METABOLOMICS 2016

12TH ANNUAL CONFERENCE OF THE METABOLOMICS SOCIETY

METABOLOMICS 2016

12TH ANNUAL CONFERENCE OF THE METABOLOMICS SOCIETY

June 27-30, 2016
Dublin, Ireland

METABOLOMICS SOCIETY

Monday

	The Auditorium	The Liffey A	The Liffey B
09:00 19:00	**Registration Open**		
10:30 - 12:00	**Workshop 1:** EMN Career Session	**Workshop 2:** Data Sharing and Standardisation	**Workshop 3:** Metabolite Profiling in Population-Based Studies
12:00 - 13:30	**Box Lunch Available - Level 1 & Level 3 Foyer**		
12:15 - 13:15		Sponsor Presentation SCIEX	Sponsor Presentation Bruker
13:30 - 15:00	**Workshop 4:** EMN The Importance of Experimental Design	**Workshop 5:** metaRbolomics: The R Toolbox for Metabolomics	**Workshop 6:** Computational Workflows and Workflow Engines
15:00 - 16:30	**Free Time**		
16:30 - 17:00	**Opening Ceremony**		
17:00 - 18:00	**Opening Plenary Session** Prof Jeremy Nicholson		
18:00 - 19:00	**Welcome Reception in Exhibit Hall**		

Tuesday

	The Auditorium	The Liffey A	The Liffey B
08:00 - 19:00	**Registration Open**		
07:45 - 08:30		Sponsor Breakfast Shimadzu Europa GmbH *Advance sign-up required*	
08:50 - 09:50	**Plenary Session 2** Prof Luke O'Neill		
09:50 - 10:30	**Break and Posters - Exhibit Hall**		
10:30 - 12:00	Model Organisms	Biomarkers in Nutrition Research	CVD/Diabetes
12:00 - 13:30	**Lunch and Posters - Exhibit Hall**		
12:15 - 13:15		Sponsor Presentation Agilent Technologies	Sponsor Presentation Waters
13:30 - 15:00	Network and Pathway Analysis for Metabolomics	Metabolic Phenotyping in Health	Crop Quality Improvement and Food Sustainability
15:00 - 15:30	**Break and Posters - Exhibit Hall**		
15:30 - 17:00	Nutrition and Metabolism	Environmental Metabolomics	Advances in Statistical Tools
17:15 - 18:45	**Poster Session 1 - Exhibit Hall:** Posters #1-244		
19:00 - 20:30			**EMN Reception** *Advance Sign-Up Required*

Wednesday

	The Auditorium	The Liffey A	The Liffey B
08:30 - 18:00	**Registration Open**		
08:50 - 09:50	**Plenary Session 3** Prof Ines Thiele		
09:50 - 10:30	**Break and Posters - Exhibit Hall**		
10:30 - 11:50	Early Career Session 1		Early Career Session 2
11:50 - 13:30	**Lunch and Posters - Exhibit Hall**		
12:10 - 13:10		Sponsor Presentation Biocrates Life Sciences AG	Sponsor Presentation Thermo Fisher Scientific
13:30 - 15:00	Identification of Metabolites Applying MS and NMR	Green Systems Biology	Metabolomics Profiling in Cancer
15:00 - 15:30	Break and Posters - Exhibit Hall		
15:30 - 17:00	Foodomics and Food Quality	Impact of Metabolomics in Clinical Medicine 1	Computational MS
17:00 - 18:30	**Poster Session 2 - Exhibit Hall:** Posters #245-490		
19:30 - 23:30	**Conference Dinner - Croke Park** Bus loading at the CCD begins at 19:15 for a 19:30 departure (See page 29 for additional details)		

Thursday

	The Auditorium	The Liffey A	The Liffey B
08:30 - 12:00	**Registration Open**		
09:00 - 10:30	Abiotic and Biotic Stresses in Plants	New Development in Instruments and Techniques	Impact of Metabolomics in Clinical Medicine 2
10:30 - 10:50	**Tea & Coffee Break - Level 1 & Level 3 Foyer**		
10:50 - 11:50	Metabolomics in Early Life	Metabolomic Analysis of Challenge Tests	Metabolomics for Disease Biomarkers
12:00 - 12:40	**Plenary Session 4** Prof Tsutomu Masujima		
12:40 - 13:30	**Closing Ceremony**		

Environment, Plant and Model Organisms

Metabolomics in Health and Disease

Metabolomics in Nutrition and Food Research

Advancing the Field

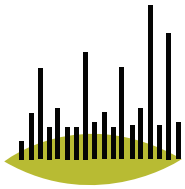
METABOLOMICS 2016

METABOLOMICS SOCIETY

METABOLOMICS SOCIETY

Contents

in partnership with



PLANT METABOLOMICS PLATFORM

Welcome

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Welcome from the Metabolomics Society

Dear Metabolomics 2016 Participant,

On behalf of the Board of Directors of the Metabolomics Society, the International and the Local Organising Committees, it is our very great pleasure to welcome you to Dublin and to Metabolomics 2016, the 12th Annual Conference of the Metabolomics Society. We would particularly like to welcome the many new members of the Society.

The annual conference of the Society has grown tremendously with many hundreds of researchers from academia, governments and industry gathering to enjoy a stimulating environment to exchange new developments and applications of the metabolomics sciences, including fundamental and applied research, and most importantly bringing together the community to share ideas and outcomes.

This year we again start the conference with a series of workshops for beginners and advanced metabolomics scientists and continue with a diverse spread of scientific sessions ranging from methodology and technology developments to topics from all areas of the biological and computational sciences. We wish to thank everyone for contributing to the cutting-edge scientific content of all presentations, whether they be posters or talks. This year there are 35 travel awards and prizes available, many to support the attendance of our early-career members, including postdoctoral fellows and PhD students. The Metabolomics Society provides twenty of these travel awards. The Metabolomics Society Board of Directors wish to extend our sincerest gratitude to the local organising committee of Metabolomics 2016, with special thanks to Co-chairs Professor Lorraine Brennan and Aifric O'Sullivan and their team, for their dedication and significant contributions. The Board of Directors, on behalf of the community, also wish to thank our loyal and committed sponsors for their continued financial support. Your support makes the conference financially feasible and enables us to keep registration costs to a minimum, which particularly assists the ability of young scientists to be part of this exciting network.

Finally, as a Society with ambitions to grow and serve our community, we want to highlight the activities and expanding portfolio of benefits to individual members, corporate members and international organisations. The membership of the Society continues to grow, in line with increasing attendance at the annual international conference. The Society has recently launched support mechanisms for smaller regional and/or science-focused metabolomics meetings, a very active early-career members network and new international partnerships between the Society and national/regional metabolomics networks. We continue to develop new awards schemes for members, task groups to facilitate international cooperation and standardisation for specific aspects of metabolomics science, online webinars and training content. One of the most exciting developments coming in the near future will be a new environment for publication of cutting-edge metabolomics research – watch this space! Thank you for renewing your membership and thereby supporting these activities.

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

Ute Roessner, President
Dan Bearden, Treasurer
Tim Ebbels, Secretary

On behalf of the Board Members of the Metabolomics Society

Welcome from the Metabolomics 2016 Hosts University College Dublin

It is our pleasure to welcome you to Dublin for Metabolomics 2016, the 12th Annual International Conference of the Metabolomics Society. We have an exciting programme planned that covers a range of metabolomics research topics under four broad themes: Metabolomics in Food and Nutrition, Metabolomics in Health and Disease, Environmental, Plant and Model Organisms and Advancing the Field. The programme blends plenary and keynote lectures by leading international scientists, parallel oral and poster sessions highlighting the latest research and dedicated sessions for early career scientists.

We would like to take this opportunity to thank all of the invited speakers and all delegates who submitted abstracts for both oral and poster presentations this year. We had a wonderful selection of abstracts that reflect the excellent science being carried out in this field. The number and quality of abstracts submitted has allowed us to develop this excellent programme. Thanks to members of the Local and International Organising Committees for their time and commitment to preparations. We would also like to thank our sponsors for their financial support for this event. Finally, we would also like to thank the Metabolomics Society for giving Dublin the opportunity to host this meeting.

We hope that you enjoy your time at Metabolomics 2016, and all that Dublin has to offer.

Professor Lorraine Brennan

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School of Agriculture and Food Science
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Dr Aifric O'Sullivan

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School of Agriculture and Food Science
UCD, Dublin, Ireland

Committee

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Metabolomics Society Board of Directors

	Role	Affiliation
Ute Roessner	Society President	University of Melbourne and Metabolomics Australia (Australia)
Dan Bearden	Treasurer	NIST (USA)
Tim Ebbels	Society Secretary	Imperial College, London (UK)
Robert Mistrik	Board Member	HighChem (Slovakia)
Darren Creek	Board Member	Monash University (Australia)
Masanori Arita	Board Member	National Institute of Genetics (Japan)
Steffen Neumann	Board Member	IPB – Halle (Germany)
Reza Salek	Board Member	European Bioinformatics Institute (UK)
Susan Sumner	Board Member	RTI International (USA)
Sastia Putri	Board Member	Osaka University (Japan)
David Broadhurst	Board Member	Edith Cowan University (Australia)
Krista Zanetti	Board Member	National Cancer Institute (USA)
Justin van der Hooft	Board Member, Ex officio and Early-career Members Network Chair	University of Glasgow (UK)
Mark Viant	Board Member and Immediate Past President (2012 – 2014)	University of Birmingham (UK)

International Scientific Committee

	Role	Affiliation
Lars Dragsted	Member	University of Copenhagen (Denmark)
Hannelore Daniel	Member	Technische Universität München (Germany)
Doris Jacobs	Member	Unilever R&D (The Netherlands)
Jules Griffin	Member	Medical Research Council Human Nutrition Research and University of Cambridge (UK)
Ivana Bodeldijk-Pastorova	Member	TNO (The Netherlands)
Age Smilde	Member	University of Amsterdam (The Netherlands)
Matej Oresic	Member	Steno Diabetes Center (Denmark)
Tim Ebbels	Member	Imperial College, London (UK)
Warwick Dunn	Member	University of Birmingham (UK)
Dan Bearden	Member	NIST (USA)
Oliver Fiehn	Member	University of California, Davis (USA)
David Wishart	Member	University of Alberta (Canada)
Darren Creek	Member	Monash University (Australia)
Ute Roessner	Member	University of Melbourne and Metabolomics Australia (Australia)
Kazuki Saito	Member	RIKEN Plant Science Centre (Japan)
Guowang Xu	Member	Dalian Institute of Chemical Physics (China)
Choong Hwan Lee	Member	Konkuk University (Korea)

Local Organizing Committee

	Role	Affiliation
Lorraine Brennan	Chair	University College Dublin (Ireland)
Aifric O Sullivan	Deputy-Chair	University College Dublin (Ireland)
Louise Kenny	Member	University College Cork (Ireland)
Aoife O' Gorman	Member	University College Dublin (Ireland)
Carl Ng	Member	University College Dublin (Ireland)

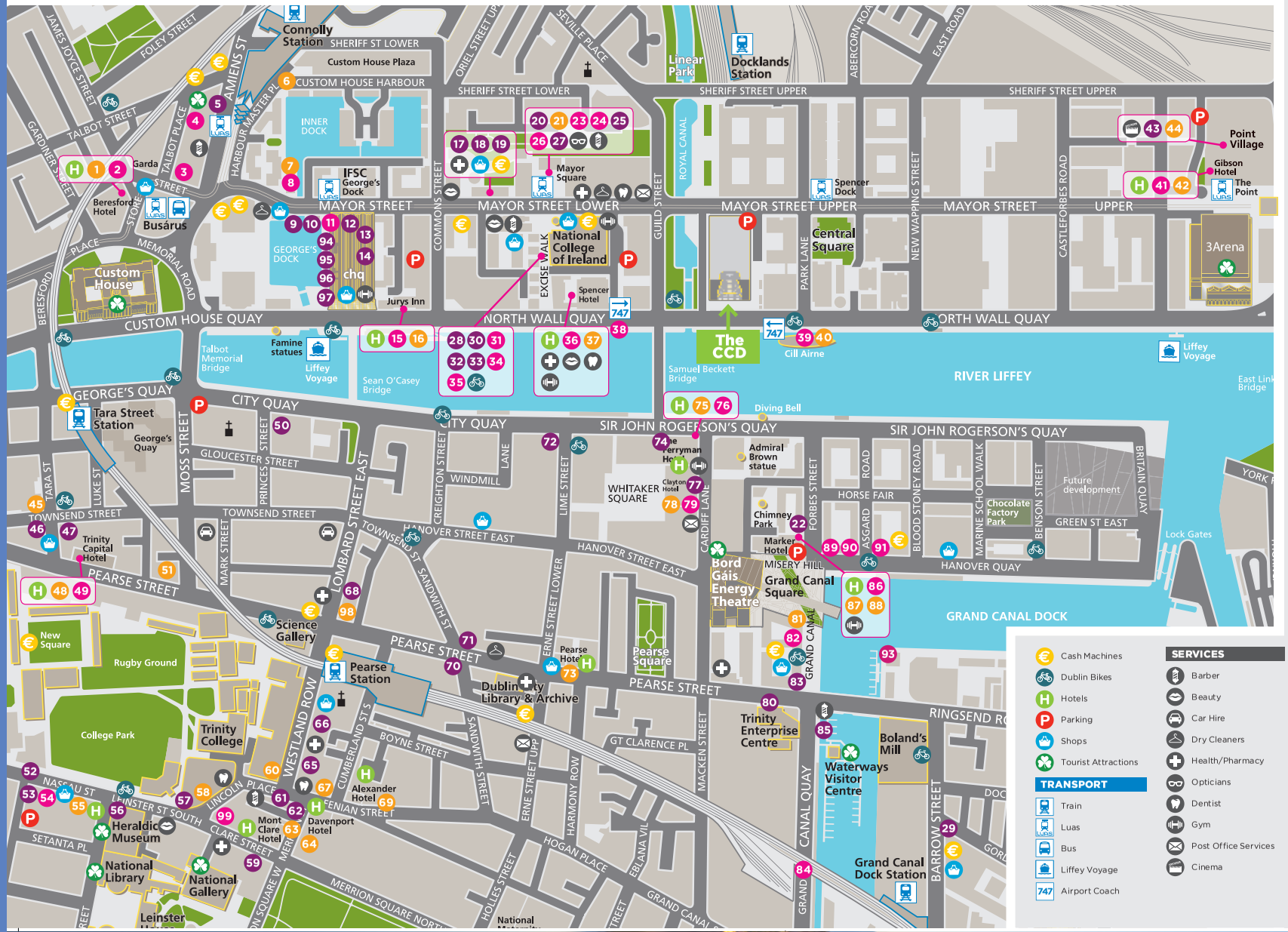

Luan - Sath
07.00 - 10.00
12.30 - 19.00
MON - SAT

Map of Local Area

Your quick guide to key services within 15 minutes walk of **The CCD**

THE CONVENTION CENTRE DUBLIN

@TheCCD
TheConventionCentreDublin



RESTAURANTS

2 Il Vignardo at The Beresford Hotel
3 The Good Bits
4 Thai Spice
8 Harbour Master Bar & Restaurant
11 Ely Bar & Brasserie
15 Oly's at Jurys Inn IFSC
23 Musashi Noodles & Sushi Bar
24 Dublin Wine Rooms
26 La Corte
31 Borlottie
34 Milano
35 J2 Grill & Sushi
36 East Restaurant at The Spencer Hotel
38 Rockets
39 Quay 12 at Cill Airne
41 Coda Eatery at The Gibson Hotel
49 Café Cairo at The Trinity Capital Hotel
54 The Pig's Ear
76 The Southbank at The Ferryman Hotel
79 Stir at The Clayton Hotel
82 Crystal Boat
84 Osteria Lucio
86 The Brasserie at The Marker Hotel
89 HQ Restaurant and Gastro Bar
90 Herbstreet
91 Milano
93 Mourne Seafood Bar
99 Blackboard Bistro

