to be involved in the stress response in mammal’s metabolism. The untargeted approach performed using an LC-FT-ICR, followed by statistical analyses suggested that several tens of compounds were involved in the stress response.

O5B-4
METABOLIC PROFILING OF CANCER AND CHILD-MOTHER COHORTS TO IDENTIFY BIOMARKERS OF EXPOSURE AND DISEASE: RESULTS FROM THE ENVIROGENOMARKERS STUDY.

Alexandros Siskos
Imperial College London, London, UK, 1NHRF, Athens, Greece

This paper summarises the main findings of the metabonomics study within the EnviroGenoMarkers Project. The EnviroGenoMarkers Project is a nested matched case-control prospective study within two pre-existing cohorts (NSHDS/Sweden and EPIC/Italy) aimed to study the role of environmental agents in Breast Cancer and Lymphoma. EnviroGenoMarkers applies the “meet in the middle” approach to identify -omics biomarkers associated with both exposure and disease, and characterise the total human exposome.
O6A-1
UTILISATION OF METABOLOMICS TO STUDY THE PRODUCTION OF SECONDARY METABOLITES IN BACTERIAL ENDOSYMBIONTS ISOLATED FROM MARINE SPONGES.
Lynsey MacIntyre
Strathclyde Institute of Pharmacy and Biomedical Sciences, University of Strathclyde, Glasgow, UK
The metabonomic methods of dereplication and metabolic profiling were used to identify pharmacologically relevant secondary metabolites from sponge-associated endosymbiotic bacteria using LC-FTMS and NMR spectroscopy. Following taxonomic identification and bioassay screening, multivariate statistical analysis methods were employed for bioactive compound discovery. Several species of Vibrionaceae showed activity against Mycobacterium marinum. Differences in the mass spectrometry and NMR spectra from active and inactive bacterial extracts were probed using multivariate analysis to uncover bioactive metabolites.

O6A-2
CAN METABOLOMICS HELP TO ELUCIDATE THE BIOACTIVE COMPOUNDS CONTRIBUTING TO THE HEALTH BENEFICIAL PROPERTIES OF POMEGRANATES?
Rachel Amir1,2
1Tel Hai Collage, Galil Elion, Israel, 2Migal, Research Institute, Kiryat Shmona, Israel
By performing metabolic profiling to peels of 29 pomegranate accessions, by measuring antioxidant activity of the peels, and by using statistical tools, we have identified the compounds that contribute to this activity. The chemical nature of most of these compounds was identified by HPLC Q-TOF. Once the data set of this metabolic profiling is organized, it will enable the identification of most of the bioactive compounds contributing to this and other activities of interest.

O6A-3
METABOLOMICS AS A TOOL IN THE IDENTIFICATION AND PRODUCTION OF NEW MARINE-DERIVED ANTIBIOTICS FROM SPONGES AND ENDOSYMBIOTIC BACTERIA
Christina Viegelmann
Strathclyde Institute of Pharmacy and Biomedical Sciences, Glasgow, UK
Metabolomic methods can be utilised to screen biological systems such as marine sponges and endosymbiotic bacteria for sustainable sources of antibiotics. 24-methylenecholesterol and two novel steroids, all significantly active against Trypanosoma brucei, were isolated from the sponge Haliclona simulans. HR-LCFTMS assisted in identifying antimycins as the anti-fungal compounds from a Streptomyces sp. isolated from H. simulans. Metabolomics was used to identify and trace biomarkers in the optimisation of the cultivation of a sponge-derived Microbacterium sp.

O6A-4
DOES ANTIBIOTIC IONISATION STATUS AFFECT THE MICROBIAL METABOLOME: AN INVESTIGATION INTO ESCHERICHIA COLI K12 CHALLENGED WITH TRIMETHOPRIM AT VARYING PH
Haitham AlRabaih
School of Chemistry and Manchester Institute of Biotechnology, Manchester, UK
Understanding the mode of action of antibiotics is paramount for future therapeutic developments. MS-based metabolomics was used to investigate trimethoprim action on E. coli. Trimethoprim is a dihydrofolate reductase inhibitor and can be ionised at different levels depending on the pH of its environment. We modulated the pH to mimic acidity in urine, and performed GC-MS on these bacteria to understand the effect of the drugs as well as their ionisation status on cellular metabolism.

O6A-5
EVALUATION OF URINARY ENDOGENOUS METABOLITES AS MARKERS FOR CYP3A INHIBITION AND INDUCTION IN HUMAN USING LC-TofMS
Kwang-Hee Shin
Seoul National University, Seoul, Republic of Korea
This study identified the urinary endogenous markers for CYP3A activity in healthy subjects. Each subject received a 1 mg of midazolam in each of 3 study periods: midazolam alone; midazolam after pretreatment with 400 mg ketoconazole once daily for 4 days; and midazolam after pretreatment with 600 mg rifampicin once daily for 10 days. Metabolomic approach using LC-TofMS could provide markers for CYP3A4 activity and insight about variability in CYP-mediated drug metabolism.

O6A-6
ULTRAFAST STATISTICAL PROFILING: FT-ICR BASED PROFILING OF MYXOBACTERIA NATURAL PRODUCTS FOR RAPID DETECTION AND IDENTIFICATION OF MARKER COMPOUNDS
Aiko Barsch
Bruker Daltonik GmbH, Bremen, Germany
The presented “Ultrafast Statistical Profiling” workflow enables a rapid profiling of complex metabolite extracts and identification of relevant marker compounds by making use of the ultrahigh resolution and the wide dynamic range provided by the FT-ICR technology - addressing two of the major bottleneck in metabolomics, sample throughput and compound identification.
O6B-1
TOWARDS A GENERATIVE MODEL OF LC/MS DATA TO IMPROVE METABOLITE IDENTIFICATION.
Rónán Daly
University of Glasgow, Glasgow, UK
Metabolome identification has become a pressing concern due to the recent surge of interest in metabolomics. In this work, we present a generative, probabilistic model of liquid chromatography coupled to mass spectrometry, geared towards the identification of metabolites. Based on a previous model that simultaneously groups related chromatographic peaks and assigns the groups to chemical formulas, this model utilises predicted retention times and metabolic network information to distinguish metabolites with the same formula.

O6B-2
GLOBAL METABOLOMICS OF STRESSED CAENORHABDITIS ELEGANS USING ISOTOPIC RATIO OUTLIER ANALYSIS
Gregory S. Stupp
Department of Biochemistry & Molecular Biology, University of Florida, Gainesville, FL, USA
The nematode Caenorhabditis elegans is exposed throughout its life to a variety of stressful conditions which makes it an ideal host to study stress response. We examined worms' metabolomic stress responses using a technique called Isotopic Ratio Outlier Analysis (IROA) which allows the discrimination between biological molecules and artifacts, along with fold-change quantification and molecular formula determination. This approach allows for precise quantification of the changes of hundreds of compounds in a global, untargeted manner.

O6B-3
METABOLOMICS-BASED ASSOCIATION NETWORKS: A CRITICAL DISCUSSION
Margriet Hendriks1,2
1Analytical BioSciences, Leiden University, Leiden, The Netherlands, 2Netherlands Metabolomics Centre, Leiden, The Netherlands
Although inference of association networks is done routinely some questions remain: to what extent is the network reliable and really revealing underlying biology? Two fundamental aspects concerning the validity of correlation-based metabolic association networks are discussed: i) the influence of measurement error correlation and ii) the reproducibility of the network. This will be illustrated with both dynamic and static human lipidomics data also illustrating that validated biochemical (pathway) information can be obtained.

O6B-4
METABOLOMICS APPLICATIONS OF THE BioCyc DATABASES AND PATHWAY TOOLS SOFTWARE
Dan Weaver
SRI International, Menlo Park, CA, USA
The BioCyc.org database collection provides metabolic reconstructions for 3,000 sequenced organisms. These Pathway/Genome Databases (PGDBs) integrate information on metabolic pathways, reactions, metabolites, genes, and proteins, providing a whole-organism context for interpreting metabolomics datasets. BioCyc PGDBs include information from tens of thousands of publications, accessible via the web and Pathway Tools software. Metabolomics analysis tools available in BioCyc include monoisotopic mass search, metabolite over-representation analysis, flux balance analysis, atom mapping, metabolic route search, and visualization tools.

O6B-5
APPROACHES FOR THE RAPID PROCESSING AND ANNOTATION OF MASS SPECTROMETRY DATA
Jan Stanstrup
Department of Nutrition, Exercise and Sports, University of Copenhagen, Frederiksberg C, Denmark
Compound identification is a major bottleneck in metabolomics. We have created an identification pipeline which automatically schedules MS/MS acquisitions for all features of interest. The spectra are then submitted to computer assisted annotation tools and retention times predicted for each candidate. This leads to a rapid and semi-automated ranking of compound candidates and limits the amount of manual structure elucidation drastically.

O6B-6
COMPUTER ASSISTED IDENTIFICATION OF URINE METABOLITES ORIGINATING FROM GREEN TEA
Lars Ridder1,2
1Laboratory of Biochemistry, Wageningen University, Wageningen, The Netherlands, 2Netherlands eScience Center, Amsterdam, The Netherlands
We present an in silico workflow for automatic chemical annotation of LC-MSn based metabolic profiles. It is based on in silico fragmentation of candidate molecules from chemical databases and their in silico biotransformation products to include potentially novel human metabolites. The workflow is applied to entire LC-MSn datasets of green tea and of urine after tea consumption, demonstrating the potential of our approach to support annotation of unknown metabolites.
O7A-1
INTERPRETING MECHANISM FROM METABOLIC FOOTPRINTING DATA OF SINGLE-GENE PSEUDOMONAS AERUGINOSA KNOCKOUTS
Jake Bundy
Imperial College London, London, UK
We have carried out a proof-of-principle metabolic footprinting study on around 80 bacterial single gene mutants, chosen to include metabolic enzymes as well as regulatory proteins. Using a package for automated fitting of NMR peaks gave enough information to distinguish functionally related clusters of genes. In addition, we elucidated the mechanism underlying a novel phenotype of a regulatory gene, and showed that this phenotype was relevant to clinical strains.

O7A-2
IMPROVED BIOPROCESS BY METABOLITE PROFILING AND MODELLING ON THE CELLULAR LEVEL
Dierk Pöther
Metabolomic Discoveries GmbH, Potsdam, Germany, 2Insilico Biotechnology AG, Stuttgart, Germany
Strains are used for the production of compounds and the production of complex molecules. Metabolomics in combination with predictive network models allows the quantitative analysis of the cellular mechanisms and identification of over-expression and attenuation targets. Here, we will provide an example of this approach in recombinant protein production using E. coli. The example shows how combining dynamic network models and metabolite profiling provides new information on limitations in nutrient supply and targets for metabolic engineering.

O7A-3
SEARCHING FOR THE NEW ZEALAND SAUVIGNON BLANC JUICE AND WINE TERROIR THROUGH METABOLOMICS
Farhana Pinu1 2
1New Zealand Institute of Plant and Food Research, Auckland, New Zealand, 2School of Biological Sciences, University of Auckland, Auckland, New Zealand
As the major wine variety of New Zealand (NZ), Sauvignon blanc plays a vital role in New Zealand economy. This study was the first application of metabolomics in NZ wine research that aimed to determine the biochemical reasons behind the large variation in wine quality by using a global metabolomics approach that involved the use of different analytical techniques, such as mass spectrometry and nuclear magnetic resonance. The results are promising and highly applicable to the wine industry.

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**PARALLEL SESSION 7B:**

**METABOLOMIC PROFILING IN DIABETES AND HEART DISEASE**

**09.00 – 10.25: LOMOND AUDITORIUM**

**O7B-1**

DIFFERENTIAL FATTY ACID PROFILES IN LPS-TREATED MICE LIVER USING STABLE ISOTOPE LABELLING AND GAS CHROMATOGRAPHY-MASS SPECTROMETRY WITH SINGLE SAMPLE ANALYSIS

Guan-yuan Chen¹ ²

¹ School of Pharmacy, College of Medicine, National Taiwan University, Taipei, Taiwan, ² The Metabolomics Core Laboratory, Center of Genomic Medicine, National Taiwan University, Taipei, Taiwan

This study proposed a new method to rapidly screen differential fatty acids in biological samples with single sample analysis. The approach involved stable isotope labeling and gas chromatography-mass spectrometry analysis. Differential FAs can be identified by comparing peak intensities of d₀ and d₃-methyl esters. The proposed method has been successfully applied to investigate the effect of lipopolysaccharide induced lipid peroxidation in mice liver.

**O7B-2**

A NOVEL LIPIDOMIC STRATEGY TO INVESTIGATE THE DYNAMICS OF INTRACELLULAR LIPID PATTERN IN SKELETAL MUSCLE CELLS UNDER LIPOTOXIC CONDITIONS

Rainer Lehmann¹ ²

¹ Division of Clinical Chemistry and Pathobiochemistry, Department of Internal Medicine IV, University Hospital Tuebingen, Tuebingen, Germany, ² German Center for Diabetes Research (DZD), Tuebingen, Germany

The novel lipidomics strategy presented here allows to follow the synthesis, transformation and degradation of individual lipid species. We performed stable isotope-labelling cell culture experiments, UHPLC-Orbitrap-MS lipidomics and data processing by a new software tool for global isotopomer filtering and matching. The lipotoxic effects of [U-¹³C]-palmitate and the associated changes of individual lipid species were studied in human skeletal muscle cells isolated from muscle biopsy material.

**O7B-3**

FROM BLIND FINGERPRINTING TO FUNCTIONAL PROFILING: CERAMIDE AND RELATED COMPOUNDS IN EXPERIMENTAL MODELS OF OXYGEN SENSING

Francisco J. Rupérez

Center for Metabolomics and Bioanalysis (CEMBIO), Universidad CEU San Pablo, Boadilla del Monte, Madrid, Spain

There are several methods for profiling different families of lipids, although for some studies the valuable information comes from differential displays of the fingerprints. A strategy to study the changes in signaling molecules such as sphingolipids in experimental models of different exposures to oxygen is presented. The combination of high throughput LC-MS with searches into public databases permits to obtain not only the profile of sphingolipids but also other compounds of interest.
O8A-1
DIFFERENT METABOLIC RESPONSES OF CAFFEINATED AND DECAFFEINATED GREEN TEA EXTRACT DURING REST AND MODERATE INTENSITY EXERCISE
Doris M. Jacobs
Unilever R&d, Vlaardingen, The Netherlands
This study compared the effects of caffeinated (cGTE) and decaffeinated (dcGTE) supplementation of green tea extract on numerous plasma metabolites at rest and during moderate intensity exercise. At rest, cGTE led to metabolite changes reflecting aerobic energy utilization, while dcGTE only increased 3-hydroxybutyrate. During exercise, cGTE caused changes indicative of anaerobic energy utilization, while no significant effects were observed for dcGTE.
Our results highlight the significant contribution of caffeine to the metabolic effects of GTE.

O8A-2
METABOTYPING IN CARDIOVASCULAR RISK SUBJECTS REVEALS DIFFERENCES IN THEIR URINARY PROFILES AFTER WINE INTAKE
Rafael Llorach-Asuncion
1Nutrition and Food Science Department, XaRTA, INSA, Pharmacy Faculty, University of Barcelona, Barcelona, Spain,
2INGENIO-CONSOLIDER Program, Fun-c-food CSD2007-063, Ministry of Science and Innovation, Barcelona, Spain
Diet has been shown to influence metabolism and to impact on the cardiovascular-disease risk. The aim was to classify the subjects in different phenotypes attending to their anthropometric-clinical characteristics and subsequently, to evaluate the changes on urinary metabotypes by 1H-NMR metabolomics approach in response to red wine, dealcoholized red wine and gin intake. The results suggested that individuals with different clinical phenotype show different response to the beverages intakes, translated in different metabolic profiles.

O8A-3
NEW BIOMARKERS OF COFFEE CONSUMPTION IDENTIFIED BY NON-TARGETED METABOLOMIC PROFILING IN COHORT STUDY SUBJECTS
Yoann Fillâtre
Human Nutrition Unit, UMR1019 INRA/University of Auvergne, Clermont-Ferrand, France,
Metabolomic profiling of urines from 20 high coffee consumers and 19 non-consumers selected in the SU.VI.MAX2 cohort was performed using UPLC-ESI-QTOF-MS. Of the 1111 ions detected, 132 had statistically different intensities between the two groups. In addition to many caffeine derived compounds, three promising new biomarkers of coffee intake were tentatively identified, which showed excellent performance in the ROC curve test.

O8A-4
DISCOVERY BIOMARKERS OF BREAD INTAKE IN CARDIOVASCULAR HIGH-RISK PARTICIPANTS. A MASS SPECTROMETRY-BASED METABOLICS APPROACH.
Cristina Andres-Lacueva
1Nutrition and Food Science Department, XaRTA, INSA, Pharmacy Faculty, University of Barcelona, Barcelona, Spain,
2INGENIO & CONSOLIDER Program, Fun-C-Food CSD2007-063, Ministry of Science and Innovation, Barcelona, Spain
Bread is a component of the Mediterranean-Diet which provides important amounts of bioactive compounds. A metabolomics strategy designed to discover new biomarkers of food consumption was applied classifying participants according their reported bread-consumption. Urinary profile showed differences between regular-bread consumers and no-bread-consumers in food and endogenous metabolome. The results reinforce the capacity of metabolomics to explore the impact of dietary components and the ability to obtain new biomarkers of intake combining epidemiological data and metabolomics.
O8B-1
FROM METABOLITE PROFILING TO BIOMARKERS, GLYOXYLATE AND TYPE 2 DIABETES
Dietrich Rein
Metanomics Health GmbH, Berlin, Germany
Metabolic changes occur several years prior to a clinical diabetes phenotype. We discovered metabolites associating with the development of diabetes through broad profiling. Metabolite profiling in different models and large clinical studies allowed the generation of mechanistic hypothesis regarding their function. Glyoxylate associated with important diabetic pathway changes. Our quest for new diagnostic diabetes markers led to the discovery of metabolites with prominent physiological significance. Metabolites involved in physiologically relevant mechanisms will be discussed.

O8B-2
A METABOLOMICS EVALUATION OF SHORT AND LONG TERM EFFECTS OF DIFFERENT MACRONUTRIENT INTAKE IN OVERWEIGHT AND OBESE POSTMENOPAUSAL WOMEN
Elin Chorell
1,2
1Public Health and Clinical Medicine, Umeå, Sweden, 2Computational Life Science Cluster, Umeå, Sweden
With menopause there is an increased risk of central obesity associated with insulin resistance and cardiovascular disease, for partly unclear reasons. Thus, there is a need for intervention studies, with concomitant biochemical analyses, to develop effective treatment of postmenopausal obesity. We performed a global evaluation of plasma metabolic responses using GC-TOF/MS from 66 obese and overweight postmenopausal women consuming a Paleolithic-type diet or a diet according to the Nordic Nutrition Recommendations for 24 months.

O8B-3
DISCOVERY OF NOVEL BIOMARKERS FOR FABRY DISEASE USING A MASS SPECTROMETRY METABOLOMICS APPROACH
Christiane Auray-Blais
Université de Sherbrooke, Sherbrooke, Quebec, Canada
Fabry disease is an X-linked lysosomal storage disorder characterized by the accumulation of glycosphingolipids in biological fluids, and different organs. A metabolomic approach was devised using time-of-flight mass spectrometry for biomarker discovery. Our results confirmed the detection and chemical structure elucidation of 7 novel lyso-Gb₃ analogues presenting modifications on the sphingosine moiety. Relative quantification of these promising urinary biomarkers revealed that they are excreted in variable quantities in patients, suggesting complex biochemical and physiological profiles.

O8B-4
EXAMINING RESPONSE TO ASPIRIN THERAPY USING A PHARMACOMETABOLOMICS-INFORMED-PHARMACOGENOMICS APPROACH
Anastasia Georgiades
Duke University School of Medicine, Durham, USA
The mechanisms responsible for variation in response to aspirin therapy are poorly understood. Combining metabolomics and genomics allows for a comprehensive interrogation of mechanisms of variation in aspirin response. Mass spectrometry (MS)-based metabolomic profiling was performed on serum samples collected before and after low-dose aspirin therapy to characterize the metabolomic signature of aspirin exposure and identify important pathways affected. We then used our established pharmacometabolomics-informed-pharmacogenomics approach to identify genetic variants associated with aspirin response.
O9A-1
VITAMIN B-6 RESTRICTION IN HEALTHY MEN AND WOMEN AFFECTS METABOLITE PROFILES REFLECTING ALTERED ONE-CARBON METABOLISM AND TRYPTOPHAN CATABOLISM

Jesse Gregory
1University of Florida, Gainesville, FL, USA

Vitamin B6 participates in many aspects of human metabolism through the coenzymic role of pyridoxal phosphate. However, there is a distinct need for biomarkers that reflect functional consequences of vitamin B6 deficiency. We report here metabolic profile analysis of plasma samples from a controlled dietary study in healthy adults. Changes in the profiles of constituents from one-carbon metabolism and tryptophan catabolic pathways clearly identified functionally important metabolic effects of marginal vitamin B6 deficiency.

O9A-2
AN EXPLORATION OF THE URINARY METABOLOME IN THE EUROPEAN PROSPECTIVE INVESTIGATION ON CANCER AND NUTRITION (EPIC) COHORT TO IDENTIFY NOVEL DIETARY BIOMARKERS

William Edmands
International Agency for Research on Cancer, Lyon, France

An efficient fully automated data-analysis pipeline for high-throughput and high-resolution mass spectrometry data was created to identify novel urinary biomarkers of nutritional intake in 481 samples from the EPIC study cohort. A combination of pre-acquisition normalisation, QC-based signal correction, automated chemometric analysis, data-dependent auto MS/MS and accurate mass database matching were applied. We have so far detected over 300 polyphenol metabolites correlated to reported intakes of polyphenol rich foods in this sample set.

O9A-3
ANALYTICAL STRATEGIES TO IDENTIFY LOW ABUNDANT METABOLITES IN COMPLEX SAMPLE MATRICES: BIOAVAILABILITY OF POLYPHENOLS AS SHOWCASE

Justin van der Hooft1,2
1Plant Products and Human Nutrition Group, School of Medicine, University of Glasgow, Glasgow, UK, 2Netherlands Metabolomics Centre, Leiden, The Netherlands

The complete structural elucidation of polyphenol glycosides in food and especially their conjugated breakdown products in human fluids is still a tedious task. The examples provided show that the combined use of LC-MSn, 1D-1H-NMR, and HPLC-MS-SPE-NMR serves as an efficient identification and quantification approach for small metabolites present in complex matrices. Automation of metabolite annotation and identification will be discussed as well. Thus, recent technological and software developments open up new routes in bioavailability research.

O9A-4
USING LIPIDOMICS TO STUDY THE METABOLISM OF DIETARY LIPIDS AND THE EFFECT ON CANDIDATE MARKERS FOR CARDIO METABOLIC DISEASES

Albert Koulman
MRC HNR, Cambridge, UK

The risk for Insulin resistance has been associated with specific plasma phosphatidylcholines and triglycerides. These studies were unable to show that dietary factors contributed the concentrations of these candidate markers. Our lipidomics analysis of selected dietary interventions studies showed that diet significantly changed the levels of intact lipid that are associated with the risk for insulin resistance and that there are strong correlations between intact lipid and hydrolysed fatty acid as measured by GC.

O9A-5
EFFECTS OF MARGINAL SELENIUM DEFICIENCY IN MICE ON LIVER METABOLISM

Kerstin Geillinger1,2
1Technical University of Munich, Freising, Germany, 2ZIEL - Abteilung Biochemie, Freising, Germany

Selenium (Se) is an essential trace element in mammals. In Europe, the majority of the population does not reach the recommended amount of Se supply, thus suboptimal Se status prevails. Se deficient liver was characterized by significantly elevated levels of hypotaurine, taurine, homocysteine (Hyc) and glutamic acid, while methionine levels were unaltered. Elevated Hyc levels in the liver of Se deficient animals are most likely caused by an impaired transsulfuration pathway indicated by lower cystathione-β-lyase expression.
O9B-1
DEVELOPMENT OF A GENERAL METHOD FOR THE HPLC/MS-BASED ANALYSIS OF COENZYME A DERIVATIVES AND COFACTORS FROM CELL EXTRACTS
Katrin Müller
Technische Universität Braunschweig, Braunschweig, Germany
Coenzyme A derivatives play key roles in the metabolism and are characteristic for many complex catabolic pathways. Due to their properties, they are not covered by standard analytical methods. Previous publications analyzed 1-5 different CoA derivatives in a few organisms and were restricted by the limited availability of pure standards. In contrast, our method aims to cover the full range of CoA metabolites within samples from highly organisms. The effectiveness is demonstrated on different metabolic pathways.

O9B-2
DISSECTION OF THE CARBON AND ENERGY METABOLISM OF APICOMPLEXAN PARASITES IMPORTANT FOR VIRULENCE USING 13C-STABLE ISOTOPE RESOLVED METABOLOMICS
Malcolm McConville1,2
1Department of Biochemistry and Molecular Biology, Bio21 Institute of Molecular Science and Biotechnology, University of Melbourne, Parkville, Victoria, Australia, 2Metabolomics Australia, University of Melbourne, Parkville, Victoria, Australia
Analysis of central carbon metabolism in the protozoan parasites, Plasmodium falciparum and Toxoplasma gondii using 13C-stable isotope resolved metabolomics approaches have led to a substantial reassessment of the carbon and energy metabolism of these important parasites. In particular, they highlight the importance of a complex mitochondrial metabolism, including an unanticipated GABA shunt, as being key determinants of the virulence of these pathogens.

O9B-3
PLASMODIUM FALCIPARUM PHOSPHOENOLPYRUVATE CARBOXYLASE IDENTIFIED AS A KEY ENZYME IN REDOX MAINTENANCE AND ENERGY GENERATION
Sonal Sethia
University of Glasgow, Glasgow, UK
Phosphoenolpyruvate carboxylase (PEPC) is a crucial enzyme known to fix atmospheric carbon dioxide (CO₂) and replenish tricarboxylic acid (TCA) cycle intermediates. CO₂ fixation is essential for intra-erythrocytic survival of Plasmodium falciparum. To investigate the role of PEPC in P.falciparum, parasitized red blood cells with a pepc gene deletion were metabolically labelled with 13C-labelled bicarbonate and glucose and 13C,15N-labelled glutamine. Our data provide evidence that PEPC is involved in maintenance of metabolic homeostasis in the parasite.

O9B-4
ABSOLUTE QUANTIFICATION OF METABOLITES FOR FLUX ANALYSIS IN TRYPANOSOMES USING ORBITRAP-BASED LC-MS
Dong-Hyun Kim1
1College of Medical, Veterinary and Life Sciences, University of Glasgow, Glasgow, UK
Human African Trypanosomiasis is a parasitic disease caused by Trypanosoma brucei, which is fatal if untreated. New drugs and new targets for chemotherapy are urgently required due to the emergence of resistance and unacceptable side effects of existing treatments. We present the first global quantitative analysis of metabolite concentrations and metabolic fluxes in trypanosomes in order to understand the metabolism of this system, with aim of developing optimised anti-parasite drugs.

O9B-5
METABOLOMICS-GUIDED ADVANCES IN CELL CULTURE AND DRUG DISCOVERY FOR TRYPANOSOMIASIS AND MALARIA
Darren Creek1,2
1University of Melbourne, Victoria, Australia, 2University of Glasgow, Glasgow, UK
New approaches are urgently needed to discover novel drugs for parasitic tropical diseases. We demonstrate the application of metabolomics for rational development of an optimised in vitro culture medium for T. brucei. This medium demonstrated significantly improved sensitivity in standard drug screening assays for the identification of novel trypanocidal compounds. In addition, metabolic targets of anti-parasitic drugs were identified by an unbiased metabolomics approach in T. brucei and P. falciparum.

O9B-6
TRICHOMONAS VAGINALIS PRODUCES S-methyl-L-cysteine USING CYSTEINE SYNTHASE.
Gareth Westrop
Strathclyde University, Glasgow, UK
LC/MS analysis revealed that Trichomonas vaginalis cell extracts contain S-methyl-cysteine (SMC), identified by fragmentation analysis and comparison with a standard. The intracellular concentration of SMC was determined using a standard curve and published values for cell volume. SMC was exported into the medium during growth of the culture and levels were greatly reduced when cells were grown under conditions previously shown to down-regulate cysteine synthase activity. Recombinant cysteine synthase produced SMC from phosphoserine and methanethiol.
O9B-7
NEW METABOLITE MARKERS IMPLICATING ADAPTIONS OF THE HUMAN HOST TO MYCOBACTERIUM TUBERCULOSIS AND VISA VERSA
Du Toit Loots
Centre for Human Metabonomics, School for Physical and Chemical Sciences, North-West University, Potchefstroom, South Africa
To date, the majority of the tuberculosis research has been done using genomics and proteomics, and limited to investigating various aspects of the microbe only. Until only recently, due to metabolomics, the interaction of the host and bacteria, and the adaptions that each makes in response to each other, can be investigated. In this study, a GCxGC-TOFMS metabolomics research approach was used to identify new metabolite markers better characterizing this phenomenon.

O9B-8
METABOLIC RESPONSE OF CANDIDA ALBICANS TO PHENYLETHYL ALCOHOL UNDER HYPHAE-INDUCING CONDITIONS AND ITS ROLE ON MORPHOGENESIS
Silas Villas-Boas
The University of Auckland, Auckland, New Zealand
Phenylethyl alcohol is a quorum sensing molecule identified in C. albicans. This metabolite inhibits C. albicans morphogenesis. We have applied metabolomics and isotope labelling experiments to investigate the metabolic changes in C. albicans in response to phenylethyl alcohol. Our results showed a global upregulation of central carbon metabolism in response to phenylethyl alcohol, and we short-listed 7 pathways that appear to be associated with C. albicans morphogenesis. Phenylethyl alcohol is uptaken and is converted to NADH/NADPH molecules.

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P1-1
METABOLOMICS UNVEILS THE MOLECULAR PHENOTYPE OF “OMEGA-3” TRANSGENIC MICE
Giuseppe Astarita
Waters, Milford, MA, USA, Mass General Hospital, Boston, MA, USA
The fat-1 transgenic mouse model is able to convert omega-6 into omega-3 fatty acids. Such mouse is protected against a wide variety of diseases related to inflammation. In this study, we used a state-of-the-art, high-throughput assays for the analysis of metabolites in tissue samples from fat-1 and wild-type mice, providing new clues to the pathways and mechanisms that may be involved in the health benefits associated with alterations of the omega-6/omega-3 fatty acids ratio.

P1-2
THE PSEUDOXANTHOMA ELASTICUM MOUSE MODEL: UNTARGETED METABOLOMICS TO SEARCH FOR THE Abcc6 SUBSTRATE
Mie Rostved Rasmussen
Department of Biomedicine, Aarhus University, Aarhus, Denmark
Pseudoxanthoma elasticum (PXE) is a serious genetic disorder of ectopic mineralization. PXE patients display mutations in the gene encoding ABCC6, but the physiological function of this protein as well as the PXE pathomechanism remain unknown. The Abcc6 knockout mouse represents a useful animal model to study PXE, and in the present study an untargeted metabolomics-based screening approach demonstrated that the hepatic metabolic profile of the PXE mouse model differed from that of wildtype mice.

P1-3
METABOLITE PROFILING OF MYCOBACTERIUM SPP.: BIOCHEMICAL DIVERSITY AND ADAPTION
Marigot Drapal
Royal Holloway University of London, Egham, Surrey, UK, Animal Health and Veterinary Laboratories Agency, Weybridge, Surrey, UK
The increasing occurrence of drug-resistant Mycobacterium tuberculosis (Mtb) strains has resulted in an interest for metabolic profiling approaches leading to better understanding of complete cellular processes underlying phenotypes in Mtb and related Mycobacterium species. The metabolite profiling platform developed for the model organism M. smegmatis and Bacillus Calmette-Guérin (BCG) include quenching and extraction procedures for GC-MS analysis and HPLC and was applied to monitor metabolic changes during different growth stages of both model organisms.

P1-4
METABOLIC SCREENING FOR IDENTIFYING THE OXIDATIVE STRESS TARGETING ENZYMES
Daiki Setoyama
Kyushu University, Fukuoka, Japan
Based on the LC-MS-based metabolomics, we explored the oxidative H$_2$O$_2$-sensitive enzymes tightly linked to the cellular metabolism in human cells. We identified a key mitochondrial metabolic enzyme as a novel target for oxidative inactivation.

P1-5
UNTARGETED AND TARGETED APPROACHES FOR METABOLOMICS BASED ON ULTRA HIGH PERFORMANCE LIQUID CHROMATOGRAPHY–MASS SPECTROMETRY
Xinyu Liu
Dalian Institute of Chemical Physics, Dalina, China
Untargeted and targeted approaches based on ultra high performance liquid chromatography–mass spectrometry were developed and validated respectively for global metabolite profiling and free amino acid profiling of haemolymph. The robustness of the method was confirmed by the stable relative standard deviation of overwhelming majority metabolites in QC samples. Combination of untargeted and targeted approached has a major significance for distinguishing different varieties of silkworm and uncovering further biological mechanism.

P1-6
COMBINED NMR-BASED METABOLIC ANALYSES IN TROUT NUTRITION STUDIES.
Catherine Deborde
INRA, UMR1332 Fruit Biology and Pathology, Centre INRA de Bordeaux, Villenave d’Ornon F-33140, France, Metabolome Facility of Bordeaux Functional Genomics Center, IBVM, Centre INRA de Bordeaux, Villenave d’Ornon F-33140, France
In a context of limited marine resources and continuous development of world aquaculture, developing aquafeeds with a reduced content of fish-meal and fish-oil, using alternative protein and lipid sources, is a real challenge. NMR-based metabolomic profiling of aquafeed polar extracts were implemented to characterize classic “marine” and new “vegetable” diet and assess their effect on rainbow trout metabolism through $^1$H-NMR profiling of plasma.
P1-7
METABOTYPING OF THE C. ELEGANS SIR-2.1 MUTANT USING IN VIVO LABELING AND 
$^{13}$C-HETERONUCLEAR MULTIDIMENSIONAL NMR METABOLOMICS
Sujin Lee
College of Pharmacy, Seoul National University, Seoul, Republic of Korea
The roles of sir-2.1 in C. elegans lifespan extension is controversial. We applied an efficient workflow for in vivo $^{13}$C-labeling of C. elegans and $^{13}$C-heteronuclear NMR. The metabolomic analysis defined the sir-2.1 mutant metabotype as the decoupling between enhanced catabolic pathways and ATP generation as well as the increases in glycolysis, nitrogen catabolism and initial lipolysis. We also suggested the relationship between the branched chain amino acids and the roles of sir-2.1 in the lifespan.