PUBS

1 Café Le Monde at The Beresford Hotel
6 The Vaults
7 Harbour Master Bar & Restaurant
16 Oly's Bar at Jurys Inn IFSC
21 Lagoona Bar & Restaurant
37 The Spencer Cocktail Bar
40 Blue River Bistro Bar at Cill Airne
42 Hemi Bar at The Gibson Hotel
44 Harry's Bar
45 Macturcaills
48 The Trinity Capital Hotel Bar
51 O'Neill's Pub & Townhouse
55 The Blarney Inn
58 Lincoln Inn
60 Kennedy's
63 O'Callaghan Mont Clare Hotel Bar
64 O'Callaghan Davenport Hotel Bar
67 The Ginger Man
69 O'Callaghan Alexander Hotel Bar
73 Pearse Hotel Bar
75 The Ferryman Hotel Bar
78 Vertigo Bar at The Clayton Hotel
81 Café Bar H
87 The Marker Bar at The Marker Hotel
88 The Rooftop Lounge at The Marker Hotel
98 The Lombard Pub & Townhouse

CAFÉS

5 The Pig & Heifer
9 Munchies
10 O'Brien's
12 Starbucks
13 Insomnia
14 Toss'd Noodles & Salads
17 Burritos & Blues
18 Subway
19 Insomnia
20 Il Fornaio Cafe Bar
22 Lolly and Cooks
25 Broadway Pizza Parlour
27 Swedish Food Co
28 Café Nero
29 Flavours
30 Foodie
32 Seven Wonders
33 Bagel Bar
43 Costa Coffee
46 McCabes Deli
47 The Espresso Corner
50 The Pig & Heifer
52 O'Brien's
53 BrewBaker Café
56 Café Crepe
57 Insomnia
59 Café Sol
61 Café Tri via
62 Café Sol
65 The Westland Café
66 Il Caffe di Napoli
68 Lunch!
70 The Pig & Heifer
71 BG Café & Deli
72 Café Parigi
74 Munchies
77 V-Deli
80 KC Peaches
83 Il Valentino
85 The Art of Coffee
94 Freshii
95 Seven Wonders
96 The Bakehouse Express
97 J2 Sushi & Tea

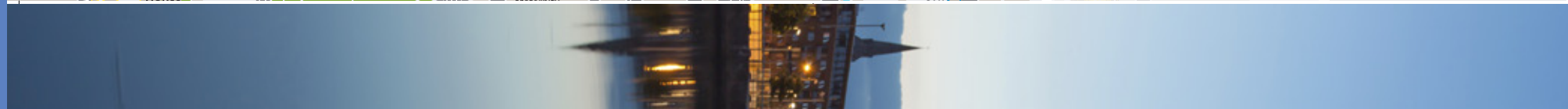
Cash Machines
Dublin Bikes
Hotels
Parking
Shops
Tourist Attractions

TRANSPORT

Train
Luas
Bus
Liffey Voyage
747 Airport Coach

SERVICES

Barber
Beauty
Car Hire
Dry Cleaners
Health/Pharmacy
Opticians
Dentist
Gym
Post Office Services
Cinema



Conference Policies

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METABOLOMICS SOCIETY CONFERENCE POLICIES

The following policies will be in place for meetings provided by the Metabolomics Society to assure the comfort and privacy of all conference participants and to encourage scientific discussions and presentation of novel data.

1. No photography, videotaping or recording is allowed in oral sessions or in the Poster-Exhibit Hall except by the official Society photographer or Society approved Audio-visual vendor. This includes cameras, cell phones and all other devices.
2. All conference attendees acknowledge and consent that pictures will be taken by the official Society Photographer and may be used for Society purposes such as marketing.
3. Name badges are required for all conference sessions, including the exhibit hall.
4. No smoking is permitted in the conference venue.
5. Cell phones must be turned off in oral sessions.
6. Material presented or displayed at the Conference, including but not limited to orals, posters, workshops, exhibit booths and hospitality suites, is the intellectual property of the presenter and may not be recorded, photographed, quoted, disseminated or transmitted in any form without the express approval of the author of the material presented. Such materials must contain appropriate credits for all content used.
7. The placement of exhibitor advertising in the meeting area is strictly limited to the booths and tables of corporate members in the Exhibit Hall.
8. No organized activities (even off-site) other than those approved by the local organising committee and the Society are allowed during the conference week (currently Noon on Sunday through 6:00 pm on Thursday).

Presentation policies

9. Each attendee may only submit one abstract for poster or oral presentation in the scientific sessions as the presenting author.
10. Poster presenters must be present at their posters for their dedicated session within 10 minutes after the start of the session.
11. Commercial logos on posters should not be larger than 20 cm x 20 cm.
12. Posters and presentations should acknowledge all authors and affiliations
13. Posters and oral presentations should describe original research and include appropriate structural elements such as summary, introduction, methods, results and conclusions.
14. Poster presenters are encouraged to provide handouts, e.g., preprints, extended abstracts, copies of poster panels, etc. No hardware, computers, books, accessories, or saleable items may be displayed.
15. Posters and oral presentations should acknowledge funding mechanism(s), and declare any conflict of interest.
16. Posters and oral presentations should affirm that research with human subject samples received appropriate Institutional Review Board approval or exemption.
17. Posters and oral presentations should refrain from using photographic or schematics of animal models unless absolutely necessary for describing the study.

Corporate Sponsorship

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Corporate Sponsorship for Metabolomics 2017

Invitation from the Industry Engagement Task Group (IETG)

Corporate Sponsors of the annual international meeting of the Metabolomics Society provide valuable support to the Society and provide attendees with opportunity to see the latest advances in the field of metabolomics with regard to software, instruments and tools. Indeed, Corporate Sponsor booths are a key feature of EVERY Metabolomics Society Annual Meeting!

Opportunities are now available for Corporate Sponsorship of the 2017 Metabolomics Society meeting in Brisbane. Please contact info@metabolomics2016.org for the latest information and updates on this exciting meeting!

Dan Bearden

Chair, IETG

Sponsors Listing

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PLATINUM SPONSORS

Agilent Technologies

Website: www.agilent.com
Booth: B8

Agilent Technologies, a global leader in life sciences, diagnostics and applied chemical markets, is the premier laboratory partner for a better world. We can partner with you in your metabolomics research by providing comprehensive tools including sample preparation, instrumentation and software programs to process and analyze your samples to gain insight into the biological system that you are studying.

Biocrates Life Sciences AG

Website: www.biocrates.com
Booth: B4

Biocrates offers targeted metabolomics kits and services. The technology provides quantitative and highly reproducible results as well as high throughput, making it perfectly suited for epidemiological and clinical research. Biocrates' metabolomics platform has been featured in hundreds of scientific publications. Biocrates is the partner of choice for targeted metabolomics projects in academia and pharmaceutical industry.

Bruker

Website: www.bruker.com
Booth: B5

Bruker is one of the world's leading analytical instrumentation companies. Thanks to our latest innovations in hyphenated NMR, LC-MS and GC-MS, Bruker remains the leader in integrated solutions for metabolomics that can be used for a broad variety of targeted and non-targeted studies. Allowing to detect, identify, and measure molecules covering the entire metabolomics chemical space, Bruker provides all hardware and software "puzzle pieces" to give a complete picture of the metabolome.

SCIEX

Website: www.sciex.com
Booth: B7

SCIEX delivers advanced analytical technologies and software that contribute to the understanding and research of human disease. Innovative LC/MS, LC-MS/MS and CE solutions enable deeper analysis of complex biological systems by providing comprehensive quantitation and characterization required across proteomics, lipidomics and metabolomics - leading to advances in systems biology and biomarker discovery.

Thermo Fisher Scientific

Website: www.thermofisher.com
Booth: B6

Thermo Fisher Scientific Inc. is the world leader in serving science. Our mission is to enable our customers to make the world healthier, cleaner and safer. Through our premier brands – Thermo Scientific, Applied Biosystems, Invitrogen, Fisher Scientific and Unity Lab Services – we offer an unmatched combination of innovative technologies, purchasing convenience and comprehensive support.

Waters

Website: www.waters.com/metabolomics
Booth: B3

Waters Corp. holds worldwide leading positions in complementary analytical technologies - liquid chromatography, mass spectrometry, rheometry and microcalorimetry.

Specifically, the company designs, manufactures, sells and services ultra performance liquid chromatography (UPLC), high performance liquid chromatography (HPLC), chromatography columns and chemistry products, mass spectrometry (MS) systems, thermal analysis and rheometry instruments.

GOLD SPONSORS

Veritomyx, Inc

Website: www.veritomyx.com
Booth: E1

PeakInvestigator™ advanced signal processing software from Veritomyx® detects and deconvolves overlapped MS peak data, effectively increasing MS resolution by 3-4x, and revealing critical hidden information with large sensitivity and precision improvements. More accurate, complete and precise information accelerates correct metabolomic and proteomic biomolecular IDs. PeakInvestigator works with raw profile MS data from ion trap, TOF, Orbitrap and FTICR mass analyzer outputs from 3,000-3,000,000+ resolution. See what you're missing!

BRONZE SPONSORS

Anatune Ltd

Website: www.anatune.co.uk
Booth: D5

Anatune provides complete analytical solutions for sample preparation, chromatography and mass spec; providing fully automated platforms that deliver improved productivity, performance and data quality. We're currently working with researchers to deliver targeted and untargeted platforms for metabolomics, synthetic biology and metabolic phenotyping. Anatune are an Agilent Value Added Reseller and the distributors for GERSTEL, ITSP Solutions, MIDI Inc and Syft Technologies in UK and Ireland.

Avanti Polar Lipids, Inc.

Website: Avantilipids.com
Booth: A2

Avanti has the tools to help you succeed in Lipidomics. Our mass spec standard line includes deuterium labeled lipids available in complex standard mixtures or as individual compounds. We have been supplying mass spec standards to the LipidMAPS consortium and many others for 15 years. Our Analytical Services Division is also available to perform targeted or broad range Lipidomic analysis for a fee. Please visit our new website for more information.

Beckman Coulter UK Ltd

Website: www.beckmancoulter.com
Booth: A7

For over 75 years Beckman Coulter has built a global reputation with academic and biopharmaceutical laboratories by providing reagents, instrumentation, and labware. Beckman Coulter offers a complete range of technologies such as flow cytometry, centrifugation, liquid handling, particle characterization, and genomic analysis to streamline workflow for the life sciences laboratory.

Biolog

Website: www.biolog.com
Booth: A4

Biolog is a world leader in cell-based phenotypic testing technologies and assays. It has focused its efforts on developing products to cost effectively test metabolic properties of cells (phenotypes) very simply and efficiently. The OmniLog® Phenotype MicroArray™ System employs custom cell-based assays to determine1400 metabolic phenotypes of mammalian cells.

Cambridge Isotope Laboratories, Inc.

Website: www.isotope.com
Booth: A3a

Cambridge Isotope Laboratories, Inc. is the world leader in the manufacture and separation of stable isotopes and stable isotope labeled compounds. CIL offers an array of highly pure compounds that are uniformly or selectively enriched in 13C, 15N, D, 18O or 17O. Our labeled reagents are used across scientific fields including proteomics, metabolomics, metabolism and environmental applications for quantitative mass spectrometry.

Chenomx Inc

Website: www.chenomx.com
Booth: A1

Chenomx specializes in mixture analysis for applications in life sciences such as metabolomics, food, and cell culture research. Chenomx is known as the 'Gold Standard' for reliable, routine, and quantitative mixture analysis of samples using NMR. Software Licenses enable scientists to perform the work themselves or Services are available to outsource the analysis steps.

GERSTEL GmbH & Co.KG

Website: www.gerstel.com
Booth: D4

GERSTEL develops and produces automated solutions for GC–MS and LC–MS including sample preparation and sample introduction. The GERSTEL MultiPurpose Sampler (MPS) automation platform performs derivatization, addition of standards and generates dilution series and calibration standards. Sample clean-up includes SPE; online SPE with exchangeable cartridges; Filtration; Centrifugation and Vortexing – all operated with MAESTRO PrepAhead efficiency.

LECO Corporation

Website: www.leco.com
Booth: D3

LECO instruments provide the speed, sensitivity, resolution, and data-handling tools necessary for the characterization of complex metabolite profiles. High performance TOFMS allows you to collect high integrity qualitative and quantitative data in one injection. The different qualitative and quantitative functions are accomplished post hoc with on-board data analysis as well as exporting to your favorite statistical package. For application information, visit www.leco.com/metabolomics.

Lipotype GmbH

Website: www.lipotype.com
Booth: D2

Lipotype delivers comprehensive, absolutely quantitative lipid analysis services for clinical and biological samples on a high-throughput scale. Lipotype is a spin-off from the Max-Planck-Institute in Dresden, Germany.

Lipotype offers high quality lipid analysis services for different customers/applications including biomarker identification (clinical researchers, pharma/biotech companies), functional food development (food industry) and small-scale profiling needs for academic researchers.

Phenome Centre Birmingham partnered with Birmingham Metabolomics Training Centre

Website: www.birmingham.ac.uk/research/activity/phenome-centre
Booth: A6

Phenome Centre-Birmingham was established through an £8m award by the MRC, industry and University of Birmingham to provide capacity and capability for metabolic phenotyping in human health. Comprising of LC-MS and NMR, it offers a complete collaborative metabolomics service from experimental design to data analysis. In partnership, the Birmingham Metabolomics Training Centre offers a wide range of face-to-face and on-line training courses for both novice and experienced metabolomics scientists

Proteome Software

Website: www.proteomesoftware.com
Booth: A5

Proteome Software sets the standard in MS/MS analytics with our proteomics and metabolomics software. Our developers and technical specialists work to bring you the most intuitive, highest-quality products possible. From customer-focused design and development to specific, clear technical support and documentation, our dedicated employees work to create a satisfying user experience. Researchers and core labs around the world rely on Proteome Software for performing complex MS/MS analysis.