P1-8
COMPREHENSIVE METABOLOCIC ANALYSIS REVEALS MAJOR DIFFERENCES IN THE MACROPHAGE 
INFLAMMATORY RESPONSE BETWEEN YOUNG AND AGED MICE
Fan Fei
McMaster University, Hamilton, Ontario, Canada
Inflammation is an immune response to foreign pathogenic infections and tissue injury. Aging is linked to an increased susceptibility to infection and systemic inflammation; however, the cause of this dysregulated response is not known. This is the first comprehensive metabolic analysis to explore age-associated differences in the inflammatory response to LPS (bacterial lipopolysaccharide) exposure and LPS tolerance using murine macrophages obtained from old and young mice.

P1-9
METABOLIC PROFILING OF MALE AND FEMALE DROSOPHILA MELANOGASTER BY DIFFERENT 
CHROMATOGRAPHIC METHODS IN COMBINATION WITH HIGH RESOLUTION MS
David Watson
University of Strathclyde, Glasgow, UK, University of Glasgow, Glasgow, UK
Genes that are present in the single male X chromosome have to be compensated in order to attain similar levels of expression to those present in females who have two X chromosomes. Metabolomic profiling revealed elevated levels of methylated RNA nucleosides in male Drosophila melanogaster suggesting that methylation may have a role in gene compensation. This hypothesis was supported by the observation of a highly elevated levels of a novel metabolite decarboxy S-adenosylmethionine in males.

P1-10
PROFILING MULTIPLE AUXOTROPHIC YEAST STRAINS USING UNTARGETED METABOLIC WORKFLOW BY HIGH 
RESOLUTION LC-MS/MS
Lekha Sleno
UQAM, Montreal, Canada
An untargeted metabolomics approach was used for investigating a series of auxotrophic yeast strains. Previous analysis of the auxotrophic mutant used in most chemical genomics studies showed perturbations in tryptophan degradation in comparison to its prototrophic counterpart. In order to better study the involvement of the auxotrophic mutations, a series of new mutants were analysed to pinpoint which implicated the disruption of tryptophan metabolism, as well as other metabolic pathways disrupted.

P1-11
OXIDATIVE STRESS-INDUCED ADAPTIVE CHANGES IN METABOLISM IN G6PD-DEFICIENT ERYTHROCYTES
Hsiang-Yu Tang
Graduate Institute of Biomedical Sciences, Chang Gung University, Tao-Yuan, Taiwan
G6PD deficiency is associated with increased susceptibility of erythrocytes to reactive oxygen species, which can cause hemolytic anemia. In this study, we studied the changes in metabolic responses of erythrocytes to oxidative stress. Diamide induced disturbances in glutathione homeostasis, nucleotide pool, and accompanied AMPK activation in G6PD-deficient erythrocytes. These findings suggest that anomalous redox homeostasis in G6PD-deficient erythrocytes after diamide treatment, and AMPK is activated as an attempt of cells to compensate for energy deficit.

P1-12
METABOLITE ALTERATIONS IN ENU MUTAGENESIS DERIVED Asgr1-KO MICE AS A MODEL FOR HUMAN 
IDEOPATHIC HYPERPHOSPHATASEMIA
Cornelia Prehn
1Helmholtz Zentrum München, Institute of Experimental Genetics, Neuherberg, Germany
We describe the quantification of 163/186 metabolites (lipids, amino acids, acylcarnitines, carbohydrates) out of 10 μL plasma using the Biocrates AbsoluteIDOTS™ kits p150/p180, respectively. We present the metabolomic measurement results of the phenotypic characterization of a C3HeB/FeJ mouse line that was generated within a genome-wide ENU-mutagenesis screen. The isolated mouse line revealed significantly elevated levels of alkaline phosphatase activity carrying a dominant biallelic missense mutation in the Asgr1 (asialoglycoprotein receptor 1) gene (c.815A>G, p.Tyr272Cys).
P1-13 FILLING IN THE ‘GAPS’ OF DROSOPHILA MELANOGASTER METABOLIC MAP USING METABOLIC APPROACHES

Dominika Korzekwa
University of Glasgow, Glasgow, Lanarkshire, UK

A computer-annotated metabolic map of Drosophila has been predicted by KEGG. However, ‘gaps’ still remain with no identified Drosophila orthologues for metabolic enzymes. One of these gaps is Drosophila gene CG30016. Based on sequence homology it is hypothesised to be a homologue of 5-hydroxyisourate hydrolase (5-HIUH) involved in purine metabolism. Enzyme defects within purine metabolism in humans result in IEMs including hyperuricemia. Here, we propose a method for identifying metabolic ‘gaps’ using metabolomics approaches.

P1-14 METABOLIC PROFILING OF MULTIFUNCTIONAL PROTEIN 2 (MFP-2) KNOCKOUT MOUSE

Anna Artati
Helmholtz Zentrum München, Institute of Experimental Genetics, Neuherberg, Germany

Multifunctional protein-2 (MFP-2) is responsible in peroxisomal beta-oxidation. Deficiency of this enzyme in human causes severe developmental syndrome with multiple abnormalities. Most of affected individuals die within the first year of life. To understand the affected pathway of this disease, we analyzed metabolomics of MFP-2 knockout mouse (MFP2 KO) which partly phenocopies the human disease using UPLC-MS/MS method. This study shows for the first time difference metabolic profile between MFP-2 KO and wild type mice.

P1-15 THE EFFECTS OF HYDROGEN PEROXIDE ON CELLULAR METABOLISM OF HEPATOMA CELLS USING UPLC/Q-TOF MS

Cheng-Yu Hung
Metabolomics Core Laboratory, Healthy Aging Research Center, Chang Gung University, Tao-Yuan, Taiwan

Metabolomics provides a powerful platform for discovering the changes of the cellular metabolites involved in redox homeostasis with H2O2 treatment. In this study, the metabolic profiles of HepG2 cells showed in a dose-dependent change by PCA distribution. The major alterations in the metabolome included glutathione and purine metabolism based on the VIP analysis. Our findings suggest that glutathione acts as a H2O2 scavenger, and purine metabolism provides a compensatory mechanism to protect H2O2-induced oxidative damage.

P1-16 MS-BASED METABOLITE PROFILING REVEALS CIS-UROCANIC ACID AND CHOLESTEROL AS TIME-DEPENDENT SKIN BIOMARKERS IN UVB-RADIATED MICE

Hye Min Park
Kon-Kuk University, Seoul, Republic of Korea

Amino acids, organic compounds, fatty acids, lipids, nucleosides, carbohydrates, lysoPCs, lysoPEs, urocanic acids and ceramides were determined to be discriminators that characterized the differences in hairless mice skin following UVB irradiation for 6 and 12 week using UPLC-Q-TOF-MS, GC-TOF-MS, and Nanomate tandem-MS as well as multivariate analysis. Especially, cis-uurocanic acid and cholesterol showed potential as time-dependent candidate biomarkers of histological changes in UVB-induced skin.

P1-17 NMR-BASED METABOLOMICS TO INVESTIGATE NAPHTHALENE TOXICITY USING THE URINE OF A NAPHTHALENE TOLERANT MODEL

Ching-Yu Lin
National Taiwan University, Taipei, Taiwan

Naphthalene, the most common polyaromatic hydrocarbons, exists widely in the environment with significant human exposure. Naphthalene exposure resulted in Clara cell tolerant to further injury. We investigated naphthalene toxicity by analyzing the urinary metabolome of the tolerant mice by NMR-based metabolomics. The urine recorded NA metabolism and NA-induced metabolic turbulences which can be monitored and associated with cell injury.

P1-18 WHEN INFORMATION FORM URINE AND BLOOD ISNT ENOUGH - SYSTEMIC AND ORGAN SPECIFIC METABOLOMICS OF MTKO MICE

Zander Lindeque
Centre for Human Metabonomics, North-West University, Potchefstoom Campus, Potchefstroom, South Africa

Blood, urine and several tissue samples from metallothioneins 1+2 knockout mice were screened for metabolic variation. The brain metabolome content of these mice differed markedly from wild-type mice while urine and blood samples were comparable. This important finding would have been overlooked if urine and blood were solely screened for metabolic differences in these model animals.

P1-19 METABOLOMICS OF THOROUGHBRED RACEHORSES: A PILOT STUDY

Ebony Escalona
Imperial College, London, UK, University of Liverpool, Liverpool, UK

Some types of intestinal disease in the horse are strongly associated with equine oral stereotypy (EOS), a behavioural phenotype which has interesting similarities with human autism spectrum disorder. Metabolic profiles of horses demonstrating EOS revealed gut microbial co-metabolite differences compared to neurotypical horses. This study demonstrates the utility and sensitivity of 1H NMR metabonomic approaches to investigating equine intestinal microbiota.
P1-20
CHARACTERIZING A NOVEL E. COLI AMINO ACID N-ACETYLTRANSFERASE USING METABOLOMICS
Hitoshi Iuchi1, 2
1Systems Biology Program, Graduate School of Media and Governance, Keio University, Fujisawa, Kanagawa, Japan, 2Institute for Advanced Biosciences, Keio University, Tsuruoka, Yamagata, Japan
A large number of enzymes remain uncharacterized even in E. coli K-12. Here, we combined classical enzyme assays and metabolite profiling to characterize the activity of orphan enzyme YhhY. Our results demonstrate that YhhY is an acetyltransferase displaying activity on several amino acids.

P1-21
A POOLED SAMPLE APPROACH TO DIFFERENTIAL METABOLOMICS USING GCxGC TOFMS - STANDARDIZED METHODS AND A REFERENCE FEATURE FOR BIOMARKER SCREENING IN ETHANOL FED MICE
Lorne Fell
LECO Corporation, Saint Joseph, Michigan, USA, 2LECO Gmbh, Monchengladbach, Germany
This research presents a standardized approach for metabolomic GCxGC-TOFMS analysis using standardized sample preparation and optimized analysis of population pools to leverage the capabilities of GCxGC-TOFMS as a means of rapid evaluation. GCxGC-TOFMS analysis of pooled samples combined with data processing by means of a software-driven “Reference” feature show substantial numbers of biologically-relevant metabolites to be differentially expressed in the populations.

P1-22
CAENORHABDITIS ELEGANS, AN EXCELLENT MODEL ORGANISM FOR METABOLOMICS
Ramadan Ajredini
University of Florida, Gainesville, Florida, USA
The nematode Caenorhabditis elegans is a free-living animal that lives in soil and composting fruit. Although, C. elegans is one of the best-studied animals genetically, less attention has been given to its metabolism. This poster will describe the methods that we have developed to generate high-quality synchronized samples of both the exo- and endo-metabolomes. These methods provide the material for IROA and NMR studies that are described in other posters in this meeting.

P1-23
THE APPLICATION OF METABOLOMICS TO INVESTIGATE THE BURDEN OF RECOMBINANT PROTEIN PRODUCTION ON YEAST CELLS
Catherine Winder
University of Manchester, Manchester, UK
Recombinant proteins are important industrial products, with a vast number of existing and potential applications. The synthesis of recombinant proteins requires complex systems that can only be found in living cells. The application of metabolomic approaches to understand the burden of recombinant protein production on host cells will facilitate the development of alternative feeding strategies, to improve protein yields and the predictability of protein production.

P1-24
POTENTIAL BIOMARKERS OF DISEASE IN THE SERUM AND URINE OF MICE INFECTED WITH SCRAPIE AT PRECLINICAL STAGE
Seyed Ali Goldansaz
Department of Agricultural, Food & Nutritional Science, University of Alberta, Edmonton, Alberta, Canada
The objective of this study was to search for potential metabolites in the serum and urine of mice infected with scrapie prion agents. Quantitative metabolic profiling was conducted using Nuclear Magnetic Resonance (NMR) spectroscopy. Comparisons were made in a longitudinal manner using different time points to study the metabolite trend over time. Results showed alterations in different organic metabolites (i.e., organic acids, lipids, aromatic heteropolycyclic compounds, aliphatic homomonocyclic/acyclic compounds, amino acids, carbohydrates and carbohydrate conjugates).

P1-25
HYALURONIC ACID-DEPENDENT PROTECTION AGAINST UVB-DAMAGED HUMAN CORNEAL CELLS
Ji-Min Li
Institute of Bioinformatics and Structural Biology, National Tsing Hua University, Hsinchu, Taiwan
Many previous reports suggested that exposure to the UVB irradiation causes corneal pathologies due to the direct damage on DNA molecules and the generation of reactive oxygen species (ROS) which interfere downstream signaling cascades via post-transcription modifications of cysteine-residues in target proteins resulting in losing their biological functions. The aim of this study is to in vitro investigate if hyaluronan is able to decrease UVB-induced toxicity and promote cell repair system.
**P2-1**

**MEASURING NITROGEN FLUX IN PRIMARY AND SECONDARY AMINE CONTAINING METABOLITES USING LABELLING WITH THE 15N STABLE ISOTOPE.**

*Damien Callahan*

*The University of Melbourne, Parkville, Vic, Australia, Deakin University, Melbourne, Vic, Australia*

This paper will describe a new approach to flux measurements through the use of the labelling with the 15N stable isotope. This stable isotope labelling approach can be applied to N-containing metabolites and has been used in proteomics but rarely in metabolomics. This approach can be applied to a range of biological systems. The methodology including the challenges as well as the application of both low and high resolution mass spectrometry instrumentation will be described.

**P2-2**

**IN VIVO 13C STABLE ISOTOPE TRACING OF PRIMARY METABOLISM DURING LEAF DEVELOPMENT**

*Frederik Dethloff*

*Max Planck Institute of Molecular Plant Physiology, Potsdam, Germany*

We developed an *in vivo* plant feeding method where labelled precursors, such as U-13C-sucrose, are fed into the plant using a reverse petiole assay (Lin *et al.* 2011). This assay is suitable for plants grown on soil in a phytotron, but could equally be applied to plants growing in a greenhouse or even in the field.

**P2-3**

**USE OF BIOINFORMATICS TOOLS FOR FLUXOMICS ANALYSIS OF THE METABOLIC CHANGES DURING ADIPOCYTE DIFFERENTIATION**

*Anibal Miranda*

*Universitat de Barcelona, Barcelona, Spain*

The formation of new adipocytes from the differentiation of pre-adipocytes is accompanied with important metabolic changes. Stable isotope tracer data is used to reveal the metabolic flux profile in cells under studied conditions, and thus to provide an insight into the cell phenotype. The de novo adipocyte differentiation and the associated changes of metabolic flux profile were studied on the 3T3-L1 cell line incubated with stable isotope tracers and bioinformatics analysis.

**P2-4**

**ACUTE EFFECT OF CIGARETTE SMOKE ON HUMAN BRONCHIAL EPITHELIAL CELL METABOLOME IS REVERSIBLE BY UPF1**

*Arno Aug*

*Department of Biochemistry, The Centre of Excellence for Translational Medicine, University of Tartu, Tartu, Estonia*

We assessed protective capacity of glutathione analogue UPF1 (4-methoxy-L-tyrosinyl-y-L-glutamyl-L-cysteinyl-glycine) against cigarette smoke condensate (CSC)-induced alterations in metabolic profile of human bronchial epithelial cells (HBEC) with mass spectrometer. Signals affected by CSC with/without UPF1 formed 3 major clusters of metabolites following similar changing pattern within each group over time. Among metabolites in cluster 1 species of phosphatidylcholines were identified. Glutamine and glutamic acid were identified in cluster 2. UPF1 inverts the effect of CSC.

**P2-5**

**TIME-DEPENDENT METABOLIC VARIANCE IN MOUSE KIDNEY UPON CISPLATIN-INDUCED ACUTE KIDNEY INJURY**

*Miho Irie*

*Kyushu University, Fukuoka, Japan*

To find some clues of the potential mechanism(s) of CDDP-induced AKI, we examined time-dependent comprehensive metabolic variance in CDDP-administrated mouse kidney. By tracing complex metabolic behaviors, we succeeded in visualizing a subtle alteration of renal states, which could not be traced by the general biochemical evaluation such as BUN.

**P2-6**

**PATHWAY-WIDE METABOLITE ANALYSIS OF CENTRAL CARBON METABOLISM USING THREE COMPLEMENTARY LC-ESI-MS METHODS AND ITS APPLICATION**

*Christoph H. Borchers*

*University of Victoria-Genome BC Proteomics Centre, Victoria BC, Canada, Department of Biochemistry and Microbiology, University of Victoria, Victoria BC, Canada*

Central carbon metabolism (CCM) is a complex enzyme-mediated network containing several dozens of metabolic precursors, intermediates and end products. We developed three UPLC-MS-based methods including improved ion-pairing UPLC-(−)ESI-MS using tributylamine (TBA) as the paired ion, a new UPLC-(+)ESI-MS method combining reductive amination and polar PFP LC with efficient tail sweeping, and another new UPLC-(−)ESI-MS method using 3-nitrophenylhydrazine for pre-analytical derivatization, for isotope-resolving metabolic profiling and quantitation of >55 CCM metabolites in various biological samples.

**P2-7**

**IMPROVING BIOPROCESS FERMENTATIONS BY STABLE ISOTOPE LABELING AND FLUX ANALYSIS**

*Dierk Pöther*

*Metabolomic Discoveries GmbH, Potsdam, Germany*

Combining metabolomics with stable isotope labeling provides a detailed analysis of the metabolic flux and active pathways. The physiological state can be deeply characterised by the analysis of different biochemical pathways. Furthermore, identification of biochemical bottlenecks or highways illustrate the hidden metabolic capabilities of an organism. Flux analysis was applied
P2-8
THE COMPLETE TARGETED PROFILE OF THE ORGANIC ACID INTERMEDIATES OF THE CITRIC ACID CYCLE USING A SINGLE STABLE ISOTOPE DILUTION ANALYSIS, SODIUM BORODEUTERIDE REDUCTION AND SELECTED ION MONITORING GC/MS
Daina Avizonis
McGill University, Montreal, Quebec, Canada
This paper presents a methodology that allows for the complete targeted quantitation of the citric acid cycle intermediates (CAC) using stable isotope dilution and sodium borodeuteride to quickly reduce and stabilize the α-keto acids. By reducing pyruvic to D:-lactic, oxaloacetic to D:-malate, α-ketoglutaric to D:-α-hydroxyglutaric and oxalosuccinic to D:-isocitric acid, we are able to quantify them in along with Lactic, malic, α-hydroxyglutaric using commercially available isotopically labeled standards by GC/MS.

P3-1
URINARY METABOLOMIC ANALYSIS OF BLADDER CANCER BY UPLC-FTMS AND UPLC-ION TRAP MS
Chiun-Gung Juo
Chang Gung University, TaoYuan, Taiwan
124 bladder cancer and 65 hernia urine samples were analyzed using a metabolomic platform coupling UPLC-FTMS and UPLC-ion trap MS. The platform improved retention time, mass accuracy and signal stability. The product spectra obtained from ion trap MS were useful for elucidating the metabolite structures, especially when authentic standards were not available. Using this technology platform, two metabolite panels were used to differentiate BCa from hernia and to differentiate early stage BCa and hernia, respectively.

P3-2
FINGERPRINTING OF BREAST CANCER CELLS VS. NORMAL MAMMARY CELLS BY SECONDARY ELECTROSPRAY IONIZATION MASS SPECTROMETRIC ANALYSIS OF VOLATILE COMPOUNDS FROM THE CULTURE MEDIUM
Jingjing He
1Department of Chemistry and Applied Biosciences, ETH Zurich, Zurich, Switzerland, 2State Key Laboratory of Bioactive Substance and Function of Natural Medicines, Institute of Materia Medica, Chinese Academy of Medical Sciences and Peking Union Medical College, Beijing, China
We directly fingerprinted the volatile metabolic signature of three types of human breast cancer cells versus normal human mammary cells by secondary electrospray ionization-mass spectrometry. Different samples can be classified by using feature selection followed by principal component analysis (PCA). Moreover, high resolution mass spectrometry and fragmentation can give clues to the chemical structure of the most discriminant molecules. The identification of such volatile metabolic compounds may provide potential biomarkers for early diagnosis of cancers.

P3-3
EXPOSURE TO CARCINOGENIC POLYCYCLIC AROMATIC HYDROCARBONS THROUGH TOBACCO SMOKE
Xue Li
1Shanghai University, Shanghai University, China, 2ETH Zürich, Zürich, Switzerland
Exposure to carcinogenic polycyclic aromatic hydrocarbons (PAHs) through tobacco smoke was investigated. 2-Naphthol (2-OHNap) and 2-hydroxyfluorene (2-OHFlu) were found to be dominant hydroxylated metabolites of PAHs in smoker urine samples, and probably selective PAHs biomarkers of tobacco smoke. Meanwhile, 2-OHNap, 2-OHFlu, 1-hydroxypyrene (1-OHPyr), 3-/9-hydroxypheanthrene (3-/9-OHPhe) and 6-OHChr increased with the increase of cigarette consumption over time, further evidencing smoker’s exposure to PAHs through tobacco smoke.

P3-4
DEVELOPMENT & OPTIMIZATION OF GC-MS BASED GLOBAL METABOLITE PROFILING OF ADHERENT MAMMALIAN CELLS
Rahul Vijay Kapoore
The University of Sheffield, Sheffield, UK
To discern molecular mechanisms of tumour progression through metabolomics, it is essential to optimize a metabolomic method. Initially, the effect of trypsinization and cell scraping treatment on leakage of internal metabolites was compared for harvesting adherent cell lines. Both the treatments caused significant metabolite leakage providing it inadequate for metabolomics studies. Later we have developed a novel method with no trypsinization treatment, which resulted in identification of 93 unique metabolites with minimal leakage internal metabolites.

P3-5
SERUM METABOLOME ANALYSIS IN PANCREATIC CANCER PATIENTS
Masaru Yoshida
Kobe University Graduate School of Medicine, Kobe, Hyogo, Japan
To develop the efficient diagnostic method for pancreatic cancer (PC), we used gas chromatography/mass spectrometry (GC/MS)-based serum metabolomics with multiple logistic regression analysis. The constructed model possessed high sensitivity and specificity for PC in not only the training set but also the validation set. Furthermore, the model showed higher sensitivity for resectable PC and lower false-positive rate in the case of chronic pancreatitis than these conventional tumor markers.
**P3-6**

**AN NMR METABOLIC APPROACH FOR THE DIAGNOSIS OF LEPTOMENINGEAL CARCINOMATOSIS**

**He Wen**

*College of Pharmacy, Seoul National University, Seoul, Republic of Korea*

Leptomeningeal carcinomatosis (LC) is the third most common metastatic complication of the central nervous system. However, current diagnosis, such as Cytological diagnosis and MR imaging, are not satisfactory. NMR-based metabolomics on CSF of rat LC model presented differences between normal and LC groups. Predictions based on multivariate model provided sensitivity, specificity and overall accuracy of 88-89% in LC diagnosis. Overall, we demonstrated that metabolomics approach provided both earlier and more accurate diagnosis than current use.

**P3-7**

**EFFECT OF EXTERNAL BEAM AND 131I-MIBG THERAPIES ON HUMAN GLIOMA CELL METABOLISM**

**Shazia Khan**

*Strathclyde Institute of Pharmacy and Biomedical Sciences, University of Strathclyde, Glasgow, UK*

Many studies have been done on tumour metabolism to diagnose several types of tumour only few are for assessment of treatment effect. In present work we examined the metabolic pathway associated with external beam γ-radiation and internal β-radiation therapy on direct and indirect irradiated human glioma cells in vitro that might be used to predicting or monitoring cellular response, toxicity and resistance to these treatments. These radiations significantly impact on cell metabolism in different ways.

**P3-8**

**LIPIDOMIC ANALYSIS DEMONSTRATES THAT THE ANTI-LEUKEMIC THERAPY OF BEZAFIBRATE AND MEDROXYPROGESTERONE ACETATE REDUCES DE NOVO PHOSPHOLIPID SYNTHESIS**

**Andrew Southam**

*University of Birmingham, Birmingham, UK*

Previously we demonstrated that the combination of the lipid lowering drug, Bezafibrate, And the contraceptive, medroxyProgesterone acetate, (BaP) kills acute myeloid leukaemia (AML) cells in vitro. Here, we utilised mass spectrometry-based lipidomics to investigate 24-hour BaP treatment on HL60 and K562 AML cell lines. BaP induced highly consistent changes to cellular phospholipid profiles in both cell lines, including a widespread increase in unsaturation of phospholipid fatty acyl residues and reduced phospholipid synthesis from glucose.

**P3-9**

**METABOLIC CHARACTERIZATION OF A METASTATIC PROSTATE CANCER STEM CELL SUBPOPULATION**

**Marta Cascante**

*Department of Biochemistry and Molecular Biology, CSIC associated unit, Faculty of Biology, Universitat de Barcelona, Biomedicine Institute of the Universitat de Barcelona (IBUB), Barcelona, Spain*

Characterization of the metabolic profiles of two distinct prostate cancer cell subpopulations which cooperate in the establishment of metastases. These cell subpopulations show a differential behaviour regarding their invasive and metastatic capacities. We aim to study the relationship between the metabolism and the acquisition of the abovementioned properties which are essential in the metastatic process.

**P3-10**

**PROGNOSTIC VALUE OF 1H NMR SPECTROSCOPY IN THE TREATMENT OF NON-SMALL CELL LUNG CANCER**

**Evelyne Louis**

*Universiteit Hasselt, Hasselt, Belgium,
Lung cancer is the leading cause of cancer mortality worldwide. Despite progress we experience unacceptable toxicities without survival benefit. Clinical trials do not answer the question of who will benefit and who may be harmed by treatment. We aim to distinguish a metabolic profile that differs between responders and non-responders. There was no significant difference between the metabolic profiles of the 2 groups, probably due to the heterogeneous composition of the small subgroups.

**P3-11**

**LC-HRMS BASED METABOLIC AND LIPIDOMIC PHENOTYPING FOR THE STUDY OF MAMMARY CANCER SIGNATURE IN CANINE SERUM.**

**Frédérique Courant**

*Oniris - LABERCA, Nantes, France; Oniris - AMaROC, Nantes, France*

Comprehensive LC-HRMS metabolomic/lipidomic approach has been developed for global characterization of serum samples. After a fractionation of the sample, the polar metabolites are characterized by complementary C18 and HILIC-based LC-HRMS methods while the analysis and identification of lipids is achieved using a versatile LC-HRMS/MS acquisition. The information provided by the different proposed methods has been applied to the study of mammary cancer signature in canine serum samples.

**P3-12**

**TARGETING CELL CYCLE REGULATION IN CANCER THERAPY**

**Miriam Tarrado-Castellarnau**

*Universitat de Barcelona, Barcelona, Spain*

Cell division is orchestrated by a complex network of interactions between proteins, metabolism and microenvironment aiming to enable cell proliferation only in response to specific stimuli and under adequate conditions. There are three main players in cell cycle regulation: i) The cell cycle protein machinery, ii) The metabolic enzymes and related metabolites and iii) The reactive-oxygen species (ROS) and cellular redox status. Cancer development has been associated to defects in all of them.
P3-13
DETERMINATION OF AMINO ACID IN URINE SAMPLES COLLECTED FROM PATIENTS WITH PROSTATE CANCER AND BENIGN PROSTATE HYPERPLASIA, BEFORE AND AFTER DIGITAL RECTAL EXAMINATION
Wiktor Sroka
Department of Medicinal Chemistry, Ludwig Rydzygier Collegium Medicum., Bydgoszcz, Poland
Prostate cancer (PCa) is the second most common cause of cancer related death and leading type of cancer diagnosed in men. The aim of our research is to find an improved biomarker for PCa. Our strategy involved identifying and quantifying a number of amino acids in urine samples collected in the morning prior to and after digital rectal examination. We observed that patients with PCa present with higher urinary levels of arginine, homoserine, proline and tyramine.

P3-14
BREATH ANALYSIS BY GAS CHROMATOGRAPHY-MASS SPECTROMETRY IN THE DETECTION OF LUNG CANCER AND CHRONIC OBSTRUCTIVE PULMONARY DISEASE
Roldán Cortés
Department of Biochemistry and Molecular Biology, IBUB, University of Barcelona, Barcelona, Spain
Organic Volatile Compounds (VOCs) generated in metabolism can be detected in exhaled air. Several diseases entail altered patterns of exhaled VOCs due to an alteration in normal metabolism. Specifically, abnormal pulmonary and systemic metabolism in lung disorders is expected to result in an altered exhaled VOCs pattern. Therefore, we analyzed the pattern of exhaled VOCs in the breath of healthy subjects, COPD patients and lung cancer patients to assess the diagnostic potential of breath analysis.

P3-15
IDENTIFICATION OF THE CHEMICAL SHIFTS OF A SERIES OF METABOLITES APPEARING IN THE ‘1H-NMR SPECTRUM OF BLOOD PLASMA BY SPIKING
Liene Bervoets1,2
1Faculty of Medicine and Life Sciences, Diepenbeek, Belgium 2Institute for Materials Research (IMO), Diepenbeek, Belgium
Instead of using ‘1H-NMR chemical shifts reported in literature for metabolites appearing in the plasma, chemical shifts were determined by spiking with known metabolites. Spiking experiments seem necessary in order to more accurately identify the chemical shifts of plasma metabolites. Moreover, it could lead to an enhancement of the discriminative power of the cluster analysis and a better understanding and/or explanation of the clinical relevance of study findings.

P3-16
OPTIMIZATION AND VALIDATION OF A METABOLOMIC METHOD FOR ANALYSIS OF PROSTATE CANCER CELL CULTURES (LNCaP) USING EXACTIVE-ORBITRAP MASS SPECTROMETER
Manal Alossaimi
University of Strathclyde, Glasgow, UK
A method for carrying out metabolomics profiling of tissue cultures with an optimized extraction procedure and validation of an analytical method using LC/MS. Cell culturing, quenching, metabolite extraction, and the LC/MS settings were optimized aiming at a reliable, unbiased, sensitive, and high throughput metabolomic protocol. This approach was validated using ~ 200 standard compounds and LNCaP. An MS/MS library was obtained for both. Effects of storage conditions on metabolite profiles and stability study were assessed.

P3-17
METABOLOMICS STUDIES INTO THE REGULATION OF METABOLISM BY THE p53 PATHWAY
Celia Berkers
CR-UK Beatson Institute, Glasgow, UK
Increasing evidence suggests that the tumour suppressor p53 plays a key role in the regulation of metabolic homeostasis. However, the metabolic roles of many p53 target genes, such as TIGAR, and of oncogenic mutant p53 proteins are less well understood. We have developed LC/MS-based metabolomics methods to examine how these less-studied players in the p53 pathway affect metabolism. Our approach aids in understanding how (mutant) p53 may help cells to survive metabolic stresses.

P3-18
A NMR METABONOMIC APPROACH TO EXPLORE EARLY BIOMARKERS OF HEPATOCellular CARCINOMA IN THE EUROPEAN PROSPECTIVE INVESTIGATION INTO CANCER AND NUTRITION (EPIC)
Anne Fages
Université de Lyon (CNRS/ENS Lyon/ UCB Lyon 1), Institut des Sciences Analytiques, Centre de RMN à très hauts champs, Villeurbanne, France
We present a 800 MHz 1H NMR metabonomic study of a case-control liver cancer cohort (1case: 2controls) nested within EPIC (European Prospective Investigation into Cancer and Nutrition). We investigated early or etiologic biomarkers related to HCC occurrence on 336 serum samples. We propose a method to explore systematic sources of variation in the dataset. Metabolic patterns discriminating matched cases and controls from a stratified analysis were identified.

P3-19
NMR-BASED METABOLITE PROFILING FOR EARLY DETECTION AND NON-INVASIVE DIAGNOSIS OF GASTRIC CANCER
Jeeyun Jung1,2
1Korea Basic Science Institute, Seoul, Republic of Korea; 2College of Oriental Medicine, Wonkwang University, Iksan, Republic of Korea
This study suggests that the urinary metabolic profiles can be a potential alternative non-invasive tool for the clinical diagnosis of gastric cancer, and metabolomic investigation of gastric tissue and urine can provide new insights into the metabolic alterations in gastric adenocarcinoma.
P3-20  
**NMR METABONOMIC INVESTIGATION OF A E3N MATCHED CASE-CONTROL BREAST CANCER PROSPECTIVE COHORT**  
Elodie Jobard1,2  
1Université de Lyon, CNRS/ENS Lyon/UCB-Lyon-1, Institut des Sciences Analytiques UMR5280, Centre de RMN à Très Hauts Champs, Villeurbanne, France, 2Université de Lyon, Département d’oncologie médicale, Centre Léon Bérard, Lyon, France  
A 1H-NMR metabolomic study of the E3N breast cancer sub-cohort was carried using a matched case-control design on 1,602 plasma samples. The main objective is to identify early or predictive biomarkers of breast cancer in this prospective study, where blood was collected on volunteers healthy at the time of inclusion. We present a descriptive statistical analysis of the breast-cancer sub-cohort together with an exploration of main sources of systematic variation in the NMR metabolomic dataset.

P3-21  
**DETERMINATION OF HETES IN PROSTATE CANCER SERUM SAMPLES USING UHPLC-MS/MS**  
Giovanny Rodriguez Blanco  
Erasmus Medical Center, Rotterdam, The Netherlands  
HETEs are bioactive molecules produced along the arachidonic (AA) acid pathway and they have been associated with different diseases including cancer. In this study we aimed to determine concentrations of 5- HETE, 8- HETE, 11- HETE, 12- HETE, 15- HETE and AA using UHPLC-MS/MS in serum samples from patients diagnosed with prostate cancer (PCa) and controls. Results indicate a possible relationship between concentration of HETEs and PCa in a reduced group of patients.

P3-22  
**IDENTIFICATION AND QUANTIFICATION OF INTRACELLULAR METABOLITES INVOLVED IN TRICARBOXYLIC ACID CYCLE METABOLISM**  
Khalid Al-Qahtani1,2  
1Department of Chemistry, University of Oxford, oxford, UK, 2Metabolic Screening Laboratory, King Faisal Specialist Hospital and Research Center, Riyadh, Saudi Arabia  
The chiral differentiation and quantification of L-2-hydroxyglutarate (L-2HG) and D-2-hydroxyglutarate (D-2HG) is key to characterizing neuro-metabolic disorders and the effect of IDH1 and IDH2 mutations on the reduction of 2-ketoglutarate to D-2 Hydroxyglutarate. The ability to distinguish and quantify the enantiomers of L/D-2-HG is therefore an important for characterising changes in the metabolic pathways associated with wild type and modified cancer cell lines.

P3-23  
**USING METABOLOMICS TO INVESTIGATE THE INDUCTION OF NON-ALCOHOLIC FATTY LIVER DISEASE IN A RAT MODEL OF HEPATOCELULAR CARCINOGENESIS**  
Yajing Chu1,2  
1Department of Biochemistry, University of Cambridge, Cambridge, UK, 2Medical Research Council Human Nutrition Research, Cambridge, UK  
A rat model of non-alcoholic fatty liver disease (NAFLD) induced by a choline deficient (CD) diet was studied to elucidate the multiple pathogenic mechanisms of NAFLD. In addition animals were treated with an analogue of the thyroid hormone, GC-1, to investigate the potential reversal of fatty liver by this intervention. A comprehensive metabolomic strategy combining NMR spectroscopy, GC-MS, UPLC-MS and MS imaging techniques was employed, demonstrating perturbations of lipid and amino acid metabolism.

P3-24  
**ASSOCIATIONS BETWEEN IN VITRO SURVIVAL TO CHEMOTHERAPY, MINIMAL RESIDUAL DISEASE AND CONDITIONED CULTURE MEDIA METABOLOME OF PRIMARY ACUTE LYMPHOBLASTIC LEUKEMIA**  
Rafael Canevarolo1,2  
1Boldrini’s Children Hospital, Campinas, SP, Brazil, 2Brazilian Biosciences National Laboratory, Campinas, SP, Brazil  
Twenty one patients newly-diagnosed with acute lymphoblastic leukemia had their blasts cultured in vitro for 24h, in the absence or presence of asparaginase or prednisolone. The metabolic profile of the conditioned media in which leukemia cells were cultured was determined by 1H-NMR, and associations between metabolite’s concentration, leukemia cells in vitro survival and patient’s minimal residual disease status were found.

P3-25  
**ROLE OF TGF-β INDUCED EPITHELIAL MESENCHYMAL TRANSITION (EMT) IN Pancreatic Cancer METABOLISM**  
Amrita K Cheema  
Departments of Oncology and Biochemistry, Georgetown University Medical Center, Washington, USA  
Pancreatic cancer is an aggressive disease in large part due to lack of diagnostic and prognostic biomarkers. According to American Cancer Society the five year survival rate for patients diagnosed with pancreatic cancer is 4%. The malignancy of cancer cells has been attributed to a phenomenon called EMT which is induced by TGF-β. This study aims to elucidate the metabolic changes that accompany the induction of EMT in pancreatic cancer cell lines.

P3-26  
**GLUTATHIONE SUCCINATION IN FUMARATE HYDRATASE DEFICIENT CELLS**  
Leon Zheng  
Cancer Research UK, Beatson Institute for Cancer Research, Glasgow, UK  
Fumarate Hydratase (Fh1) deficient cells accumulate high levels of fumarate, which can covalently bind to glutathione (GSH) leading to the formation of succinincGSH. The formation of this adducts deplete cells of reducing power, leading to oxidative stress in Fh1−/−cells and the activation of an antioxidant response. By using stable isotopologue analysis, we have demonstrated that...
the biosynthesis rate of glutathione and cystine uptake are increased in Fh1−/− cells, making these cells more sensitive to cystine deprivation.

P3-27
USE OF MASS SPECTROMETRY IMAGING COMBINED WITH METABOLOMICS STUDY TO EVALUATE DRUG EFFICACY AND IMPACT ONTO BIOLOGICAL ENVIRONMENT
David Bonnel
ImaBiotech, MS Imaging Department, Lille, France
Presentation of a new process which combines mass spectrometry imaging and metabolomics to follow drug distribution, quantification and “read-out” information for pharmacokinetics and pharmacodynamics.

P3-28
STANDARDIZING THE SAMPLE HANDLING PROTOCOL FOR METABOLIC PROFILING OF A HeLa CELL CULTURE
Eleni C. Kafkia1,2
1Laboratory of General Biology, Medical School, University of Patras, Patras, Greece, 2Metabolic Engineering & Systems Biology Laboratory, Institute of Chemical Engineering Sciences, Foundation for Research & Technology - Hellas, Patras, Greece
Effective metabolic profiling of immortalized mammalian cell cultures requires the standardization of the sample handling protocol to minimize its effect on cell physiology. We evaluated three handling protocols performed with combinations of PBS and saline washing solutions at different durations by interpreting the metabolomic measurements in the context of cancer metabolism. The analysis indicated as mildest the protocol in which cell detachment before quenching is avoided and the fastest effective washing procedure is pursued.

P3-29
SECRETOMIC ANALYSIS OF POTENTIAL RESISTANT MARKERS IN HUMAN UTERINE CANCER CELLS
Szu-Ting Lin
National Tsing-hua university, Hsinchu, Taiwan
Drug resistance has been the obstacle in chemotherapy. In this study, we used doxorubicin-sensitive uterine sarcoma cell and self-developed two different levels of doxorubicin-resistant cells for secretomic analysis. These secreted proteins mainly involve in cell proliferation, metabolism and redox homeostasis. RNA interference and overexpression strategies will be applied to verify the roles of the identified proteins in drug resistance. The current work will be extended into a metabolomics analysis for further drug resistant research.

P3-30
DISCOVERY OF NEW METABOLIC BIOMARKERS FOR THE DIAGNOSIS OF Pancreatic Ductal Adenocarcinoma (PDAC)
Regina C. Reszka
Metanomics Health GmbH, Berlin, Germany
A retrospective study was conducted and plasma as well as serum samples from pancreatic cancer, chronic pancreatitis and liver cirrhosis patients and matched healthy blood donors were collected. Metabolomic profiles of plasma and serum samples were generated applying high quality polar and lipid GC-MS and LC-MS/MS technology. The multimarker panel identified by Random Forest consisted of 10 metabolites and provided an AUC=0.85 when discriminating between pancreatic cancer and pancreatitis (including CA19-9 an AUC= 0.94 was reached).

**THEME: PLANT PHYSIOLOGY AND CROP IMPROVEMENT**

P4-1
IMPACT OF DROUGHT STRESS ON THE METABOLITE PROFILES OF BARLEY KERNELS
Alexandra Wenzel
Technische Universität München, Chair of General Food Technology, Freising-Weihenstephan, Germany
A gas chromatography-mass spectrometry (GC-MS)-based metabolite profiling method was applied to investigate changes in the metabolite profiles of barley kernels in response to drought stress. Multivariate and univariate statistical analyses revealed a differently pronounced impact of drought stress on the barley metabolites depending on the genotype. The profiles of the polar constituents were strongly influenced by drought conditions. The metabolic responses to drought stress were strongly dependent on the growing year.

P4-2
METABOLITE PROFILING OF CROPS: ASSESSMENT OF FOOD QUALITY AND SAFETY
Thomas Frank
Technische Universität München, Freising, Germany
Different crops including cereals (maize, rice, barley) and legumes (soybeans, mung beans) were subjected to a metabolite profiling approach based on GC/MS. The employed extraction and fractionation methodology allowed a comprehensive coverage of a broad spectrum of low molecular weight metabolites ranging from lipophilic to hydrophilic compounds. The objective was to investigate the impact of genetic background, breeding strategy, environmental conditions, farming practice, stress, and food processing on the respective crop metabolic phenotype.
P4-3 MULTI-RESPONSE OPTIMIZATION OF METABOLOMICS PROTOCOL BASED ON RESPONSE SURFACE METHODOLOGY
E.A. Bekele
KU Leuven, Leuven, Belgium
We applied a multi-response optimization approach based on Derringer’s desirability function to optimize the derivatization step of the GC-MS protocol. This method allows searching for optimal parameters while simultaneously considering gross detection enhancement of various metabolic classes. Linear and interactions of factors revealed the effect of the derivatization parameters on its performance. Based on global desirability values, the best optimal set of derivatization parameters were selected and validated on apple tissue.

P4-4 METABOLOMIC DIVERSITY IN THE LEAVES OF DIFFERENT VARIETIES OF PIPER BETLE
Swagata Karak
University of Calcutta, Kolkata, West Bengal, India
A total ninety nine metabolites could be identified from eight varieties of *Piper betle* L. leaf which is used as a masticatory in South East Asian countries. Principal component Analysis revealed that some varieties differ from the others based on their metabolite content. A few metabolites responsible for the variation could be identified. Hierarchical cluster analysis also illustrated heterogeneity between the varieties. Varieties could also be differentiated on the basis of their essential oil constituents.

P4-5 COMPARATIVE METABOLIC PROFILING OF RICE GRAINS REVEALS PRIMARY METABOLITES ARE CORRELATED WITH SECONDARY METABOLITES
Jae Kwang Kim
National Academy of Agricultural Science, Rural Development Administration, Suwon, Republic of Korea
Gas-chromatography coupled with time-of-flight mass spectrometry (GC-TOFMS) was used to analyze the relationships between primary metabolites and phenolic acids in rice, including six black cultivars and one white cultivar. PCA could fully distinguish between the cultivars. HCA of these metabolites resulted in clusters derived from common or closely related biochemical pathways. PLS was applied to predict the total phenolic content based on primary metabolite profiles from rice grain. The predictive model showed good predictability.

P4-6 METABOLIC PROFILING OF Lycium chinense FRUITS USING GAS CHROMATOGRAPHY-TIME-OF-FLIGHT MASS SPECTROMETRY FOR QUALITY ASSESSMENT BASED ON VARIETY
Joon-Soo Sim
1National Academy of Agricultural Science, Rural Development Administration, Suwon, Republic of Korea
Lycium species have become increasingly popular in Europe and North America because of their health-enhancing effects. However, its functional components have not been elucidated. In this study, the levels of health-promoting lipophilic compounds and 42 hydrophilic metabolites were determined in *L. chinense* fruit from 11 cultivars. PCA showed that the Cheongdang (LM-3) cultivar was distinct from the others. The correlation results of metabolites revealed strong correlations between metabolites that participate in closely related pathways.

P4-7 THE DETERMINATION OF SUBSTANTIAL EQUIVALENCE FOR CAROTENOID BIOFORTIFIED RICE USING COMPARATIVE ANALYSIS OF METABOLIC PROFILING
Chang-Muk Lee
National Academy of Agricultural Science, Rural Development Administration, Suwon, Republic of Korea
Safety assessment of genetically modified (GM) food is based on the concept of substantial equivalence (SE). To investigate substantial equivalence among carotenoid-biofortified GM rice and conventional rice cultivars, profiles of polar metabolites were analyzed using GC-TOFMS. The GM rice is more comparable to its non-transgenic counterpart rice variety according to the closer co-separation than for other cultivars tested. Profiling of polar metabolites could be a useful tool to reveal SE of GM rice.

P4-8 A NEW METHOD FOR PLANT METABOLOMICS STUDY BASED ON CAPILLARY ELECTROPHORESIS-TIME-OF FLIGHT MASS SPECTROMETRY
Jieyu Zhao
Dalian Institute of Chemical Physics, Dalian, China
A new method based on CE-TOF-MS was developed and validated to investigate polar metabolic profiling in plant. The optimal extraction solvent system was achieved by design of experiments. The reliability of the method was guaranteed by high reproducibility and well linearity. The current CE-TOF-MS metabolic profiling can significantly discriminate tobacco leaves of different flavors and geographical origins. It holds promising for studying complex polar compositions in plant.

P4-9 METABOLOMICS OF DEFENSIVE CHEMISTRY: MS-BASED CHARACTERIZATION OF SESQUITERPENE LACTONE- AND HYDROXYBENZENEA C IDERIVED DEFENSIVE METABOLITES OF TARAXACUM OFFICINAL E ROOT LATEX
Gabriela Zurek
Bruker Daltonik, Bremen, Germany
We studied the chemical composition of the root latex of *Taraxacum officinale* as a first step to identify metabolites important for plant resistance against herbivores and pathogens. We found two major classes of secondary metabolites: Sesquiterpene lactone
glycosides and inositol-4-hydroxybenzeneacetic acid derivatives. The established workflow, solely based on mass spectrometry, speeds up metabolite re-identification in new biological matrices and is readily extendable, after preliminary fragmentation studies, to many more compound classes.

P4-10
ANALYSIS OF BARLEY (HORDEUM VULGARE L.) PROTEOME AND METABOLOME SUBJECT TO DROUGHT STRESS WITH MASS SPECTROMETRIC METHODS.
Maciej Stobiecki
Institute of Bioorganic Chemistry PAS, 61-704 Poznan, Poland
The aim of the conducted research was to compare changes in proteome and metabolome of four barley varieties (Maresi CamB1, Sebastian and Stratus) subjected to water deficit. These changes were monitored using 2D gel electrophoresis and Maldi ToF and GC/MS mass spectrometry. This approach enabled us to identify proteins and metabolites, belonging to different classes of natural products involved in the stress response. An attempt of linking metabolites synthesis with corresponding enzymes expression was undertaken.

P4-11
TOWARD BETTER ANNOTATION OF PLANT METABOLOME: ISOLATION AND STRUCTURE ELUCIDATION OF SECONDARY METABOLITES FROM ORYZA SATIVA (RICE)
Zhigang Yang
RIKEN Center for Sustainable Resource Science, Yokohama, Japan
For the better annotation of plant metabolome in general, we aim to elucidate structures of isolated compounds from the model plants using MS/MS and NMR methods. In the present study, we have investigated the isolation and identification of secondary metabolites from Oryza sativa (rice), which is the best world-important crop. Thirty six compounds including three novel flavonoids were isolated from the leaf of O. sativa.

P4-12
METABOLOMICS AND CHEMOMETRICS STUDY TO MONITOR THE BIOCHEMICAL CHANGES AND α – AMYLASE INHIBITORY ACTIVITY DURING POST-HARVEST RIPENING IN ACHRAS SAPOTA L. FRUITS
Susmita Das
University of Calcutta, Kolkata, West Bengal, India
Biochemical changes during post-harvest ripening in Achras sapota fruit were monitored by GC-MS based metabolomics approach. A variety of chemometric analyses were done to identify the metabolic differences between ripening stages and the metabolites influencing α- amylase activity. Based on the VIP Citric acid, malic acid, raffinose and sucrose influenced most in modulating α – Amylase inhibitory activity in the fruits and the least contribution of proline, glycine, 4-guanidinobutyric acid and valine were exerted.

P4-13
METABOLIC EXPLORATION OF ANOXIA-INDUCED WAX-ESTER SYNTHESIS IN EUGLENA GRACILIS
Daisaku Ohta
Osaka Prefecture University, Sakai, Japan
Euglena strains produce a battery of saturated wax esters under limited oxygen supply. We report a metabolic profiling study exploring key events underlying the metabolic shift toward the lipid biosynthesis. Profiling of 56 different wax esters demonstrated the clear initiation of wax ester fermentation within four hours of anoxia, implicating a quick metabolic response leading to the wax ester fermentation independent of altered gene expression levels.

P4-14
THE EFFECT OF GENETICS AND ENVIRONMENT ON THE METABOLOME OF COMMERCIAL MAIZE HYBRIDS USING LC/MS: A MULTISITE STUDY
Jan Hazebroek
DuPont Pioneer, Johnston, IA, USA
We report on supplementing earlier GC/TOF-MS metabolomics data with LC/FT-ICR MS metabolomics data to elucidate biological variation due to environment and genotype in maize forage and grain samples collected from non-GMO DuPont Pioneer commercial maize hybrids grown at six North America locations. The results will further our understanding of the biological context that must be placed on metabolomics data if used to supplement compositional analysis for substantial equivalence assessments.

P4-15
THE GC-MS METABOLOMICS APPROACH TO FIND BIOACTIVE COMPONENTS OF BLUEBERRY, RASPBERRY AND BLACKBERRY
Jeongae Lee
Korea Institute of Science and Technology, Seoul, Republic of Korea
This study was applied metabolomics approaches to develop metabolic profiling in blueberry, raspberry and blackberry with gas chromatography-mass spectrometry and mass profiler professional. PCA score plot was obtained from hexane and ethyl ether extracts with good discrimination between berries. Loading plot analysis performed to increase accuracy of data processing was collected 139 peaks. A hierarchical cluster analysis using ANOVA test (p<0.001) was categorized 28 peaks. Fatty alcohols and fatty acids were found in berries.
P4-16
METABOLOMIC FINGERPRINTING EMPLOYING UPLC-TOFMS FOR THE IDENTIFICATION OF THE ORIGIN OF AGRICULTURAL PRODUCTION SYSTEMS
Elena Cubero-Leon
Standards for Food Bioscience Unit, European Commission Joint Research Centre - Institute for Reference Materials & Measurements (IRMM), Geel, Belgium
In this study, the metabolite fingerprint of organic and conventional carrots (Daucus carota L.) was analysed using ultraperformance liquid chromatography-time-of-flight-mass spectrometry. Using this method, the metabolome of organically and conventionally grown carrots revealed significant differences. Our study shows that a UPLC-TOFMS fingerprinting methodology is a valuable approach to investigate and understand specific metabolic alterations as a result of changes in environmental conditions such as the influence of different agricultural production systems in the plant physiology.

P4-17
DISCRIMINATIVE ANALYSIS OF OIL PALM SPEAR LEAF METABOLOME OBTAINED FROM OIL PALM GROWN UNDER DIFFERENT PLANTING CONDITIONS
Noor Idayu Tahir
1Malaysian Palm Oil Board (MPOB), Kajang, Selangor, Malaysia, 2Universiti Putra Malaysia, Serdang, Selangor, Malaysia
The presence and level of an organism's metabolome reflects the phenotypic response to environmental condition and changes while describing its genotype. A sound and systemic corroboration is required to discriminate environmental effects on oil palm planted on different settings. LC-MS-based metabolomics and multivariate statistical analysis were carried out on oil palm clones to allow the discovery of patterns discriminating the specimens under study.

P4-18
METABOLIC FINGERPRINTING FOR OIL PALM BASAL STEM ROT DISEASE DIAGNOSTICS
Nurazah Zain
Malaysian Palm Oil Board, Kajang, Selangor, Malaysia
To gain a better understanding on oil palm defense mechanism to basal stem rot (BSR) caused by the wood-rotting fungal pathogen Ganoderma boninense, metabolite profiles of oil palm root tissues from partially tolerant and susceptible parental palms were compared using LC-MS and analysed using multivariate analysis. These findings generated a substantial amount of metabolites data and contributed to the identification of compounds related to oil palm tolerance, thus improving the current understanding of BSR.

P4-19
METABOLITE PROFILE IN SUGARCANE VARIETIES, HYBRIDS AND SPECIES WITH HPLC-DAD COMBINED WITH MULTIVARIATE ANALYSIS
Isabel Coutinho
Instituto de Química - UNESP, Araraquara, São Paulo, Brazil
We described the application of a method developed by our group for the metabolomics analysis of sugarcane, where sixteen genotypes of sugarcane were analyzed by HPLD-DAD and the metabolite fingerprint obtained was subjected to multivariate analysis. With respect to that, we identified that main discrimination between genotypes was due more abundance of chlorogenic acids in sugarcane wild species than noble species and modern varieties.

P4-20
IMPROVED LEGUME CROPS FOR A SUSTAINABLE FUTURE
Adrian Charlton
1Food and Environment Research Agency, York, North Yorkshire, UK
The integration of metabolomics and a robust genetic approach has been used to prioritise genetic resources for breeding of more competitive European legume crops with better quality and performance traits. European legumes will be of critical importance to a sustainable food supply chain due to their high protein content and low nitrogen requirements.

P4-21
METABOLOMICAL ANNOTATION IN BIOMASS CROPS: uHPLC-MS, AND NMR STUDIES OF SECONDARY METABOLITES IN WILLOW
John Baker
Rothamsted Research, Harpenden, Herts, UK
The poster will present the metabolic complexity of secondary metabolism in high biomass genotypes of Salix viminalis as revealed by uHPLC-FT-MS (Orbitrap Elite). 25% of the top 500 retention-time/empirical formula features in willow uHPLC-MS can be identified by MS-MS and correlation of the MS data with that from 1H NMR. This platform now forms an integral part of a metabolomics operation that is focussed on gene and biomass/bioenergy trait discovery in Willow.

P4-22
CROPPING CARBON - A STRATEGIC RESEARCH PROGRAMME, USING METABOLOMICS, TO OPTIMISE WOODY BIOMASS CROPS FOR BIOENERGY AND INDUSTRIAL APPLICATIONS
Claudia Harflett
Rothamsted Research, Harpenden, Hertfordshire, UK
Increasing global energy consumption has led to concerns over energy security and environmental impacts such as rising greenhouse gas emissions. The UK aims to obtain 15% of its energy needs from renewable resources by 2020. We describe the Cropping Carbon strategic programme at Rothamsted Research, detailing metabolomic approaches to optimise and understand biochemical pathways and C-flow in woody biomass crops. The project will model both above- and below-ground carbon status using a systems approach.
P4-23
METABOLITE PROFILING STUDY OF BURDOCK ROOTS IN RESPONSE TO COPPER STRESS
Youngae Jung
Korea Basic Science Institute, Seoul, Republic of Korea
Arctium lappa L. (Asteraceae), known as burdock, has long been cultivated as a popular vegetable for dietary use and folk medicine worldwide. In this study, metabolite profiling coupled with multivariate analysis was applied to achieve a holistic view of the copper stress response in burdock roots using 1H NMR and GC-MS analysis. These results showed not only the increased phenols and unsaturated fatty acids but also decreased primary metabolites and sterols.

P4-24
DE NOVO RNA SEQUENCING AND METABOLITE PROFILING TO IDENTIFY GENES INVOLVED IN ANTHOCYANIN BIOSYNTHESIS IN KOREAN BLACK RASPBERRY (RUBUS COREANUS MIQUEL)
Sarah Lee
Division of Bioscience and Biotechnology, Konkuk University, Seoul, Republic of Korea
De novo RNA sequencing and metabolite profiling of Korean black raspberry (Rubus coreanus Miquel) were performed to identify genes involved in anthocyanin biosynthesis and to analyze biochemical changes during ripening process. We have annotated the transcriptomes and identified primary and secondary metabolites such as sugars, organic acids, amino acids, anthocyanins, and proanthocyanidins of fruits. The positive correlation between the expression of anthocyanin biosynthetic genes and the anthocyanin accumulation during ripening of fruit was also demonstrated.

P4-25
TOBACCO SEEDS EXPRESSING A MUTATED FORM OF ARABIDOPSIS CYSTATHIONINE γ-SYNTHASE EXHIBIT HIGHER LEVEL OF METHIONINE AND ALTERED LEVELS OF SEVERAL METABOLITES
Yael Hacham
Migal Galilee Technology Center, Kiryat-Shmona, Israel
We have expressed an unregulated form of Arabidopsis Cystathionine g-synthase (AtCGS) under the control of a seed-specific promoter in tobacco. Although the level of soluble methionine did not change significantly in these seeds, total methionine content was significantly elevated, as well as the levels of other amino acids incorporated to seeds storage proteins.

P4-26
CHANGES IN METABOLITE PROFILE IN FODDER GRASSES IN PLANT ADAPTATION TO COLD
Mariusz Czyżnielewski
Institute of Plant Genetics Polish Academy of Science, Poznań, Poland
Quality and quantity of metabolites are changing in fodder grasses in plant adaptation to cold stress conditions. Plant samples were collected on the third, fifth and twelfth day of the adaptation to cold. Monosaccharides were observed in higher amounts than oligosaccharides at the first two time-points with no significant changes of GC-MS studied metabolite profiles. A dramatic increase of sucrose level and amounts of phenylalanine, tyrosine and lysine were observed at the last time point.

P4-27
IDENTIFICATION OF 6-C-(6"-O-glycosyl)-GLYCOSIDE OF FLAVONES AND TRIACYLATED POLIAMINES PRESENT IN TRACE AMOUNTS IN BARLEY (HORDEUM VULGARE)
Anna Piasecka
Institute of Plant Genetics Polish Academy of Science, Poznań, Poland
In order to establish the detailed chemical profile of barley leaves, extract from a large amount of material from variety Maresi was submitted to preparative polyamide column chromatography and reversed phase C18 HPLC. Collected eluent containing trace compounds was analyzed by HPLC-MS. Such analytical approaches enable to identify 109 metabolites including phenylpropenoic derivatives of flavone apigenin, luteolin and chrysoeriol glycosides and polyamines putrescin, hydroxyputrescin, describe for the first time in barley.

P4-28
THE EFFECT OF GENOTYPE AND ENVIRONMENT ON STEROL CONCENTRATION IN TOBACCO
Qiansi Chen
Zhengzhou Tobacco Research Institute, Zhengzhou, Henan, China
The sterols in tobacco leaves of three cultivars which were planted in three different regions were determined by GC-MS. The results showed that the sterols concentration in tobacco of three regions were obviously different, while sterols concentration in three cultivar from same region was roughly the same. The results suggested that the effect of environment play a more important role on sterol concentration in tobacco than genotype factor.

P4-29
METABOLITE PROFILING AND HYPERSPECTRAL IMAGING FOR SCREENING OF PATHOGEN RESISTANT SUGAR BEET GENOTYPES
Nadja Arens
1Leibniz Institute of Plant Genetics and Crop Plant Research IPK, Gatersleben, Germany
Phenotyping of three sugar beet pathosystems with the help of a hyperspectral imaging system measuring signals in Short Wave Infrared Range (SWIR) and metabolite profiling by LC-PDA-Q-TOF-MS to identify molecular markers for disease resistance in various genotypes. There will be a focus on the characterization of metabolites of the phenylpropanoid pathway.
P4-30
EFFECT OF HEREDITY, ENVIRONMENTS AND DEVELOPMENTAL STAGE ON ALKALOIDS CONCENTRATION IN TOBACCO
Pingping Liu
Zhengzhou Tobacco Research Institute, Zhengzhou, Henan, China
The alkaloids concentration in tobacco leaves from five developmental stages of three cultivars which were planted in three different regions were analyzed by GC-MS. As a result, the tobacco alkaloids concentration went down at first and then went up from vigorous growth period to mature period with the minimum point appearing at squaring stage, and risen sharply after topping, and the environmental deviation performed a greater impact on alkaloids concentration than genotype differences.

P4-31
METABOLITE AND GENE EXPRESSION PROFILES OF RICINUS COMMUNIS SEEDLINGS REVEAL A COORDINATED SHIFT IN CARBON-NITROGEN METABOLISM IN RESPONSE TO AN INCREASE IN TEMPERATURE
Paulo Roberto Ribeiro
1Wageningen Seed Lab, Laboratory of Plant Physiology, Wageningen University, Wageningen, The Netherlands, 2Laboratory of Biochemistry, Biotechnology and Bioproducts, Department of Biofunction, Federal University of Bahia, Salvador, Bahia, Brazil
Metabolite and gene expression profiles were performed to determine metabolic changes during seedling establishment in R. communis in response to an increase in temperature. The variation in carbohydrate and amino acid content suggest that a shift in carbon-nitrogen metabolism happens in R. communis seedlings in response to an increase in temperature. Relative gene expression of the elongation factor 1-beta (EF1B), which plays a central role during protein biosynthesis, suggests that protein biosynthesis is indeed up-regulated.

P4-32
GENOTYPE AND OZONE TREATMENT GENERATED DIFFERENCES IN PHENOLIC PROFILES OF EURAMERICAN POPLAR
Sarita Keski-Saari
University of Eastern Finland, Department of Biology, Joensuu, Finland
Tropospheric ozone is a phytotoxin that causes oxidative stress in plants. We studied mechanisms of ozone tolerance in three Euramerican poplar (Populus deltoides x nigra) genotypes (Cima, Robusta and Carpaccio) that were exposed to filtered air or 120 ppb ozone. Ozone reduced the growth of Cima the most, while Robusta showed most intensive visible injuries. The genotypes clearly differed from each other in their leaf phenolic profiles. Ozone induced increases in concentrations of some phenolics.

P4-33
UNTARGETED STABLE ISOTOPE-ASSISTED METABOLIC PROFILING BY LC-HRMS REVEALS NOVEL CONJUGATES OF THE MYCOTOXIN DEOXYNIVALENOL IN WHEAT
Bernhard Kluger
University of Natural Resources and Life Sciences, Vienna (BOKU), Tulln, Austria
A novel approach for untargeted profiling of metabolisation products of xenobiotics in plants using liquid chromatography - high resolution mass spectrometry (LC-HRMS) is presented. By the use of non-labelled and 13C15 fully-labelled mycotoxin deoxynivalenol (DON) as precursor, the efficient distinction between xenobiotic derived MS signals and signals resulting from wheat matrix background is feasible. The software algorithm MetExtract was used to automatically detect DON derived LC-HRMS signals, resulting in the assignment of novel DON conjugates.

P4-34
GC-MS BASED TARGETED PROFILING OF FUSARIUM - WHEAT INTERACTIONS
Alexandra Parich
University of Natural Resources and Life Sciences, Vienna (BOKU), Tulln, Austria
Fungal virulence and plant resistance mechanisms in the Fusarium head blight (FHB) disease were investigated using a targeted GC-MS based metabolomics approach. Two parent and four FHB resistance-related near isogenic wheat lines were treated with (i) F. graminearum, (ii) deoxynivalenol or (iii) water. The differentially expressed metabolites after 0, 12, 24, 48 and 96h were identified and linked to the different treatments as well as to the wheat genotypes.

P4-35
TARGETED METABOLIC ANALYSIS OF DIURNAL CHANGES IN CENTRAL CARBON METABOLISM TO IMPROVE BIODEGRADABLE PLASTIC PRODUCTION IN TRANSGENIC SUGARCANE
Mark Hodson
Metabolomics Australia, Australian Institute for Bioengineering and Nanotechnology, University of Queensland, St Lucia, Queensland, Australia
Polyhydroxyalkanoate production in plants would decrease petroleum dependency by producing a renewable supply of biodegradable plastics. Previously we have shown that carbon storage compounds such as starch and sucrose are decreased in transgenic sugarcane lines producing high levels of polyhydroxybutyrate (PHB). Here we have used targeted quantitative analysis of central carbon and amino acid metabolism to identify differences in primary metabolism between a wild-type and transgenic PHB-producing lines of sugarcane across a diurnal time course.
P4-36
SEED-SPECIFIC EXPRESSION OF A FEEDBACK-INHIBITION INSENSITIVE FORM OF CYSTATHIONINE-γ-SYNTHASE (CGS) INCREASES THE PRODUCTION OF MET AND OTHER AMINO ACIDS IN TRANSGENIC ARABIDOPSIS THALIANA SEEDS
Hagai Cohen1,2
1MIGAL - Galilee Research Institute, Kiryat Shmona, Israel, 2Technion - Israel Institute of Technology, Faculty of Biology, Haifa, Israel
In order to study the regulation and importance of methionine (Met) in plant seeds, Arabidopsis plants were transformed with the Met/SAM feedback insensitive Arabidopsis thaliana cystathionine-γ-synthase (AtCGS) gene fused to a seed-specific promoter. AtCGS is the main regulatory enzyme in Met synthesis through the Asp-family pathway. GC-MS-metabolite profiling and microarray analysis were performed to identify novel metabolic networks and gene expression programs influenced by altered Met metabolism.

P4-37
ON-GOING METHOD DEVELOPMENTS IN BORDEAUX METABOLOME FACILITY
Stéphane Bernillon1,2
1INRA Bordeaux, UMR1332, F-33140 Villenave d'Ornon, France, 2Metabolome Facility of Bordeaux Functional Genomics Center, F-33140 Villenave d'Ornon, France
Bordeaux Metabolome Facility (BMF) is dedicated to plant metabolomics analysis and data analysis. Besides routine analyses, this facility has developed three methods to improve lipidome coverage, identify secondary metabolites by LC-MS and LC-NMR, and increase 1H-NMR analysis throughput by robotized extraction and titration followed by automated data processing by binning automation of NMR spectra and suggestion of candidate compounds for annotation.

P4-38
METABOLOMICS APPLICATIONS TO ELUCIDATE THE ROLE OF METABOLITES IN BI-/MULTITROPHIC PLANT INTERACTIONS
Roland Mumm1,2
1Plant Research International, Business Unit Bioscience, Wageningen UR, Wageningen, The Netherlands, 2Centre for BioSystems Genomics, Wageningen, The Netherlands
Plants are continually challenged by pests and pathogens and, being sessile, must be able to respond and fight their ground. Many plants have developed a very sophisticated 'chemical arsenal' against these threats. We are using metabolomics to define this chemical arsenal. We will give an overview on where metabolomics can help to detect key metabolites involved in defence mechanisms of crops and how this knowledge is used to better understand the molecular basis of resistance.

P4-39
EFFECTS OF INFLUENTIAL FACTORS (GERMPLASM, ENVIRONMENT, TRANSGENES) ON METABOLITE VARIABILITY IN COMMERCIAL CROPS
Steven Halls
Monsanto, St Louis, USA
Influential experimental factors such as environment stress, growing location, germplasm, tissue type, development stage, and specific transgenes all affect crop metabolism. There is a need in commercial crop development to quantify the relative contributions to metabolite variability of these different factors and potential interactions. We have employed newer statistical tools to rank and make key conclusions about the effect size and impact of environmental, genetic, and transgenic effects on metabolite variability.

P4-40
MOLECULAR AND MORPHOLOGICAL INSIGHTS INTO POLYPLOIDY OF POPLAR TREES
Lena Fragner
Dep. of Molecular Systemsbiology, University of Vienna, 1090 Vienna, Austria
Poplar is a highly adaptive, robust and fast growing tree widely cultivated in short rotation plantations as non-food crop for the production of biofuels. Leaf extracts of diploid, tetraploid and mixoploid trees were subjected to metabolite profiling using a combined GC-MS and LC-MS platform covering primary as well as secondary metabolites. Metabolomics, proteomics and morphological data were integrated to obtain insights into mechanisms of polyploidy.

P4-41
PROFILING FREE AND WALL BOUND METABOLITES OF PHOENIX SYLVESTRIS FRUIT
Bratati De
University of Calcutta, Kolkata, West Bengal, India
Phoenix sylvestris (L.) Roxb. fruit is an underutilized fruit of West Bengal, India. The metabolite profiles of the free and wall bound constituents from the mesocarp tissue were analyzed by GC-MS. 23 Metabolites could be identified from the 50% methanolic extract. The cell wall bound metabolites included 22 ester linked metabolites and 17 ether linked metabolites. All the fractions were tested for α-glucosidase and α-amylase inhibitory activities. Ether linked fraction showed highest activity.
APPLICATION OF METABOLOMICS TOOLS IN DIFFERENTIATION OF FRUITING BODIES OF AMANITA MUSCARIA AND THE CORRELATION WITH TYPE OF TOP-SOIL.