Shimadzu Europa GmbH

Website: www.shimdazu.eu/analytics
Booth: D1

Since its creation in 1875, Shimadzu has been a worldwide leading manufacturer of analytical instrumentation. Its equipment contain many “industry first” technologies and products, which lead to Koichi Tanaka being awarded the 2002 Nobel Prize for Chemistry for his outstanding contributions in the field of mass spectrometry. Shimadzu is offering powerful and smart solutions based on UFMS (Ultra Fast Mass Spectrometry) as well as software tools for the Metabolomics field. Discover the benefits of the comprehensive technology GCxGC coupled to MS and the multimode analysis possibilities on the LCMS triple quad range.

Sigma Aldrich

Website: www.sigmaaldrich.com
Booth: E3

MilliporeSigma is the U.S. life science business of Merck KGaA, Darmstadt, Germany. With 19,000 employees and 72 manufacturing sites worldwide, MilliporeSigma's portfolio spans more than 300,000 products enabling scientific discovery. MilliporeSigma has customers in life science companies, university and government institutions, hospitals and industry. The company is committed to solving the toughest problems in life science by collaborating with the global scientific community. Visit us at www.emdmillipore.com and www.sigma-aldrich.com.

SpectralWorks Limited

Website: www.spectralworks.com
Booth: A3

SpectralWorks Ltd is a leading UK based software development company dedicated to providing innovative solutions for markets within the life sciences industry. We believe we have the right balance between scientific and software development expertise to provide the best scientific solutions for the end user.

We want to improve the way software is integrated within the laboratory environment by providing the correct solutions to increase productivity and reduce overheads.

UNIVERSITY/NON-PROFIT

Metabolomics Australia

Website: www.metabolomics.com.au
Booth: T7

Metabolomics Australia offers high throughput metabolomics services to all life science researchers. Services are offered through a consortium of Australian universities and research institutes with world class facilities and expertise in small molecule analysis. Metabolomics Australia can provide specific detection and quantification services and cater to complex investigations and systems wide analyses.

OTHER PARTNERS

Science Foundation Ireland

Website: www.sfi.ie

Science Foundation Ireland funds oriented basic and applied research in the areas of science, technology, engineering, and mathematics (STEM) which promotes and assists the development and competitiveness of industry, enterprise and employment in Ireland. The Foundation also promotes and supports the study of, education in and engagement with, STEM and promotes an awareness and understanding of the value of STEM to society and in particular to the growth of the economy.

#ScienceRising supporting Innovation 2020 – a Science Foundation Ireland campaign creating the connection for individuals and industry with science and innovation in Ireland.

GigaScience

Website: www.gigasciencejournal.com

CONFERENCE HOST

Metabolomics Society

Website: www.metabolomicssociety.org
Booth: T8

The Metabolomics Society is dedicated to promoting the growth, use and understanding of metabolomics in the life sciences. It 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 a 1,000 members in more than 40 countries.

Floor plan of the Exhibit Hall is on Page 31.

Sponsor Booth Listing

Company	Booth
Chenomx Inc	A1
Avanti Polar Lipids, Inc.	A2
SpectralWorks Limited	A3
Cambridge Isotope Laboratories, Inc.	A3a
Biolog	A4
Proteome Software	A5
Phenome Centre Birmingham Birmingham Metabolomics Training Centre	A6
Beckman Coulter UK Ltd	A7
Waters	B3
Biocrates Life Sciences AG	B4
Bruker	B5
Thermo Fisher Scientific	B6
SCIEX	B7
Agilent Technologies	B8
Shimadzu Europa GmbH	D1
Lipotype GmbH	D2
LECO Corporation	D3
GERSTEL GmbH & Co.KG	D4
Anatune Ltd	D5
Veritomyx, Inc	E1
Sigma Aldrich	E3
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Metabolomics Society	T8
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General Information

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METABOLOMICS 2016
GENERAL INFORMATION

Date

- From Monday 27th June to Thursday, 30th June.

Venue

The 12th Annual Conference of the Metabolomics Society will be held at the Convention Centre Dublin (CCD), Spencer Dock, North Wall Quay, Dublin 1, Ireland. The CCD sits at the heart of Dublin's transport hub with excellent air, road, rail and sea connections, meaning the CCD is only minutes from the airport, motorway network, Port Tunnel, rail stations and ferry terminals. Increased availability of taxis in Dublin means that it is easy to travel to and from Dublin city, day or night. For more information on how to get to the Convention Centre Dublin, please visit: **www.theccd.ie**

Registration Desk Hours

- Monday, 27th June – 09:00 – 19:00
- Tuesday, 28th June – 08:00 – 19:00
- Wednesday, 29th June – 08:30 – 18:00
- Thursday, 30th June – 08:30 – 12:00

Speaker Presentations

All presentations must be dropped off at the Presentation Table, located next to the Registration Desk on the ground level. Your presentation should be dropped off the day before your talk. You are welcome to drop your presentation off earlier, during the posted times. Please note, it is not possible to load the presentations in the meeting rooms, they must be brought to the Presentation Table to be loaded centrally. Once your presentation has been dropped off you will not be able to make changes.

Presentation Table Hours

- Monday, 27th June – 13:30 – 16:00
- Tuesday, 28th June – 08:00 – 09:00 and 17:00 – 18:00
- Wednesday, 29th June – 08:00 – 09:00 and 17:00 – 18:00
- Thursday, 30th June – Not open, all presentations loaded by Wednesday, 29 June.

Name Badge

Delegates must wear their name badge at all times to gain access to conference activities, including the Exhibit Hall. If you lose your badge, please visit the Registration Desk on the ground level outside of The Forum. You will be required to show photo ID to have a new badge printed. Please notice the QR code located on the back of your badge. This can be scanned with any QR code reader, available for download in most app stores. Sponsors or other attendees may request to scan your QR code using their smart phone, which will provide them with your name, phone, and e-mail address. If you do not wish to share this information, you should politely decline the scan.

Internet Access

WI-FI access is available throughout the Convention Centre Dublin.

Delegates should select the CCDGuest option, open their browser and hit "Connect". You may be disconnected after 1-2 hours, to keep the signal available for those using it currently. If disconnected, you may use the same instructions to reconnect.

Poster Presentations

Posters will be on display in the Exhibition Hall on Tuesday (Poster Session 1) and Wednesday (Poster Session 2). You can find a list of posters in this abstract book on page 107. Complete poster abstracts are available on the conference website.

Catering

During the week, morning and afternoon Tea/ Coffee Breaks will be provided. A box lunch will be provided on Monday, Tuesday and Wednesday. Check the agenda for the location of refreshments, on most days they will be served in the Exhibit Hall. Please note: Food & Beverage is not permitted inside the Plenary Session Room (The Auditorium).

OTHER DETAILS

Banking

Bank opening hours are generally from 10:00 – 16:00. There are numerous ATMs located within walking distance of the CCD. The closest ATM is located on Mayor Street, in both MACE and Spar retail outlets, and both stores are open between 07:00 and 22:00 daily. Visa and MasterCard are accepted in almost all restaurants, bars, cafes and shops.

Cloakroom

A cloakroom is available on the ground floor of the CCD. There is a charge of €2 per item.

- Monday, 27th June – 09:00 – 19:30
- Tuesday, 28th June – 07:30 – 19:30
- Wednesday, 29th June – 08:30 – 17:00
- Thursday, 30th June – 08:30 – 14:00

Currency

The currency in Ireland is Euro (€). Most Banks offer a foreign exchange facility and generally offer the best exchange rates. It is important to remember that traveller's cheques are not generally accepted for everyday transactions so we recommend cashing them at the beginning of your trip.

Electricity Supply

Throughout Ireland 220V is the standard supply. Flat three-pin plugs are used.

Emergency Contact Details

During the conference, in case of an emergency of any kind, please contact the registration desk located on the ground floor foyer near The Forum hall. If you require medical services while residing in your hotel/accommodation, please contact your hotel/accommodation front desk who will be able to arrange a doctor on call. Please ensure to pay attention to any hotel alarms and announcements.

Fire/Ambulance and Emergency Number in Ireland is 999

Facilities

The venue is fully accessible for delegates - If you have any particular requirements, please advise any of the staff who will be able to make appropriate arrangements should they be required.

Food and Beverage

A box lunch will be provided to all attendees on Monday, Tuesday and Wednesday. On Monday the lunch will be set-up on Level 1 and Level 3 Foyers. On Tuesday and Wednesday the lunch will be available in the Exhibition Hall. We welcome you to pick-up a lunch and then visit with sponsors in the Exhibit Hall or take your lunch with you to a Platinum Sponsor Presentation, located on Level 1. No Food or Beverage will be allowed inside The Auditorium on Level 3 at any time.

Liability and Insurance

The organisers of the 12th Annual Conference of the Metabolomics Society reserve the right to alter any

of the programme or other arrangements for the meeting including cancellation or postponement of any part of the event should the unforeseen circumstances require it. The organisers accept no responsibility for resulting costs or inconvenience to participants in this case. The organisers of the 12th Annual Conference of the Metabolomics Society accept no liability for participant personal injuries or loss/damage to property while in attendance or as a result of the workshop or social events. Participants are requested to have their own travel insurance in place and are responsible for all travel arrangements including visa applications, if required.

Lost and Found

During the conference any lost property should be turned in to the registration desk. All unclaimed items at the end of the week will be turned over to CCD Security.

Parking

There are 321 low-ceiling underground public car parking spaces on The CCD site. Spaces can be reserved directly with the operators Park Rite by telephone on +353 (0) 1 542 5600. If the public car park below the CCD is full, the nearest car park is located at the National College of Ireland, approximately a two-minute drive away and the Irish Financial Services Centre (IFSC) is about a five-minute drive away.

Access: On Guild Street (coming from Samuel Becket Bridge) take the first right turn and then right turn down the ramp to the car park under the Convention Centre building. Along North Wall Quay past the front of the Convention Centre and take the next left turn, take the next left and then left turn down the ramp to the car park.

Photography and Recording

No photography, videotaping or recording is allowed in oral sessions or in the Poster-Exhibit Hall except by the official Society photographer or Society approved Audio Visual vendor. This includes cameras, cell phones and all other devices. All conference attendees acknowledge and consent that pictures will be taken by the official Society Photographer and may be used for Society purposes such as marketing.

Smoking Policy

Smoking is not permitted in Ireland in any building, and there is no smoking allowed in any of the meeting rooms or public spaces. There are designated smoking areas outside the buildings, and delegates are requested not to litter in these areas. The smoking ban applies to restaurants, bars, cafes and all public venues.

Shopping

Shops in Ireland are generally open from 09:00 -18:00 on Monday-Saturdays with later hours on Thursday evenings. Most major stores/shops open on Sunday – some with reduced opening times from 12:00 – 18:00.

Tipping

It is generally customary to leave a small gratuity for services in restaurants if good service is provided. Tips for taxis and any porter service are at your discretion.

Social Events and Tours

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Social Events and Tours

Welcome Reception

Monday, 27th June 18:00 – 19:00

The Welcome Reception will take place in the The Forum Exhibition Hall. Please join us for light refreshments and beverages while greeting your fellow Metabolomics colleagues and meeting the sponsors for the first time. You will need a badge to enter the Exhibit Hall, so please stop by the Registration Desk before attending the Reception.

Early Career Members Network Reception

Tuesday 28th June 19:00 – 20:30

The EMN Reception will take place at the CCD following the evening Poster Session on Tuesday. This will be a more formal, interactive gathering in which the EMN outline the aims and outreach events that the network offers alongside a presentation from a high-level metabolomics PI. Refreshments will be provided! The EMN are also hosting Workshops and chairing the Early Career Sessions during the conference itinerary. We encourage you to attend these sessions and support our early career colleagues in their work.

Conference Dinner, Croke Park

Wednesday, 29th June
Buses will depart the CCD at 19:30
Dress Code: Smart/Casual

Upon arrival at the stadium, guests will follow in the footsteps of Ireland's sporting legends with an interactive Gaelic Games display, guests will try their hand at Hurling and Gaelic Football skills. This will be an unforgettable Irish experience in a uniquely Irish venue!

The event is scheduled until 23:30, however a bus will be available for early departures at 22:30. After the event, the buses will return directly to guest hotels, keep an eye out for your stop. Buses will also stop at the CCD and this is where you should depart the bus if you are not staying at one of the Metabolomics room block hotels.

The cost to attend is included in your full-conference registration fee and transportation will be provided. Note: Single Day Pass or Exhibit Hall Only passes, do not include access to the Conference Dinner. Additional tickets can be purchased from the registration desk. Ticket price: $105.00 USD. Prices include an informal dinner, drinks and entertainment. There are a limited number of guest tickets available.

Tourism Activities

Make the most of your stay in Dublin and enjoy one of the local Tours available. There are half day and full day options available. Information can be found on the website: **http://metabolomics2016.org/registration/local-tours**

Information sheets are also provided at the Registration Desk. Advance sign-up and payment is required. Do not delay, as some tours sell out quickly!