Piotr Mlynarz

1Department of Chemistry, Wroclaw University of Technology, Wroclaw, Poland

The objective of these metabolomics studies were Amanita Muscaria mushrooms in relation to their ecosystem (soil). The 1H NMR studies of A.M. homogenate, soil characterization together with chemometric tools were applied. The differentiation between cap and stem were performed based on the metabolite quantitative and qualitative content in both morphological part of A.M. and combined with soil description parameters.

NMR BASED TAXONOMICAL IDENTIFICATION OF HALLUCINOGENIC AND POTENTIALLY HALLUCINOGENIC MUSHROOMS.

Stanislaw Deja

1Faculty of Chemistry, Opole University, Oleska 48, 45-051 Opole, Poland, Opole, Poland

Eight hallucinogenic fungi species belonging to the four most popular hallucinogenic and potentially hallucinogenic genera (Coprinus, Gymnopilus, Amanita and Stropharia) were analyzed by means of 1H NMR spectroscopy. Mushroom metabolic fingerprints were found to be characteristic not only for genera but also for particular species. This results show metabolomics as a competitive approach to the currently practiced morphological studies and should be considered as useful technique in forensics mycology related sciences.

ANALYSIS OF ISOPRENOID PATHWAY METABOLITES BY LC-MS

Bernhard Schönenberger

Sigma-Aldrich, Buchs, Switzerland

The quantitative analysis of a whole range of synthetic metabolites of isoprenoid pathways by newly developed LC-MS methods has been performed. Isoprenoidphosphates and isoprenoidpyrophosphates with one isoprene unit have been well separated by a cycloextrine-based stationary phase and a buffer/acetonitrile eluent in HILIC mode, whereas the corresponding isoprenoidphosphates and isoprenoidpyrophosphates up to 3 isoprene units have all been analysed on a C8 column by ICP-LC-MS using dihexylamine acetate.

THE METABOLOMICS STUDY OF DIFFERENT NICOTINE CONVERSION TOBACCO LEAF AND FLOWERS

Lifeng Jin

Zhengzhou Tobacco Research Institute of CNTC, Zhengzhou, China

Nicotine conversion is undesirable process because it will produce nornicotine, which is the precursor of a well characterized carcinogen N’-nitrosonornicotine. At the same time, nicotine conversion will cause tobacco leaf quality to reduce. So the nicotine conversion is a concerned point. Based on UPLC-Q-TOF/MS, a high nicotine conversion mutant and the wide type was analysis and a series of quality related compounds were detected, which may be the key metabolites of the tobacco leaf.

TARGETED METABOLOMICS EMPLOYED FOR THE STUDYING OF ‘PINOT NOIR’ GRAPE SKIN PHENOLICS AS INDUCED BY CANOPY MICROCLIMATE MANIPULATION

Urska Vrhovsek

IASMA Research and Innovation Centre, Edmund Mach Foundation, Food Quality and Nutrition Department, San Micehele all Adige, Italy

Earlier research efforts to reveal the effect of canopy microclimate manipulation on grape quality parameters were mainly focused only to few targeted compounds. Metabolomics is offering much wider possibilities to study plant secondary metabolism within purposely-induced microclimate shifts. A field trial was thus designed in ‘Pinot Noir’ vineyard in order to reveal related alternations of multiple classes of skin phenolics, including some very rarely studied ones to date.

CHEMOTYPING UNDER FIELD CONDITIONS: ANALYSIS OF METABOLOME DIVERSITY IN THE BIOENERGY CROP Miscanthus

Thomas Wilson

IBERS, Aberystwyth University, Aberystwyth, UK

Mass spectrometry (MS) metabolite fingerprinting methods, in conjunction with supervised data mining, were used to validate leaf sampling methods before exploring the metabolome differences associated with genotype in a novel population of wild Miscanthus. Major inter-specific differences (M. sinensis versus M. sacchariflorus) were evident in flow infusion-MS fingerprints, with geographic origin identified as a major source of variation within the M. sinensis group.
**Theme: New Developments in Instrumentation and New Techniques**

**P5-1**
WHERE CAN YOU BENEFIT FROM EXTREMELY HIGH RESOLUTION MASS SPECTROMETRY IN METABOLOMICS RESEARCH - ONLY A NUMBER’S GAME?
Timm Wiebke
Bruker Daltonik GmbH, Bremen, Germany
Recent developments in FT-ICR-MS instrumentation demonstrated mass spectral resolution of > 20 Million. This presentation highlights the impact offered by the capability to resolve isotopic fine structures for several metabolomics related applications. Aim is to trigger a discussion about possible other metabolomics related questions that might be answered by ultra-high resolution MS and which software tools will be required to quickly access the isotopic fine structure and link it into different workflows.

**P5-2**
UNDERSTANDING HUMAN METABOLISM AND HEALTH BY NMR-BASED METABOLOMICS
Sofia Moco
Nestle Institute of Health Sciences, Lausanne, Switzerland
The emergence of large cohorts in clinical studies rises the demand of technologies able to generate a large number of measurements. We will describe in detail the establishment of a flow injection system coupled to a NMR in the analysis of thousands of urine samples by metabolomics. From the obtained profiles, metabolite quantification, from central carbon metabolism and gut microbial host co-metabolism, is feasible.

**P5-3**
ETHNIC DIFFERENCE IN CERAMIDE PROFILES OF SKIN STRATUM CORNEUM
Kwang-Hyeon Liu
Kyungpook National University, Daegu, Republic of Korea
Ceramides are sphingolipids consisting of sphingolipid bases, which are amide-linked to fatty acids. Up to now, 16 ceramide subclasses have been identified in human stratum corneum. In this study, we developed the lipidomic platform for the skin lipid profiling and identification using chip-based direct infusion nanoelectrospray tandem mass spectrometry. Using this platform, we identified 21 skin ceramides in human skin stratum corneum, and compared ceramide composition among three ethnic groups.

**P5-4**
EXHALED BREATH METABOLOMICS: ADDING TO DISEASE DIAGNOSIS, CHRONOBIOLOGY AND INDIVIDUALIZED HEALTHCARE
Pablo M-L Sinues
ETH, Zurich, Switzerland, 2University Hospital, Zurich, Switzerland
Although the analysis of exhaled metabolites is appealing for metabolomics studies, this approach remains in its infancy in comparison with the analysis of other biofluids and tissue specimens. We present some examples of how the in vivo, real-time mass spectrometric analysis of human breath may contribute to address open issues in lung disease diagnosis, chronobiology and individualized healthcare.

**P5-5**
CRYSTALLOGRAPHIC SCREENING OF METABOLITE BINDING AS A TOOL FOR DETERMINATION OF UNKNOWN PROTEIN FUNCTIONS (AND, POSSIBLY, NOVEL METABOLITES).
Igor A. Shumilin1, 2
1University of Virginia, Charlottesville, VA, USA 2Midwest Center for Structural Genomics, Argonne, IL, USA
A method for determination of unknown protein functions based on crystallographic screening of metabolite library binding to target proteins was developed. This method was successfully applied to proteins from three different families. Metabolic substrates and biochemical function were established for one protein family and metabolic substrate analogs were identified for the members of two other families, leading to experimentally testable hypotheses about their functions. The suggested approach has potential applications in both proteomics and metabolomics.

**P5-6**
METHOD DEVELOPMENT AND VALIDATION FOR RAT SERUM FINGERPRINTING WITH CE-MS: APPLICATION TO VENTILATOR-INDUCED-LUNG-INJURY STUDY
Magdalena Rusak1, 2
1Medical University of Bialystok, Bialystok, Poland, 2CEMIO, Madrid, Spain
High ventilation in critical care units may induce lung injury. The effect of this has been studied through the development and validation of a method for serum fingerprinting with CE-TOF-MS. The method was validated using eight different compounds across the electropherogram and was applied to serum samples to study the effect of high ventilation in a rat model of ventilator induced lung injury (VILI). Five statistically significant compounds were identified classifying VILI and control group.

**P5-7**
A STUDY OF THE PROPERTIES OF SILICON HYDRIDE BASED COLUMNS IN RELATION TO METABOLITE PROFILING.
Sami Bawazeer
Strathclyde university, Glasgow, UK
In comparison with silica gel the properties of silicon hydride are very different. Three silicon hydride columns, Silica C, Phenyl Hydride and UDC Cholesterol, were studied for their ability to retain standard mixtures and for profiling the urinary metabolome. The Silica C column provided best performance in HILIC mode whereas as the Phenyl Hydride column offered good selectivity in reversed phase mode for steroid glucuronide conjugates and the glucuronides and sulphates of phenolic acids.
P5-8
NON-TARGETED METABOLIC PROFILING OF HUMAN URINE SAMPLES
Baljit Ubhi
AB SCIEX, Warrington, UK, AB SCIEX, Foster City, USA
Metabolite profiling LC/MS data was acquired from urine samples using the TripleTOF (R) 5600+ mass spectrometer. Data were opened into MarkerView™ Software for statistical analysis. The MS and MS/MS data were evaluated using Formula Finder and the Structural Elucidation tool within PeakView™ Software. Metabolite changes amongst a healthy group of individuals are presented and demonstrate the power of a high resolving MS/MS system.

P5-9
THE METABOLITES ANALYSIS OF SERUM USING FAST-GC-MS/MS WITH TANDEM COLUMN
Shuichi Kawana
SHIMADZU CORPORATION, Kyoto, Japan
To increase the sample throughput, we have tried to shorten the analysis time of serum by fast GC-MS/MS using a short medium-bore capillary column with a thicker stationary phase in place of the inactive retention gap and a short narrow-bore capillary column. The fast GC-MS/MS system can shorten the analysis time of serum from 30-60 minutes (Conventional GC-MS) to 5.5 minutes and quantifies the 20 targeted metabolites accurately.

P5-10
UNTARGETED METABOLOMICS WORKFLOW USING UHPLC/Q EXACTIVE ORBITRAP MASS SPECTROMETER AND SIEVE 2.1
Junhua Wang
ThermoFisher Scientific, San Jose, CA, USA
Metabolomics is a rapidly growing field of post-genomic biology, aiming to comprehensively characterize the small molecules in biological systems. Here we present a workflow using a UHPLC/benchtop quadrupole Orbitrap platform and automated data analysis software for untargeted metabolomic profiling of plasma samples for biomarker discovery from the Zucker diabetes fatty (ZDF) rat model. The optimal conditions for sample preparation, LC, column, MS and data processing parameters in SIEVE are explored.

P5-11
A PLATFORM TO IDENTIFY ENDOGENOUS METABOLITES USING A NOVEL HIGH PERFORMANCE ORBITRAP AND THE mzCloud LIBRARY
Yingying Huang
Thermo Fisher Scientific, San Jose, California, USA
Metabolite identification is a bottleneck in metabolomics study. Presented here is a new platform to identify endogenous metabolites using a novel high performance Orbitrap hybrid instrument in conjunction with UHPLC and an MS
library. This platform allows compound identification that goes beyond identifying the exact same metabolites in the library, to discovering additional unknown but biologically relevant compounds in metabolomics studies.

P5-12
ANALYTICAL PLATFORM FOR METABOLOME/LIPIDOME ANALYSIS OF MICROBIAL CELLS
Sakda Khoomrung
Systems and Synthetic Biology, Chalmers University of Technology, Kemivägen 10, 41296, Gothenburg, Sweden
We present here several analytical methods that we have developed/set up in-house and apply routinely for yeast metabolomics research.

P5-13
DEVELOPMENT OF A HYDROPHILIC INTERACTION CHROMATOGRAPHY - MASS SPECTROMETRY (HILIC-MS)
METHOD FOR IMPLEMENTATION AND EXPANSION OF A NON-TARGETED METABOLICOMICS PLATFORM SCREENING HUMAN URINE AND PLASMA.
Wendelin Koch
Research Unit Analytical BioGeoChemistry, Helmholtz Zentrum München, German Research Center for Environmental Health (GmbH), 85764 Neuherberg, Germany, Chair of Analytical Food Chemistry, Technische Universität, 85354 Freising-Weihenstephan, Germany
In this work the development of a HILIC-MS method is presented. The method is finally integrated to a non-targeted metabolomics RP-LC-MS platform. The platform will be applied to screen for biomarkers in human urine and plasma samples.

P5-14
A STANDARDIZED METHOD FOR BREATH MOLECULAR PROFILING TO DISCOVER DISEASE SPECIFIC BIOMARKER
Mrinal Kumar Das
Biomarker Team, Immunology Group, International Centre for Genetic Engineering and Biotechnology (ICGEB), New Delhi, India
Exhaled breath is a rich source of various metabolites, which represents health status of a subject, getting attention as a matrix for disease diagnosis. This has been accelerated due to the tremendous developments in matrix for capturing molecules and gas chromatography mass spectrometry (GC-MS) techniques. In this report we are discussing a method standardized by our team for exhaled breath sample collection and separation using multidimensional GC-MS to identify breath based biomarkers for different diseases.
P5-15
A COMPREHENSIVE EVALUATION OF VARIOUS PRECIPITATION AND EXTRACTION PROCEDURES FOR UNTARGETED BLOOD PLASMA PROFILING BY UPLC-MS
Magali Sarafian
Imperial College London, London, UK
Prior to untargeted UPLC-MS profiling of blood, sample preparation is critical for successful analysis of high and low-molecular weight species. The present study aims to compare eight methods of sample preparation for lipid profiling by UPLC-MS. These procedures were appraised by characterization of a set of qualitative and quantitative criteria. Based on our results isopropanol is the optimal method of sample preparation for lipid profiling by UPLC-MS.

P5-16
COMPARING DIFFERENT ANTICOAGULANTS FOR SAMPLING BLOOD PLASMA USING GC-TOF-MS AND LC-QTOF-MS/MS METABOLOMICS
Joyce Wong
University of California, Davis, Davis, CA, USA
We examined the different anticoagulants and their effects in metabolomics profiles for blood plasma. Blood were taken from a single model animal Sus domesticus using four different blood withdrawal methods: citrate, EDTA, heparin anticoagulations and serum clotting as positive control. GC-TOF-MS was used for primary metabolism while LC-QTOF-MS/MS was used for complex lipids profiling. Statistical assessments, biochemical pathway annotation and metabolome coverages will then used for data analysis for each anticoagulants.

P5-17
USING CAPILLARY ION CHROMATOGRAPHY MASS SPECTROMETRY FOR METABOLIC APPLICATIONS
Linda Lopez
Thermo Fisher Scientific, Sunnyvale, CA, USA
Capillary ion chromatography (IC) coupled with MS provides complementary analysis of ionic and charged small molecules important to metabolomic research. Capillary IC has lower system noise, higher stability and requires smaller sample injection, whereas MS provides confirmatory structural information, and higher sensitivity. The analytes were separated by capillary IC using electrolytically generated gradient and detected in selected reaction monitoring mode. Here we demonstrate the targeted analysis of metabolites and isobaric sugar phosphates.

P5-18
MUSCLE: A NOVEL MULTI-PLATFORM, USER-FRIENDLY SOFTWARE TOOL FOR THE ROBUST, OBJECTIVE AND AUTOMATED OPTIMISATION OF TARGETED LC-MS ANALYSES
James Bradbury
University of Birmingham, Birmingham, UK
This paper presents the development of a software tool called MUSCLE which provides robust evolutionary closed loop optimisation of targeted LC-MS/MS metabolite analyses autonomously. We demonstrate the key features of the software, specifically the ability to optimise analyses across different instrument manufacturers, as well as results which show that MUSCLE was able to find an optimal set of LC and MS parameters that offered a faster analysis of a multi-steroid sample than achieved manually.

P5-19
NON-TARGETED SCREENING IN AQUEOUS MEDIA USING GC×GC-TOFMS
Martin Almstetter
Philip Morris International R&D, Neuchatel, Switzerland
A novel non-targeted GC×GC-TOFMS screening approach was developed to tackle compound profiling in aqueous samples. Aqueous trapping solutions (e.g. cigarette aerosol trapped in phosphate buffered saline) are directly injected on-column and analyzed by GC×GC-TOFMS using a combination of water resistant ionic-liquid based analytical columns. Avoiding the use of organic solvent facilitates the detection of constituents that would be otherwise masked and therefore expands the coverage of the compound profile without the need for supplementary analysis.

P5-20
LIPIDOMIC ANALYSIS USING HIGH RESOLUTION TIME OF FLIGHT MASS SPECTROMETRY - LOOK NO COLUMN NEEDED
Juergen Wendt
LECO Gmbh, Monchengladbach, Germany
Plasma samples are investigated using direct infusion with ultra-high resolution (R > 100,000) ESI-TOFMS analysis to differentially profile lipids from diseased and control rats in the Zucker model. Specifically the ability to investigate the “unsaturome” (unsaturated forms of the same lipid classes) is demonstrated. The power and simplicity of direct analysis as a screening tool for metabolic analysis is demonstrated and its strengths, values and limitations discussed.

P5-21
QUANTITATIVE METABOLITE PROFILING IN PICHIA PASTORIS-METHOD DEVELOPMENT AND VALIDATION
Gunda Koellensperger
University of Natural Resources and Life Sciences-BOKU, Vienna, Austria
We present LC-MS based analytical workflows for comprehensive metabolite profiling of Pichia pastoris. The potential of on-line two-dimensional chromatography in combination with MS/MS detection will be discussed. Validation is an integral part of any analytical method development; however in this specific application, it is highly challenging to follow principles of metrology. We will show a critical validation, including the assignment of measurement uncertainty and accuracy of quantification. Accuracy was addressed by an interlaboratory comparison study.

87
P5-22
METHOD DEVELOPMENT FOR PEPTIDOME CHARACTERIZATION
Estelle Pujos-Guillot
INRA, Plateforme d’Exploration du Métabolisme, F-63000 Clermont-Ferrand
The purpose of this study was to develop the analytical tools required for peptide isolation, characterization and identification by mass spectrometry, in plasma and serum samples. After protein precipitation, peptide profiles were determined using UPLC/LTQ-Orbitrap. Two approaches depending on masses were developed to perform the data processing and the identification: peptides of masses between 400-800 m/z were identified with proteomic tools, whereas a metabolomic approach was used for bioactive peptides of lower masses (100-500 m/z).

P5-23
TOF-SIMS LIPID PROFILING OF ACUTE MYELOID LEUKAEMIA CELLS TREATED WITH A NOVEL COMBINATION THERAPY
Joanna Denbigh
1University of Manchester, Manchester, UK
Time of flight secondary mass spectrometry (ToF-SIMS) is a powerful surface analysis technique which has seen much development in biological applications in recent years due to significant advances in instrumention; in particular with cluster/polyatomic primary ion beams. This poster presents the lipid profiles obtained by cluster ion bombardment of mammalian acute myeloid leukaemia cells treated with a combination drug therapy allowing an assessment of the application of novel technology in this important area.

P5-24
THE AUTHENTICATION AND QUALITY CONTROL OF NATURAL PRODUCTS BY USING A NON-TARGETED AND TARGETED NMR SCREENING TOOL
Jimmy Yuk
Bruker BioSpin, Billerica, MA, USA
The analysis of various natural products using a non-targeted and targeted profiling approach was achieved using an automated NMR screening tool. Results showed that it was possible to gain both qualitative and quantitative results on different natural products using this approach. The application of an automated NMR-based screening tool shows promise for a high-throughput method to measure the quality and authentication of natural products.

P5-25
STRATEGY FOR EXPANDING A METABOLOMICS SERVICE CORE USING GOOGLE DOCUMENTS
Angela Beliveau
University of California, Davis, Davis, CA, USA
The West Coast Metabolomics Center (WCMC) is testing a new strategy in using Google Documents as a Laboratory Information Management System. We will show the advantages and disadvantages in using the Google Doc system by describing its use in the laboratory work flow, customer interactions, and more. The Google Doc system has allowed the WCMC to avoid costly investments in ulterior LIMS software, while still allowing the laboratory to keep pace with rising service demand.

P5-26
IDENTIFICATION OF LIPIDS BY LC COUPLED ION MOBILITY MASS SPECTROMETRY USING IMS-QTOF
Theodore Sana
Agilent Technologies, Santa Clara, CA, USA
New analytical techniques are continuously being developed to facilitate analysis of complex classes of molecules such as lipids. A prototype IMS-QTOF system was evaluated for the separation and identification of lipid isomers from extracts of pooled rat spinal cords. Following LC and drift space separation, the peaks were fragmented. Identification of lipid isomers or unannotated lipids was accomplished using an Agilent/METLIN accurate mass lipid database, an MS/MS mass spectral library of standards and SimLipid software.

P5-27
COMPREHENSIVE METABOLOME ANALYSIS OF SMALL VOLUME SAMPLES BY TWO COMPLEMENTARY UPLC-NANOESI-MS METHODS
Endre Laczko
University of Zurich, Zurich, Zurich, Switzerland
Metabolomics, thought as a complement to proteomics and transcriptomics, is still at need for a comprehensive as well as efficient identification and quantification of the metabolites especially in small volume samples. Here we like to present a complementary set of two capillary scale UPLC-nanoESI-HRMS methods for the comprehensive analysis of metabolites, ranging from very polar (sugars) to very non-polar (lipids) biochemical classes and ranging in concentration levels over several orders of magnitude.

P5-28
NON-TARGETED METABOLOMIC ANALYSIS OF FRESH WATER AND MARINE STICKLEBACK FISH
Manhong Wu
1Department of Anesthesia, Stanford University School of Medicine, Stanford, CA, USA
Three spine stickleback fish (Gasterosteus aculeatus) are found in both freshwater and marine environments and have evolved mechanisms for osmoregulation. We have used an untargeted LC and GC/Q-TOF based metabolomics approach to identify metabolomic differences from tissues obtained from lab raised freshwater and marine fish. The focus is on the GC/QTOF workflow since there is significant overlap between the GC and LC/MS results.
P5-29
LIPIDOMIC PROFILING USING Sub-2µm PARTICLE CO\textsubscript{2} BASED SUPERCritical CHROMATOGRAPHY MASS SPECTROMETRY
Robert Tonge
Waters Corporations, Milford, MA, USA
We have developed rapid, high throughput and efficient method for the separation and analysis of free fatty acids and neutral lipids using sub-2µm particle CO\textsubscript{2} based supercritical chromatography. The organic extract from the matrix containing lipids is directly injected onto the system showing a significant saving in solvent, cost and sample preparation time. The separation mechanism is mainly based on the number of carbon chains and the number of double bonds on the acyl chain.

P5-30
ELECTRON IMPACT AND CHEMICAL IONIZATION HIGH RESOLUTION TIME-OF-FLIGHT MASS SPECTROMETRY ANALYSES OF BLOOD PLASMA SAMPLES
David Alonso
LECO Corporation, Saint Joseph, Michigan, USA
The unique capabilities of GC with high resolution time-of-flight mass spectrometry (HRT) make it an essential tool for metabolomics. The workflow in this study includes EI and CI analyses of derivatized blood plasma samples from lean, fatty and obese Zucker rats. Mass spectral data was collected in high resolution mode and chromatography was adjusted to maximize the number of metabolites identified. Pseudomolecular ions and mass accuracy < 1.0 ppm facilitated unknown metabolite identification from formula determination.

P5-31
A GCXGC/TOFMS METABONOMICS STUDY FOR LIVER TISSUES IN D-GALACTOSAMINE/LIPOPOLYSACCHARIDE INDUCED ACUTE HEPATIC FAILURE MICE
Fangting Dong
National Center of Biomedical Analysis, bei jing, China
A new comprehensive method of two-dimensional gas chromatography coupled to time-of-flight mass spectrometry (GCxGC/TOFMS) was established for the study of metabolomics in acute hepatic failure. 982 peaks were obtained from the approach of GCxGC/TOFMS, 89 metabolites were identified, among them 47 metabolites were differentially determined, while 43 peaks from GC/TOF-MS, 51 metabolites were identified. For complex metabolite profiles compared with the traditional GC/TOFMS, GCxGC/TOFMS would be a better way for the characterization of metabonomic profiles.

P5-32
AUTOMATED JUST IN TIME ONLINE DERIVATIZATION FOR GC-MS AND GC MS/MS ANALYSIS OF PHOSPHORYLATED METABOLITES
Christina Haberhauer-Troyer\textsuperscript{1,2}
\textsuperscript{1}Austrian Center of Industrial Biotechnology (ACIB), Vienna, Austria, \textsuperscript{2}University of Natural Resources and Life Sciences, Department of Chemistry, Division of Analytical Chemistry, Vienna, Austria
The capabilities of two step just-in-time online derivatization prior to GC-MS and GC-MS/MS analysis were exploited for the analysis of 14 phosphorylated metabolites of the central carbon metabolism. This automated derivatization strategy was used along with uniformly \textsuperscript{13}C labeled cell extract as internal standard in order to compensate errors from sample preparation. Excellent selectivity of the GC-MS/MS method was achieved by improving gas chromatographic separation as well as by making use of selective MS/MS transitions.

**Theme: Metabolomic Profiling in Neuroscience**

P6-1
PROFILING NEUROPROTECTION MECHANISMS IN NEURONAL CELLS FOLLOWING ACUTE ADMINISTRATION OF METHAMPETAMINE
Garth Maker
Murdoch University, Perth, Western Australia, Australia
To study the biochemical effects of a high dose of the illicit psychostimulant drug methamphetamine, rat cortical neurons were cultured and exposed to 1 mM for 48 hours. Metabolites were profiled using GC-MS. Key changes included perturbation of amino acid homeostasis, excitotoxicity and oxidative stress. Multiple amino acid neuroprotective mechanisms were observed, several of which have not been previously associated with methamphetamine exposure. Comparison was also made with caffeine exposure, which caused some similar effects.

P6-2
ALTERATIONS IN METABOLIC PATHWAYS AND NETWORKS IN ALZHEIMER’S DISEASE: METABOLOMICS INFORMS GENOMICS
Rima Kaddurah-Daouk
Duke University, Durham, NC, USA
A targeted electrochemistry based metabolomics platform revealed major perturbations within tryptophan, tyrosine, pruine and one carbon metabolism pathways in patients with Alzheimer’s disease (AD). A partial correlation network linked some of the metabolic changes to amyloid-beta (Ab42) a protein marker for AD. Metabolomics data was used to inform GWAS data and both metabolic and genetic findings highlighted enzymes implicated in AD pathogenesis.
P6-3
DEVELOPMENT OF AN IN VITRO METABOLOMIC APPROACH FOR ENHANCED NEUROTOXIC EFFECTS BY ENVIRONMENTAL CONTAMINANTS, WITH EMPHASIS ON NEUROTRANSMITTER PATHWAYS
Pim Leonards
VU University, Amsterdam, The Netherlands
This paper presents the development of a metabolomic and neurotoxicity approach for the SH-SY5Y cell line. The focus is on four neurotransmitter pathways: Dopamine, Serotonin, Gaba, and Acetylcholine. Analytical methods were developed to detect and quantify the precursors, neurotransmitters and metabolites in the SH-SY5Y cells using a 12 well based system and LC-MS/MS. An LC-HRTOF system was used for untargeted analysis. SH-SY5Y cells were exposed to pesticides to investigate the effects on the neurotransmitter pathways.

P6-4
LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY BASED ANALYSIS OF THE CEREBROSPINAL FLUID METABOLOMOME FOR THE STRATIFICATION OF PATIENTS WITH UNEXPLAINED ENCEPHALOPATHIES.
Christophe Junot
CEA/DSV/iBiTec-S/SPi/LEMM, Gif-sur-Yvette, France
This work deals with the development of a liquid chromatography coupled to high resolution mass spectrometry based method for the analysis of the cerebrospinal fluid (CSF) metabolome. It emphasizes the relevance of CSF metabolomics for the study and characterization of inborn errors of metabolism involving the nervous system. At last, it shows that CSF metabolomics enables the stratification of patients having unknown encephalopathies.

P6-5
2,4 DIHYDROXYBUTANOIC ACID AS A POTENTIAL MARKER OF ALZHEIMER’S DISEASE
Marko Sysi-Aho
VTT Technical research centre of Finland, Espoo, Finland
Our findings show that 2,4-DHBA is a potential marker for AD which compares favorably against the tau protein and β-amyloid risk markers. Further studies are needed to understand biochemistry of 2,4-DHBA and to elucidate the potential link between hypoxia and AD progression.

P6-6
UNTARGETED METABOLOMICS METHODS FOR THE EARLY DETECTION OF ALZHEIMER’S DISEASE (AD): POTENTIAL FOR DEVELOPING NEW DIAGNOSTICS?
Stewart Graham
Queen’s University Belfast, Belfast, UK
High resolution mass-spectrometry (UPLC-QTof-MS) was combined with chemometrics to analyse human plasma from patients with mild cognitive impairment (MCI), patients with MCI who later developed Alzheimer’s disease, and healthy age-matched controls. Using this profiling method 2443 ions were used to build the multivariate model (R2=0.95 Q2=0.75) and from the S-plots we were able to identify a small subset of ions which produce a model capable of predicting the disease with a high-degree of accuracy.

P6-7
METABOLIC SIGNATURES OF HUMAN ALZHEIMER’S DISEASE (AD): 1H NMR ANALYSIS OF THE POLAR METABOLOME IN POST-MORTEM BRAIN TISSUE
Brian Green
Queen’s University Belfast, Belfast, UK
1H NMR metabolomics studies were conducted on polar extracts of human post-mortem brain tissue (n=15; age-matched controls; n=15 AD) using a Bruker 400 MHz NMR spectrometer. Principal component analysis (PCA) and orthogonal partial least squares discriminant (OPLS-DA) plots correlated closely with disease status and the statistical model distinguished (R2=0.75; Q2=0.40) tissue of AD patients from age-matched controls and predictions were further enhanced by using NMR data to train an artificial neural network (ROC=0.99).

P6-8
METABOLIC PROFILING OF BRAIN REGIONAL VARIATION UNDER ADULT-ONSET HYPOTHYROIDISM USING A MOUSE MODEL
Caterina Vasilopoulou
1,2
1Metabolic Engineering and Systems Biology Laboratory, Institute of Chemical Engineering Sciences (ICE-HT), Foundation for Research & Technology - Hellas (FORTH), RIO-PATRAS, ACHAIA, Greece, 2Laboratory of Animal and Human Physiology, Department of Biology, University of Patras, RIO-PATRAS, ACHAIA, Greece
Although mammalian brain has been considered the main target tissue of thyroid hormones, the current knowledge about the effect of adult onset hypothyroidism (AOH) on brain physiology remains fragmented. We present a systematic metabolomic study of the cortex, cerebellum and midbrain physiology under AOH in a mouse model. The observed differences in response to AOH among brain regions provide clues connecting the metabolic physiology to the role of each region in brain function.
P6-9
FROM EPIGENETICS TO METABOLOMICS: TARGETED AND UNTARGETED MASS SPECTROMETRY-BASED METHODS FOR EXAMINING METAOMETRIC DIFFERENCES ASSOCIATED WITH ALTERED STRESS RESPONSE DUE TO EARLY LIFE STRESSORS
Constance A. Sobsey
1University of Victoria, Victoria, BC, Canada
Early life stressors have been associated with altered methylation patterns and differences in hypothalamic-pituitary adrenal axis function. To examine what other systemic changes may be associated with this model, we applied high-sensitivity target and untargeted mass spectrometry techniques to perform comprehensive metabolomics analysis on serum from human participants in an early life stress-exposure cohort. The metabolomics data is examined in the context of methylation status, trends in HPA activity, and extensive clinical data.

THEME: ENVIRONMENTAL

P7-1
A METABOLIC APPROACH TO INVESTIGATE ALLELOPATHIC INTERACTIONS OF UNICELLULAR ALGAE
Katharina Eick
Friedrich-Schiller-Universität, Institute of Inorganic and Analytical Chemistry, 07743 Jena, Germany
Using the stimulatory allelopathic effect of Sceletonema costatum on Thalassiosira weissflogii, GC/Tof-MS based metabolic profiling of the two interacting diatoms was conducted. In this poster we introduce release and uptake dynamics of chemical compounds between unicellular algae. We substantiate named changes in both the endo- and exometabolome, present first propositions of involved chemical substances and by using \(^{13}\)C labelled algae, will introduce hypothesis of chemical flux between the communicating diatoms S. costatum and T. weissflogii.

P7-2
PATTERNS OF CHEMICAL DIVERSITY IN SPONGE ASSOCIATED MARINE BACTERIA
Utpal Bose
School of Pharmacy, The University of Queensland, Brisbane, Australia
We investigate the chemical diversity of two sponge associated Salinispora species distributed over 3500 km of north east coast of Australia. We test whether host specificity influences secondary metabolites production – using three sponge species as a classifier – through chemometrics approaches. To measure the lower level diversities which depend on multiple factors, we have broken down the total population into rational subsets and used chemometrics to explore the patterns of metabolites production.

P7-3
HIGH-THROUGHPUT NMR-AND LC-MS/MS-BASED METABOLOMICS: INSIGHT OF THE RESPONSES OF VARIOUS ORGANS AFTER NAPHTHALENE INTERVENTION
Hao-Jan Liang
1Institute of Toxicology, College of Medicine, National Taiwan University, Taipei, Taiwan,
Naphthalene induced injuries onto Clara cell in lungs was perviously studied via intraperitoneal injections. However, the overview of the injuries mechanisms onto lung, liver and kidney were limited. This study, NMR- and LC-MS/MS-based metabolomics was applied to elucidate the injuries mechanisms after naphthalene exposure. Results demonstrating energy and antioxidative stress related metabolites as well as polar lipids (phosphatidylcholine and ceramides) were perturbed. High-throughput metabolomics enabled the visualization of the responses in organs after toxicant intervention.

P7-4
METABOLOMICS STUDY OF CAENORHABDITIS ELEGANS FOR THE TOXICITY EVALUATION OF SUB-LETHAL RESPONSES TO TITANIUM DIOXIDE NANOPARTICLES USING GAS CHROMATOGRAPHY - MASS SPECTROMETRY COMBINED WITH PATTERN RECOGNITION APPROACH AND INGENUITY PATHWAY ANALYSIS
Ratnasekhar Ch
Analytical Chemistry section, CSIR- Indian Institute of Toxicology Research, Lucknow, India,
In the present study, we employed a GC-MS based metabolomic approach to identify the metabolome responses to TiO\(_2\) nanoparticles exposure. Pattern recognition analysis and ingenuity pathway analysis were used to determine the global alterations in metabolite profiles of C. elegans after their responses to TiO\(_2\) nanoparticles. Both bulk and nano sized TiO\(_2\) particles with two different concentrations (1/10\(^{th}\) and 1/2 of LC\(_{50}\)) were taken in to consideration for the present study.

P7-5
NMR-BASED METABOLOMICS TO STUDY NAPHTHALENE TOXICITY IN A TOLERANT MOUSE MODEL
Feng-Peng Huang
Institute Of Environmental Health College of Public Health National Taiwan University, Taipei, Taiwan,
Naphthalene is a common PAH in environment. Studies indicated naphthalene caused Clara cell damage. However, mice are repeat exposed to naphthalene for seven days, the Clara cell become refractory to injury. Naphthalene tolerant animal provides a good model to investigate the mechanisms of naphthalene toxicity. NMR-based metabolomics was applied to exam metabolome of the BALF and tissues in mice. Results showed that numerous amino acid and energy-related metabolites are important in response to naphthalene toxicities.
Poster Abstracts

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P7-6
GLYCEROPHOSPHOCHOLINE PROFILING OF THE CORAL SERIATOPORA CALIENDRUM IN RESPONSE TO COPPER-INDUCED OXIDATIVE STRESS
Chuan-Ho Tang1,2
1Institute of Marine Biodiversity and Evolutionary Biology, National Dong Hwa University, Pingtung, Taiwan; 2National Museum of Marine Biology and Aquarium, Pingtung, Taiwan
In loss process of coral symbionts, the cells experience a variety of membrane deformation according to the mechanisms involved. For diagnosing coral bleaching, it is useful to characterize the membrane lipids modulation. Glycerophosphocholine profiling in the coral of exposure to copper was examined in this study. The results were correlated with cellular accommodation in necrotic process, and suggested that dose-dependent exocytosis of symbionts share with cell necrosis in the lipids metabolism in copper-induced coral bleaching.

P7-7
DISCRIMINATING THE ACUTE TOXICITIES OF ETHION AND BIFENOX IN RAT LIVER BY NMR-BASED METABOLOMICS
Sheng-hun Lee
Institute of Environmental Health, National Taiwan University, Taipei, Taiwan
We intend to classify different classes of pesticides by NMR-based metabolomics approach. Dose-response experiments were conducted in rats treated with two pesticides (ethion: organophosphate insecticide, and bifenox: diphenyl-ether herbicide) via ip. Hydrophilic metabolome from the liver were analysed by 1H and J-resolved NMR followed by multivariate analysis. The results demonstrated a unique classification pattern between two pesticides. This is a proof-of-concept study to show that metabolomic effects reflect mode of toxic action.

P7-8
THE ROLE OF MASS SPECTROMETRY IN THE METABOLOMICS STUDY OF TOXICOLOGICAL EFFECTS OF METAL TOXICITY IN LABORATORY MICE. EXPERIMENTS EXPOSURE TO As, Cd AND Hg UNDER CONTROLLED CONDITIONS
Tamara Garcia-Barrera1,2
1Department of Chemistry; University of Huelva, Huelva, Spain; 2Research Center of Health and Environment (CYSMA). University of Huelva, Huelva, Spain
Metals have a central role in biological systems, regulating and participating in numerous cellular processes, as well as presenting toxic or deleterious effects on the metabolism. In this work we use a combination of metallomic (SEC-ICP-MS) with metabolomics (DI-ESI-QqQ-TOF-MS) approaches to study exposure experiments to metal of model mice Mus musculus evaluating metabolite profiles changes caused by toxic metals in different mice organs and fluids. Altered metabolites were quantified by gas chromatography-mass spectrometry (GC-MS).

P7-9
CROSS-PLATFORM METABOLIC PROFILING OF THE AQUATIC MODEL ORGANISM LYMNAEA STAGNALIS FOR NEUROTOXICITY ASSESSMENT
Sara Tufi
Vrije Universiteit, Amsterdam, The Netherlands
The pond snail Lymnaea Stagnalis is a model organism in neurobiology that can be employed to assess environmental neurotoxicity. A comprehensive cross-platform metabolic profiling based on complementary analytical techniques has been carried out for characterizing the central nervous system, albumen gland, and digestive gland of L. Stagnalis and, in order to investigate the neuronal metabolism, a targeted approach focusing on the main neurotransmitters, their metabolites and precursors has been developed.

P7-10
UNDER THE SEA --- METABOLOMIC RESPONSE OF THE SEAGRASS HALOPHILA OVALIS TO NICKEL INDUCED ABIOTIC STRESS
Gregory King
The University of Tokyo, Tokyo, Chiba prefecture, Kashiwa City, Japan
Seagrasses are the only known ecological group of fully submerged marine angiosperms. In terms of biodiversity they are similar in magnitude to mangroves and coral reefs, which make them an essential source of livelihood and food for many. In recent years, seagrass populations worldwide have been decreasing. In this study, we utilize GC-MS based metabolomics to gain insight regarding the response of the seagrass, Halophila ovalis, to nickel induced stress.

P7-11
STUDY ON HEAT TOLERANCE IN STONEFLY NYMPHS AT DIFFERENT OXYGEN LEVELS BY FT-ICR MS AND NMR BASED METABOLOMICS
Ulf Sommer
NERC Biomolecular Analysis Facility - Metabolomics Node (NBAF-B), School of Biosciences, University of Birmingham, Birmingham, UK
We tested if oxygen limitation occurred at thermal extremes on stonefly nymphs treated with varying temperature and oxygen pressures, using direct infusion FT-ICR mass spectrometry and 1-D and 2-D J-resolved NMR. The concept of oxygen limitation applies to stoneflies; under normoxia and especially hypoxia, oxygen limitation was indicated by increases in anaerobic metabolites, perturbations of the TCA cycle, and a lower energy status. Hyperoxia alleviated anaerobic metabolism and improved heat tolerance.
P7-12
SURVIVING STARVATION: LIPIDOMIC ANALYSIS OF ALGAE UNDER NUTRIENT DEPRIVATION
Phillip Whitfield
University of the Highlands and Islands, Inverness, UK
The unicellular green picoalgae Ostreococcus tauri is the most primitive known free-living eukaryote. In this study the effect of low nitrogen and low phosphorous environments on the lipid metabolism of O. tauri was investigated. Algal lipids were solvent extracted and analysed by liquid chromatography-mass spectrometry (LC-MS). Multivariate data analysis identified an elevation of triglycerides in algae cultured in nitrogen-limiting conditions, whilst betaine lipids were increased when the algae were depleted of phosphorous.

P7-13
IDENTIFICATION OF METABOLOMIC BIOMARKERS INDICATIVE FOR CO-EXPOSURE OF HUMAN CELLS TO PAHs AND HEAVY METALS
S. Potratz
German Federal Institute for Risk Assessment (BfR), Department of Product Safety, Max-Dohrn Strasse 8-10, 10589 Berlin, Germany
Risk assessment is predominantly based on single compound exposure scenarios which do not account for synergistic or antagonistic mechanisms within compound mixtures. Therefore, we looked into the co-exposure of MCF-7 cells to the heavy metal cadmium in combination with the genotoxic PAH benzo[a]pyrene. Cells were treated with these toxicants and analyzed by a combination of a targeted and untargeted metabolomics approach. Our results indicate a synergistic effect of BP and Cd in cells upon co-exposure.

P7-14
CLOUD METABOLOMICS - RESPONSE TO COLD SHOCK IN BACTERIA ORIGINATING FROM CLOUDS
Cyril Jousse1,2
1Clermont Université, Université Blaise Pascal, Institut de Chimie de Clermont-Ferrand, Clermont-Ferrand, France, 2Plateforme d’Exploration du Métabolisme, Université Blaise Pascal & I.N.R.A. site de Theix, Clermont-Ferrand, France
The presence of metabolically active microorganisms in clouds raise questions about their implication in physico-chemical processes. In such harsh conditions, they could contribute to transform organic compounds and to precipitation. In this highly dynamic context, we are focusing on -omics approaches to lift the veil on physiological peculiarities.
In this study, Pseudomonas syringae was challenged with temperature downshifts. Using Metabolic Profiler facility and multivariate analyses, we highlighted numerous significant biomarkers involved in cold stress metabolism.

P7-15
SCREENING OF ENVIRONMENTAL POLLUTANTS IN WATER BY GCxGC-TOFMS
Bob Green
1ALMSCO International, Llantrisant, South Wales, UK
Two-dimensional gas chromatography with time-of-flight mass spectrometry (GCxGC-TOFMS) is an enhanced separation technique which provides highly sensitive detection and accurate mass spectral identification of trace analytes; making it an ideal choice for the analysis of complex environmental samples. This work demonstrates the use of passive sampling of watercourses in conjunction with GCxGC-TOFMS to provide a method suitable for investigative work, such as screening for emerging contaminants, in addition to target-focused studies.

P7-16
1H-NMR BASED PROFILING OF ORGANIC COMPONENTS IN LEACHATE FROM ANIMAL CARCASS DISPOSAL SITE OVER TIME.
Hyun-Whee Bae1,2
1Graduate School of Analytical Science and Technology, Chungnam National University, Daejeon, Republic of Korea, 2Seoul center, Korea Basic Science Institute, Seoul, Republic of Korea
Leachate, is generated by decomposition of animal carcass, has many environmental, sanitary and food safety hazards. However, there is a lack of research on characteristic of leachate. In this study, we performed 1H-NMR based profiling of leachate from different animal species and two types of soil over time. PCA from NMR data is showed similar pattern between species and soil types, and major components including organic acids, amino acids and phenols, were identified and quantified.

P7-17
HUMAN RELEVANT DOSE OF ENDOCRINE DISRUPTING CHEMICALS EFFECT ON THE RAT PLASMA METABOLOME
Kasper Skov
DTU FOOD, Markhøj, Denmark
Endocrine disrupting chemicals (EDCs) are compounds which interfere with normal hormone homeostasis. So far the main concern has been on their effect on reproduction and development. The present study has been conducted to evaluate the effect of EDCs on the rat plasma metabolome.
The study evaluated the difference between four groups of rat exposed to EDCs. It was shown that metabolites in the lipid synthesis were changed when exposing the rats to an EDC.
P7-18
“BOTTOM'S UP!” - UNDERSTANDING GLOBAL METABOLIC REGULATION THROUGH METABOLOMIC CHARACTERISATION OF ANIMAL SYSTEMS
Horst Joachim Schirra
The University of Queensland, Centre for Advanced Imaging, Brisbane, Queensland, Australia
We aim to understand global metabolic regulation. Here we present results from several projects that highlight different aspects of this puzzle: Characterisation of phosphine toxicity and resistance allowed us to identify the core metabolic enzyme dihydrolipoamide dehydrogenase as resistance factor. This study is exceptional in that systems biology identified a single cause of phenotype change which can subsequently be studied with classical methods. Further systems discussed are the callipyge mutation in sheep and periconception overnutrition.

P7-19
FROM AIRBORNE EXPOSURE TO BIOLOGICAL EFFECTS: MONITORING METABOLIC RESPONSES TO CERIUM OXIDE NANOPARTICLES IN LUNG EPITHELIAL CELLS USING UNTARGETED MASS SPECTROMETRY-BASED METABOLOMICS
Ralf J. M. Weber
University of Birmingham, Birmingham, UK
Cerium oxide nanoparticles (CeO₂ NPs) are increasingly being used to increase fuel efficiency in internal combustion engines. The resulting environmental exposure has raised concerns about the impact of CeO₂ NPs on human health, in particular via inhalation. Here we report a mechanistic investigation into the uptake and mode of action of CeO₂ NPs in lung cells (A549 and BEAS-2B) using a variety of microscopy imaging techniques and untargeted mass spectrometry-based metabolomics.

P7-20
ADAPTATION OF THE PHOTOHETEROTROPHIC MARINE BACTERIUM DINOROSEOBACTER SHIBAE DFL12 T TO CHANGING LIGHT REGIMES: A SYSTEMS BIOLOGY APPROACH
Nelli Bill
Technische Universität Braunschweig, Braunschweig, Germany
Marine microorganisms have to cope with a poor nutrient availability. The ability of microorganisms to perform aerobic anoxygenic photosynthesis for additional energy formation in marine environments is a benefit. We investigated the metabolic adaptation of the photoheterotrophic bacterium Dinoroseobacter shibae DFL12T, a member of the globally abundant marine Roseobacter clade, to changing light regimes in a systems biology approach. Metabolome and transcriptome results showed a distinct metabolic response of D. shibae to light.

P7-21
METABOLIC AND PROTEOMIC ADAPTATIONS OF PHAEOBACTER INHIBENS DSM 17395 TO VARIOUS NUTRIENT CONDITIONS IN MARINE ENVIRONMENTS
Michael Hensler
Technische Universität Braunschweig, Bioinformatics and Biochemistry, Braunschweig, Germany
Heterotrophic bacteria in marine environments are challenged by changing nutrient conditions (diversity and seasonal variations of dissolved organic matter). To unravel the metabolic adaptation to such conditions, we cultivated Phaeobacter inhibens DSM 17395, a model organism for the marine alphaproteobacterial Roseobacter clade, with different substrate mixtures. Applying detailed metabolome and proteome analyses the response of P. inhibens to these distinct nutrient conditions was investigated showing a specific adaptation on metabolic and proteomic level.

P7-22
EVALUATION OF PACIFIC WHITE SHRIMP (LITOPENAEUS VANNAMEI) HEALTH DURING A SUPERINTENSIVE AQUACULTURE GROWOUT USING NMR-BASED METABOLOMICS
Tracey Schock
National Institute of Standards and Technology, Charleston, USA
NMR-based metabolomic techniques can improve and expand the aquaculture industry. This technology was used to assess shrimp health during a full growout cycle from the nursery phase through harvest in a minimal-exchange, superintensive, biofloc system. The results provided physiological insight into common environmental stresses that may limit growth or better explain reduced survival and production.

P7-23
INVESTIGATING THE MOLECULAR RESPONSE OF DAPHNIA MAGNA TO SILVER NANOPARTICLES USING A MULTI-OMICS APPROACH
Alex Gavin
School of Biosciences, University of Birmingham, Birmingham, UK
The most common nanomaterials in use today are silver nanoparticles (AgNPs), which are known to be released into aquatic environments. Here, we employed a multi-omics approach to characterise the molecular mechanism of AgNPs in D. magna, and determine if they induce similar metabolic and transcriptional responses as dissolved Ag⁺ ions. Our preliminary conclusions are that at the concentrations studied, AgNP and Ag⁺ ions share similar modes of action, but AgNPs show a considerably enhanced response.
P7-24
A METABOLOMICS APPROACH FOR ANALYSING MODE-OF-ACTION OF TRICLOSAN IN MICROALGAE
Mechthild Schmitt-Jansen
Helmholtz-Centre for Environmental Research - UFZ, Department Bioanalytical Ecotoxicology, Leipzig, Germany
A metabolomics approach was used to identify potential modes-of-action of the bactericide triclosan in the microalga Scenedesmus vacuolatus. A concentration-dependent test design was chosen to be able to identify metabolites responsive at low concentrations, pointing to sensitive metabolic pathways. Lipophilic metabolites, like hexadecanoic acid, oleic acid and octadecanoic acid were affected significantly at the lowest tested concentration indicating inhibition of the fatty acid biosynthesis, a mode-of-action of the toxicant, known from bacteria.

P7-25
TRANSCRIPTOMIC AND METABOLOMIC ANALYSES OF MOLECULAR RESPONSES OF HUMAN CELL LINES TO A COMMONLY USED BROMINATED FLAME RETARDANT: HEXABROMOCYCLODODECANEA
Jinkang Zhang
School of Biosciences, University of Birmingham, Birmingham, B15 2TT, UK
As one of widely used brominated flame retardants, hexabromocyclododecane (HBCD) has been detected in various environments. In this study, A549 cells and HepG2/C3A cells were employed as in vitro models to investigate molecular responses to HBCD, using metabolomic and transcriptomic approaches. Few changes at gene expression and metabolic levels after 24 hours exposure indicated that there are limited adverse effects of HBCD exposure to these cells at concentrations as high as ca.8% of EC50 values.

P7-26
UNDERSTANDING LIPID METABOLISM IN THE MICRO-ALGA CHLAMYDOMONAS FOR BIODIESEL PRODUCTION
Matthew P. Davey
Department of Plant Sciences, Cambridge, UK
In order to improve the economic cost of microalgal biofuels we need to understand how changes in the availability of nutrients to the algae can influence the triggers that underpin triacylglyceride (TAG) metabolism and production. The rationale of this research was to study the effect of carbon supply (acetate or CO2) on TAG production and membrane autophagy in Chlamydomonas reinhardtii (wild type and the starch-less mutant strain sta6) grown under low N availability.

P7-27
EFFECTS OF IONIC SILVER ON THE GREEN ALGAE CHLAMYDOMONAS REINHARDTII
Nadia Lamari
Eawag, Swiss Federal Institute of Aquatic Science and Technology, Dübendorf, Switzerland
Silver (Ag) have long been known as antimicrobial agent moreover ionic silver is also among the most toxic metals for various aquatic organisms. Using unicellular alga Chamydomonas reinhardtii, the aim of this work is to assess stress response to metal toxicity. As the metabolome represents the ultimate response of an organism to genetic and environmental changes, effects of silver toxicity were investigated at the metabolic level of the algae using high-resolution mass spectrometry.

P7-28
METABOLOMATIC ANALYSIS OF HONEY BY MASS SPECTROMETRY: CHEMICAL CHARACTERIZATION AND DETECTION OF POLLUTANTS.
Jerome Cotton1,2
1 CEA Saclay, Gif-Sur-Yvette, France, 2 Profilomic, Boulogne, France
The aim of this study is to analyze 91 pollutantsin honey. Our approach focuses on a metabolomic analysis with acquisition of chemical fingerprint by LC/FTMS while maintaining specificity. The results for the contaminants analysis showed that 74 of 76 honeys are polluted by at least one molecule. The added value of this work lies in the acquisition of a global chemical fingerprint for the achievement of multivariate statistics on all signals generated during the analysis.

P8-1
USE OF LC-Orbitrap-FTMS AND MZmine SOFTWARE FOR IDENTIFICATION OF NEW COMPOUNDS FROM BRAZILIAN RED PROPOLIS: APPLICATION IN A FINGERPRINTING ASSAY OF PROPOLIS
Ticiano Gomes do Nascimento1,2
1 Federal University of Alagoas, Maceió, Alagoas/Brazil, Brazil, 2 University of Strathclyde, Glasgow, UK
The abstract to be presented at the conference will discuss the use of LC-Orbitrap-FTMS and MZmine software for fingerprint studies and discovery of new compounds from Brazilian red propolis. It was detected presence of new compounds (isoflavonoid, flavonoid, terpenoid and flavonosides coupled to p-coumaryl groups). Multivariate statistical analysis were useful for evaluating the similarities and differences in the chemical profile of propolis. LC-FTMS and MZMine software are useful to assess intra-specific variability of propolis.
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P8-2
MOUSE MODEL OF FETAL GROWTH RESTRICTION SHOWS AN ALTERED SERUM METABOLIC PROFILE WHICH IS REVERSIBLE FOLLOWING TREATMENT WITH SILDENAFIL CITRATE
Karolina Sulek
University of Auckland, Auckland, New Zealand
Fetal Growth Restriction (FGR) is strongly associated with longer-term health consequences. In order to further investigate Sildenafil citrate (Viagra) therapeutic potential for FGR, we looked for its mechanism(s) of action responsible for rescue of fetal growth via aberration of the global metabolic profile in COMT−/− mice. Metabolic profiling provided insights into pathogenesis of FGR as well as potential therapeutic mechanisms.

P8-3
THE USE OF LC-MS PROFILING AND BIOASSAY IN THE ISOLATION AND IDENTIFICATION OF ANTI-TRYPANOSOMAL DITERPENES FROM LIBYAN PROPOLIS
Weam Siheri
University of Strathclyde Glasgow, Glasgow, UK
Propolis is collected by bees from plants as a defensive substance in response to environmental pressures which include a range of microorganisms and parasites. The ethanolic extracts of Libyan propolis were profiled by using LC-FTMS. The samples were then fractionated by using open and flash column chromatography and the fractions were tested for activity against Trypanosoma brucei. Metabolite profiling using MZmine and data base searching assisted, along with bioassay, in the isolation of active compounds.

P8-4
DROSOPHILA, METABOLOMICS AND INSECTICIDE ACTION
Robert A. Brinzer
University of Glasgow, Glasgow, Scotland, UK
Invertebrate pests pose threats to human and animal health and property, driving a need for effective pesticides. To prevent resistance from rendering active ingredients in pesticides ineffective, synergists can be added. Pest populations are becoming insensitive to existing synergists, which can also be detrimental to human health. Metabolomics offers the potential to discover new targets by identifying metabolic bottlenecks. In Drosophila, the tryptophan catabolism pathway was found to impact survival on permethrin challenge.

P8-5
FUNDAMENTAL PROPERTIES OF HUMAN BLOOD AS SAMPLES FOR APPROPRIATE LIPID BIOMARKER EXPLORATION
Masaki Ishikawa
National Institute of Health Sciences, Setagaya-ku, Tokyo, Japan
Understanding on fundamental properties of human blood is important for ensuring proper biomarker discovery and its qualification. We performed a lipidomic analysis of fasting human blood from 60 Caucasian healthy volunteers using LC-MS/MS. Obvious gender- and age-differences in blood metabolite levels were observed in some lipid species. Furthermore, our results suggest that plasma might be suitable for the exploration because of its irrelevance to coagulation process. Repeated freeze-thaw cycles of blood samples should be avoided.

P8-6
CHEMICAL PROFILING OF AFRICAN PROPOLIS BY LC-UV-ELSD, HIGH RESOLUTION LC-MS AND GC-MS AND CORRELATION TO BIOLOGICAL ACTIVITY.
Tong Zhang
Strathclyde Institute of Pharmacy and Biomedical Sciences, Glasgow, UK
In order to investigate the chemical properties of African propolis the ethanol extracts of 46 samples collected from 10 African countries were analysed by liquid chromatography (LC) coupled with different detection techniques including evaporative light scattering detector (ELSD), ultraviolet and visible (UV) detector and a high resolution mass spectrometer (HRMS). By applying this dereplication strategy it is possible that the novel compounds can be discovered at the earliest stage before any purification work is started.

P8-7
A METABOLOMICS AND GENETIC POLYMORPHISM TO ASSESS PHARMACOKINETIC VARIABILITY IN HEALTHY VOLUNTEERS
Dongseong Shin
Seoul National University College of Medicine and Hospital, SEOUL, Republic of Korea
In a clinical pharmacokinetic study for an investigational drug, variability of some pharmacokinetic parameters was found. A metabolomics approach using QTOF MS was used to investigate the metabolic pathway which effect on the pharmacokinetics. Cystein glycine conjugation and cystein conjugation were detected in slowly eliminated and high plasma concentration group. Slowly eliminated group had zero copy of GSTM1. Metabolomics approach may be successfully applied to find a candidate metabolizing enzyme which have clinical significance.
P8-8
THE UTILIZATION OF A METABOLOMICS APPROACH TO INVESTIGATE TROGLITAZONE TOXICITY IN A CELL CULTURE SYSTEM.
Alfred Thumser
University of Surrey, Guildford, Surrey, UK
We have shown that (1) a metabolomics approach is more sensitive than standard cell viability assays for the determination of cellular toxicity, while also being more informative, and (2) troglitazone hepatotoxicity can be studied in the HuH-7 cell-line at concentrations equivalent to levels found in human liver samples, apparently without further metabolism. It is proposed that troglitazone toxicity is due to inhibition of energy-generating processes and increased oxidative stress.

P8-9
METABOLOMICS STUDIES OF ENDOPHYTIC METABOLITES FROM MALAYSIAN MANGROVE PLANT IN THE SEARCH FOR NEW POTENTIAL ANTIBIOTICS
Noor Wini Mazlan¹ 2
¹Strathclyde Institute of Pharmacy and Biomedical Sciences, University of Strathclyde, The John Arbuthnott Building, 161 Cathedral Street, Glasgow, Scotland, UK, ²Department of Chemistry, Faculty of Sciences and Technology, University of Malaysia Terengganu, Kuala Terengganu, Terengganu, Malaysia
Chemical investigation of Avicennia lanata, a mangrove plant which collected from the East coast of Malaysia along with two fungi isolated from this plant; Aspergillus aculeatus and Lasiodiplodia theobromae yielded some unknown and known compounds. Prior to this study, metabolomics has been applied to identify and optimize the production of bioactive secondary metabolites by using both high resolution mass spectrometry and NMR spectroscopy. Some of these compounds exhibited interesting activity against anti-trypanosomal assay.

P8-10
IDENTIFICATION OF BIOMARKERS FOR NON-STEROID ANTI-INFLAMMATORY DRUGS INDUCED GASTRIC ULCER BY CE-MS BASED METABOLIC ANALYSIS
Kenichiro Takeuchi
Drug Safety Research Laboratories, Astellas Pharma Inc., Osaka, Osaka, Japan
Non-steroid anti-inflammatory drugs (NSAIDs) are among the most frequently used drugs in the world and enhance the risk of serious gastric ulcer complications. In this study, we performed CE-MS-based metabolic profiling in stomach and serum from rats which was induced gastric ulcer by NSAIDs. We found four biomarker candidates in serum which can predict gastric injury induced by NSAIDs in rats. These candidates may facilitate the development of serum biomarkers.

THEME: DATA EXTRACTION AND INTERPRETATION

P9-1
POTENTIAL METABOLOMICS BIOMARKERS FOR EARLY DIAGNOSIS OF ENDOMETRIOSIS USING SERUM ¹H NMR
Sudha Srivastava
Tata Institute of Fundamental research, Mumbai, India
Present study focuses on identification of biomarkers for endometriosis using ¹H-NMR based metabonomics. PLS-DA modeling of bins obtained from spectra of serum discriminated endometriosis patients from controls with sensitivity and specificity levels of about 80% and 90% respectively. Endometriosis patients showed large changes in the concentration level of several compounds. Our work offers information for non-invasive diagnosis of the disease and may be of potential benefit to understand the pathogenesis of endometriosis.

P9-2
METABOLITE PROFILING OF LIPID AND NUCLEOTIDE METABOLISMS IN A MARINE BACTERIUM DEGRADING AND METABOLIZING SEAWEED COMPONENTS
Eun Ju Yun
School of Life Sciences and Biotechnology, Korea University, Seoul, Republic of Korea
Seaweeds are recently emerging for producing biofuels and industrial chemicals. A marine bacterium degrading and metabolizing seaweeds, was isolated from a coast side. Biochemical pathways of metabolizing seaweed components are hardly known. We have investigated the metabolite profiling of the isolated bacterium on the components of seaweeds concentrating on the metabolism of lipids and nucleotides. These results will lead us to the better understanding of marine bacteria metabolizing seaweeds in the ocean environment.

P9-3
COMBINING NON-TARGETED AND METABOLIC PATHWAY DRIVEN TARGETED METABOLOMICS BASED ON THE SAME LC-QTOF DATA SET - EXEMPLIFIED ON COFFEE METABOLOMICS
Heiko Neuweger
Bruker Daltonik GmbH, Bremen, Germany
A proof of concept study for coffee metabolic profiling using a novel workflow for combined non-targeted and targeted metabolomics based on the same high resolution QTOF data files will be presented. Non-targeted data evaluation pointed to metabolites as being characteristic for particular coffee types. Creating a target compound list derived from related metabolic pathways enabled to quickly screen for their presence and revealed several metabolic changes not directly assessed by non-targeted data evaluation.
P9-4
HIGHLY ACCURATE CHEMICAL FORMULA PREDICTION TOOL UTILIZING HIGH-RESOLUTION MASS SPECTRA, MS/MS FRAGMENTATION, HEURISTIC RULES, AND ISOTOPE PATTERN MATCHING
Tomáš Pluskal
Okinawa Institute of Science and Technology Graduate University, Onna, Okinawa, Japan
We developed a universal software tool for predicting chemical formulas of small molecules from high-resolution mass spectrometry data. The tool is based on the use of a combination of heuristic techniques, including MS/MS fragmentation analysis and isotope pattern matching. Its performance was evaluated using a real metabolomic dataset obtained with the Orbitrap MS detector. The program is now freely available as part of the open-source MZmine 2 framework.

P9-5
RECONSTRUCTION OF INSULIN SIGNAL FLOW IN GLOBAL PHOSPHORYLATION AND METABOLIC NETWORKS
Katsuyuki Yugi
1The University of Tokyo, Bunkyo-ku, Tokyo, Japan
Starting from time-series metabolomic and phosphoproteomic measurements, we found where an insulin signal flowed through a global network; the insulin signal flowed through pathways that involves 26 protein kinases, 76 phosphorylated metabolic enzymes, and 80 allosteric effectors, resulting in quantitative changes of 97 metabolites. We also found when specific phosphorylation and allosteric regulation selectively control metabolites using kinetic models. Altogether, we demonstrate a global landscape of the insulin signal flow that regulates metabolic homeostasis.

P9-6
GLOBAL METABOLOMIC ANALYSIS OF MIXTURES USING 13C-DETECTED NMR TECHNIQUES
Chaevien Clendinen
University of Florida, Gainesville, Florida, USA
We present an approach to 13C metabolomics using natural abundance and enriched 13C-detected NMR. In conjunction with statistical techniques, we demonstrate the use of 1D 13C NMR to conduct a global metabolomic analysis of natural abundance 13C synthetic mixtures and apply this method to the serum of mice afflicted with muscular dystrophy. In addition, we are also developing a method for analyzing 1D 13C and 2D-INADEQUATE data using the 13C-enriched metabolome of C. elegans.

P9-7
INTEGRATED PROTEOMIC AND METABOLIC PROFILING OF GILTHEAD SEABREAM LIVER TO TRACK INTERACTIONS BETWEEN DIETARY FACTORS AND SEASONAL TEMPERATURE VARIATIONS.
Ana M Rosa da Costa
CIQA-Algarve Chemistry Research Centre & Department of Chemistry and Pharmacy, University of Algarve, Faro, Portugal
This work describes the results of an experiment with gilthead seabream, where liver proteome and metabolome were assessed for each subject using DIGE and FTIR spectroscopy, for the purpose of assessing possible interactions between nutritional and seasonal stress factors. Results confirmed that it is possible to use nutritional strategies to mitigate the impact of seasonal stress on gilthead seabream metabolism.

P9-8
IONS FUSION OF HIGH-RESOLUTION LC-MS-BASED METABOLOMICS DATA TO DISCOVER MORE RELIABLE BIOMARKERS
Zhongda Zeng
Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian City, China
A systematic approach is developed for ion fusion of high-resolution LC-MS-based metabolomics data. Less redundant features help to discover more reliable biomarkers. The knowledge applied includes mass change of ion between theoretical calculation and precise measurement, such as isotope distribution, adducts ion and neutral loss. Correlation analysis is also used for the fusion. A metabolomics data with liver cancer and Cirrhosis is employed to deliver the strategy.

P9-9
MetaboHUB: A FRENCH INFRASTRUCTURE DEDICATED TO METABOLOMICS AND FLUXOMICS
Dominique Rolin1,2
1French MetaboHUB, INRA-Bordeaux, France, 2French MetaboHUB, University-Bordeaux, France
MetaboHUB project aims at creating a national infrastructure that will provide tools and services to academic research and industrial partners in the fields of nutrition, health, agriculture, environment and biotechnology. MetaboHUB will be established by implementing and up-grading 4 existing facilities (Bordeaux, Paris-Saclay, Toulouse and Clermont-Ferrand) into a unique infrastructure sharing common regulations and complementary metabolomics and fluxomics tools.

P9-10
ERVA METHOD FOR 1H-NMR METABOLOMICS DATA: A NOVEL BINNING STRATEGY HIGHLIGHTING CHEMICAL INFORMATION
Daniel Jacob1,2
1INRA, Bordeaux, France, 2Metabolome Facility of Bordeaux Functional Genomics Center, Bordeaux, France
An improved method of data reduction called ERVA is proposed for proton NMR 1D spectra processing. This new method, by providing buckets centred on resonance peaks and rid of any non-significant signal, helps to recover the chemical fingerprints of metabolites. Then, taking advantage of the concentration variability of each compound from a complex-mixture series of samples, chemical information is highlighted through bucket clustering, and candidate compounds are proposed for spectra annotation.
P9-11
ANALYSIS OF LONGITUDINAL METABOLOMIC DATA FROM ENDOCRINE DISRUPTION STUDIES: THE A-SCA METHOD
Marie Tremblay Franco1,2
1INRA, UMR 1331, Toxalim, Toulouse, France, 2Université de Toulouse, INP, UMR1331, Toxalim, Toulouse, France
Methods usually used to analyze metabolomics data are not appropriate to treat longitudinal data. We applied the A-SCA method, taking into account both the experimental design and the relationship between variables, to study the effects of low doses of bisphenol A on global metabolism in SD rats exposed during the perinatal period. Serum samples of the F1 generation collected at 5 time-points were submitted to 1H NMR spectroscopy. Time effects were demonstrated.

P9-12
DEVELOPMENT OF THE GOLM METABOLOMEx DATABASE TOWARDS BIG DATA
Jan Hummel
Max Planck Institute of Molecular Plant Physiology, Potsdam, Germany
We report an update of the Golm Metabolome Database (GMD, http://gmd.mpimp-golm.mpg.de/), a database harbouring primarily GC-MS datasets in plants. In our developments, we focused on the agile integration of multiple metabolomic gas chromatography (GC) -mass spectrometry (MS) data sets, paving the way towards ‘Big Data’ applications including searching and data mining across multiple GC-MS based metabolite profiling data sets.

P9-13
UNTARGETED METABOLOMICS FOR TOXICITY PROFILING OF HUMAN KIDNEY CELLS USING HPLC-ESI-MS AND DIRECT-INFUSION Nano-ESI-MS
Christina Ranninger
University of Salzburg, Salzburg, Austria
The aim of this study was to screen the effects of nephrotoxic drugs on cultured cells to observe the impact of drug treatment on metabolite abundance. In these studies, three different drug doses were applied to three biological replicates at three different time points. For toxicity profiling two different approaches were chosen, namely RP-HPLC-ESI-MS and direct-infusion nano-ESI-MS. Data evaluation involved univariate and multivariate statistical approaches to determine differentially regulated metabolites.