Fáilte Ireland Tourism office is located on Suffolk Street in Dublin City Centre. For the Fáilte Ireland Tourism website, visit: **www.discoverireland.ie**

CCD Floor Plan

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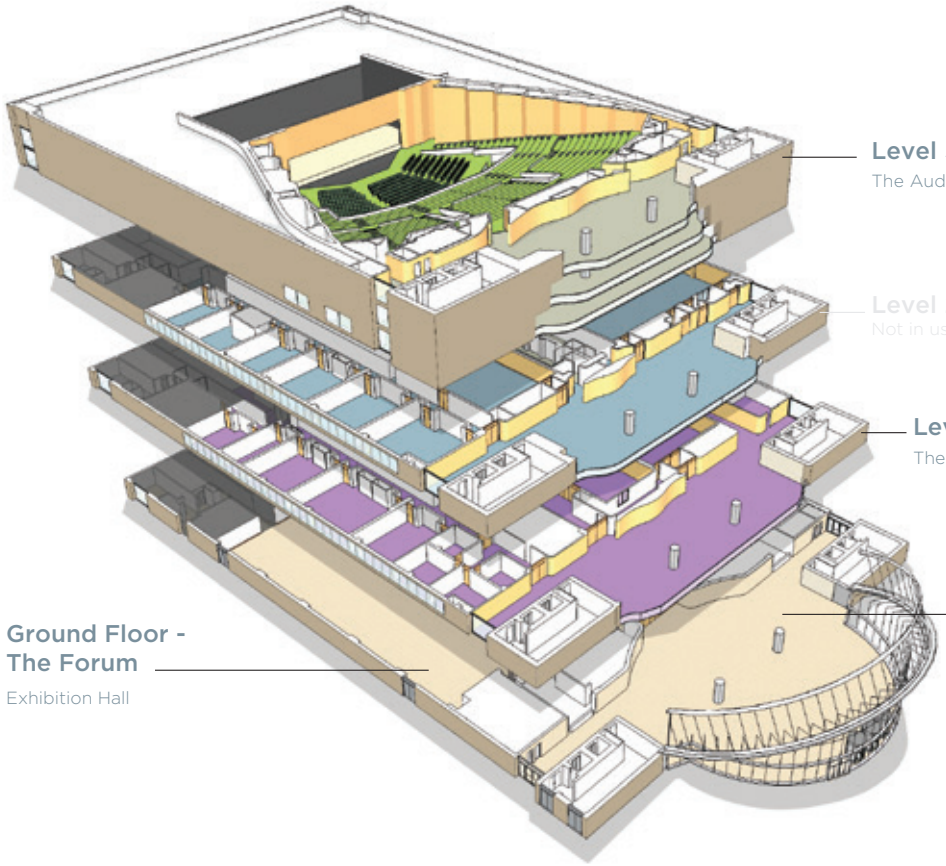
CCD Floor Plan

Levels



Exhibitions Floor Plan and Guide

Monday

	The Auditorium	The Liffey A	The Liffey B
09:00 19:00	**Registration Open**		
10:30 12:00	**Workshop 1:** EMN Career Session	**Workshop 2:** Data Sharing and Standardisation	**Workshop 3:** Metabolite Profiling in Population-Based Studies
12:00 13:30	**Box Lunch Available - in Foyer**		
12:15 13:15		Sponsor Presentation SCIEX	Sponsor Presentation Bruker
13:30 15:00	**Workshop 4:** EMN The Importance of Experimental Design	**Workshop 5:** metaRbolomics: The R Toolbox for Metabolomics	**Workshop 6:** Computational Workflows and Workflow Engines
15:00 16:30	**Free Time**		
16:30 17:00	**Opening Ceremony**		
17:00 18:00	**Opening Plenary Session** Prof Jeremy Nicholson		
18:00 19:00	**Welcome Reception in Exhibit Hall**		

Tuesday

	The Auditorium	The Liffey A	The Liffey B
08:00 19:00	**Registration Open**		
07:45 8:30		Sponsor Breakfast Shimadzu Europa GmbH *Advance sign-up required*	
08:50 09:50	**Plenary Session 2** Prof Luke O'Neill		
09:50 10:30	**Break and Posters - Exhibit Hall**		
10:30 12:00	Model Organisms	Biomarkers in Nutrition Research	CVD/Diabetes
12:00 13:30	**Lunch and Posters - Exhibit Hall**		
12:15 13:15		Sponsor Presentation Agilent Technologies	Sponsor Presentation Waters
13:30 15:00	Network and Pathway Analysis for Metabolomics	Metabolic Phenotyping in Health	Crop Quality Improvement and Food Sustainability
15:00 15:30	**Break and Posters - Exhibit Hall**		
15:30 17:00	Nutrition and Metabolism	Environmental Metabolomics	Advances in Statistical Tools
17:15 18:45	**Poster Session 1 - Exhibit Hall** Posters #1-244		
19:00 20:30			**EMN Reception** *Advance Sign-Up Required*

Environment, Plant and Model Organisms

Metabolomics in Health and Disease

Wednesday

	The Auditorium	The Liffey A	The Liffey B
08:30 18:00	**Registration Open**		
08:50 09:50	**Plenary Session 3** Prof Ines Thiele		
09:50 10:30	**Break and Posters - Exhibit Hall**		
10:30 11:50	Early Career Session 1		Early Career Session 2
11:50 13:30	**Lunch and Posters - Exhibit Hall**		
12:10 13:10		Sponsor Presentation Biocrates Life Sciences AG	Sponsor Presentation Thermo Fisher Scientific
13:30 15:00	Identification of Metabolites Applying MS and NMR	Green Systems Biology	Metabolomics Profiling in Cancer
15:00 15:30	Break and Posters - Exhibit Hall		
15:30 17:00	Foodomics and Food Quality	Impact of Metabolomics in Clinical Medicine 1	Computational MS
17:00 18:30	**Poster Session 2 - Exhibit Hall** Posters #254-490		
19:30 23:30	**Conference Dinner - Croke Park** Bus loading at the CCD begins at 19:15 for a 19:30 departure (See page 29 for additional details)		

Thursday

	The Auditorium	The Liffey A	The Liffey B
08:30 12:00	**Registration Open**		
09:00 10:30	Abiotic and Biotic Stresses in Plants	New Development in Instruments and Techniques	Impact of Metabolomics in Clinical Medicine 2
10:30 10:50	**Tea & Coffee Break - in Foyer**		
10:50 11:50	Metabolomics in Early Life	Metabolomic Analysis of Challenge Tests	Metabolomics for Disease Biomarkers
12:00 12:40	**Plenary Session 4** Prof Tsutomu Masujima		
12:40 13:30	**Closing Ceremony**		

Metabolomics in Nutrition and Food Research

Advancing the Field

Schedule

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Monday 27th June

Time	Session	Location
09:00 - 19:00	Registration	
10:30 - 12:00	Workshops (See page 67)	
12:00 - 13:30	Lunch	
12:15 - 13:15	Platinum Sponsor Presentations	
13:30 - 15:00	Workshops	
16:30 - 17:00	Opening Ceremony	The Auditorium
17:00 - 18:00	**Plenary Speaker: Jeremy Nicholson** Metabolic Profiling in Systems Medicine	The Auditorium
18:00 - 19:00	Welcome Reception	Exhibition Hall

Tuesday 28th June

Time	Session	Location
07:45 - 08:30	Sponsor Breakfast Presentation (Advanced sign-up required)	The Auditorium
08:50 - 09:50	**Plenary Speaker: Luke O'Neill** The intersection between inflammation and metabolism	
09:50 - 10:30	Tea/Coffee/Posters	Exhibition Hall
10:30 - 12:00	Parallel Session 1: Model Organisms	
10:30 - 10:55	**2459** When NMR spectroscopy is not such a DOSY alternative – using NMR to model complex formation and the origins of metabolism **Julian Griffin, University of Cambridge, UK**	The Auditorium
10:55 - 11:10	**2304** Mapping metabolism in the parasite Trypanosoma brucei using U-13C-labelled amino acids and LC-MS **Fiona Achcar, University of Glasgow, UK**	
11:10 - 11:25	**2551** The Time is Right to Focus on a Model Organism Database **Christoph Steinbeck, European Bioinformatics Institute, UK**	
11:25 - 11:40	**2071*** The role played by CYP6G1 in the metabolism of imidacloprid and its 5-hydroxy and olefin metabolites in Drosophila melanogaster **Roberto Fusetto, The University of Melbourne, Australia**	
11:40 - 11:55	**2237*** Spatio-temporal metabolomics of tumor organoids treated with chloroquine **Andrew Palmer, EMBL, Germany**	

Tuesday 28th June

Time	Session	Location
10:30 - 12:00	**Parallel Session 2: Biomarkers in Nutrition Research (Chairs: Kati Hanhineva and Henrik Antti)**	
10:30 - 10:55	**2298** A Metabolome Wide Association Study of fruit intakes **Linda Oude Griep, Imperial College London, UK**	The Liffey A
10:55 - 11:10	**2365** Large-scale metabolomics to assess pharmacokinetics of conjugated black tea catabolites in human plasma **Ric de Vos, Plant Research International, Wageningen-UR, Netherlands**	
11:10 - 11:25	**2597*** New classification and validation system for intake biomarkers to improve assessment of food intake and nutritional status – A FoodBAll project goal **Giulia Pratico, University of Copenhagen, Denmark**	
11:25 - 11:40	**2134** An integrated approach for the identification of predictive markers of type 2 diabetes **Estelle Pujos-Guillot, INRA, Clermont-Ferrand, France**	
10:30 - 12:00	**Parallel Session 3: CVD/Diabetes (Chairs: David Wishart and Oscar Yanes)**	
10:30 - 10:55	**2111** Metabolomic Profiling of Patients with Congenital Adrenal Hyperplasia Reveals Novel Biomarkers for Glucocorticoid Action **David Watson, University of Strathclyde, Scotland**	The Liffey B
10:55 - 11:10	**2338** Metabolomics and proteomics analysis of vitreous humor from healthy, non-proliferative and proliferative diabetic retinopathy patients **Miriam Navarro, University of Rovira and Virgili, Spain**	
11:10 - 11:25	**2358*** Identification of serum metabolites associated with risk of type 2 diabetes by untargeted metabolomics approach: A nested case control study **Lili Xiu, Academia Sinica, Taiwan**	
11:25 - 11:40	**2532** Metabolite profiling of plasma and tissues from mouse models of diabetes at different stages of disease development **Pieter Giesbertz, Technical University of Munich, Germany**	
11:40 - 11:55	**2090*** Metabolomics reveals the importance of the pre-conception metabolic state for pregnancy metabolism and programming offspring health **Christian Hellmuth, Ludwig Maximilian University of Munich, Germany**	
12:00 - 13:30	Lunch/Posters	Exhibition Hall
12:15 - 13:15	Platinum Sponsor Presentations	

Tuesday 28th June

Time	Session	Location
13:30 - 15:00	**Parallel Session 4: Network and Pathway Analysis for Metabolomics (Chairs: Fabien Jourdan and Egon Willighagen)**	
13:30 - 14:00	**Keynote Speaker** Building the Killer App for Modeling Metabolism: from ModelSEED to KBase **Matt DeJongh, Hope College, Michigan, USA**	The Auditorium
14:00 - 14:15	**2345** Isotope tracer-based metabolomics applied to non-steady state circadian systems **Seth Rhoades, University of Pennsylvania, USA**	
14:15 - 14:30	**2403** Carbon Flux Signatures of Mycobacterium tuberculosis **Katharina Nöh, IBG-1: Biotechnology, Forschungszentrum Jülich, Germany**	
14:30 - 14:45	**2153** TTFD: a metabolic network-based guidance tool for the setup and interpretation of stable isotope metabolomics experiments **Dries Verdegem, VIB-KU Leuven, Netherlands**	
14:45 - 15:00	**2346*** Evidence for a chemically enabled non-enzymatic origin of the Krebs cycle **Markus Keller, Division of Biological Chemistry, University of Innsbruck, Austria**	
13:30 - 15:00	**Parallel Session 5: Metabolic Phenotyping in Health (Chairs: Matej Oresic and Nichole Reisdorph)**	
13:30 - 14:00	**Keynote Speaker** Personalized Medicine in Human Space Flight: What Elite Athletes can Teach us About Molecular Deficits that affect Astronaut Health and Performance **Michael Schmidt, George Washington University, US**	The Liffey A
14:00 - 14:15	**2563** Metformin metabolomic profiles to inform pharmacogenomic discovery **Matthew Breitenstein, Mayo Clinic, USA**	
14:15 - 14:30	**2591** Pharmacometabolomics: Enabling Tool for Precision Medicine **Rima Kaddurah-Daouk, Duke University Medical Center, USA**	
14:30 - 14:45	**2311** Lipid mediator profiling for identifying sub-phenotypes of respiratory disease **Craig Wheelock, Karolinska Institute, Sweden**	
14:45 - 15:00	**2328** Metabolomics profiling identifies gender-enhanced upregulation of oxidative stress in COPD **Shama Naz, Karolinska Institute, Sweden**	

Tuesday 28th June

Time	Session	Location
13:30 - 15:00	**Parallel Session 6: Crop Quality Improvement and Food Sustainability (Chairs: Robert Hall and Doris Jacob)**	
13:30 - 14:00	**Keynote Speaker** Variability in fruit metabolites in tomato: leads for understanding the underlying biology and to improve fruit quality **Tony Granell, Polytechnic University, Valencia, Spain**	The Liffey B
14:00 - 14:15	**2388** Application of LC - Data independent acquisition (DIA) - digital archiving (DA) mass spectrometry for mycotoxin and metabolite profiling of silage **Mark Sumarah, Agriculture and Agri-Food Canada**	
14:15 - 14:30	**2300** Multi-platform metabolomics analyses of a broad collection of fragrant and non-fragrant rice varieties reveals the high complexity of grain quality characteristics **Roland Mumm, Wageningen University and Research, Business Unit, Netherlands**	
14:30 - 14:45	**2054** Fruit position within pear trees impacts ripening and associated metabolism after harvest **David Rudell, USDA-ARS, USA**	
14:45 - 15:00	**2173** Metabolomics to assess the potential of fermented fruit/vegetable by-products as a new source of functional foods **Ninna Granucci, The University of Auckland, New Zealand**	
15:00 - 15:30	Tea/Coffee/Posters	Exhibition Hall
15:30 - 17:00	**Parallel Session 7: Nutrition and Metabolism (Chairs: Ines Thiel and Jules Griffin)**	
15:30 - 16:00	**Keynote Speaker** Process Metabolomics: living systems under “direct” observation. **Soren Engelsen, University of Copenhagen, Denmark**	The Auditorium
16:00 - 16:15	**2506** Evolution of Gut Microbiota:Host co-metabolic processes determined both by term and mode of birth in the INFANTMET Cohort **Cian J. Hill, University College Cork, Ireland**	
16:30 - 16:45	**2088** The effect of plant sterols and different low doses of omega-3 fatty acids from fish oil on lipoprotein subclasses **Doris Jacobs, Unilever R&D, The Netherland**	
16:45 - 17:00	**2398** The application of lipid profiling to understand dietary fat metabolism in breast-fed infants **Albert Koulman, MRC Human Nutrition Research, UK**	