P9-14
GRAPE ISOPRENOIDS: AUTOMATED DATA ANALYSIS IN MORE THAN 500 SAMPLES
Elisabete Carvalho
Fondazione Edmund Mach, San Michele all’Adige, Trento, Italy
The isoprenoid profiling of more than 500 grape samples was done using HPLC-DAD as part of a system-wide untargeted metabolomics analysis. By using a pipeline based on Multivariate Curve Resolution (MCR) we were able to process all data automatically, obtaining estimates of pure spectra, elution profiles, and accurate estimations of peak area for each of the analysed metabolites in each grape sample.

P9-15
MetAnnoDB, A DATABASE OF HUMAN METABOLITE ANNOTATIONS BASED ON ACCURATE MASS AND MS/MS SPECTRA
Dinesh Barupal
International Agency for Research on Cancer, Lyon, France
MetAnnoDB is a database of annotated ions in human plasma and urine samples analyzed using a UPLC-QTof mass spectrometer. The database contains 2,000 MS/MS spectra with accurate masses, out of which up to 500 have been confidently annotated as unique metabolites. Database would assist in the generation of MSI-compliant metabolomics dataset using high-resolution mass spectrometers. It can be accessed at www.metannodb.org.

P9-16
DIFFERENTIATION OF ANALYTICAL AND BIOLOGICAL VARIABILITY IN METABOLOMICS USING STANDARD REFERENCE MATERIALS AND MULTIVARIATE STATISTICS
Yamil Simón-Manso
National Institute of Standards and Technology (NIST), Gaithersburg, Maryland, USA
NIST has long developed and provided standard reference materials (SRMs) to assist others in making reliable measurements. SRMs of urine from smokers and non-smokers were used to compare the analytical and biological variability of the extracted profiles of the nicotine pathway metabolites and also the global profiling of the material. We discuss a protocol to evaluate the analytical variability associated with LC-MS measurements of biological fluids using SRMs and multivariate statistics.

P9-17
METABOLIGHTS: A CROSS-SPECIES REPOSITORY FOR METABOLOMICS EXPERIMENTS AND DERIVED INFORMATION
Kenneth Haug
EMBL-European Bioinformatics Institute, Cambridge, UK
MetaboLights is a database for metabolomics experiments and the associated metadata. It is the first comprehensive, cross-species, cross-platform/technique database which combines curated reference data of pure metabolites, curated information about their occurrence and concentration in species, organs, tissues and cell types under various conditions with data characterizing the experiment which lead to these findings and allows ready cross-referencing between experiments. The MetaboLights database is completely open to the public, including open access to the data.
P9-18
A SYSTEMATIC APPROACH TO OBTAIN VALIDATED PLS MODELS FOR PREDICTING LIPOPROTEIN SUBCLASSES FROM SERUM NMR SPECTRA
Velitchka Mihaileva1,2
1Wageningen University, Wageningen, The Netherlands, 2Netherlands Metabolomics Centre, Leiden, The Netherlands
PLS models were established for estimation of cholesterol/triglyceride concentrations in lipoprotein subclasses from diffusion edited 1H-NMR spectra of fasting serum from healthy humans. The PLS models were calibrated on HPLC derived lipoprotein subclasses. Significant models for 5 VLDLs, 4 LDLs, 4 HDLs, and the total VLDL, LDL, and HDL lipids we found. The lipoprotein subclass resolution in the predicted lipoprotein profiles proved to be suitable for assessing dietary effects and modeling lipoprotein turnover.

P9-19
GENOME SCALE METABOLIC RECONSTRUCTION OF T BRUCEI USING GENOMIC INFORMATION AND COMMUNITY-BASED ANNOTATION.
Sanu Shameer
INRA-TOXALIM, Toulouse, France
10,000 cases of African trypanosomiasis have been reported every year and many more go undiagnosed. With metabolic network reconstruction we plan to study the T.brucei parasite and its metabolic response to gene deletions, medium perturbation, etc. We are developing a compartmentalized metabolic network by merging Trypanocyc community based annotated model with manually curated metabolic models of L.major and E.coli. We have also been able to integrate metabolomic data onto this network using MetExplore web server.

P9-20
THE RETENTION TIME ALIGNMENT FOR NON-TARGETED LC/MS ANALYSIS USING KERNEL DENSITY ESTIMATION WITH NOVEL BANDWIDTH ESTIMATOR
Jiawei Liu
Graduate Institute of Networking and Multimedia, National Taiwan University, Taipei, Taiwan
Goal: Align the retention time to identify compounds and increase reliability of detected compounds.
Observation: Retention time in LC-MS data contains unknown scale deviation, which makes compounds with similar m/z indistinguishable. The statistical approach would be a good solution.
Method: Kernel density estimation based on the spectrum similarity is used to align with m/z and retention time information. Parameters estimation method is also included.
Result: This approach shows better bandwidth estimation than traditional ones.

P9-21
METABOLOMICS TECHNOLOGY VALIDATED QUALITY MARKERS FOR BIOBANK PLASMA SAMPLES
Dietrich Rein
Metanomics Health GmbH, Berlin, Germany, 2metanomics GmbH, Berlin, Germany
Research in healthcare often starts with the analysis of existing biobank samples. The quality of these biobank samples can be impaired by various pre-analytical sample processing steps that will confound the analytical results and decrease the value of results. We performed experiments to analyse the impact of various pre-analytical processes on the human blood plasma metabolome. Several metabolites suited as Quality Markers for human EDTA plasma were identified and validated.

P9-22
BN server: A WEB-BASED SERVICE FOR LC/TOFMS-BASED METABOLOMICS DATA NORMALIZATION AND STATISTICAL ANALYSIS
San-Yuan Wang1,2
1Department of Computer Science and Information Engineering, National Taiwan University, Taipei, Taiwan, 2The Metabolomics Core Laboratory, Center of Genomic Medicine, National Taiwan University, Taipei, Taiwan
BN server is implemented as an integrated web-based platform to normalize and analyze the liquid chromatography/time-of-flight mass spectrometry-based metabolomics data. It is designed for the scientists with little or without background in programming and statistics. After users uploading the metabolomics data to BN server, BN server will automatically remove the batch and injection order effects, perform the preliminary hypothesis test and principal component analysis.

P9-23
A HIGH-THROUGHPUT AND ROBUST QUANTUM MECHANICAL TOTAL LINE SHAPE FITTING APPROACH FOR QUANTITATIVE PROFILING OF THE SERUM METABOLOME
Jacques Vervoort1,2
1Wageningen University, Wageningen University, The Netherlands, 2Netherlands Metabolomics Centre, Leiden, The Netherlands
Quantum Mechanical Total Line Shape (QMTLS) fitting model was implemented for quantitative profiling of 43 metabolites in 1H-NMR spectra of ultra filtrated serum samples covering a large concentration range. With the proposed procedure 90% to 98% of the signal intensities of the selected regions in the experimental spectrum were explained by the calculated spectrum. The QMTLS model can be performed in automated manner and is suitable for a high-throughput analysis of large sets of samples.
P9-24
ASSESSING THE REPEATABILITY AND STATISTICAL ADVANTAGES OF HOMONUCLEAR 2D-NMR SPECTRA: A CLUSTERING APPROACH
Baptiste Feraud1,2
1UCL, ISBA, Louvain-la-Neuve, Belgium, 2UCL, Machine Learning Group, Louvain-la-Neuve, Belgium
A large amount of recent scientific and statistical works are available concerning 1D NMR spectra. More recently, two-dimensional NMR spectroscopy techniques have been investigated. Commonly, users accept that additional dimension means more predictive power. But, until now, no statistical study proved this clearly. Is supplementary information equivalent to crucial information? Accurate multivariate clustering tools will be shown to respond to this question, to test the repeatability and to compare with classic 1D method.

P9-25
ADAPTATION OF RANK PRODUCT STATISTICS FOR METABOLOMICS STUDIES
Andris Jankevics
University of Manchester, Manchester, UK
Metabolomics aims at understanding biology by comprehensive metabolite profiling. Very often, lists of extracted features or metabolites have to be compared between different conditions, e.g. two different treatments or cell lines. Classical statistical methods (e.g. t-tests) have been shown to be unreliable in this setting.
In this work we present an adaptation of the rank products statistical test for metabolomics data sets, introducing a necessary modification of the original algorithm for handling unpaired data.

P9-26
EXTRACTION OF METABOLOMICS DATA TO DISCLOSE MINOR PATHWAYS OF ORGANIC ACID METABOLISM IN ISOVALERIC ACIDEMIA
Carolus J. Reinecke
Centre for Human Metabonomics, North-West University, Potchefstroom, South Africa
Here we present a protocol used to evaluate a hypothesis on minor metabolites presumed to be present in isovaleric acidemia (IVA), an inherited disorder of leucine catabolism. Data extraction from the matrix used for the investigation of IVA, but excluding previously identified diagnostic biomarkers of IVA, was followed by univariate and multivariate analyses. This disclosed a number of novel markers which indicate the profile of metabolic homeostasis present in the IVA patients.

P9-27
METABOLOMICS CHARACTERISATION OF ANGELICA SPECIES BY COMPREHENSIVE TWO-DIMENSIONAL GAS CHROMATOGRAPHY COUPLED WITH TIME-OF-FLIGHT MASS SPECTROMETRY (GCxGC-TOFMS).
Nai-Wen Chang1,2
1The Metabolomics Core Laboratory, Center of Genomic Medicine, Taipei, Taiwan, 2Graduate Institute of Biomedical Electronics and Bioinformatics, National Taiwan University, Taipei, Taiwan
Due to the difference of GCxGC-TOFMS data among three types of Angelica samples, Japan, Hualien and ChungHua, is not obvious, we propose a method to improve the performance of classification. 2D chromatograms were first aligned and the supervised learning method was used for identifying major components and relative quantities of each species in 75 Angelica samples. Major components of each species, which is used to separate three type of Angelica, were identified in our approach.

P9-28
MRMPROBS: DATA ASSESSMENT AND METABOLITE IDENTIFICATION TOOL FOR LARGE-SCALE MRM-BASED WIDELY TARGETED METABOLICS
Hiroshi Tsugawa1,2
1RIKEN Center for Sustainable Resource Science, Yokohama, Kanagawa, Japan, 2Department of Biotechnology, Graduate School of Engineering, Osaka University, Suita, Osaka, Japan
We developed novel software, MRMPROBS, for widely targeted metabolomics by using the large-scale multiple reaction monitoring mode. The traditional method of assessing measured metabolomics data without probabilistic criteria is not only time-consuming, but is often subjective and makeshift work. Our program overcomes these problems by detecting and identifying metabolites automatically, by separating isomeric metabolites, and by removing background noise using a probabilistic score defined as the odds ratio from an optimized multivariate logistic regression model.

P9-29
COMPARATIVE ANALYSIS OF SAMPLE PREPARATION METHODS FOR LC-ESI-qToF-MS-DRIVEN PLASMA FINGERPRINTING. LESS IS MORE WHEN HANDLING THE COMPLEXITY OF THE BLOOD FLUIDS METABOLOME
Sara Tulipani1,2
1Biomarkers and Nutritional & Food Metabolomics Research Group, Nutrition and Food Science Dpt, XaRTA, INSA, Pharmacy Fac., University of Barcelona, Barcelona, Spain, 2INGENIO-CONSOLIDER Program, Barcelona, Spain
We applied a LC-ESI-qToF-MS-driven metabolomic workflow and multiple chemometric techniques to evaluate five methods of plasma sample preparation (three solvent extractions, a membrane-based solvent-free technique, a novel hybrid method combining solvent extraction and SPE-mediated phospholipid removal) in terms of biomatrix effects minimization, reproducibility, metabolite coverage and detection of real-life diet-dependent metabolomic changes. The phospholipid selective removal determined the minimization of matrix effects and was the most suitable method to handle the complexity of plasma metabolome.
P9-30
A NEW LIPID SOFTWARE WORKFLOW FOR PROCESSING ORBITRAP-BASED GLOBAL LIPIDOMICS DATA IN TRANSLATIONAL AND SYSTEMS BIOLOGY RESEARCH
Madalina Oppermann
Thermo Fisher Scientific, Stockholm, Sweden
The content presented describes a new software for identification of lipid differences in benchmark phenotype for Type II diabetes on data generated using an LC-MS/MS-based workflow on a high resolution, accurate mass quadrupole-Orbitrap mass spectrometer. Lipid identification is carried out in a vast, >10^6 entries, database, and it is accompanied by a relative quantitative comparison of the samples in the analysis set.

P9-31
FULLY AUTOMATED NMR SPECTRAL PROFILING FOR METABOLOMICS - BAYESIL
David Wishart
University of Alberta, Edmonton, Alberta, Canada
A fully automated and quantitative NMR spectral profiling system, BAYESIL, for metabolomics is presented. It uses a variety of novel phasing and baseline correction methods to automatically process 1D NMR spectra. Based on extensive testing with defined mixtures and real biological samples BAYESIL consistently performs with sensitivity and specificity greater than 98% for compound identification and quantification (down to 10 µM). This may open the door to routine applications of NMR in a clinical setting.

P9-32
ESTABLISH TARGETED LIPIDOMICS WORKFLOW USING Tipick WITH ADJUSTED PARAMETERS ON DENOISE AND PEAK PICKING STAGES
Tien-Chueh Kuo
1Graduate Institute of Biomedical Electronics and Bioinformatics, National Taiwan University, Taipei, Taiwan, 2The Metabolomics Core Laboratory, Center of Genomic Medicine, Taipei, Taiwan
Targeted lipidomics analysis aims at identified known lipid species from cells. Tipick is a denoising/peak picking algorithm developed to extract true ion signals from LC/MS data. To establish workflow for targeted lipidomics analysis, parameters of Tipick are adjusted for lipidomics use. Extracted ion chromatograms of 237 lipid standards are used to examine noise level and detect peaks using Tipick. We have successfully established workflow for targeted lipidomics by adjusting suitable parameters of Tipick.

P9-33
A FULLY AUTOMATED UNTARGETED LIPID DATA PROCESSING METHOD USING MZmine COMPARED TO AGILENT RECURSIVE ANALYSIS
Mark Silveria
University of California, Davis, Davis, Ca, USA
A comparison of multiple untargeted LC-MS data processing software to find the best fit for a reverse phase lipidomic method. We discuss potential problems with untargeted data processing and ways to avoid them along with differences between methods. Our automated data processing methods are available online as a download.

P9-34
DENOISE METHOD TO REMOVE SCAN-BASE NOISE AND AUTOMATIC DRAIN ALGORITHM THRESHOLD DETERMINING PRE-PROCESSING METHOD APPLY ON GC-TOFMS
Chung Yu-Yen
The Metabolomics Core Laboratory, Graduate Institute of Biomedical Electronics and Bioinformatics, National Taiwan University, Taipei, Taiwan
Remove noise-like intensity to improve the result of identification and decrease data size. Noise level depends on scan in our GC-TOFMS data. Drain algorithm is commonly used for picking region with compounds co-eluted, however threshold tuning is difficult. Evaluate threshold in each scan by regression model. Threshold of drain algorithm determined by the number of cluster automatically. We find the number of identified compounds increase especially in higher match factor threshold.

P9-35
REST ARCHITECTURE FOR MASSBANK DATABASE SERVICE
Ramon Francisco Mejia
RIKEN Center for Sustainable Resource Science, Yokohama, Kanagawa, Japan
This poster proposes a Representational State Transfer (REST) approach for MassBank. We introduce the next version of the MassBank database service which implements different network topologies: a master node orchestrates critical operations through a star topology, major nodes are regularly crawled, integrated (e.g., integrated standard spectra), and shared through a partially-connected topology, and minor nodes representing transient users sharing metabolomic data through a fully-connected topology.

P9-36
BIPACE - A GENERIC RETENTION TIME ALIGNMENT ALGORITHM FOR GAS-CROMATOGRAPHY MASS- SPECTROMETRY DATA
Nils Hoffmann
Genome Informatics, Faculty of Technology, Bielefeld University, Bielefeld, Germany,
We present BIPACE, a generic algorithm for retention time alignment of multiple datasets from one and two-dimensional chromatography, coupled to FID, MS, or in principle, arbitrary detectors. We demonstrate BIPACE’s ability to support various similarity functions for retention time and mass spectral similarity on a set of publicly available GCxGC-MS datasets and compare BIPACE’s performance using symmetric and asymmetric retention time similarity functions to previously published algorithms.
P9-37
MAMBO-MS: A WEB-BASED GC-MS AND LC-MS MASS SPECTRAL LIBRARY MANAGEMENT SYSTEM
Saravanan Dayalan1,2
1Bio21 Molecular Science and Biotechnology Institute, The University of Melbourne, Parkville, Victoria, Australia, 2Metabolomics Australia, The University of Melbourne, Parkville, Victoria, Australia
MAMBO-MS is a downloadable and installable framework for a web-based mass spectral library management system for GC-MS and LC-MS. It is made up of a Lab Management System through which labs are able to access the system, User Management System, which defines different user groups and privileges to users and a Data Management System that defines the metadata of the system along with how the different mass spectral libraries are stored, curated and accessed.

P9-38
NOVEL SOFTWARE SOLUTIONS FOR LIQUID CHROMATOGRAPHY-HIGH RESOLUTION MS (LC-HRMS) METABOLITE PROFILING OF LEGUMES UNDER DROUGHT AND FUNGAL INFECTION CONDITIONS.
Michael Dickinson
The Food and Environment Research Agency, York, UK
This work describes preliminary metabolomics data from the EU FP7 five-year project ABSTRESS (www.abstress.eu). Progenesis Comet software was used to interpret high resolution MS data files from a Thermo Exactive. A range of metabolites potentially associated with fusarium infection and drought stress have been identified from leaf and root samples of stressed legume plants using the software.

P9-39
EVALUATION AND CORRECTION OF BATCH VARIATION IN METABOLOMIC WORKFLOWS USING DIRECT INFUSION MASS SPECTROMETRY (DIMS).
Jennifer Kirwan
1University of Birmingham, Birmingham, UK
Minimising and correcting for analytical variation is of particular concern in large scale, multibatch studies. We report results from a purpose-designed study of mammalian heart tissue constructed to characterise and correct the intra and inter-batch analytical variation. The findings objectively demonstrate that our workflow reduces analytical variation and increases the percentage of significantly different mass features. Analysing samples across seven days and eight different batches we report an overall analytical precision of 15.9% median RSD.

P9-40
FUSION OF METABOLICMS DATA FROM DIFFERENT PLATFORMS USING PLATFORM SPECIFIC MEASUREMENT ERRORS
Oksana B. Korobko
University of Amsterdam, Amsterdam, The Netherlands
Problem of fusion of different platforms of metabolomics data can be solved in respect to measurement errors. Maximum-Likelihood Fusion method was developed to manage such problems. This method consists of a step in which measurement error structure is derived from replicate metabolomics data and the error structure is used as an input for ML PCA to obtain the principal components model.

P9-41
HYPOTHESIS-FREE IDENTIFICATION OF GENETICALLY INFLUENCED NMR SPECTRAL FEATURES AND THEIR INTERPRETATION USING MASS SPECTROMETRY DERIVED METABOLIC TRAITS
Johannes Raffler1,2
1Helmholtz Zentrum Munich, Neuherberg, Germany, 2Ludwig Maximilian University, Munich, Germany
NMR spectroscopy is a robust platform often used in metabolomics studies. We present an approach to derive features of biomedical interest from raw NMR spectra using genetic associations as a selection criterion. These spectral features can be characterized using data from mass spectrometry (MS). Conversely, NMR features can help to annotate metabolites of unknown chemical identity detected on MS platforms. These knowledge transfers might pave the way to harmonize metabolic data gathered on different platforms.

P9-42
UNTARGETED METABOLICMS OF FUSARIUM GRAMINEARUM: COMPARISON OF STABLE ISOTOPIC LABELLING ASSISTED AND CONVENTIONAL DATA PROCESSING STRATEGIES
Christoph Bueschl
University of Natural Resources and Life Sciences (BOKU), Tulln, Austria
We present a novel data processing strategy for stable isotope-assisted metabolomics experiments and compare the results with conventional strategies. Processing algorithms were exemplified with 13C and 12C cultures of Fusarium graminearum. The total number of extracted features (including isotopologues) was 5-6 times higher with the labelling-free approach. Quantitative comparison of selected features showed a high correlation of the obtained peak areas. Both strategies showed were clearly suited to differentiate between the two cultivated fungal strains.
NOVEL STABLE ISOTOPIC LABELLING-ASSISTED WORKFLOWS FOR IMPROVED LC-HRMS BASED METABOLOMICS OF FUNGI AND PLANTS
Rainer Schuhmacher
University of Natural Resources and Life Sciences, Vienna (BOKU), Tulln, Austria
Here we present novel, stable isotopic labelling-assisted workflows for improved untargeted metabolite profiling by LC-HRMS. MetExtract and FragExtract, powerful data processing tools for global metabolome characterisation, tracer metabolisation and MS/MS spectrum evaluation are illustrated. We give a description of the data processing concepts and discuss their performance and limitations. The workflows will be exemplified with the characterisation of the wheat metabolome as well as untargeted profiling of biotransformation products of xenobiotic and endogenous tracers.

FRAGEXTRACT: A NOVEL SOFTWARE TOOL FOR MS/MS SPECTRUM EVALUATION FOR STRUCTURE ELUCIDATION IN METABOLOMICS RESEARCH
Nora Neumann
University of Natural Resources and Life Sciences, Vienna (BOKU), Tulln, Austria
We present a novel data processing tool, FragExtract, for liquid chromatography tandem mass spectrometry (LC-MS/MS) data obtained from measurements of fully labelled and corresponding non-labelled samples. The algorithm is able to reliably extract MS/MS fragment signals, calculate their number of carbon atoms and provide meaningful suggestions for elemental formulas of each fragment ion. Therefore FragExtract shows high potential to assist in structural elucidation and annotation of unknown compounds in SIL-assisted untargeted metabolomics studies.

UNDERSTANDING THE COMPLEX INTERACTIONS INSIDE THE HOST-MICROBIOME-METABOLOME AXIS IN INFLAMMATORY BOWEL DISEASES VIA (ULTRA)HIGH RESOLUTION SPECTROMETRIC TECHNIQUES
Kirill Smirnov
Research Unit Analytical BioGeoChemistry, Helmholtz Zentrum München, German Research Center for Environmental Health (GmbH), Neuherberg, Germany
The composition of the gut microbiota can have a great influence on the humans’ health. However, it is little known how changes in the microbial composition affect the metabolism of the host. Via (ultra)high resolution spectrometric techniques we want to setup metabolite maps and correlate them to the nutritional, clinical, and microbiological data regarding human inflammatory bowel disease etiology.

WORKFLOWS FOR THE CREATION OF LIBRARIES OF RECURRING MASS SPECTRA (GC/MS, LC/MS/MS) FROM BIOLOGICAL MATERIAL INCLUDING STANDARD REFERENCE MATERIALS
John M. Halket1,2
1Mass Spectrometry Facility, King’s College London, London, UK, 2Department of Medicine, Imperial College, London, UK
Workflows are being developed to process large numbers of data files and provide quality spectra with well characterized retention parameters, resulting in searchable libraries of recurring components. GC/MS libraries of identified and unidentified recurring spectra from urine extracts and essential oils are available for download. Problems encountered during development of the automated procedures such as retention index variations, molecular weight estimations, peak overloading and perfectly overlapping components are described and discussed with examples.

HUMAN PLASMA METABOLITE PROFILING: THE IMPACT OF CHROMATOGRAPHY AND DATA ACQUISITION METHODS ON METABOLITES DETECTED BY LC-MS
Alan Barnes
1Shimadzu Corporation, MSBU Overseas, Manchester, UK
The diverse compound classes present in human plasma require careful consideration when performing untargeted global metabolite profiling. In these experiments NIST standard reference material of human plasma (SRM-1950) was analysed. Reversed phase chromatographic separation accommodated both rapid elution of polar compounds (amino acids, fatty acids) whilst balanced with later elution of non-polar compounds (diacylglycerophosphocholines, triacylglycerols). Data acquisition on the LCMS-IT-TOF was designed to maximise sensitivity whilst simultaneously acquiring MSn data to enable metabolite identification.

METABOLIGHTS REFERENCE LAYER: A COMPREHENSIVE KNOWLEDGE BASE OF METABOLITES
Tejasvi Mahendrakar
EMBL-EBI, Cambridge, UK
The MetaboLights Reference Layer is a comprehensive knowledge with a Metabolite-centric view. It includes elements such as reference spectra of various types, biological and chemical reference data, protocols and cross-references to other worldwide resources.
P9-49
THE USE OF MASS DEFECT FOR UNKNOWN BIOMARKERS RECOGNITION, CLASSIFICATION AND CHEMICAL FORMULA PREDICTION WITHIN LC-MS UNTARGETED EXPERIMENTS
Luca Narduzzi
Edmund Mach foundation, Trento, Trentino, Italy
Automatic annotation of the unknown signals extracted from LC-MS untargeted experiments is improving, but the chemical identification is still a complex and error-prone process. We employed a further step of data visualization to classify the unknown biomarkers signal using the mass defect ratio (MDR) and the retention time (RT) to create a 2D plot that helps in excluding improbable formulas/structures, giving a satisfactory tentative identification especially when compared to a reference standards 2D plot.

P9-50
EVALUATING THE PREDICTION RELIABILITY OF COMMERCIALY AVAILABLE SOFTWARE TOOLS DEVELOPED FOR TANDEM MASS SPECTRAL FRAGMENTATION SIMULATION
Florian Pitterl
1Institute of Legal Medicine and Core Facility Metabolomics, Innsbruck Medical University, Innsbruck, Austria
We evaluated the prediction reliability of two software tools developed for MS/MS simulation by comparing computational spectra of 600 compounds to experimental spectra. Predicted spectra were used as input for library search and for establishing libraries against which the corresponding experimental spectra were matched. Applying computational data as library spectra proved to be a convenient method for fast compound identification which may streamline metabolite identification in cases where reference spectra of authentic standards are absent.

P9-51
FUTURE OF METABOLOMICS STANDARDS; ROLE OF COSMOS
Reza Salek
EMBL- European Bioinformatics Institute, Hinxton, Cambridge, UK
An EU coordination action for developing metabolomics standards, called COordination of Standards in MetabolomicS - COSMOS (http://cosmos-fp7.eu), was launched in October 2012, initiated by EBML-EBI. This consortium of 14 European partners, with MetaboLight (http://www.ebi.ac.uk/metabolights/) playing a central role. COSMOS aims to develop efficient policies ensuring that metabolomics data is encoded in open standards, tagged with community-agreed complete set of metadata, supported by communally developed standards and disseminated in open-access databases.

P9-52
FLEXIBILITY VERSUS STANDARDIZATION TRADE-OFF IN LC/MS DATA PRE-PROCESSING OF LIPIDOMICS EXPERIMENTS
Mia Pras-Raves
AMC, Bioinformatics Laboratory, Amsterdam, The Netherlands
A workflow for the processing and analysis of LC-MS lipidomics datasets should be both standardized to enable routine processing of large datasets, and flexible enough to allow for differences in approach for different datasets or deal with specific problems. Based on the XCMS R-package, we constructed a workflow with extensions for the identification of phospholipids, isotope correction and normalization, in order to yield a more reliable list of metabolites with embedded plots for quality assessment.

P9-53
PROBABILISTIC ANNOTATION OF LC-MS BASED METABOLOMICS
Ricardo Silva
University of São Paulo, Ribeirão Preto, São Paulo, Brazil
Here we present the adaptation and extension of a previous probabilistic method to provide further insights in the compound annotation process. We build on well established preprocessing steps to maximize the utilization of information from those steps and create an extensive framework to model prior knowledge as information, resulting in an analysis flux that allow a higher quality annotation. We show the feasibility of this analysis implementing the R package probmetab.

P9-54
METABOLOMICAL CHARACTERIZATION OF THE RELATIONSHIP BETWEEN THE HYPERTHERMOPHILIC IGNICOCOCUS HOSPITALIS AND NANOARCHAEUM EQUITANS
Michelle Tigges
1Montana State University, Bozeman, MT, USA
Few microbes live in functional or spatial isolation, yet interactions between microbes are complex and multifaceted making them difficult to understand. Organisms that live at the extremes of life, however, may represent simplified systems from which we can gain insight into metabolic interdependences between microbes. We use untargeted metabolic profiling to describe the simplest symbiotic system known, which occurs between two hyperthermophilic archaeal organisms, to provide a basis for understanding multi-organism interactions.
P9-55
mzCLOUD: A KEY CONCEPTUAL SHIFT TO UNDERSTAND “WHO’S WHO” IN UNTARGETED METABOLOMICS
Robert Mistrik
HighChem, Bratislava, Slovakia
Untargeted metabolomics, in combination with novel mass spectrometric techniques, allow the detection of thousands of low-concentration compounds that can provide important insights into physiologically relevant processes. However, the majority of detected components remain unknown. To address this major obstacle in untargeted metabolomics, a novel library concept has been developed and implemented in a web-based interface that relies on powerful computational techniques and contributions of spectral trees from the metabolomics’ community.

P9-56
AUTOMATED OPERATION OF MASS FRONTIER TO CONSTRUCT IN-SILICO MASS SPECTRAL MS\textsuperscript{n} LIBRARIES
Mark R. Viant
\textsuperscript{1}School of Biosciences, University of Birmingham, Birmingham, UK
Multi-stage (MS\textsuperscript{n}) mass spectrometry is often applied to increase the specificity of metabolite annotation. However, experimental MS\textsuperscript{n} mass spectral libraries currently do not adequately cover metabolite space. In-silico MS\textsuperscript{n} libraries can provide putative data for MS\textsuperscript{n} libraries where experimentally determined MS\textsuperscript{n} data of authentic standards are unavailable. Here we present freely-available software to allow automated operation of Mass Frontier fragmentation software (HighChem), ultimately enabling generation of an MS\textsuperscript{n} in-silico fragmentation library in a high-throughput fashion.

P9-57
A MULTIVARIATE APPROACH TO REVEAL BIOMARKER SIGNATURES IN INSTRUMENTAL PROFILES OF BODY FLUIDS
Tarja Rajalähti\textsuperscript{1,2}
\textsuperscript{1}The Norwegian Multiple Sclerosis Competence Centre, Department of Neurology, Haukeland University Hospital, Bergen, Norway, \textsuperscript{2}KG Jebsen Multiple Sclerosis Research Centre, Department of Clinical Medicine, University of Bergen, Bergen, Norway
A general recipe for interpretation and for revealing patterns of predictive biomarkers in multicomponent profiles is presented. The approach is based on multivariate techniques and will be illustrated on proton NMR profiles of serum samples.

P9-58
IMPROVING QUANTITATIVE MASS SPECTROMETRY BASED METABOLOMICS
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\textsuperscript{1}LACDR, ABS, Leiden, The Netherlands, \textsuperscript{2}NMC, Leiden, The Netherlands
Both the data preprocessing and measurement design are important steps in the whole metabolomics workflow that, if properly handled, can improve the way how high quality quantitative mass spectrometry based metabolomics data is obtained. We introduce a new untargeted feature extraction and integration method and we demonstrate the effective use of (pooled) quality control, blank and transfer samples to emphasize their value to correct for within and between analytical batch and cross study variations.

P9-59
BUILDING A POLYPHENOL AND METABOLITE ION DATABASE FOR HIGH MASS ACCURACY LC-MS METABOLOMICS EXPERIMENTS
Stephen Barnes
\textsuperscript{1}University of Alabama at Birmingham, Birmingham, AL, USA
Polyphenols are abundant in diets used for animal experiments and vary enormously in human diets by region. As their physiological forms and metabolites, they are underrepresented in mass spectrometry metabolite databases. The goal of the present study was to data mine polyphenol-rich databases and generate accurate mass values for the molecular ions of polyphenol and their metabolites in order to supplement existing metabolite databases.

P9-60
IMPACT ON HUMAN METABOLITE PROFILES OF METHODOLOGICAL DECISIONS RELATING TO THE ANALYSIS OF PLASMA AND URINE.
Evangelia Daskalaki
\textsuperscript{1}Strathclyde Institute of Pharmacy and Biomedical Sciences, University of Strathclyde, Glasgow, UK
Longitudinal metabolomics screening approaches are frequently being used in biomarker discovery, yet no standardized and validated methods exist for analysis. The aim of the present study is to determine the impact on human metabolite profiles of methodological decisions relating to the analysis of plasma and urine. Preliminary results indicate great complexity within the metabolic profiles with correlations existing between groups of metabolically linked metabolites within individuals.

P9-61
VISUAL METABOLOMICS CORRELATION ANALYSIS: A NOVEL METHODOLOGY FOR ELUCIDATING CO-REGULATION AND METABOLIC PATHWAY ABERRATIONS IN RADIATION METABOLOMICS DATASETS
Tytus D. Mak
Lombardi Comprehensive Cancer Center, Georgetown University Medical Center, Washington, USA
The majority of statistical methods used for analyzing post-processed metabolomics data focuses on analyzing changes in excretion levels of various metabolites in biofluids. These methodologies generally examine metabolites as independent biomarkers, without any consideration for the complex correlation structure that exists between them. By ignoring this, many biologically significant patterns and mechanisms can be overlooked. As such, a new methodology, called Visual Metabolomics Correlation Analysis (ViMCA), has been developed to specifically explore this correlation structure.
P9-62
STATISTICAL ANALYSIS OF GCXGC-TOFMS METABOLOMICS DATA TO INVESTIGATE TRAUMATIC BRAIN INJURY
Alec Kettle
LECO UK, Stockport, Cheshire, UK
In this study, we investigate the metabolic changes in a mouse model related to traumatic brain injury relative to a control group. Metabolites were extracted from plasma and derivatized for GC×GC-TOFMS analysis. We present a data analysis approach Statistical Compare software that allowed for the characterization and comparison of these data and samples. Processing provided alignment across multiple samples and a Fisher-Ratio-based feature selection algorithm to determine class distinguishing analytes to gain insight to traumatic brain injury.

P9-63
A CRITICAL REVIEW OF DATA ANALYSIS METHODS AND REPORTING IN METABOLOMICS DISEASE PREDICTION STUDIES
Elizabeth Considine
University College Cork, Cork, Ireland
This review assessed all available literature where predictive algorithms were employed on metabolomics datasets for disease prediction. The studies were assessed under a range of criteria including the potential for bias by inappropriate use of quality control measures and validation techniques; and the quality of data reporting, including the interpretability of performance metrics used and if sufficient information is provided to enable replication of the analysis. Results: Minimum standards are not being adhered to.