Tuesday 28th June

Time	Session	Location
15:30 - 17:00	**Parallel Session 8: Environmental Metabolomics (Chairs: Carl Ng and Annick Moing)**	
15:30 - 16:00	**2246** MetFish: A suite of chemoselective tags combined with tandem mass spectrometry for quantitative and comprehensive metabolomics analyses in extreme environments **Thomas Metz, Pacific Northwest National Laboratory, USA**	The Liffey A
16:00 - 16:15	**2044*** High resolution mass spectrometry for understanding biochemical impacts in fish exposed to complex mixtures of environmental contaminants **Jonathan Mosley, US Environmental Protection Agency, USA**	
16:15 - 16:30	**2069*** Mass spectrometry-based lipidomics to study effects of naphthalene on various organs of mice **Ping-Chun Hsieh, National Taiwan University, Taiwan**	
16:30 - 16:45	**2203** Towards a fully-automated extraction of polar and apolar metabolites from low mass tissue samples **Jelena Sostare, University of Birmingham, UK**	
16:45 - 17:00	**2030** Responses in the metabolome & lipidome of marine copepods induced by climate-related food deprivation **Ulf Sommer, University of Birmingham, UK**	
15:30 - 17:00	**Parallel Session 9: Advances in Statistical Tools (Chairs: Age Smilde and David Broadhurst)**	
15:30 - 16:00	**2330** A Novel Method for Power Analysis and Sample Size Determination in Metabolic Phenotyping **Tim Ebbels, Imperial College London, UK**	The Liffey B
16:00 - 16:15	**2193** Exploring metabolomic data from designed experiments using ANOVA-Multiblock Orthogonal Partial Least Squares **Julien Boccard, University of Geneva, Switzerland**	
16:15 - 16:30	**2035** Batch correction in the presence of non-detects **Ron Wehrens, Wageningen UR, Netherlands**	
16:30 - 16:45	**2194** Dealing with sample dependency in metabolomics studies **Pär Jonsson, Umeå University, Sweden**	
16:45 - 17:00	**2286** Batch correction strategies to reduce non-biological variation in large-scale metabolic profiling **Fumiaki Imamura, University of Cambridge, UK**	
17:15 - 18:45	Poster Session 1 - Posters #1-244	Exhibition Hall
19:00 - 20:30	EMN Reception, for early career members (Advanced sign-up required)	Liffey B

Wednesday 29th June

Time	Session	Location
08:50 - 09:50	**Plenary Speaker: Ines Thiel** Modelling of Human Metabolism	The Auditorium
09:50 - 10:30	Tea/Coffee/Posters	Exhibition Hall
10:30 - 11:50	Parallel Session 10: Early Career Session 1 (Chairs: Aoife O'Gorman and Fidele Tugizimana)	
10:30 - 10:45	**2154** Metabolic profiling of total physical activity and sedentary behavior in community-dwelling men **Kota Fukai, Keio University, Japan**	The Auditorium
10:45 - 11:00	**2284** Metabolomic profiles in different models of hepatocytes proliferation: partial hepatectomy and mitogen-induced hyperplasia **Laura Tronci, University of Cagliari, Italy**	
11:00 - 11:15	**2548** NMR spectroscopy detects metabolite differences between culture media of hepatitis C virus negative and positive cells after harvest **Gaëlle Diserens, DCR & DIPR, University of Bern, Switzerland**	
11:15 - 11:30	**2524** Stable isotope assisted evaluation of different extraction solvents for metabolomics of cereals using LC-HRMS **Maria Doppler, University of Natural Resourses and Life Sciences, Vienna, Austria**	
11:30 - 11:45	**2366** High quality metabolomics Mass Spectrometry Imaging using sputtered gold nanolayers **Sonia Torres, Institut Investigacio Sanitaria Pere Virgili, Spain**	
10:30 - 11:50	Parallel Session 11: Early Career Session 2 (Chairs: Stacey Reinke and Justin van der Hooft)	
10:30 - 10:45	**2415*** Metabolomic based identification of clusters that reflect dietary patterns **Helena Gibbons, University College Dublin, Ireland**	The Liffey B
10:45 - 11:00	**2040*** **D**etermination of the differences in metabolite profile in Sclerocarya birrea from different geographical origin and the effect on in-vitro glucose uptake activity **Cynthia Marokane, University of South Africa**	
11:00 - 11:15	**2424** In the quest of robust biomarkers for inflammatory bowel disease phenotypes using GCÐGC-HRTOFMS **Nicolas Di Giovanni, University of Liège, Belgium**	
11:15 - 11:30	**2229*** Crosstalk between astrocytes and motor neurons: a metabolomics study **Blandine Madji Hounoum, Université François-Rabelais, France**	
11:30 - 11:45	**2368*** Novel indicators of severe acute malnutrition in a cohort of Nigerian children identified through untargeted metabolomics **Amy McMillan, University of Western Ontario, Canada**	
11:50 - 13:30	Lunch/Posters	Exhibition Hall
12:10 - 13:10	Platinum Sponsor Presentations	

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with metabolomic analysis

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Wednesday 29th June

Time	Session	Location
13:30 - 15:00	**Parallel Session 12: New Approaches for Identification of Metabolites Applying NMR and MS (Chairs: Michael Witting and Rick Dunn)**	
13:30 - 14:00	**Keynote Speaker** New approaches for NMR-based, hybrid NMR/MS, and nanoparticle-assisted metabolomics **Rafael Brüschweiler, The Ohio State University, US**	The Auditorium
14:00 - 14:15	**2106** New Approaches to NMR-Based Metabolite Identification **Jeremy Everett, University of Greenwich, UK**	
14:15 - 14:30	**2447** mzCloud: An online substructural database of spectral trees for the identification of metabolites **Robert Mistrik, HighChem, Slovakia**	
14:30 - 14:45	**2109** Discovery of regulated metabolite families in untargeted metabolomics studies **Gerd Balcke, Leibniz Institute of Plant Biochemistry, Germany**	
14:45 - 15:00	**2397** FDR-controlled metabolite annotation for high-resolution imaging mass spectrometry **Theodore Alexandrov, EMBL, Germany**	
13:30 - 15:00	**Parallel Session 13: Green Systems Biology (Chairs: Wolfram Weckwerth and Darren Creek)**	
13:30 - 14:00	**Keynote Speaker** The integration of physiological, proteomic, and metabolomic levels reveals new adaptive and stress-responsive mechanisms in Pinus **Luis Valledor, University of Oviedo, Spain**	The Liffey A
14:00 - 14:15	**2168** Metabolomics and methanogenic potential - reducing agricultural greenhouse gases **Simone Rochfort, AgriBio, La Trobe University, Australia**	
14:15 - 14:30	**2383** Novel pathways, metabolites and bioactivity – A fresh look at salicinoid biosynthesis through NMR-MS metabolomics **Jane Ward, Rothamsted Research, UK**	
14:30 - 14:45	**2441** Metabolomics and inverse modelling of the AMPK-TOR crosstalk in plants and animals **Wolfram Weckwerth, University of Vienna, Austria**	
14:45 - 15:00	**2192** Metabolic mapping in plants: LAESI-MS imaging **Robert Hall, Wageningen UR, Netherlands**	

Wednesday 29th June

Time	Session	Location
13:30 - 15:00	**Parallel Session 14: Metabolomics Profiling in Cancer (Chairs: Lars Dragsted and Krista Zanetti)**	
13:30 - 14:00	**2119** Serum metabolomic profiling of prostate cancer risk in the Prostate, Lung, Colorectal and Ovarian Cancer Screening (PLCO) Trial **Demetrius Albanes, US National Cancer Institute, USA**	The Liffey B
14:00 - 14:15	**2287** Brain tumour: Can LC-MS-based metabolomics reveal the tumour invasive margin? **Dong-Hyun Kim, University of Nottingham, UK**	
14:15 - 14:30	**2594** DESI-Imaging of inflammatory markers for cancer **Renata Soares, Imperial College London, UK**	
14:30 - 14:45	**2041** Metabolomics study of early hepatocarcinogenesis from mice model: role of methylation and energy metabolism **Peiyuan Yin, Dalian Institute of Chemical Physics, China**	
14:45 - 15:00	**2500*** Myc linked to aberrant lipid metabolism in lung cancer by mass spectrometry imaging **Zoe Hall, University of Cambridge, UK**	
15:00 - 15:15	**2353** Plasma metabolomics for prognostic biomarker development in pancreatic cancer **Amrita Cheema, Georgetown University, USA**	
15:00 - 15:30	Tea/Coffee/Posters	Exhibition Hall
15:30 - 17:00	**Parallel Session 15: Foodomics and Food Quality (Chairs: Karsten Hiller and Cristina Andres Lacueva)**	
15:30 - 16:00	**Keynote Speaker** Combining metabolomics and genomics to dissect rice quality, and provide robust and trait-relevant tools to rice breeders **Melissa Fitzgerald, University of Queensland, Australia**	The Auditorium
16:00 - 16:15	**2410** Global untargeted metabolomics approach to reveal metabolic shifts during postharvest cold storage of 'Kinnow' Mandarin **Manpreet Saini, National Agri-Food Biotechnology Institute, Mohali, India**	
16:15 - 16:30	**2138** What makes a peanut, a peanut? Elucidating the metabolome of the raw peanut seed **Claire Klevorn, North Carolina State University, USA**	
16:30 - 16:45	**2068** Wine and grape juice lipidomics: the impact of juice lipids on wine properties **Silas Villas-Boas, University of Auckland, New Zealand**	
16:45 - 17:00	**2222** Real time detection of fish fraud using rapid evaporative ionisation mass spectrometry (REIMS) **Connor Black, Queens University Belfast, UK**	

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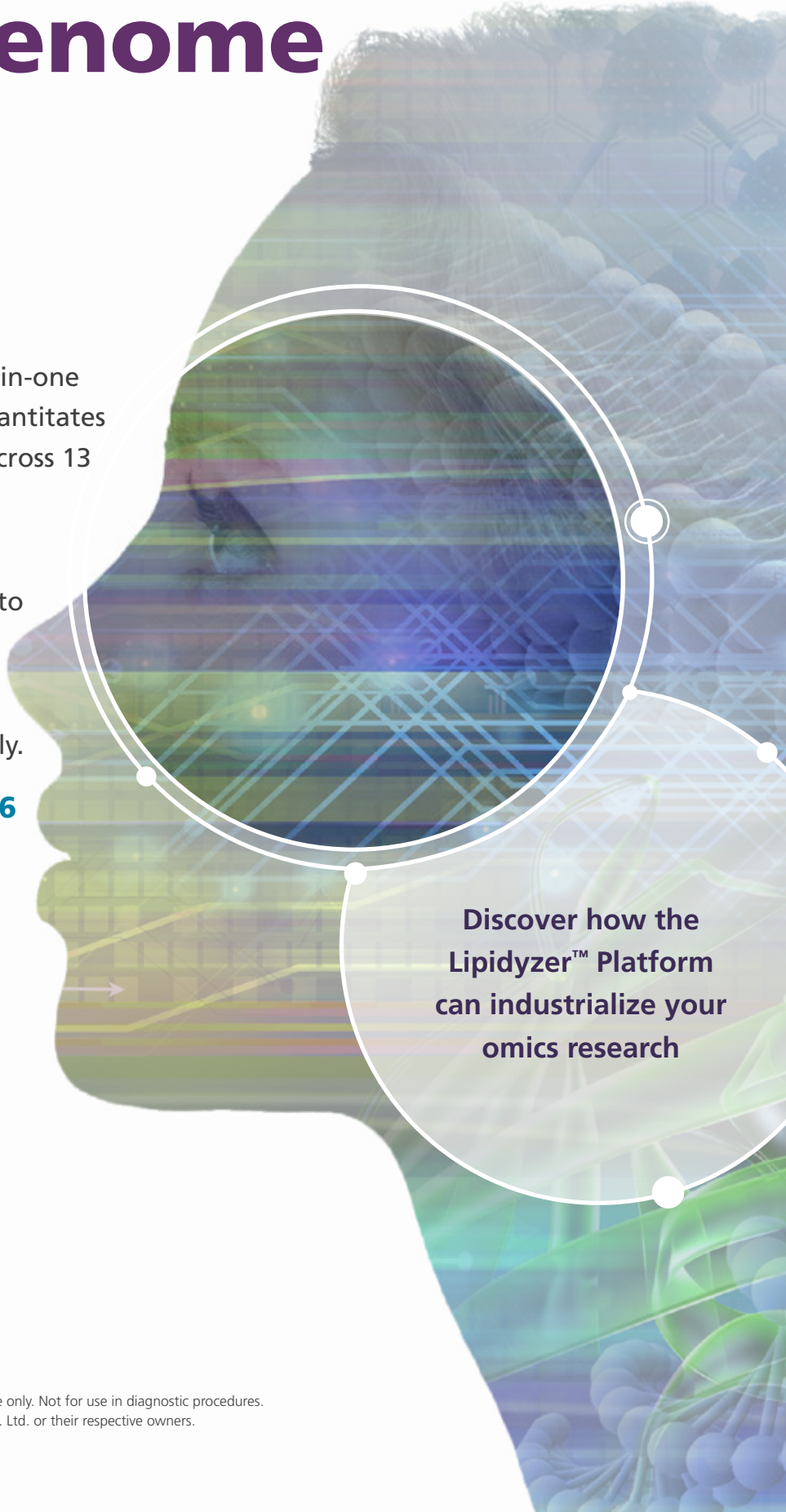

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Wednesday 29th June

Time	Session	Location
15:30 - 17:00	**Parallel Session 16: Impact of Metabolomics in Clinical Medicine 1** (Chairs: Louise Kenny and Jerzy Adamski)	
15:30 - 16:00	**Keynote Speaker** Metabolomics and Epidemiology: Building Infrastructure and Leveraging Resources to Accelerate Scientific Discovery **Krista Zanetti, National Cancer Institute, US**	The Liffey A
16:00 - 16:15	**2565** Direct from Sample Microbial Metabolomics using Rapid Evaporative Ionisation Mass Spectrometry (REIMS) **Simon Cameron, Imperial College London, UK**	
16:15 - 16:30	**2285** The metabolic signature of stored red blood cells can be used for assessing the quality of red cell concentrate units during the storage **Giuseppe Paglia, European Academy of Bolzano/Bozen, Italy**	
16:30 - 16:45	**2561*** Linking the gut microbiome, blood metabolites and Volatile organic compounds in breath **Agnieszka Smolinska, Maastricht University, Netherlands**	
16:45 - 17:00	**2503** How humanisation of the liver affects metabolism in the mouse brain **Kate Bennett, AcureOmics AB, Sweden**	
15:30 - 17:00	**Parallel Session 17: Computational MS** (Chairs: Steffen Neumann and Sebastian Böcker)	
15:30 - 16:00	**Keynote Speaker** Generalized methods for targeted 13C metabolic flux analysis **Nicola Zamboni, ETH, Switzerland**	The Liffey B
16:00 - 16:15	**2326** IFrID: A Novel In-Source Fragmentation Detection and Deconvolution Algorithm for LC-MS Metabolomics Data **Tytus Mak, National Institute of Standards and Technology, USA**	
16:15 - 16:30	**2416** Towards enhanced plant metabolomics by combining 13C-labeling assisted workflows to study the metabolic defense of wheat against Fusarium **Christoph Bueschl, BOKU University Vienna, Austria**	
16:30 - 16:45	**2023** Significance of metabolite identifications from searching mass spectral libraries **Franziska Hufsky, Friedrich Schiller University Jena, Germany**	
16:45 - 17:00	**2077** Confidence score for metabolite identifications from structural library search **Marcus Ludwig, Friedrich Schiller University Jena, Germany**	
17:00 - 18:30	Poster Session 2: Posters #245-490	Exhibition Hall
19:15 - 23:30	Conference Dinner – Bus Loading at the CCD begins at 19:15 for a 19:30 departure. (See page 29 for additional details)	