P9-64
PILOT METABOLOME PROFILE STUDY OF INBORN ERROR OF METABOLISM WITH H\textsuperscript{1} NMR
Fatemeh Dorosti
Dept. of Biochemistry, Pasteur Institute of Iran, Tehran, Iran
Inborn errors of metabolism are a rare group of genetic disorders that can produce serious clinical consequences if undiagnosed and untreated. The most common metabolic disease in Iran is Phenylketonuria (PKU). Tandem mass spectrometry (LC/MS) and nuclear magnetic resonance spectroscopy (NMR) are new in neonatal screening for inborn errors of metabolism. We study the metabolome profile of PKU patient and compare with that of normal with the help of H\textsuperscript{1} NMR Spectroscopy.

P9-65
AN INTEGRATED NMR AND MS BASED COMPLEMENTARY METABONOMICS APPROACH FOR NON-INVASIVE DIAGNOSIS OF ENDOMETRIOSIS
Mainak Dutta
Indian Institute of Technology, Kharagpur, West Bengal, India
The present study focuses on the use of NMR and MS based metabonomics approach to determine novel biomarkers for the diagnosis of endometriosis. Serum from women with endometriosis were subjected to NMR and MS analysis. Our preliminary findings suggest that NMR based metabonomics is highly reproducible whereas MS is very sensitive. It is, therefore, concluded that an integrated metabolomics approach using both NMR and MS instrumentation is necessary to provide complementary information for biomarkers discovery.

P9-66
NEW APPROACH FOR AUTOMATED XCMS PARAMETER OPTIMIZATION
Gunnar Libiseller
JOANNEUM RESEARCH Forschungsgesellschaft mbH HEALTH Institute for Biomedicine and Health Sciences, Graz, Styria, Austria
Untargeted metabolomics has to rely on automated peakdetection- and peakpicking-software. Often the default parameters for these tools do not produce the best possible results. Therefore automated parameter tuning is an important issue to receive good data to work with. For getting the best possible results of the XCMS software, we tried to identify reliable target values and implement an automated workflow optimizing them.

P9-67
QUANTILE REGRESSION-BASED DRIFT CORRECTION APPLIED TO METABOLOMICS DATA FROM HUMAN SERUM SAMPLES
Sophie Narath
JOANNEUM RESEARCH Forschungsgesellschaft mbH HEALTH Institute for Biomedicine and Health Sciences, Graz, Austria
Our aim was to compose a workflow to identify and compensate bias from various sources. A quantile regression approach was applied to QC-pool samples. Success criteria for this approach are overall reduced variation of the QCs, graphical representations of drift features and multivariate modelling. In the present project, metabolite fingerprints of 106 human deproteinized serum samples from diabetes patients were generated using a HILIC-FTMS setup (LTQ Orbitrap XL).
P10-1

METABOLIC PROFILES AND FREE RADICAL SCAVENGING ACTIVITY OF CORDYCEPS BASSIANA FRUITING BODIES ACCORDING TO DEVELOPMENTAL STAGES

Hyung-Kyoon Choi
Chung-Ang University, Seoul, Republic of Korea

The metabolic profiles of Cordyceps bassiana according to fruit body developmental stages were investigated using GC-MS. Relative levels of amino acids, purine nucleosides, and sugars were higher in development stage 3 than the other stages. The free radical scavenging activities, which were significantly higher in stage 3 than the other stages, showed positive correlation with purine nucleosides. These results represented metabolic profiles and suggested the metabolism associated with fruiting body development in C. bassiana.

P10-2

INVESTIGATION OF THE FACTORS CAUSING CESSION OF 1-PROPANOL PRODUCTION BY MASS SPECTROMETRY-BASED METABOLIC PROFILING

Sastia Putri
Osaka University, Suita, Osaka, Japan

We conducted GC/MS and LC/MS-based metabolic profiling to investigate the factors causing the cessation of 1-propanol production. Cultivation of Escherichia coli in fed-batch culture was performed and metabolite changes that occurred was monitored. The results of time course metabolic profiling revealed phosphoenolpyruvate (PEP) and pyruvate accumulation coincided with a decrease in glycolytic metabolites. This observation was in good agreement with a dramatic decrease in glucose uptake rate when production has reached a plateau.

P10-3

METABOLIC PROFILING REVEALS COORDINATED REGULATION OF METABOLIC PATHWAYS OF S. CEREVIAE IN A CHARDONNAY WINE FERMENTATION

Chandra Richter
E&J Gallo Winery, Modesto, CA, USA

This work describes the endo- and exo-metabolome at three discreet timepoints during a wine fermentation, providing an understanding into the regulation of metabolic pathways during an alcoholic batch fermentation process. As both the endo- and exo-metabolome were identified we are able to gain perspective on the complex relationship between yeast and grape in the winemaking process. In summary, these analyses reveal distinct regulation of metabolic pathways important in wine production.

P10-4

OPTIMIZING SAMPLE PREPARATION FOR METABOLOMICS COVERAGE IN ROBUSTNESS IN YEAST

Mimi Swe
University of California, Davis, Davis, CA, USA

Yeast cells are important for biotechnology, molecular biology, and biochemistry. While a range of metabolomic studies have already been conducted on yeast, new methods may increase coverage of metabolites and improve robustness of analysis. We developed quenching and extraction methods that optimized metabolome coverage and yielded high quantitative robustness in yeast cells. Data on primary metabolism were acquired using GC-TOF-MS and GC-CI-QTOF-MS, while complex lipids were profiled using CSH-QTOF MS/MS.

P10-5

SAUVIGNON BLANC METABOLOMICS: IMPACT OF TRACES OF LIPOS IN GRAPE JUICE ON THE DEVELOPMENT OF WINE VOLATILE THIOLS

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NZ Sauvignon Blanc wine is well recognized worldwide for its high level of volatile thiols. However, biosynthesis of these thiols during fermentation is not well understood. Recent studies showed that traces of lipids in juice can significantly influence the development of volatile thiols in the wine. We profiled lipid traces in juices from different harvest seasons. The correlation results revealed a series of lipids with both strong positive and negative correlation to volatile thiols in wines.

P10-6

ASSESSMENT OF SAMPLING STRATEGY FOR METABOLOME ANALYSIS OF LACTOBACILLUS CASEI 431®

Kristine B. Jäpelt
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A sampling strategy for quenching of Lactobacillus casei 431® to approach global analysis of changes in the metabolite fingerprint during growth is developed and validated. Different quenching procedures will be assessed by evaluation of their ability to halt metabolic activity and preserve cell integrity using GC-TOF and other methods. Remaining metabolic activity is assessed with C13 labelled glucose. We expect to show that addition of buffer to quenching solution stabilizes cells and reduces metabolite leakage.
P10-7
QUANTITATIVE DETERMINATION OF NADP+ AND NADPH USING LC-MS: WORKFLOW OPTIMIZATION IN METABOLOMICS
Karin Ortmayr
University of Natural Resources and Life Sciences, Vienna, Austria
A complete analytical workflow for the quantitative analysis of the redox cofactors NADP+ and NADPH is presented, including a thorough evaluation and validation of the process employing isotopically labeled internal standards in mass spectrometric analysis. Applied in a metabolic study in yeast, this analytical workflow using hot extraction and LC-MS/MS analysis was found appropriate and delivered data fit for biological interpretation in metabolomics.

P10-8
COMPARATIVE METABOLOME ANALYSIS OF JAPANESE FRESH AND AGED SAKE REVEALS THE DIFFERENCE OF ORGANIC ACID CONCENTRATIONS.COMPARATIVE METABOLOME ANALYSIS OF JAPANESE FRESH AND AGED SAKE REVEALS THE DIFFERENCE OF ORGANIC ACID CONCENTRATIONS.
Keita Kamezaki1, 2
1 Institute for Advanced Biosciences, Keio University, Tsuruoka, Japan, 2 Department of Environment and Information Studies, Keio University, Fujisawa, Japan
The purpose of this study is to explore the metabolite differences between Japanese fresh sake and aged sake. Capillary electrophoresis mass spectrometry (CE-MS)-based metabolome analysis on 98 fresh sake and 19 aged sake samples revealed the increase of organic acid concentrations such as succinate and malate in aged sake as compared to fresh sake. This result indicates the increment in organic acid concentrations may relate to the maturation of Japanese sake.

P10-9
DERIVATIZATION PROCEDURES FOR MICROBIAL METABOLIC FOOTPRINTING BY GAS CHROMATOGRAPHY-MASS SPECTROMETRY
Stefanie Wiese
Chr. Hansen A/S, Hoersholm, Denmark
Metabolic profiling attempts to qualify and quantify as many small metabolites as possible in order to gain insight in the functioning of biological systems. In this work a silylation procedure was optimized focusing on a compound composition representative for fermentation samples. Samples contained high amounts of glucose, lactic acid in MRS medium representing a common fermentation matrix. Derivatization efficiency, robustness and the effect on liner and column performance was tested for compounds of a broad variety of structural patterns.

P10-10
ENHANCED PHASE II DETOXIFICATIONS CONTRIBUTES TO BENEFICIAL EFFECTS OF DIETARY RESTRICTION AS REVEALED BY MULTI-PLATFORM METABOLOMICS STUDIES
Wen Jun Xu
College of Pharmacy, Seoul National University, Seoul, Republic of Korea
We investigated the metabolite profiles of urines from control and DR rats using NMR and LC-MS metabolomics. For DR group, marker signals from glucuronide and glycine conjugations pathways were identified, phase II detoxification confirmed by mRNA and protein levels of UGT and GLYAT and Nrf-2 signaling pathway were up-regulated in liver tissues. Taken together, our metabolomic and biochemical studies provide a possible metabolic perspective in understanding the complex mechanism of the beneficial effects of DR.

P10-11
CHARACTERISATION OF THE WINE METABOLOME: LINKING SENSORY ATTRIBUTES TO GENOTYPE
Jade Haggerty
The University of Adelaide, Adelaide, Australia
This project aims to identify new genes responsible for the production of the most important aroma compounds formed in the fermentation bouquet. Micro-fermentations were performed with an overexpression library using chemically defined grape juice media -leucine (CDGJM-Leu) and the aroma compounds were analysed using headspace solid-phase microextraction coupled with gas chromatography mass spectrometry (HS-SPME GC-MS). This data was then analysed using statistical software to give rise to important clones to be analysed in further experiments.

THEME: METABOLOMIC PROFILING IN DIABETES AND HEART DISEASE

P11-1
METABOLOMIC ASSESSMENT OF THE PROTECTIVE EFFECT OF CJ-1 IN HIGH FAT DIET-INDUCED HEPATOSTEATOSIS IN MICE
Jung Chao
National Yang-Ming University, Taipei, Taiwan
CJ-1, a naturally abundant plant phenolic compound in vegetables and fruits, has been shown to have potent anti-oxidative and anti-obesity activity. In this study, we first investigated the beneficial effects of CJ-1 administration on nutritional hepatosteatosis model by a more “holistic view” approach, 1H NMR-based metabolomics, to proof efficacy and to obtain information that lead to understanding the mode of CJ-1 action.
P11-2
HUMAN STUDY FOR OBESE RELATED METABOLOMIC ANALYSIS WITH DIET INTERVENTION BY UPLC-QTOF-MS
Dae Young Kwon
Korea Food Research Institute, Songnam, Kyongki-do, Republic of Korea
The aim of the work is to identify the key metabolites related to weight reduction in humans by studying the metabolic profiles of serums obtained from thirty four participants who have undergone the dietary intervention of taking one packet of soybean peptides after every meal for 12 weeks. This research enables us to better understand obesity and increased the predictability of the obesity risk by studying metabolites present in the blood.

P11-3
METABOLIC PROFILING STUDY OF CARDIOVASCULAR DISEASE USING ULTRA-PERFORMANCE LIQUID CHROMATOGRAPHY/QUADRUPOLE TIME-OF-FLIGHT MASS SPECTROMETRY
Jueun Lee
1Korean Basic Science Institute, Seoul, Republic of Korea, 2Sungkyunkwan University, Suwon, Republic of Korea
In this study, we applied ultra-performance liquid chromatography/quadrupole time-of-flight mass spectrometry (UPLC/Q-TOF MS) to investigate metabolic change in serum from healthy individuals and patients with cardiovascular disease (Angina pectoris and Myocardial infarction). The Partial least squares-Discriminant Analysis (PLS-DA) model was generated from metabolic profiles and the score plot showed the significant difference between groups. The serum of patients with cardiovascular disease was especially characterized by the decreased levels of tryptophan and acyl carnitine.

P11-4
LIPIDOMIC ANALYSIS OF HEART TISSUES FROM A HAMSTER MODEL FOR DILATED CARDIOMYOPATHY
Yoshiro Saito
1National Institute of Health Sciences, Tokyo, Japan
To understand the mechanistic basis for cardiac dysfunction of dilated cardiomyopathy (DCM), lipidomic analyses were performed using left ventricles from J2N-k cardiomyopathic hamsters and its control J2N-n. Disturbances in membrane phospholipid homeostasis (changes in phosphatidylcholine and phosphatidylethanolamine species levels) were found even at the presymptomatic phase. The potential involvement of specific eicosanoids in the cardioprotective pathways was suggested by their increases during the symptomatic phase. This study provide insight into the mechanisms for DCM pathogenesis.

P11-5
METABOLIC APPROACH IN ACUTE PULMONARY HYPERTENSION DUE TO PULMONARY EMBOLISM IN AN ANIMAL MODEL
Renata Bujak
1Center for Metabolomics and Bioanalysis (CEMBIO), Facultad de Farmacia, Universidad CEU San Pablo, Campus Montepintrue, 28668 Boadilla del Monte, Madrid, Spain, 2Department of Toxicology, Ludwik Rydygier Collegium Medicum Nicolaus Copernicus University, dr. A. Jurasza 2, 85-089 Bydgoszcz, Poland
Acute pulmonary hypertension (PH) due to acute pulmonary embolization (PE) is associated with high mortality. The diagnosis of PE is challenging due to unspecific clinical symptoms and the lack of specific diagnostic blood tests. Metabolic fingerprinting with LC-MS and GC-MS was used in animal model (Sus scrofa) to evaluate alterations of metabolites in dextran microspheres embolism of the pulmonary circulation. Metabolomics could be a powerful tool for the diagnosis and prognosis of acute PE.

P11-6
A METABOLOMICS APPROACH TO GESTATIONAL DIABETES MELLITUS THROUGH GLOBAL FINGERPRINTING
Danuta Dudzik
1CEMBIO (Center for Metabolomics and Bioanalysis), San Pablo CEU University, Faculty of Pharmacy, Madrid, Spain, 2Department of Pharmacology, Medical University of Bialystok, Bialystok, Poland
Metabolomics has provided insights into metabolite alterations and molecular mechanism of many diseases. Looking for the
compounds that can serve as early biomarkers of civilization diseases is of main interest. The combination of different analytical platforms offers great advantages to illustrate the complete metabolome. We applied LC-MS and GC-MS for serum and CE-MS for urine fingerprinting, to compare metabolite patterns occurring during GDM to get an insight on the altered mechanisms and potential diagnostic markers.

**P11-9**
**METABOLIC DIFFERENCES OF INFLAMMATORY DISEASES IN A MURINE MODEL**
Young-Shick Hong
*Korea Basic Science Institute, Cheongwon, Republic of Korea*
Myocarditis is a cause of acute heart failure, sudden death, and chronic dilated cardiomyopathy. Comprehensive metabolic mechanism on myocarditis is still unclear. We explored the holistic metabolite perturbations in blood plasma of rats whose the inflammation is induced by inflammation adjuvant (CAF) alone and myosin together with CAF, through NMR-based metabolomic approach. Furthermore, the influence of cachexia observed in the inflammatory rats on their plasma metabolome was compared with that in food-restricted rat model.

**P11-10**
**THE SULT1A1 DETOXIFICATION PROFILE IN THE SOUTH AFRICAN TSWANA POPULATION GROUP INVOLVED IN THE PURE EPIDEMIOLOGICAL STUDY**
Hlengiwe Mbongwa
*North-West University, North West Province, South Africa*
Here we present a metabolomics analysis of cardiovascular parameters determined from the South African Tswana group as part of world-wide PURE study. A genetically well-defined group (SULT1A1 genotyping and copy number variation) were primarily defined. A metabolomics approach however could not disclose a natural separation in PCA between controls and the cases, but effect size analysis highlighted markers of lipid metabolism. The polymorphisms and copy-number variations distinctly affected sulphonation ability in the samples analysed.

**P11-11**
**IMPACT OF METFORMIN ON HepG2, Hepa1-6 AND DIFFERENTIATED 3T3-L1 CELLS UNDER GLUCOSE AND GALACTOSE CONDITIONS**
Caroline Muschet
*Helmholtz Zentrum München, Institute of Experimental Genetics, Neuherberg, Germany*
This study presents the impact of the anti-hyperglycaemic drug metformin at different sugar supply (glucose or galactose) on the metabolome of hepatoma (HepG2 and Hepa1-6) and adipocyte (differentiated 3T3-L1) cell lines. Metabolomic analyses, assessing 186 metabolites, were undertaken. Metformin treatment was shown to correlate with vast changes in metabolite profiles of all challenged cell lines. The response of the metabolome to drug treatment strongly depended on the supplemented hexose.

**P11-12**
**NMR METABOLOMICS OF RODENT MODELS OF OBESITY AND LIPOATROPHY**
Simona Bartova\(^1,2\)
\(^1\)Institute of Chemical Technology, Prague, Czech Republic, \(^2\)Institute of Microbiology, Academy of Sciences of the Czech Republic, Prague, Czech Republic
Type 2 diabetes mellitus (T2DM) and lipoatrophic diabetes have common basis in insulin resistance. We characterized 2 different models using NMR urine fingerprinting: Mouse model of diet-induced obesity and transgenic model of A-ZIP lipoatrophic mice. Our results indicated the satisfactory distribution according to different diet or genetic backround.

**P11-13**
**EFFECTS OF PREBIOTICS ON INSULIN RESISTANCE AND THE GUT MICROBIOME METABOLISM: A NON-TARGETED METABOLOMICS STUDY**
Tanja Verena Maier\(^1,2\)
\(^1\)Research Unit Analytical BioGeoChemistry, Helmholtz Zentrum München, German Research Center for Environmental Health (GmbH), 85764 Neuherberg, Germany, \(^2\)Chair of Analytical Food Chemistry, Technische Universität München, 85354 Freising, Germany
Many factors can modify the gut microbiome and may therefore influence host metabolism and disease susceptibility. Therefore, the objective of this study was to assess the impact of differently digestible carbohydrates (prebiotics), evaluating the effect on insulin resistance. A non-targeted metabolomics approach was performed, using FT-ICR-MS to analyze the complex metabolic interactions of the gut microbiome in relation to the prebiotic nutrition. In this presentation we focus on the metabolomics methods used in the study.

**P11-14**
**IDENTIFYING NOVEL PATHWAYS OF ATHEROSCLEROSIS USING AN UNBIASED METABOLOMICS APPROACH UTILIZING MULTIPLE PLATFORMS**
Elizabeth Axton
*UC Davis, Davis, CA, USA*
Blood plasma from patients undergoing elective cardiac evaluations (N>10,000) was submitted to metabolomics analysis using GC-TOF-MS, UHPLC-QTOF-MS, and HILIC-TOF-MS with the intent of identifying novel pathways and biomarkers of atherosclerosis and adverse cardiovascular outcomes. This multi-platform, unbiased approach allows for identification of over 500 compounds, plus 400-500 potential unknowns, while using only 50 µL of blood plasma.
P11-15
APPLICATION OF METABOLIC ANALYSIS TO A POPULATION-BASED, PROSPECTIVE COHORT STUDY: DESIGN AND SAMPLE PREPARATION METHOD OF THE ‘TSURUOKA METABOLIC COHORT STUDY’
Toru Takebayashi
Keio University School of Medicine, Tokyo, Japan; Keio Institute for Advanced Biosciences, Tsuruoka, Japan
An epidemiologic study with high throughput technologies is of value for discovering potential biomarkers for health and disease in humans. In particular, metabolomics is relevant to profile metabolic phenotype and understand the consequences of gene-environment interaction, leading to identify early pathophysiological changes of chronic diseases and personalized preventive health care. Thus, we initiated a population-based metabolome-wide cohort study with 10,000 participants in Tsuruoka, Japan. Here, we report study design and sample preparation method.

P11-16
PLASMA METABOLITES PROFILE AND LIVER DISEASES IN COMMUNITY-DWELLING ADULTS: TSURUOKA METABOLIC COHORT STUDY
Sei Harada
Keio University School of Medicine, Tokyo, Japan; Keio Institute for Advanced Biosciences, Tsuruoka, Japan
We performed CE-MS metabolome profiling on the 2,136 plasma samples of Japanese who enrolled into a longitudinal cohort study. To determine the metabolic status associated with development of alcoholic liver disease, we fitted O-PLS models in the highest tertile of ethanol intake. Gin, Glu, and Thr had high loading scores in a valid model and significantly related to gamma-GTP in regression models (P<0.0001). These metabolites may have important roles in the pathogenesis of alcoholic hepatopathy.

P11-17
SIGNATURE LIPID BIOMARKER ANALYSIS OF NON-ALCOHOLIC LIVER DISEASE
Cristina Alonso
OWL, Parque Tecnológico de Bizkaia, Derio, Bizkaia, Spain
Nonalcoholic fatty-liver disease (NAFLD) is one of the most common liver disorders, but the understanding of its progression from steatosis to steatohepatitis (NASH) is limited. Our UPLC/MS-based platform allows the semi-quantitative determination of around 1000 lipids and 150 polar metabolites. We have used this platform to determine the sera metabolite profile of 467 biopsied individuals with normal liver histology or diagnosed with steatosis or NASH, obtaining a robust BMI-dependent lipidomic signature that reliably differentiates them.

P11-18
PHARMACOMETABOLOMIC OF ASPIRIN REVEALS NEW INSIGHTS ABOUT EFFECTS OF AN OLD DRUG
Sandrine Ellero-Simatos
Division Analytical Biosciences, Leiden Academic Centre for Drug Research, Leiden, The Netherlands; Netherlands Metabolomics Centre, Leiden, The Netherlands
Considerable inter-individual variation in response to aspirin anti-platelet therapy exists, for which underlying mechanisms are still in debate. We used targeted metabolomics in serum samples from healthy volunteers pre- and post- aspirin and correlated metabolic profiles with ex-vivo platelet aggregation measures, a clinically relevant intermediate phenotype for recurrent cardiovascular events. We identified metabolic pathways implicated in variation of response in 2 independent populations and confirmed their relevance in additional functional studies using ex-vivo platelets.

P11-19
MAPPING THE GENETIC DETERMINANTS OF TISSUE METABOTYPES PROFILED BY UPLC-MS IN CARDIOMETABOLIC DISEASES
Jessica Le Ven
Faculty of medicine, Department of Surgery & Cancer, Imperial College London, London, UK
Cardiometabolic disease (CMD) are complex and influenced by both genetics and the environment. In order to identify novel genetic determinants of metabolism underpinning CMD, we studied a panel of recombinant inbred (RI) rat lines using analytical approaches (1H NMR, UPLC-MS) and statistical genetics. We have profiled the metabolome of various organs and biofluids by UPLC-MS to gain new insights on the tissue-specific regulation of metabolic patterns.

P11-20
PROFILING PLASMA AND TISSUE METABOLOMES OF MOUSE MODELS IN DIFFERENT STATES OF DIABETES AND OBESITY
Pieter Giesbertz
Technische Universität München, Freising-Weihenstephan, Bayern, Germany
Type II diabetes develops over a range of stages starting with obesity and insulin resistance and often leading to pancreatic insufficiency. Associations between metabolites and these different stages in human plasma have been described. To identify the origins of critical metabolites marking these stages, we used metabolomics techniques and analyzed plasma and tissue of mouse models representing these stages. Major changes in metabolite groups were found between early and late stages of diabetes.

P11-21
STATE-OF-THE-ART LC-MS BASED LIPIDOMICS APPLIED IN THE STUDY OF LUNG DISEASES
Ruben t’Kindt
RICO - Metablys, Kortrijk, Belgium
The present contribution reports on the application of a powerful lipidomics method combining high resolution reversed-phase liquid chromatography with quadrupole time-of-flight mass spectrometry in the study of lung diseases. Induced lung sputum is shown to be a promising matrix for monitoring lung disease. Using our lipidomics platform, hundreds of lipids, including a vast
amount of sphingolipids, could be accurately identified. It is demonstrated that the lung lipidome is significantly affected in patients suffering from COPD.

P11-22
UNDERSTANDING THE ROLE OF METABOLITES IN HUMAN DISEASES - CLINICAL METABOLOMICS FROM A UNIVERSITY OF BIRMINGHAM PERSPECTIVE
Warwick Dunn
School of Biosciences, The University of Birmingham, Birmingham, UK
Metabolomics is increasingly being applied as an integrative systems biology tool to investigate molecular processes related to human disease. Here, we present clinical metabolomics projects performed at The University of Birmingham: (i) a study of the effect of glucocorticoids variations on endogenous metabolism, (ii) an amniotic fluid study of twin-to-twin transfusion syndrome, and (iii) a lipidomic study of fibroblast cells sampled from different areas of the body to understand metabolic similarities and differences.

P11-23
UNTARGETTED METABOLOMICS OF THE STZ MODEL OF DIABETES IN MULTIPLE TISSUE TYPES: 1 GAS CHROMATOGRAPHY-MASS SPECTROMETRY
Paul Begley
Centre for Advanced Discovery & Experimental Therapeutics (CADET), Central Manchester NHS Foundation Trust & Institute of Human Development, The University of Manchester, Manchester, UK
We present an untargeted GC-MS metabolomic study, comparing the consequences of streptozococin (STZ) - induced diabetes in a rat model, across multiple tissue types. The study identifies differential responses to STZ-induced diabetes when liver, kidney, heart and other tissue types are compared, which may reflect differences in metabolic regulation.

P11-24
13C16-PALMITIC ACID METABOLIZATION INTO CERAMIDE FOR THE DETERMINATION OF CERAMIDE SYNTHESIS IN TYPE 2 DIABETES PATIENTS.
Michel Boutin
Service of Genetics, Department of Pediatrics, Faculty of Medicine and Health Sciences, Universite de Sherbrooke, Sherbrooke, Quebec, Canada
A research protocol was developed to study the metabolism of palmitic acid into ceramide. A heavy palmitic acid tracer (13C16) was administered i.v. to patients with type 2 diabetes and healthy controls. Plasma specimens were collected at different time points to analyze (13C16)-C16:0-ceramide. The samples were purified by liquid-liquid extraction with chloroform followed by a mixed-mode cation exchange cartridge and were analyzed by ultra-performance liquid chromatography coupled to tandem mass spectrometry.

P11-25
UNTARGETTED METABOLOMICS OF THE STZ MODEL OF DIABETES IN MULTIPLE TISSUE TYPES: 2 LIQUID CHROMATOGRAPHY-MASS SPECTROMETRY
Katherine Hollywood
Centre for Advanced Discovery & Experimental Therapeutics (CADET), Central Manchester NHS Foundation Trust & Institute of Human Development, The University of Manchester, Manchester, UK
Herein we present the results of a non-targeted metabolomic-based analysis investigating the compositional variation between control and STZ-induced diabetic rats in multiple tissue types. A robust tissue extraction method had been developed which is transferable between tissue types and compatible with RP-UPLC MS/MS analysis. Our analysis indicates a wide selection of metabolite features which are significantly altered between control and diabetic animals and in addition varying responses per tissue type.

P11-26
THE INTERACTION OF DIET AND AGE TO INFLUENCE THE METABOLIC PHENOTYPE OF ADIPOSE TISSUE
Helena Matthews
University of Cambridge, Cambridge, UK
The influence of high-fat feeding on adipose tissue function at metabolic and epigenetic levels was assessed in mice from a ten-month ageing study. A metabolomics-based approach was used to define changes in lipid metabolism, and epigenetic state was assessed by analysis of DNA methylation and measurement of one-carbon cycle metabolites. Lipid metabolism was significantly altered by high-fat feeding. Investigation into the metabolic link between nutrition and epigenetics in relation to adipose tissue function is on-going.

P11-27
METABOLIC AND MOLECULAR TRAJECTORIES REVEAL THE LOSS OF METABOLIC FLEXIBILITY IN THE EARLY PROCESSES OF FRUCTOSE-INDUCED INSULIN RESISTANCE
Blandine Comte1,2
1INRA, UMR 1019, UNH, CRNH Auvergne, F-63000 Clermont-Ferrand, France, 2Clermont Université, Université d’Auvergne, Unité de Nutrition Humaine, BP 10448, F-63000 Clermont-Ferrand, France
The early phases of insulin resistance development remain unclear. To analyse these processes over time from the gene to the metabolite levels, pair-fed rats with a control or a high-fructose diets were studied over 45 days. Metabolic trajectory observed in urine metabolomics of the fructose-fed rats revealed differences in metabolic flexibility from that of the control (D30-45). At the metabolic level, the fructose-fed phenotype was characterized by an increase (DS) in lipogenic and gluconeogenic potentials.
P11-28
HIGH THROUGHPUT IMPLEMENTATION OF REVERSED-PHASE UHPLC–CSH-QTOF MS/MS FOR COMPREHENSIVE ANALYSIS OF COMPLEX LIPIDS IN BLOOD PLASMA
Brian DeFelice
University of California at Davis, Davis, CA, USA
A high throughput UHPLC-QTOFMS/MS method for the identification and quantification of >400 complex lipids, including mono-, di-, and triacylglycerols, lyso- and diacylglycerophospholipids, sphingolipids, cholesterol esters, ceramides, and fatty acids, was developed for analysis of blood plasma in clinical trials. Class specific internal standards were shown to have a quantitative linear range of 3.5 orders of magnitude. The method was optimized with 15 min run-to-run cycle times, producing information-rich chromatograms with narrow chromatographic peaks (8-17s).

P11-29
LC-MS/MS WORKFLOW FOR NON-TARGETED LIPIDOMICS: VALIDATION AND APPLICATION TO VERY LONG-CHAIN ACYL-COA DEHYDROGENASE DEFICIENT (VLCADD) MICE.
Anik Forest
Institut de Cardiologie de Montréal, Montreal, Qc, Canada
A workflow for non-targeted lipidomics of biological samples using high-resolution HPLC-quadrupole-time-of-flight was validated and applied to a mouse model of fatty acid β-oxidation defect. We found that 92 plasma lipid species differentiated VLCADD from control mice (corrected p<0.05;>2-fold change). The identification by tandem MS was achieved for LC-acylcarnitines, which are known markers of this defect, but that of other lipid species offers the promise of extending our understanding of the biological impact of VLCAD deficiency.

P11-30
EVALUATION OF T2 DIABETES DRUG TREATMENT RESPONSE BASED ON METABOLOME
Ivana Bobeldijk-Pastorova1,2
1TNO EELS, Microbiology and Systems Biology, Zeist, The Netherlands, 2TNO Triskelion, Zeist, Zeist, The Netherlands
A metabolomics approach was used to explore the variability in response to 5-year treatment of 352 screen detected type 2 diabetes patients.
GC-MS analysis of baseline plasma samples resulted in relative concentrations of 173 metabolites for each patient. Patients with a larger dysregulation of glucose metabolism were more prone to decrease in HbA1c status after 5 years. Stratification of the patients based on their medication yielded valuable insights into mechanisms of differential response to treatment.

Theme: Personalised Medicine, Nutrition and General Human Health

P12-1
GLUTAMINE, LACTATE, AND GLUCOSE AS METABOLIC MARKERS FOR METABOLOCIC STUDY USING 1H NUCLEAR MAGNETIC RESONANCE (NMR) SPECTROSCOPY
Hans Kim
1State University of New York Upstate Medical University, Syracuse, NY, USA
NMR is a versatile method to conduct metabolomic study. It has been used for decades for metabolic profiling of cells, tissues, organs, and human bodies utilizing various nuclei in metabolites. NMR-based metabolomic study will lead to discovery of new metabolic markers, therapeutic targets, and ultimately a more thorough understanding of diseases. A study was conducted to test new metabolites such as glutamine, lactate, and glucose for metabolic markers using proton NMR spectroscopy for metabolomic study.

P12-2
FOOD METABOLOMICS: CHARACTERIZATION AND AUTHENTICITY ASSESSMENT OF COFFEE BY HIGH RESOLUTION LC-MS
Verena Tellström
Bruker Daltonik GmbH, Bremen, Germany
Untargeted LC-QTOF-MS based metabolomics enabled differentiation of different coffee types according to their assigned flavour intensity and to readily identify target compounds responsible for the differentiation. The established model was successfully applied to classify coffee samples in a blind experiment.

P12-3
A CE-MS-BASED METABOLOME ANALYSIS OF THE ANTI-DIABETIC EFFECT OF PANAX NOTOGINSENG EXTRACT IN KKAY MICE
Hiroyasu Unemura
LION Corporation, Tokyo, Japan
We already revealed that Panax notoginseng extract including panaxatriol had an anti-diabetic effect on the Type2 model mice and improved fasting and postprandial blood glucose in a human study. Our several studies, to date, suggested that the underlying mechanism of the effect depends on improving insulin resistance, so we used a metabolomics approach by capillary electrophoresis mass spectrometry (CE-MS) to understand the anti-diabetic effect on the KKAY mice.
P12-4
HIGH RESOLUTION MASS SPECTROMETRIC PROFILING IN A STUDY OF THE METABOLISM OF FERULIC ACID IN RAT HEPATOCYTES.
Khaled M.K. Omar
1Omar Al-Mukhtar University, Bayda, Libya, 2Strathclyde University, Glasgow, UK
Metabolism of Ferulic acid and its impact on GSH levels was studied using rat hepatocytes. The most abundant metabolites were the sulphate of FA, glucuronide and glycine conjugates along with novel metabolites resulting from side chain oxidation and reduction of the carboxylic acid group to an alcohol. In addition a glutathione (GSH) adduct was formed which was metabolised to its glucuronide. This adduct could be formed by chemical reaction via nucleophilic addition.

P12-5
METABOLOME ANALYSIS AFTER HYPER- AND HYPOGLYCEMIC FOOD INTAKE IN HEALTHY YOUNG MEN
Hisami Yamanaka-Okumura
Institute of Health Biosciences, University of Tokushima Graduate School, Tokushima city, Japan
Postprandial serum metabolites were investigated by CE-TOFMS. We defined glucose and white rice as hyperglycemic foods, barley as hypoglycemic food, and water as control. Almost amino acids decreased at 4 hours and recovered at 6 hours after glucose and white rice intake, but the change was small after barley intake. Serum metabolites were affected by insulin secretions as results of hyper- or hypoglycemic foods.

P12-6
“WHAT’S WRONG WITH MY DECAF?” - A METABOLOMICS-BASED COMPARISON OF CAFFEINATED AND DECAFFEINATED COFFEE AND ITS IMPLICATIONS FOR ALZHEIMER’S DISEASE.
Kai Lun Chang
1Imperial College London, London, UK, 2National University of Singapore, Singapore, Singapore
Decaffeination process removes more than just caffeine from coffee, and some of these components are potential therapeutic agents against Alzheimer’s disease (AD). This is the first study to globally measure and compare small-molecule metabolites present in caffeinated and decaffeinated coffee. 73 discriminant metabolites (P<0.0001) differentiated between both coffee types and a majority of them have important implications for AD. Our findings provide important revelations about therapeutic roles of different coffee types in AD.

P12-7
ANALYSIS OF 1071 SERUM SAMPLES WITH LC-ESI/MS REVEALS AN AGE DEPENDENT LINEAR DECREASE OF DEHYDROEPIANDROSTERONE SULFATE
Aigar Ottas
University of Tartu, Tartu, Tartumaa, Estonia
In collaboration with The Centre for Translational Genomics, University of Tartu, Estonia; 1071 serum samples of voluntary men and women were analyzed with LC-ESI/MS and the obtained data was correlated with age to reveal age-dependent metabolites. The m/z value of 368 showed the highest correlation and was identified as dehydroepiandrosterone sulfate (DHEAS) - a known natural steroid prohormone that has been shown to characterize many different diseases. DHEAS measurement might characterize a subject’s biological age.

P12-8
URINARY METABOLOMICS ANALYSIS: WORKFLOW OF A POWERFUL TOOL FOR THE SCREENING OF ANABOLIC PRACTICES IN CATTLE
Cristina da Costa Jacob
ONIRIS, École nationale vétérinaire, agroalimentaire et de l’alimentation Nantes-Atlantique, Laboratoire d’Étude des Résidus et Contaminants dans les aliments (LABERCA), Nantes, France
The purpose of the present study was to set up and assess a mass spectrometry metabolomics strategy as a new tool to screen for fraudulent anabolic treatments in cattle and demonstrate the feasibility of such approach. Therefore, an urinary untargeted metabolomics approach based on liquid chromatography (reverse-phase and HILIC) coupled to high resolution mass spectrometry (LC-HRMS) was developed and applied for the screening of trenbolone acetate/ estradiol combinations in cattle.

P12-9
FOOD METABOLOMICS - VALIDATION STRATEGIES FOR MARKERS OF COMMON FOODS
Lars Ove Dragsted
University of Copenhagen, Frederiksberg, Denmark
Robust markers of food intake are necessary to reveal food-related health effects. We have explored a number of dietary intervention studies for urine markers of foods and food components. Cross-validation or separate test sets were used for primary validation. Additional validation was performed in independent studies with a different design. Only 20-30% of the markers could be confirmed. Additional demands on sensitivity, specificity, dose-response and individual variability further reduced the set. Validation strategies will be discussed.
P12-10
TRACING THE STAGES OF CHRONIC KIDNEY DISEASE (CKD) USING "H NMR-BASED SERUM METABOLITE PROFILING
Yong-Kook Kwon
Korea Basic Science Institute, Seoul, Republic of Korea
"H NMR-based metabolomics was employed to investigate the altered metabolic pattern in serum from patients with chronic kidney disease (CKD). Each type of CKD patients was divided into 3 stages by eGFR and was investigated using global profiling by "H-NMR coupled with PLS-DA. PLS-DA model showed the 70% accuracy rate. Creatinine, pyruvate, leucine, urea, and trimethylamine oxide (TMAO) were important variables for determining stage of CKD. Creatinine, TMAO and urea were consistently increased.

P12-11
PHYTOHUB: A NEW DATABASE DEDICATED TO DIETARY PHYTOCHEMICALS AND THEIR HUMAN METABOLITES FOR NUTRITIONAL METABOLICOMICS
Claudine Manach
Human Nutrition Unit, UMR 1019 INRA / University of Auvergne, Clermont-Ferrand, France
Identification of phytochemical metabolites from non-targeted analyses is often a bottleneck in metabolomics workflows. Here we describe the design and construction of PhytoHUB, an open-access web database dedicated to the phytochemical part of the food metabolome. The database will be the first to collate comprehensive information on phytochemical metabolites and their physico-chemical and spectroscopic properties. PhytoHUB should be an invaluable resource for all those investigating the links between exposure to dietary phytochemicals and health.

P12-12
IMPLEMENTATION OF METABOLOMICS TO THE HORSE BIOLOGICAL PASSPORT: MONITOTING OF GROWTH FACTORS ADMINISTRATIONS IN URINE BY UHPLC-HRMS.
Benoit Loup
Laboratoire des Courses Hippiques (LCH), Verrieres le Buisson, France
In horseracing, the use of growth factors is strictly banned. Although routine analyses have already been developed to detect these molecules, metabolomics could enable to improve doping control. Thus a strategy has been carried out consisting in the development of a statistical model which allows the suspicion of the use of growth hormones and IGF-1 by a metabolomic approach (UHPLC-HRMS), this model is then applied in a longitudinal study to establish the horse biological passport.

P12-13
THE fRAILL PROJECT - USING METABOLOMICS AS A TOOL FOR INVESTIGATING FRAILTY, RESILIENCE AND INEQUALITY IN LATER LIFE
Nicholas Rattray
The University of Manchester, Greater Manchester, UK
The fRAILL Project is a multilayer analysis of socioeconomic and biological determinants to develop an integrated understanding of processes leading to positive and negative outcomes in later life in the context of social inequalities. UHPLC-FTMS alongside GC-MS metabolomics on blood sera will contribute to genetic GWAS and empirical data in an attempt to determine a potential biological link to the wellbeing-frailty axis.

P12-14
POSTPRANDIAL FATTY ACID-SPECIFIC CHANGES IN CIRCULATING OXYLIPINS IN LEAN AND OBESE MEN AFTER HIGH FAT CHALLENGE TESTS
Katrin Strassburg¹,2
Leiden Academic Centre for Drug Research, Leiden, The Netherlands; Netherlands Metabolomics Centre, Leiden, The Netherlands
This study is the first demonstrating that circulating oxylipins are acutely affected after high-fat meal challenges. In a double-blind randomized cross-over challenge we characterized the postprandial oxylipin response after high fat challenges in lean and obese men, receiving three high-fat milkshakes differing in the composition of fatty acid types, namely saturated, monounsaturated and n-3 polyunsaturated fatty acids. Until now it was unclear which oxylipins appear in circulation after high-fat meals differing in fatty acid composition.

P12-15
IMPACT OF EXERCISE ON THE PLASMA METABOLOMЕ OF PATIENTS SUFFERING FROM MULTIPLE SCLEROSIS
Gwenaelle Le Gall
Institute of Food Research, Norwich Research Park, Norwich, NR4 7UA, UK
We have conducted a metabolomic analysis on the blood plasma from MSc patients to evaluate if physical activity has an impact on the plasma metabolome and to identify any associated biomarkers. Significant changes in several intermediates and end-products of beta-oxidation and glycolysis were observed after intervention and xanthine levels were lowered by exercise. This outcome opens an encouraging path of research focusing on the effect of exercise on the purine metabolism in MSc patients.
P12-16
APPLICATION OF QUANTITATIVE METABOLOMICS IN HUMAN MATERNAL, PRENATAL AND NEONATAL DISEASE BIOMARKER STUDIES
Rupasri Mandal
1University of Alberta, Edmonton, Alberta, Canada

Applications of metabolomics in disease biomarker studies are presented. TMIC, Canada’s National Metabolomics Platform, specializes in performing quantitative metabolomics using a wide range of technologies. Recently, TMIC has participated in several disease biomarker studies such as first trimester prediction of early-/late-onset preeclampsia and neonatal Hypoxic Ischaemic Encephalopathy. These studies will be presented in detail. Here we intend to show the potential that metabolomics holds in contributing to the understanding of maternal and neonatal health.

P12-17
GLOBAL PROFILING OF THE SKELETAL MUSCLE METABOLOME: METHOD DEVELOPMENT AND VALIDATION FOR THE ASSESSMENT OF METABOLIC CHANGES IN INTERVENTION STUDIES
Rob Vreeken1 2
1Netherlands Metabolomics Centre, Leiden, The Netherlands, 2Leiden Amsterdam Centre for Drug Research, Analytical Biosciences, Leiden, The Netherlands

Skeletal muscle tissue is the largest insulin-sensitive tissue in the body and a major user of glucose. Understanding energy metabolism in muscle tissue provides insight into the mechanisms governing muscle in health and/or disease. To this end, we have developed and validated an extraction method to detect and quantify a broad range of metabolites (organic acids, amines, nucleotides/co-enzymes, acyl-carnitines and oxylipins) from muscle tissue biopsies.

P12-18
TARGETED AND NON-TARGETED QUANTITATIVE METABOLOMICS USING MULTI-PLATFORM APPROACH
Tamara Lim
University of Alberta, Edmonton, Alberta, Canada

TMIC, Canada’s national metabolomics platform, specializes in performing quantitative metabolomics on various samples using a wide range of technologies. Recently, TMIC developed several quantitative assays for vitamins, lipoproteins, volatiles, oxylipins and steroids. TMIC also reported comprehensive metabolomic characterization of human biofluids such as measurement of 4229 metabolites in serum, 419 metabolites in cerebrospinal fluid and 2882 metabolites in urine. Description of TMIC’s new assays along with their applications in various fields will be presented.

P12-19
COMPARISON OF THE URINE METABOLOMES OF STRATIFIED SU.VI.MAX2 SUBJECTS TO IDENTIFY BIOMARKERS OF FRUIT AND VEGETABLE INTAKE.
Yoann Fillâtre
Human Nutrition Unit, UMR1019 INRA/University of Auvergne, Clermont-Ferrand, France
SU.VI.MAX2 subjects were stratified by consumption for 20 plant foods and their urine profiled by LC-QTof. A clear discrimination was observed for most foods, particularly for 10 foods that are frequently consumed and rich in phytochemicals. The low and high consumption of total F&V were also clearly distinguished. Identification of biomarkers is ongoing. The study provided useful insight into the conditions for success of the approach for rapid discovery of a range of nutritional biomarkers.

P12-20
METABOLOMICS BASED IDENTIFICATION OF PATTERNS OF DIETARY INTAKE
Eibhlin Carr
Institute of Food and Health, University College Dublin, Dublin, Ireland

In recent years, biomarkers have been suggested as a means for unbiased and objective measure of dietary intake and metabolomics has an emerging role in the identification of novel biomarkers. The objective of the research was to investigate the relationship between dietary intakes patterns and metabolic profiles. We demonstrate that urinary metabolite clusters are linked to dietary patterns.

P12-21
THE ACCUMULATION OF CEREAL BRAN DERIVED METABOLITES IN PLASMA AND TISSUES AND IMPACT ON ENDOGENOUS METABOLISM IN TWO HUMAN DIETARY STUDIES AND AN ANIMAL FEEDING TRIAL
Kati Hanhineva
University of Eastern Finland, Department of Clinical Nutrition, Kuopio, Finland

LC-MS metabolite profiling was used to characterize composition of human plasma after consumption of bran to study the circulating phytochemical metabolites and to investigate how the bran-rich diet is reflected in endogenous metabolism. Various phytochemical classes were observed, and several endogenous pathways were affected with varying response postprandially and at fasting. Additionally, samples from mouse trials have been profiled and interesting phytochemical accumulations have been observed in various organs, accompanied with endogenous metabolite changes.

P12-22
EFFECT OF NUTRITIONAL INTERVENTION AND ETHERLIPID DEPLETION ON LIPID METABOLISM IN MOUSE MODEL
Heli Nygren
1VTT Technical Research Centre of Finland, Espoo, Finland

We have investigated how lipidomic profiles are affected by etherlipid depletion and nutritional interventions (HFD and HFD+ω-3 FA:s). Global lipidomic profiles were studied in plasma, plasma HDL fractions and tissues of gnpat KO mice using a LC-MS platform. In addition to the depletion of ether lipids, upregulation of certain lipids was observed in gnpat KO mice. Dietary lipid composition affected the levels of many etherlipids showing that they are also regulated by diet.
P12-23
STUDY OF THE METABOLOMIC CHANGES IN RED WINES DURING AGING UNDER DOMESTIC AND CELLAR CONDITIONS THROUGH AN UNTARGETED-TARGETED METABOLOMIC WORKFLOW
Panagiotis Arapitsas
Fondazione Edmund Mach, San Michele all’Adige, Italy
This project evaluated the chemical implications of the appropriate storage of red wines by an untargeted-targeted workflow, highlighting a number of known and novel metabolites as markers. The data obtained following the kinetic of the markers over 24 months at two conditions of storage (cellar vs domestic), allowed us to build hypothesis about the metabolic changes in wine during storage, which can be useful for improving both the production and storage of red wines.

P12-24
BIOMARKERS OF DIETARY INTAKE - A LIPIDOMIC APPROACH
Aoife O’Gorman
Institute of Food and Health, University College Dublin, Dublin, Ireland
The aim of this study was to use a statistical approach in an attempt to link lipidomic profiles with dietary data to identify biomarkers of dietary intake. Six lipidomic patterns were identified with MUFA, PUFA and SFA intake having strong relationships with LP1 (lipidomic pattern 1). MUFA intake had a significant relationship with a glycerophospholipid and a sphingolipid. PUFA had a significant relationship with a phosphoethanolamine, whilst SFA had a significant relationship with two sphingomyelins.

P12-25
A STUDY OF METABOLOMIC CHANGES IN MATERNAL URINE BETWEEN 13-18 WEEKS OF GESTATION USING ZWITTER-IONIC HYDROPHILIC INTERACTION LIQUID CHROMATOGRAPHY COUPLE TO ION TRAP TIME OF FLIGHT MASS SPECTROMETRY
Drupad Trivedi1,2
1University of Manchester, Manchester, UK, 2Middlesex University, London, UK
The dynamic changes in maternal metabolism during pregnancy could be monitored via maternal bio-fluids. On comparison of metabolomics data from HILIC-MS analysis of normal pregnancy urine samples from 13-18th week of gestation it was found that five key metabolites were strongly expressed in pregnancy from start of second trimester compared to mid second trimester. No other published study is known to have used metabolomics as a tool for biomarker discovery in pregnancy urine.

P12-26
PATTERNS OF TIME SINCE LAST MEAL REVEALED BY SPARSE PCA IN AN OBSERVATIONAL LC-MS BASED METABOLIC STUDY
Gözde Güdeniz
University of Copenhagen, Frederiksberg 1958, Denmark
This study demonstrates the application potential of sparse PCA (SPCA) as a variable selection tool in a metabolomics study. The dataset was compromised of LC-MS plasma profiles of 270 subjects and focus was extracting patterns related to time passed since the subjects had their last meal (TSLM). SPCA provided clear variable selection advantages over PCA. Also, SPCA extracted inter-correlated variables from different biochemical classes in different sparse components, i.e. amino acids and lyso-lipids.

P12-27
NMR METABOLOMICS TO STUDY THE REGULATION OF ENERGY METABOLISM ON CHICKEN LINES DIVERGENT FOR LOW OR HIGH ABDOMINAL FAT DEPOSITION
Julie Lalande
CNRS, Chimie et Interdisciplinarité: Synthèse, Analyse, Modélisation (CEISAM), UMR 6230, Faculté des Sciences, Université de Nantes, BP 92208, 2 rue de la Houssinière, F-44322 Nantes Cedex 03, France
NMR metabolomics is suitable for studying the regulation of energy metabolism on chicken lines divergent for low or high abdominal fat deposition. It is shown that plasma metabolic profiles are different in chickens fed with high and low fat diets. New information are thus obtained on circulating nutrients, which may help in elucidating key regulators associated to variations in body fat content.

P12-28
RESVERATROL METABOLISM IN A NON-HUMAN PRIMATE, THE GREY MOUSE LEMUR Microcebus murinus BY ULTRA HIGH PERFORMANCE LIQUID CHROMATOGRAPHY-QUADRUPOLE TIME OF FLIGHT
Marie-Claude Menet
Université Paris Descartes, EA 4463, Paris, France
Microcebus murinus is a non-human primate used to study the ageing process. However, no information about resveratrol metabolism is available in this lemur. Resveratrol and its metabolites were qualitatively and quantitatively analysed in Microcebus plasma by Ultra High Performance Liquid Chromatography on line with a Quadrupole-Time Of Flight mass spectrometer used in full scan mode. Free resveratrol is measurable for several hours in Microcebus plasma and its two main metabolites are trans-resveratrol-3-O-glucuronide and trans-resveratrol-3-sulfate.

P12-29
THE PHENOL-EXPLORER DATABASE ON THE POLYPHENOL METABOLOME AS AN AID TO IDENTIFY NOVEL BIOMARKERS OF DIETARY EXPOSURE FOR NUTRITIONAL EPIDEMIOLOGY
Augustin Scalbert1
1International Agency for Research on Cancer (IARC), Nutrition and Metabolism Section, Biomarkers Group, Lyon, France
Thousands of metabolites found in blood or urine are directly derived from foods after digestion. They constitute the so-called food metabolome. We report the development of Phenol-Explorer, a specialist database on 500 dietary polyphenols and 383 metabolites with chemical structures, concentrations in biofluids and precursor-metabolite specificity. This information is used to identify in complex urine or plasma metabolic profiles the most useful biomarkers of dietary exposure.
P12-30
QUALITATIVE AND QUANTITATIVE DIFFERENTIATION OF SPECIES FROM VACCINIUM BY NMR SPECTROSCOPY IN AUTOMATION
Christian Fischer
Bruker BioSpin GmbH, Rheinstetten, Germany
The fruit of Vaccinium are widely eaten and touted for their health benefits. It is important to have methods to verify the identity and purity of Vaccinium extracts. NMR spectroscopy is a powerful tool for characterizing mixtures in full automation. Discrimination of different species, absolute identification & quantification of key compounds and verification if the determined parameters are in the allowed range is the basis for the quality control of a sample.

P12-31
IS THE SLEEP APNEA DIFFERENT FROM COPD? THE METABOLOMICS STUDIES OF SERUM AND URINE BY 1H NMR METHOD
Adam Zabek
Department of Chemistry, Wroclaw University of Technology, Wroclaw, Poland
In these studies the serum and urine from patients suffering sleep apnea (OSA) and COPD were investigated by means of NMR spectroscopy and chemometric tools. Results of OPLS-DA analysis showed that both bio-fluid contain information supporting the differences between groups of patients.

P12-32
A NMR BASED METABOLOMIC STUDY ON THE EFFECTS OF FATTY ACIDS INFLUENCE ON LIVER METABOLISM DURING OVERFEEDING
Albert Elmsjö
Department of Medicinal Chemistry, Division of Analytical Pharmaceutical Chemistry, Uppsala University, Uppsala, Sweden
Gaining weight and especially fat accumulation in liver has many adverse metabolic consequences, which makes it an excellent target for metabolic studies. In this study, we applied a comparative metabolomic analysis to investigate the consequences of increased intake of saturated or polyunsaturated fatty acids. The overall goals for the study were to investigate if there were any profile differences between the two study groups and also, if possible, correlate specific metabolites with MRI assessments.

P12-33
INTEGRATING FFQ AND BIOMARKER TECHNOLOGY: ARE ALL FOODS APPROPRIATE TARGETS FOR BIOMARKERS?
Amanda J Lloyd
Aberystwyth University, Aberystwyth, UK
The discovery and validation of food exposure biomarkers has proved to be complex and to date putative biochemical markers are available for only a small number of food components. We describe a data-driven procedure combining diet information with metabolite fingerprinting by mass spectrometry and supervised multivariate data analysis to discover urine biomarkers indicative of habitual exposure to different foods.

P12-34
METABOLOMICS IN GENOME-WIDE ASSOCIATION STUDIES: REVEALING GENE-METABOLITE-DISEASE LINKS
Rico Rueedi1,2
1University of Lausanne, Lausanne, Switzerland, 2Swiss Institute of Bioinformatics, Lausanne, Switzerland
While still in its infancy, the use of metabolic profiles in genome-wide association studies has improved the detection of, and provided biological context to, the sometimes poorly understood effects of genetic variants on clinical phenotypes. Our study, involving untargeted urine metabolites, revealed two novel gene-metabolite associations, each coupled to a suggestively causal metabolite to disease link.

P12-35
PREDICTION OF METABOLIC PROFILE OF POLYPHENOLS AFTER WINE AND WINE PRODUCTS INTAKE USING THE PHENOL-EXPLORER DATABASE
Mireia Urpi-Sarda1
1Biomarkers and Nutrimetabolomic Group, INSA, Nutrition and Food Science Department, Pharmacy Faculty, University of Barcelona, Av. Joan XXIII s/n, 08028, Barcelona, Spain
The consumption of red wine has been associated to health benefits. A wide wine polyphenol metabolome (97 metabolites) has been identified in biofluids after wine intake and pure compounds, as wine constituents, through Phenol-Explorer-2.0. This has allowed developing a global pathway and enabling analysis of the role of metabolites as biomarkers of wine consumption. This allowed displaying the whole metabolite spectrum that could be the key to understand the health effects of its consumption.
P13-1
METABOLIC FINGERPRINTS OF SERUM, BRAIN AND LIVER ARE DISTINCT FOR MICE WITH CEREBRAL AND NON-CEREBRAL MALARIA: A $^1$H NMR SPECTROSCOPY BASED METABONOMIC STUDY
Haripalsingh Sonawat
Department of Chemical Sciences, Tata Institute of Fundamental Research, Homi Bhabha Road, Mumbai-400005, India
$^1$H NMR-based metabolomics was used to investigate the metabolite alterations in serum, brain and liver in mice infected with *Plasmodium berghei* ANKA and exhibiting symptoms of cerebral malaria (CM) in comparison to the animals which had non-cerebral malaria or uninfected control. The mice with CM had differential changes in levels of triglycerides, glycerophosphorylcholine, myo-inositol, histamine and glutamine and showed perturbed ammonia detoxification, lipid and choline metabolic pathways.

P13-2
MOLLICUTES ADAPTATION TO LOW pH CONDITIONS
Anna Vanyushkina
SRI PCM FMBA Russian Federation, Moscow, Russia
Determining the change of composition of metabolites completed with proteomics and transcriptomics data provides information about the processes of cell regulation and adaptation mechanisms to environmental stresses. Our research object is a Mollicutes, unique bacteria that have a reduced genome, and simplified metabolic pathways. We present measurement of a hundred Mollicutes metabolites, including components of sugar, amino acid, and nucleotide metabolism in normal and low pH conditions, complemented by data from transcriptomics studies.

P13-3
THE METABOLIC INTERPLAY BETWEEN PLANTS AND PHYTOPATHOGENS.
Dirk Walther
Max Planck Institute for Molecular Plant Physiology, Potsdam-Golm, Germany
We studied the interaction of plant-pathogen pairs at the metabolic level. We selected five plant-pathogen pairs, for which both genomes were fully sequenced, and constructed the corresponding genome-scale metabolic networks. We present theoretical investigations of the metabolic interactions and quantify the positive and negative effects a network has on the other when combined into a single plant-pathogen pair network.

P13-4
SERUM METABOLOME CHANGES IN ADULT PATIENTS WITH PRIMARY DENGUE INFECTION
Liang Cui
Interdisciplinary Research Group in Infectious Diseases, Singapore-MIT Alliance for Research & Technology, Singapore, Singapore
Dengue virus is the most widespread arbovirus and little is known about the underlying molecular mechanisms. Serum metabolic profiling was performed on a cohort of dengue patients with three sampling time points at early febrile, defervescence, and convalescent stages via mass spectrometry-based analytical platforms. Dozens of differential metabolites were identified and major perturbed metabolic pathways included fatty acid biosynthesis and β-oxidation, phospholipid catabolism, steroid hormone pathway, etc. This advances our understanding on host and dengue virus interactions.

P13-5
TOWARDS IDENTIFYING THE FULL METABOLOME OF THE PROTOZOA PARASITE LEISHMANIA BY USING HIGH RESOLUTION LIQUID CHROMATOGRAPHY MASS SPECTROMETRY
Lijie Wang
University of Strathclyde, Glasgow, UK
Metabolomic profiling of the parasite *Leishmania* was carried out using hydrophilic interaction chromatography with high resolution mass spectrometry detection. The analysis so far has firmly identified >400 polar and non-polar metabolites by comparison with 200 authentic standards and by using MS² experiments to aid in identification of compounds where no standards were available. Metabolites of particular interest within the parasite were quantified by spiking with standards for the compounds over a calibration range.

P13-6
MULTI-PLATFORM METABOLIC FINGERPRINTING OF CANINE VISCERAL LEISHMANIASIS
Mariana Santos¹,²
¹Center for Metabolomics and Bioanalysis (CEMBIO), Faculty of Pharmacy, Universidad CEU San Pablo, Campus Montepino, Boadilla del Monte, Madrid, Spain, ²Departamento de Análises Clínicas e Toxicológicas, Faculdade de Farmácia, Universidade Federal de Minas Gerais, Belo Horizonte, Minas Gerais, Brazil
Visceral leishmaniasis (VL) is a serious public health problem. Dogs are the main reservoir of parasites and culling of seropositive animals is one of the control measures. Early diagnosis is still a problem and many aspects of disease pathogenesis are unknown. Herein, dog samples (plasma and urine) were analyzed through a multi-platform metabolomic approach. Metabolic differences between positive and negative samples were investigated aiming to identify pathways and metabolites as potential biomarkers for VL diagnosis.
P13-7
DIAGNOSIS OF ACUTE TYPHOID FEVER BY METABOLOMICS
Elin Näsström
Department of Chemistry, Computational Life Science Cluster, CLiC, Umeå University, Umeå, Sweden
There is a need for a rapid, more sensitive and specific diagnostic method for typhoid fever. Here human serum samples have been analyzed with GCxGC/TOF-MS for investigation of metabolic profiles in the search for potential diagnostic biomarker patterns for typhoid fever. Multivariate OPLS-DA models reveal a clear separation between typhoid fever and control (no detected infection) samples and interestingly, also between two closely related bacterial species causing typhoid fever (Salmonella Typhi and Salmonella Paratyphi A).

P13-8
QUANTITATIVE HIGH RESOLUTION 1H NMR URINALYSIS FOR ALGORITHMIC DIAGNOSIS OF URINARY TRACT INFECTION USING AN AUTOMATIC ANALYZER
Chun-yiu Law
The University of Hong Kong, Hong Kong, China
A new diagnostic algorithm for urinary tract infection (UTI) was proposed using urine acetic acid and trimethylamine concentrations. This algorithm could identify 97% bacterial UTI, 82% Escherichia coli-associated UTI and 86% non-UTI control with a predicted 74% reduction in workload for urine culture. We concluded urine acetic acid is a neglected metabolite for the diagnosis of UTI. We envisaged NMR based method for urine acetic acid will simplify the diagnosis of UTI and EC infection.

P13-9
METABOLOMICS STUDY OF SEPTIC SHOCK: FROM NMR AND MS DATA TO MORTALITY PREDICTION
Beata Mickiewicz
Bio-NMR Centre, Department of Biological Sciences, University of Calgary, Calgary, AB, Canada
Multivariate statistical analysis was applied to compare data obtained for human serum samples by 1H NMR, GC-MS and LC-MS. Clear separation was observed between septic shock patients and intensive care unit (ICU) controls without infection and between survivors and non-survivors. The predictive metabolomics model shows excellent accuracy compared to the conventional ICU scoring systems. Our results indicate that metabolomics could become a useful tool for the diagnosis and prognosis of septic shock in ICUs.

P13-10
COMPLETE PROFILING OF THE TRICHOMONAS VAGINALIS METABOLOME USING LC-MS, LC-MS/MS AND GC-MS AND ITS USE AS AN ANALYTICAL STANDARD
Gavin Blackburn
University of Strathclyde, Glasgow, UK
Overview: LC-MS, LC-MS/MS and GC-MS analysis of Trichomonas vaginalis allowing for mapping of the metabolome and identification of novel metabolites. Initial putative identifications were confirmed using comparison to standards and MS/MS where applicable. Current progress on the different analyses using these methods is shown.

P13-11
DIFFERENCE IN THE METABOLOME BETWEEN ESCHERICHIA COLI ISOLATED FROM PATIENTS WITH PYELONEPHRITIS AND CHOLANGITIS
Andy Chan
Department of Microbiology, The University of Hong Kong, Hong Kong
In this study, we have successfully identified 20 metabolites which are only present predominantly in blood culture E. coli isolates from patients with pyelonephritis but not isolates from patients with cholangitis or stool E. coli isolates

P13-12
METABOLOMICS ANALYSIS OF THE ENTOMOPATHOGENIC FUNGI FROM THE ISARIA FUMOSOROSEA SPECIES COMPLEX
Petr Simek
Biology Centre, Czech Academy of Sciences, Ceske Budejovice, Czech Republic
First metabolomic analysis of primary and secondary metabolites in mycelium of two entomopathogenic fungal strains from the Isaria fumosorosea species complex by seven analytical GC & MS platforms covering nonchiral & chiral profiling of L,D amino acids & organic acids, amines & purine & pyrimidine bases, sugars, sterols & steroids, phospholipids& glycerides, sugars, secondary metabolites & pigments in the extracted fractions of variable polarity and in their hydrolysates.

P13-13
IMPROVED METHODOLOGY FOR QUANTITATIVE SRM BASED LC-MS/MS FOR THE ANALYSIS OF AcylCoAs FOR RATIONAL DESIGN OF SYNTHETIC BIOLOGY PROCESSES
Laurakay Bruhn
Agilent Laboratories, Santa Clara, CA, USA
We present a rapid, reproducible, sensitive method for Acyl CoAs based on LC-MS/MS involving a novel TCA extraction methodology that allows accurate quantitation of 10 AcylCoA derivatives in 5 minutes with a run-to-run cycle time of 8 minutes and a detection limit of approximately 100fg per component. We are using this method to characterize the levels of AcylCoAs in E.coli cellular extracts with an engineered exogenous pathway transforming AcetylCoA to Butanol.
P13-14
METABOLOMICS-BASED ASSESSMENT OF AQUATIC ANIMAL HEALTH
Mark Styczynski
Georgia Institute of Technology, Atlanta, GA, USA
Metabolomics is a promising, yet underexploited, method to advance our understanding of a variety of aquatic species-specific maladies, as well as our ability to monitor and diagnose aquatic animal health. Here, we present our work in two different aquatic animal systems: the bottlenose dolphin and the Atlantic salmon. We studied the metabolic impacts of pathogenic infections and inappetance on plasma metabolite profiles, gaining significant novel biological insight into each system and identifying potential diagnostic biomarkers.

P13-15
IMPACTS OF PARASITISM IN THE ENDANGERED FLORIDA SCRUB JAY.
Berin Boughton1,2
1The University of Melbourne, VIC, Australia, 2Metabolomics Australia, VIC, Australia
The Florida Scrub-Jay (FSJ; Aphelocoma coerulescens) is an endangered species with less than 2500 breeding pairs left in the wild. Greater than 60% of the FSJ population is infected with parasitic worms whose filarids are found in blood and 20% are infected by trypanosome. This study used metabolomics approaches to examine host metabolism with the aim of combining identified changes in metabolism with demographic and environmental data to determine affects upon breeding success and survival.
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<td>Waters Corporation: New Techniques and Approaches in Metabolomics Sciences</td>
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<td>14.00 – 16.00</td>
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<td>Parallel Session 1B: Mass Spectrometry and NMR in Metabolomics</td>
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<td>12.10 – 13.10</td>
<td>AB SCIEX UK: Workflow Strategies for Metabolomics and Lipidomics</td>
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<td>Bruker Corporation: Solving the “Metabolomics puzzle” by Integrated NMR and MS Solutions</td>
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<td>Thermo Fisher Scientific: See the Real Difference in Metabolomics</td>
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<td>Parallel Session 5A: Metabolomic Profiling in Neuroscience</td>
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<td>Parallel Session 5B: Environmental Metabolomics</td>
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<tr>
<td>15.10 – 16.30</td>
<td>The Complementary Roles of Metabolomics and Proteomics in Systems Biology</td>
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<td>13.30 – 15.10</td>
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<td>18.00 – 19.00</td>
<td>Dinner/Ceilidh</td>
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The Metabolomics Society is dedicated to promoting the growth, use and understanding of metabolomics in the life sciences. Metabolomics is a newly emerging field of "omics" research concerned with the comprehensive characterization of the small molecule metabolites in biological systems. It can provide an overview of the metabolic status and global biochemical events associated with a cellular or biological system. As such, it can accurately and comprehensively depict both the steady-state physiological state of a cell or organism and of their dynamic responses to genetic, abiotic and biotic environmental modulation.

The Metabolomics Society is an independent, non-profit organization, governed by a Board of Directors composed of dedicated members of the metabolomics community but ultimately responsive to its members. The Metabolomics Society’s vision is to become the premier organization devoted to the development of metabolism-based research. Constituted in 2004, the Metabolomics Society now has more than 500 members in more than 20 countries and publishes its own journal: Metabolomics.

Our Mission
1. To promote the growth and development of the field of metabolomics internationally
2. To provide the opportunity for collaboration and association among the workers in that science and in related sciences and connections between academia, government and industry in the field of metabolomics
3. To provide opportunities for presentation of research achievements and creation of workshops
4. To promote the publication of meritorious research in the field

Society:
www.metabolomicsociety.org

Journal:
www.springer.com/life+sciences/biochemistry+%26+biophysics/journal/11306
Metabolomics 2013
9th Annual International Conference of the Metabolomics Society
1 - 4 July 2013
Scottish Exhibition & Conference Centre (SECC), Glasgow, Scotland, UK
www.metabolomics2013.org

Final Programme & Abstract Book

Metabolomics 2014
Tenth Annual International Conference of the Metabolomics Society
The Official Joint Conference of the Metabolomics Society and Plant Metabolomics Platform
June 23-26, 2014, Tsuruoka, Japan.

Health, medical, pharmaceutical, nutritional, agricultural, microbial, bioenergy, environmental and plant sciences meet biochemical, analytical and computational technologies.
Early registration and abstract submission due March 31, 2014.

http://metabolomics2014.org