Thursday 30th June

Time	Session	Location
09:00 - 10:30	**Parallel Session 18: Abiotic and Biotic Stresses in Plants (Chairs: Ute Roessner and Tsutomu Masujima)**	
09:00 - 09:30	**Keynote Speaker** Regulation of respiratory metabolism in response to flooding stress as revealed by 13C-stable isotope redistribution **Toshihiro Obata, Max-Planck-Institute of Molecular Plant Physiology, Germany**	The Auditorium
09:30 - 09:45	**2180*** Non-targeted and targeted metabolomic approaches reveal differences in legume chemistry before and after infestation with pea aphid host races **Carlos Sanchez Arcos, Max Planck Institute, Germany**	
09:45 - 10:00	**2082** Comparative metabolite profiling from growth chamber, environmental simulation chamber or field trial experiments investigating cold acclimation of 49 natural accessions of Arabidopsis thaliana **Ellen Zuther, Max Planck Institute, Germany**	
10:00 - 10:15	**2142** Metabolite profiling of shoot extracts, root extracts, and root exudates of rice under nitrogen and phosphorus deficiency **Keitaro Tawaraya, Yamagata University, Japan**	
10:15 - 10:30	**2002** A metabolomics approach to study the “war” between plants and insects - Identification of plant gene functions and their consequences in herbivory insects **Aiko Barsch, Bruker Daltonics, Germany**	
09:00 - 10:30	**Parallel Session 19: New Development in Instruments and Techniques (Chairs: Dan Bearden and Tim Ebbels)**	
09:00 - 09:30	**Keynote Speaker** Mass spectrometric strategy for clinical metabolomics **Tuulia Hyötyläinen, Steno Diabetes Centre, Denmark**	The Liffey A
09:30 - 09:45	**2226** Stable isotope-labeled yeast extracts as internal standard for LC-MS/MS based amino acid quantification in samples of human origin **Gerrit Hermann, ISOtopic solutions, Austria**	
09:45 - 10:00	**2324** Addition of drift-tube ion mobility to liquid chromatography-mass spectrometry workflows: examining the potential for cellular metabolomics **Tim Causon, University of Natural Resources and Life Sciences, Austria**	
10:00 - 10:15	**2238** Optimus + `ili: software for LC-MS based untargeted spatial metabolomics in 2D and 3D **Ivan Protsyuk, EMBL, Germany**	
10:15 - 10:30	**2466** Spatial Metabolomics: MALDI Mass Spectrometry Imaging of Plant Metabolites **Berin Boughton, University of Melbourne, Australia**	

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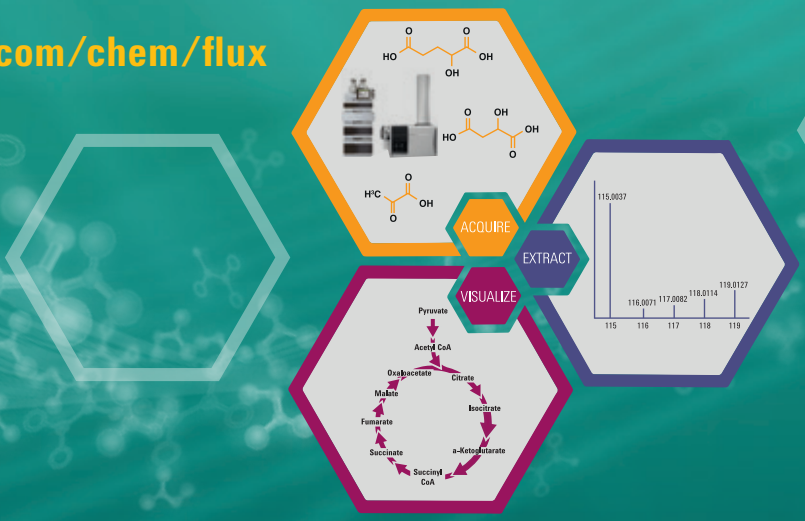

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- ***Rima Kaddurah-Daouk,*** Duke Institute for Brain Sciences

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Thursday 30th June

Time	Session	Location
09:00 - 10:30	**Parallel Session 20: Impact of Metabolomics in Clinical Medicine 2 (Chairs: Blandine Comte and Lorraine Brennan)**	
09:00 - 09:30	**Keynote Speaker** Metabolic rewiring of macrophages during inflammation: How metabolism provides antimicrobial activity and regulates inflammation **Karsten Hiller, Luxembourg Centre for Systems Biomedicine, Luxembourg**	The Liffey B
09:30 - 09:45	**2436** Origin of plasma acylcarnitines in humans during fasting and exercise **Miriam Hoene, University Hospital Tuebingen, Germany**	
09:45 - 10:00	**2390** Medium-throughput metabolomics screening identifies modes of action for novel antimalarials **Darren Creek, Monash Institute of Pharmaceutical Sciences, Australia**	
10:00 - 10:15	**2343*** Brain metabolomics identifies involvement of unsaturated fatty acid metabolism in "asymptomatic Alzheimer's disease" **Stuart Snowden, Kings College London, UK**	
10:15 - 10:30	**2453** Serine, threonine metabolic pathways associated with HDL-C response to niacin treatment **Sony Tuteja, University of Pennsylvania Perelman School of Medicine, USA**	
10:30 - 10:50	Tea/Coffee	Level 1 & 3 Foyer
10:50 - 11:50	**Parallel Session 21: Metabolomics in Early Life (Chairs: Hwang Geum-Sook and Aifric O Sullivan)**	
10:50 - 11:05	**2045*** Integration of metabolomic and genome-wide transcriptomic networks in pregnant women reveals biological pathways associated with pre-eclampsia **Rachel Kelly, Brigham and Women's Hospital Harvard Medical School, USA**	The Auditorium
11:05 - 11:20	**2384** Early serum biomarkers to predict risk of third trimester placental abruption **Susan Sumner, RTI International, USA**	
11:20 - 11:35	**2396*** The placental mitochondrial metabolome suggests the importance of lipid metabolism in pre-eclampsia **Ting-Li Han, University of Auckland, New Zealand**	
11:35 - 11:50	**2313*** Childhood obesity and insulin resistance, metabolomics strategies unveil early onset metabolic alteration and the influence of sex **Annalaura Mastrangelo, Universidad San Pablo CEU, Spain**	

Thursday 30th June

Time	Session	Location
10:50 - 11:50	**Parallel Session 22: Metabolomic Analysis of Challenge Tests (Chair: Hannelore Daniel)**	
10:50 - 11:05	**2583** Visualizing and exploring the dynamics of the human metabolome: the Humet 2.0 data repository **Gabi Kastenmüller, Helmholtz Zentrum München, Germany**	The Liffey A
11:05 - 11:20	**2589** Dynamic Response of the Human Metabolome to Environmental Stimuli through Comprehensive Metabolomic Profiling – the Humet 2.0 Study **Robert Mohney, Metabolon, Inc., USA**	
11:20 - 11:35	**2402** Stability of human plasma "metabotypes" in response to dietary challenges **Jarlei Fiamoncini, Technical University of Munich, Germany**	
11:35 - 11:50	**2477** The dynamic range of the human metabolome revealed by challenges: a non-target view **Karsten Suhre, Weill Cornell Medicine , Qatar**	
10:50 - 11:50	**Parallel Session 23: Metabolomics for Disease Biomarkers (Chair: Michael Schmidt)**	
10:50 - 11:05	**2163** Metabolic phenotyping to predict mortality and individualise treatment and transplant candidacy in patients with cirrhosis **Muireann Coen, Imperial College London, UK**	The Liffey B
11:05 - 11:20	**2128** Human serum metabolites associate with severity and patient outcomes in traumatic brain injury **Matej Oresic, Turku Centre for Biotechnology, Finland**	
11:20 - 11:35	**2375** GC-MS metabolomics towards a putative urinary biosignature for Tuberculous Meningitis in children **Shayne Mason, North-West University, SA**	
11:35 - 11:50	**2046** Integrating metabolomics and transcriptomics in the study of asthma severity **Jessica Lasky-Su, Brigham and Women's Hospital Harvard Medical School, USA**	
12:00 - 12:40	**Plenary Speaker: Tsutomu Masujima** Direct metabolomics for plant single cells	The Auditorium
12:40 - 13.:30	Closing Ceremony	

* Indicates Student and Early Career Travel Award Winners

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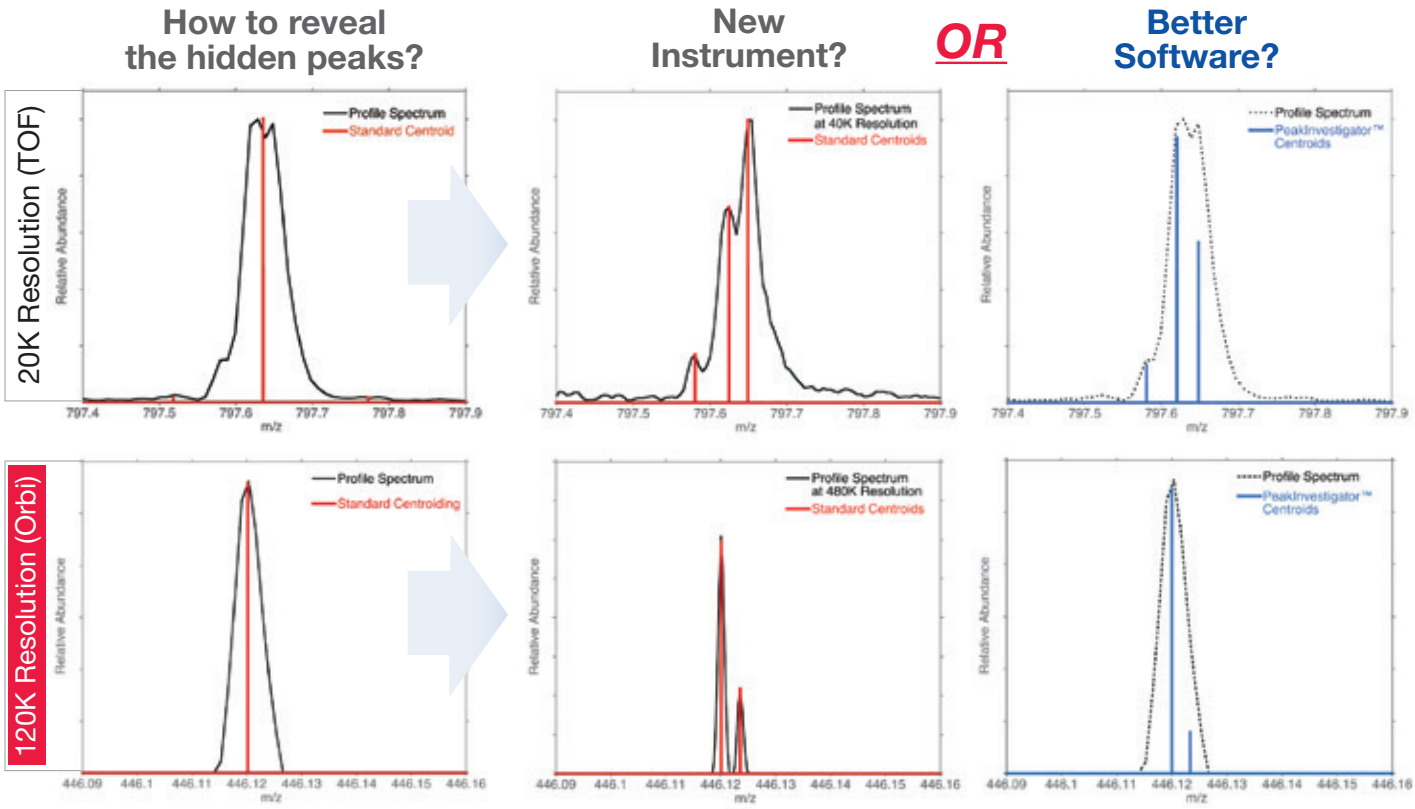

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Plenary & Keynote Speakers

10

Ines Thiele

Plenary

Professor Dr. Ines Thiele studied technical biology at the University of Stuttgart, Germany, and biotechnology at the Ecole supérieure de biotechnologie de Strasbourg, France. In 2009, she earned her PhD in bioinformatics from the University of California, San Diego. In 2009, she joined the Center for Systems Biology at the University of Iceland, as an independent group leader and Assistant Professor. In 2013, she was appointed as Associate Professor for Systems Biomedicine at the University of Luxembourg and received the ATTRACT fellowship from the Fonds National de la Recherche (Luxembourg). In 2015, she was elected as EMBO Young Investigator. Her research aims to improve the understanding on how diet influences human health. Therefore, she uses a computational modeling approach, termed constraint-based modeling, which has gained increasing importance in systems biology. Her group builds comprehensive models of human cells and human-associated microbes; then employs them together with experimental data to investigate how nutrition and genetic predisposition can affect one's health. In particular, she is interested in applying her computational modeling approach for better understanding inherited and neurodegenerative diseases. She is author of numerous international scientific papers and reviewer for multiple journals and funding agencies.

Jeremy Nicholson

Plenary

Professor Jeremy Nicholson obtained his BSc from Liverpool University (1977) and his PhD from London University (1980). After several academic appointments at London University (School of Pharmacy and Birkbeck College, London, 1981-1991) he was appointed Professor of Biological Chemistry (1992). In 1998 he moved to Imperial College London as Professor and Head of Biological Chemistry and subsequently Head of the Department of Biomolecular Medicine (2006) and Head of the Department of Surgery, Cancer and Interventional Medicine in 2009 where he runs a series of research programs in stratified medicine, molecular phenotyping and molecular systems biology. In 2012 Nicholson became the Director of world's first National Phenome Centre specialising in large-scale molecular phenotyping and he also directs the Imperial Biomedical Research Centre Stratified medicine program and Clinical Phenome Centre. Nicholson is the author of over 700 peer-reviewed scientific papers and many other articles/patents on the development and application of novel spectroscopic and chemometric approaches to the investigation of metabolic systems failure, metabolome-wide association studies and pharmacometabonomics. Nicholson is a Fellow of the Royal Society of Chemistry, The Royal College of Pathologists, The British Toxicological Society, The Royal Society of Biology and is a consultant to several pharmaceutical/healthcare companies.

Nicholson's research has been recognised by several awards including: The Royal Society of Chemistry (RSC) Silver (1992) and Gold (1997) Medals for Analytical Chemistry; the Chromatographic Society Jubilee Silver Medal (1994); the Pfizer Prize for Chemical and Medicinal Technology (2002); the RSC medal for Chemical Biology (2003); the RSC Interdisciplinary Prize (2008) the RSC Theophilus Redwood Lectureship (2008); the Pfizer Global Research Prize for Chemistry (2006); the NIH Stars in Cancer and Nutrition Distinguished Lecturer (2010), the Semelweiss-Budapest Prize for Biomedicine (2010), The Warren Lecturer, Vanderbilt University (2015).

Luke O'Neill

Plenary

Professor Luke O'Neill was appointed to the Chair of Biochemistry at Trinity College Dublin in 2008, where he leads the Inflammation Research Group. He has a PhD in Pharmacology from the University of London and carried out Post-Doctoral research at Cambridge U.K. on the pro-inflammatory cytokine IL-1 and innate immune signaling. His research is in the area of the molecular basis to inflammatory diseases. He has won numerous awards for his research, notably the Royal Irish Academy Medal for Biochemistry, The Irish Society for Immunology medal, the Royal Dublin Society/ Irish Times Boyle medal for Scientific Excellence, the Science Foundation Ireland Researcher of the Year Award and in 2014 the European Federation of Immunology Societies Medal. He was elected a member of EMBO in 2005. In 2014 he was named by Thompson Reuters as one of the world's most influential scientists, being in the top 1% in both Immunology and Pharmacology/Toxicology. He is a European Research Council Advanced Grant Holder and is co-founder and director of Opsona Therapeutics, a drug development company working in the area of Toll-like receptors.

Tsutomu Masujima

Plenary

Professor Tsutomu Masujima is the Team Leader of the Single Cell Mass Spectrometry Team in the Quantitative Biology Center (QBiC), RIKEN, Japan. His research fields include Development of New Analytical Methods for Life Sciences and Medicine. More specifically he is active in the area of Live Single Cell Mass Spectrometry and Single Cell Medicine. In 2008 he was awarded the Analytical Chemistry Award from The Japan Soc. of Analytical Chemistry. In 2014 he was awarded The Yamazaki-Teiichi Prize (in Measurement Science) and 2015 the Technology Award of the Mass Spectrometry Society of Japan. He has recekty publsied a Nature Protocols paper entitled "Direct Metabolomics for Plant Single Cells by Live Single Cell Mass Spectrometry.

Karsten Hiller

Keynote

Prof Karsten Hiller is head of the Metabolomics Group and a FNR-ATTRACT Fellow at the Luxembourg Centre for Systems Biomedicine (LCSB). He studied Biology and Computer Science at the University of Braunschweig, Germany where he also obtained his PhD in Bioinformatics and Microbiology in 2006. In 2008 he joined the Department of Chemical Engineering at the Massachusetts Institute of Technology where he performed research in stable-isotope assisted metabolomics and cancer metabolism. Since 2010 he is the Head of the Metabolomics Group at the LCSB and was holder of the FNR-ATTRACT grant from the Fonds National

de la Recherche (Luxembourg). In 2016 he was appointed as an Associate Professor for Cellular Metabolism at the University of Luxembourg. The research interest of his group covers metabolic aspects of (neuro-)inflammation and neurodegeneration. For this purpose, his team develops and applies technology at the interface of mass spectrometry, experimental and computational biology to profile cellular metabolism.

Abstract:

Metabolic rewiring of macrophages during inflammation: How metabolism provides antimicrobial activity and regulates inflammation

Having profiled the metabolome of macrophages and microglial cells under inflammation, we identified an intracellular and highly abundant metabolite: itaconic acid. By applying stable-isotope labeling experiments, we could demonstrate that this metabolite is produced in the tricarboxylic acid cycle from cis-aconitate by an enzyme encoded by immune response gene 1 (IRG1). Besides its antimicrobial function in the innate immune response, it turned out that itaconic acid is itself involved in metabolic regulation during inflammation. One key step during metabolic reprogramming in activated macrophages is the stabilization of HIF1a. Regulatory activity of this factor is known to increase the glycolytic flux towards lactic acid production and to reduce respiration. To get a better picture of the rearrangement of intracellular metabolic fluxes, we applied stable-isotope labeling and showed that a sustained flux of pyruvate through pyruvate dehydrogenase complex (PDH) is essential for macrophage polarization. A sustained and high pyruvate flux into the TCA cycle is required for the synthesis of itaconic acid and lipogenic citrate. By inhibiting the mitochondrial pyruvate transporter and thus decreasing pyruvate oxidation through PDH, we could modulate the immune response of the macrophages. This is an example on how metabolism itself is involved in cellular regulation and how detailed knowledge on such can offer therapeutic intervention points.

Krista Zanetti

Keynote

Krista Zanetti is a Program Officer in the Epidemiology and Genomics Research Program (EGRP), Division of Cancer Control and Population Sciences at the National Cancer Institute (NCI), National Institutes of Health (NIH). Dr. Zanetti earned her Ph.D. in Nutrition from Cornell University in 2003 and joined the Cancer Prevention Fellowship Program at the NCI. During the first year of her fellowship, she earned an M.P.H. at the Johns Hopkins Bloomberg School of Public Health. Dr. Zanetti then conducted primary research in the Laboratory of Human Carcinogenesis in the NCI's Center for Cancer Research from 2004 to 2010. Since joining EGRP in 2010, Dr. Zanetti's primary focus has been building infrastructure and capacity to support metabolomics in population-based studies. Most recently, she spearheaded collaborative efforts to establish the trans-NIH international COnsortium of METabolomics Studies (COMETS), which brings together 25 prospective cohorts and two consortia from the U.S., Europe, Asia and South America (http://epi.grants.cancer.gov/comets/). COMETS allows investigators from across multiple disease phenotypes to: 1.) leverage existing resources and data; and 2.) work collectively to develop methods, tools and protocols for data harmonization and sharing, quality control and data standardization.

Abstract:

Metabolomics and Epidemiology: Building Infrastructure and Leveraging Resources to Accelerate Scientific Discovery

The National Institutes of Health Common Fund has invested more than $111 million from 2012 to 2017 through the Metabolomics Program to increase the national capacity in metabolomics. With this investment and corresponding infrastructure development, it is an ideal time to expand the use of metabolomics within biomedical and public health

research to further advance biomarker discovery. In recent years, we have seen an increase in the number of epidemiologic and clinical studies using metabolite profiling to improve disease risk assessment, early detection, diagnosis, prognosis, and predictive response to therapy. However, there are a number of challenges to overcome in the field, such as the need for methods to harmonize and integrate data across laboratory platforms and analytical techniques.

These obstacles, like many others, are most effectively tackled with collaborative efforts. Towards this end, the National Cancer Institute's Epidemiology and Genomics Research Program and the Division of Cancer Epidemiology and Genetics established the International COnsortium of METabolomics Studies (COMETS). COMETS leverages resources and metabolomics data from 25 prospective cohorts and two consortia spanning the United States, Europe, Asia and South America with cardiovascular, cancer, diabetes, and aging outcomes for novel biomarker discovery. Establishing a collaborative group of prospective studies allows for increased statistical power, accelerated replication of study findings and standardized analytic methods for data across studies. This presentation will focus on the use of metabolite profiling in epidemiology studies and highlight recent collaborative efforts in this area.

Melissa Fitzgerald

Keynote

Melissa has held the Australian Food and Grocery Chair at the University of Queensland since 2012. Before that she was the head of rice quality, nutrition and value adding at the International Rice Research Institute. She was introduced to Metabolomics through collaboration on a project on metabolomics of rice, melons and broccoli, and was so impressed with the techniques, that she has embraced metabolomics to progress our understanding of the sensory experience of eating rice and other foods, by combining it with genomics and sensory profiling. Her over-arching aims are to provide selection tools to breeding programs for the traits of sensory quality of food.

Abstract:

Combining metabolomics and genomics to dissect rice quality, and provide robust and trait-relevant tools to rice breeders

Aromatic rice commands the highest prices in both domestic and international markets because consumers prize both the mouth-watering aroma and delicate flavour of the rice. The major aromatic compound in fragrant rice is 2- acetyl 1-pyrroline (2AP). Using a panel of 380 diverse varieties of rice, metabolomics profiling of volatile compounds from the grain, and genome wide association with 33000 single nucleotide polymorphisms (SNPs), the objectives of this study were to identify (i) sensory traits that describe jasmine rice; (ii) the volatile compounds that define those sensory traits, and (iii) genetic markers for those compounds. The sensory descriptors fell into three clusters, with Cluster 1 describing high quality jasmine rice, Cluster 3 describing non-fragrant rice, and lower quality jasmine rices falling between the descriptors in Clusters 1 and 2. The compounds that most strongly discriminated the high quality jasmine rices from the other samples were 2AP and four other compounds, two of which required high resolution platforms to reveal their molecular structure and annotation. These five compounds associate with the same SNP on chromosome 8, several are fragrant with a low odour threshold, and they provide new information about the pathway of 2AP synthesis. Three QTL were found that associate with high or low amounts of the five compounds. Another 20 metabolites associated either positively or negatively with high quality jasmine fragrance. Significant genetic associations could be found for some of these compounds, but for several, the structure of the phenotype data was unsuitable for valid QTL detection. By combining these platforms, we deliver new and valuable tools to breeders for

fragrant compounds and 2AP. We also deliver information and germplasm for the development of new populations targeted to provide appropriate phenotype data to identify QTLs for the other important metabolites identified here.

Michael Schmidt

Keynote

Dr. Michael A. Schmidt is the President of Sovaris Aerospace and co-chair of the Advanced Pattern Analysis & Countermeasures Group. He is also Course Director of the Clinical Genomics, Proteomics, and Metabolomics Program, at George Washington University School of Medicine and Health Sciences. Dr. Schmidt is among the leaders advancing the use of integrated Omics and personalized medicine methodologies for application in human space flight. His work also includes complex molecular profiling and countermeasure development for elite athletes across a wide range of professional and Olympic sports, including some of America's most successful teams.

Dr. Schmidt did his Ph.D. research in molecular medicine and biochemistry within the Life Sciences Division at NASA Ames Research Center, under NASA Ames Chief Medical Officer Ralph Pelligra, M.D. Dr. Schmidt also did a fellowship at NASA's Human Systems Integration Division, with an emphasis on physiologic monitoring and countermeasures aimed at raising human performance in extended microgravity, artificial gravity, sleep deprivation, night vision operations, pararescue, high altitude flight, and other stressors encountered in extreme environments. He has done additional studies at Lancaster University (neuroscience) and the Massachusetts Institute of Technology (data and models).

Dr. Schmidt is co-author of "Personalized Medicine in Human Space Flight" (Metabolomics 2013) and "Incorporation of Omics Analyses into Artificial Gravity Research for Space Exploration Countermeasure Development" (Metabolomics 2016)

Abstract:

Personalized Medicine in Human Space Flight: What Elite Athletes can Teach us About Molecular Deficits that affect Astronaut Health and Performance

For some years, we have been developing personalized medicine methodologies for human missions to the Moon, Mars, and deep space, which are based on complex molecular profiling. Core tenets of this approach have been developed in parallel through our assessment and countermeasure efforts involving elite athletes, as well as in humans working and competing in extreme conditions.

We have conducted serum chemistry, genome, gut microbiome, and gut microbiome metabolome profiling of elite athletes derived from professional football, professional basketball, track & field, Olympics, high altitude mountaineering, professional motor sports (Le Mans), and military Special Forces. This work has revealed widespread molecular deficits that are highly individualized. Our findings recognize that elite athlete and astronaut cohorts share a general vulnerability, as they encounter their unique extreme conditions.

Where elite athletes and astronauts begin to differ, however, is in the manner by which the space flight environment rapidly accelerates changes in molecular events and accentuates the influence of molecular deficits. Notably, the convergence of microgravity, space radiation, prolonged isolation, fluid shifts, muscle atrophy, bone loss, and other conditions of space travel, substantially impact adaptive mechanisms. For instance, the primary reservoirs for magnesium are bone and muscle. However, space flight associated bone and muscle loss facilitates the loss of magnesium. This has a potentially significant effects on DNA repair, since many DNA repair enzymes are either directly magnesium dependent or require ATP (which is Mg dependent). Similarly, alterations in the genes, direct nutritional inputs, or dietary components that act as transcription factors, may significantly impact one carbon metabolism, which has its own wide-ranging effects on genome stability in the radiation environment of space.

Our findings argue for detailed molecular profiling of humans entering space, and for the development of precision countermeasures that are individualized to the astronaut and to the mission.

Søren Engelsen

Keynote

Søren Balling Engelsen has a PhD in molecular modeling from The Technical University of Denmark and is professor in biospectroscopy at University of Copenhagen. His primary research topic is development and application of high-throughput quantitative spectroscopic methods (NIR, IR, Raman and NMR) for biological samples in quality control, process analytical chemistry, foodomics, and metabolomics. A key issue in this line of research is the development of multivariate chemometric methods (exploration, regression, and classification) for optimal spectral information extraction. The second research topic is molecular modeling of polysaccharide structures and their interaction with water and affinity to bioactive metabolites and in turn how to exploit these interactions to tailor functionality and health-promoting effects of food. He is author or coauthor of more than 180 published peer reviewed papers, two patents, and numerous book chapters. Søren is most recently awarded the Tomas Hirschfeld Award by the International Council for Near Infrared Spectroscopy (ICNIRS) for longstanding achievement in NIR spectroscopy. (ResearchGate: https://www.researchgate.net/profile/Soren_Engelsen).

Abstract:

Process Metabolomics: Living Systems Under "Direct" Observation

The world of analytical instrumentations is expanding continuously. Complex, hyper-sensitive and highly selective analytical instruments have become available for conducting metabolomics research. The quest for increased sensitivity has largely driven this development. Hundreds if not thousands of metabolites can be measured in a very short time. For the first time in history, we can conduct inductive research i.e. measuring first and posing the questions afterwards. Metabolomics can help answering these questions that lie beyond the powers of upstream genomics, transcriptomics and proteomics, and facilitate an understanding and assessment of the phenotype.

Plants, microbes, humans and e.g. industrial processes are not much different, and metabolomic technology is well adapted for studying down-stream consequences or different genetic makeups and environmental settings. Metabolomics technology is as such ideal for attacking global challenges such as personal health, influence of the climate, developing biopreservative foods, optimizing biofermentation processes, etc. Unfortunately, it would appear that some conservatism has sneaked in in modern metabolomics research. Many applications are conducted with the same (powerful) analytical technology and the same discriminant methods. This paper tries to line up some recent research work with focus on exploratory findings and new discriminant methods such as rPLS-DA. Examples of metabolomics research are given is diverse areas such as in vitro microbial NMR metabolomics of living lactic acid bacteria, the developing barley endosperm metabolome under different temperatures, the Lepidopteran defence droplets against predators and nutritional GC-MS plasma metabolomics comparing new Nordic diet vs. average Danish diet.

Tuulia Hyötyläinen

Keynote

Dr. Tuulia Hyötyläinen obtained a MSc degree in Chemistry at The University of Helsinki in Finland followed by a PhD in Analytical Chemistry. Dr. Hyötyläinen has a broad background in separation science, particularly in hyphenated and multidimensional chromatographic methods combined with mass spectro-

metric techniques. Her main research interests are development of novel methodologies for metabolomics and clinical diagnostics. Last seven years her main emphasis has been in the development of methods for metabolomic analyses, both for non-targeted profiling methods in discovery, as well as for targeted analysis of specific key metabolites. In non-targeted profiling methods, the goal has been to develop methods with high coverage of metabolites. One of the main goals has been the development of robust workflows from sampling, sample preparation, analysis to data preprocessing and data mining, and quality control of the each step of the workflow. Development of methodologies for the identification of unknown metabolites has also been one of the main aspects of the research.

Abstract:

Mass spectrometric strategy for clinical metabolomics

Advances in analytical techniques and bioinformatics enabled increasingly comprehensive and accurate coverage of metabolites both in tissues and biofluids, yet many challenges remain. For comprehensive coverage of the metabolome, several techniques are needed as it is not possible to analyze the complete cellular or biofluid metabolome with any single analytical technique. In addition, different methodologies are required in discovery than e.g. in clinical diagnostics. Especially in clinical studies, it is essential to consider multiple factors in the optimization of the study set-up and workflow in order to assure reliability and comparability of results across multiple studies. For example, the types of samples, sample pretreatment, storage as well as sample preparation should be taken into consideration as all these steps affect the metabolic profile. Strict quality control in all steps, including data processing is essential particularly in large-scale non-targeted metabolomics. Another challenge is the identification of unknown metabolites which are not found in the mass spectral databases. Identification of unknown metabolites requires in most cases high resolution MS measurements and often parallel techniques. This presentation will show workflow and novel analytical tools for the analysis of clinical samples and methodologies for the identification of the potential unknown metabolic biomarkers. Selected examples in biomarker discovery and clinical applications in diabetes and traumatic brain injury are presented.

Antonio Granell Richart

Session Keynote

Research Professor of the Spanish National Research Council (CSIC), leads the Plant Genomics and Biotechnology Group at the Plant Molecular and Cellular Research Institute in Valencia, Spain after working for several years in USA and Canada - Plant Science Institute in Philadelphia (PA, USA), Queens University (Kingston, ON, Canada). His research activities during the last few years have been directed to understand the molecular genetics of fruit quality traits, their variability and improvement, with an emphasis in those traits resulting from the levels of primary and secondary metabolites. Results have been published in over 120 papers in ISI journals, 40 book chapters and about 12 patent, several genomic and biotech databases, and to the generation of tools and plant materials for the scientific community. His main interest now is directed to the characterization, valorization and increase resilience of traditional tomato varieties, increase tomato tolerance to high temperatures and to develop tools and study case in the plant biotec field (http://www.ibmcp.upv.es/FGB/).

Luis Valledor

Session Keynote

Luis Valledor obtained his Ph.D in the field of Plant Biology from the University of Oviedo in 2009, obtaining a deep background in plant proteomics. Dr. Valledor was then awarded with a Marie Curie-IEF grant

to join Prof. Weckwerth's lab at the University of Vienna where he developed new proteomic and metabolomic-based approaches for studying abiotic stress responses in microalgae and pines. After working several years in the Academy of Sciences of the Czech Republic he returned to the University of Oviedo where he is a PI. His main research interest is based on the study of the adaptive process to temperature and UV stresses in conifers. To this purpose, novel workflows and analytical methods have been developed aiming to integrate environment, natural variation, ecophysiology, and omics. The goal of these studies is the employ "population" proteomics and metabolomics to deepen in our knowledge of stress biology as a basis for providing novel tools for plant selection and forest management. Understanding how microalgae respond to abiotic stresses, and particularly its signalling mediated by SnRK family, is also an important aspect of the research at his lab.

Matthew DeJongh

Session Keynote

Matthew DeJongh received his Ph.D. in Computer Science from The Ohio State University in 1991. He entered the field of Bioinformatics in 1998 as a Software Engineer for NetGenics, Inc., subsequently LION bioscience Inc. In 2002 he moved to Hope College in Holland, Michigan, USA, where he is currently Professor of Computer Science, and conducts research in bioinformatics with undergraduate students. His research interests lie in the creation of software to automate the reconstruction of metabolic and regulatory models of bacteria based on their genome sequences, and the application of these models to the analysis of phenotypic data. Since 2005 he has participated in the SEED genome annotation project, development of the RAST annotation service, the ModelSEED project for automated reconstruction of metabolic models, and the United States Department of Energy's Systems Biology Knowledgebase (KBase) project. In 2016 he is a visiting researcher in the Thiele lab at the Luxembourg Centre for Systems Biomedicine through a Fulbright Research Scholar grant.

Abstract:

Building the Killer App for Modeling Metabolism: from ModelSEED to KBase

In 2003, The Fellowship for Interpretation of Genomes initiated The Project to Annotate 1000 Genomes. The explicit goal was to develop a system for accurate, high-volume annotation of microbial genomes, and to provide superior annotations for the first 1000 sequenced genomes. The resulting system provided a platform for the ModelSEED project, which automates prediction of the metabolic capabilities of annotated microbes by constructing flux-balance analysis models of their biochemical reaction networks. The ModelSEED has been used by scientists worldwide to generate tens of thousands of metabolic models, and has been incorporated into the U.S. Department of Energy's Systems Biology Knowledgebase (KBase: http://kbase.us) project. KBase is an open platform for comparative functional genomics and systems biology for microbes, plants and their communities, and for sharing results and methods with other scientists. The recently released KBase Software Development Kit (SDK) is a framework for dynamically adding applications to KBase. It is currently in use by KBase developers for adding new functionality to KBase, but also fully accessible for use by external developers. The SDK provides access to data types including genomic reads, contigs, genomes, annotations, genes, proteins, flux-balance analysis models, trees, alignments, comparative genomics, and transcriptomics. Plans to add metabolomic data types and analyses are under development. We discuss the project's approach, outline areas of current and future development, and demonstrate how metabolic modeling analyses can be performed using the KBase Narrative Interface, the graphical user interface for accessing KBase's functionality and data.

Nicola Zamboni

Session Keynote

Nicola Zamboni graduated in the group of Jay Bailey at the Institute of Biotechnology of ETH Zurich in the field of metabolic engineering and 13C metabolic flux analysis. As a PostDoc in Stanford, he developed and applied metabolomics-based approaches for unraveling metabolic changes in eukaryotic cells. Since 2005, he's an independent PI at the Institute of Molecular Systems Biology in Zurich. His lab focuses on the development of mass spectrometry and computational methods to characterize metabolic dynamics in complex systems and reverse engineer cellular regulation.

- 1999 - M.Sc. Biotechnology, ETH Zürich
- 2003 - Ph.D. Biotechnology, ETH Zürich
- 2004 - 2005 Postdoctoral fellow, Stanford Genome Technology Center, Stanford University, USA
- 2005 – Principal Investigator, Institute of Molecular Systems Biology, ETH Zürich

Abstract:

Generalized methods for targeted 13C metabolic flux analysis

Metabolic flux analysis with stable isotopic tracers is the method of choice to investigate cellular metabolism. A variety of labeling strategies and computational frameworks have been devised and used to quantify the motion of metabolites through the biochemical network in simple systems, i.e. microbial networks. However, classical methods fail in complex systems with e.g. multiple substrates, larges networks, compartments, dynamic systems.

To gather quantitative flux information in complex systems, we advocate for the use of targeted 13C metabolic flux methods. Rather than attempting to resolve all fluxes at once, targeted methods are tailored to robustly quantify a specific metabolic flux regardless of rest of network. We present two computational approaches that we developed for targeted flux studies. One relies on parameter estimation using dynamic data and differential models. The second builds on surrogate modeling and machine learning applied to stationary labeling data. The two methods are complementary, generally applicable, compatible with MS and tandem MS data, support optimal experimental, and allows for high-throughput analyses.

Rafael Brüschweiler

Session Keynote

Rafael Brüschweiler received his Bachelor's and Master's degrees in Physics from ETH, Zürich, Switzerland, and his Ph.D. in Chemistry from the Laboratorium für Physikalische Chemie at ETH under the supervision of Prof. Richard R. Ernst. He was then a postdoctoral fellow at the Department of Molecular Biology at the Scripps Research Institute, La Jolla, California. After obtaining tenure as the Carlson Chair of Chemistry & Biochemistry at Clark University, Worcester, Massachusetts, he became the George Matthew Edgar Professor of Chemistry and Biochemistry at Florida State University and the Associate Director of Biophysics at the National High Magnetic Field Laboratory in Tallahassee, Florida. In 2013 he moved to the Ohio State University as an Ohio Research Scholar to build and lead the new CCIC NMR center. His interest in metabolomics started in 2004 while developing Covariance NMR. His laboratory's metabolomics research currently focuses on the development of novel methods for the deconvolution and analysis of 2D NMR spectra of metabolomics mixtures, such as TOCSY, HSQC, and HSQC-TOCSY, the establishment of customized databases and the COLMAR suite of web servers to efficiently analyze and query such spectra, the exploration of hybrid NMR/MS methods, and the screening of additives, including nanoparticles, for the simplified and improved analysis of NMR spectra.

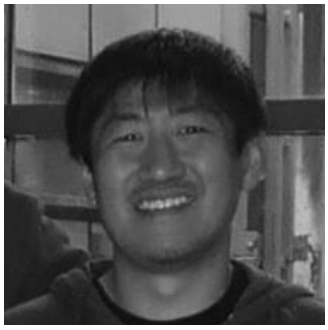
Abstract:

New approaches for NMR-based, hybrid NMR/MS, and nanoparticle-assisted metabolomics

Some of the key challenges in metabolomics concern the comprehensive, rapid and reliable identification of large numbers of metabolites in complex mixtures without the need for extensive purification. We will present new multidimensional NMR methods that significantly help accomplish this task, some of which are being implemented in our COLMAR suite of web servers (http://spin.ccic.ohio-state.edu/index.php/colmar). It is demonstrated how the addition of certain additives, such as silica nanoparticles, to the NMR sample further simplify this task by either quenching the NMR signals of metabolites with certain physical-chemical properties or by eliminating proteins as will be demonstrated for human serum. The characterization of "unknown" metabolites is another key challenge for which an approach is presented that synergistically combines NMR with mass spectrometry in a novel way.

Toshihiro Obata

Session Keynote



Toshihiro Obata is a postdoc in the Central Metabolism Group (directed by Alisdair Fernie) at the Max-Planck-Institute of Molecular Plant Physiology. He employs GC-MS based metabolite profiling and metabolic flux analysis for investigating the diversity and environmental responses of primary metabolism in plants and microalgae. He is also interested in the molecular mechanism of metabolic flux regulation with special focus on the plant mitochondrial metabolism.

Abstract:

Metabolite profiles of field grown maize leaves subjected to combined abiotic stresses and its relationship to grain yield performance

Maize is one of the most important staple crops in tropical and subtropical regions. However grain yield is severely compromised by drought and heat stresses especially when these occur simultaneously. The knowledge on metabolic responses to combined drought and heat stresses is necessary for improving the plant resistance against stress combinations. Furthermore the metabolites which show correlation to grain yield under stress conditions are potential metabolic markers for breeding of stress resilient genotypes. In this study, ten tropical maize genotypes were grown under well watered (control), drought, heat and combined drought/heat conditions in the field trials in 2010 and 2011 seasons. Metabolite profiles of leaves were analysed by GC-MS. The accumulation of amino acids under drought stress condition, which has been previously reported in greenhouse experiment, was also observed in this field trial, suggesting this is a robust metabolic response against drought stress. Combination of drought/heat stresses invoked only a few specific metabolic responses. For most of the metabolites, sum of the responses to single drought and heat treatments showed correlation to those to stress combination. These results suggest that the general metabolic response in stress combination should be considered as the sum of individual stresses in the field. Further correlation analysis between metabolite levels and grain yield revealed that the accumulation of glycine and myo-inositol was significantly correlated to grain yield under drought stress condition. The levels of myo-inositol under control condition were also correlated to the grain yield under drought stress condition. These results make this metabolite a promising candidate of a metabolic marker for breeding of maize genotype showing better yield performance under drought conditions.

Workshop Details

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Workshop 1:

EMN Workshop - Career Development

Organisers

Nicola Gray (Shimadzu UK) and Justin van der Hooft (University of Glasgow)

Abstract

This session will focus on job prospects for early-career scientists considering career pathways in both academia and industry, and discuss the challenges and opportunities in transitioning between these sectors. We will be joined by experts from academia (Jules Griffin, University of Cambridge) and non-academic scientific recruitment (Sinead Cullen, Life Science Recruitment) who will discuss how to develop a skill set for career progression within various sectors and activities to aid successful career progression. The session will cover skills and qualities sought after by recruiters in these sectors, including tailored CV writing, finishing with a discussion and Q&A session.

Workshop Objectives

This workshop is targeted at the early-career scientists of the Metabolomics Society and will provide information on career options in both academia and industry. The session will allow attendees to gain an insight into career progression within academia, with advice on honing a skill set for career progression. This will be balanced by information on alternative career choices with a focus on industry, with advise on how to transition between different sectors.

Learning Outcomes

By the end of this session, attendees will have been received information about:

- The current status of the scientific workforce in academia and industry
- Opportunities and challenges in switching between academic and industry career pathways
- Advise on developing a skill set for a career in academia or industry and how to transition between one sector and another
- CV writing for academia and industry – some concrete tips on what recruiters look for

Schedule

Time	Speaker	Topic
00.00 00.05	Nicola Gray and Justin van der Hooft	Introduction
00.06 00.31	**Dr Jules Griffin** (MRC HNR, University of Cambridge, UK)	Career Progression in Academia
00.35 01.00	**Sinead Cullen** (Life Science Recruitment, Ireland)	Career Pathways in Industry
01.00 01.30	Nicola Gray and Justin van der Hooft	Open discussion and questions

Workshop 2:

Data Sharing and Standardisation

Organisers and Speakers

Reza Salek (Chair), Steffen Neumann, Philippe Rocca-Serra, Tim Ebbels, Mark Viant, Saravanan Dayalan, Oliver Jones, Juan Antonio Vizcaíno, Andrew Jones, Masanori Arita.

Abstract

There is still a great need in standardisation and data sharing in the metabolomics field. The metabolomics community saw its first round of standardisation efforts, culminating in a set of publications, in 2007. We now have several data sharing platforms such as MetaboLights and Metabolomics Workbench that aim to make use of such standards to promote data-sharing but they are not as wll used as they could be. We will

discuss data sharing as well as metabolomics data formats, much of which are adopted from the efforts in the proteomics HUPO-PSI initiative. We will also discuss the importance of capturing metadata in an electronic, sharable format. We hope to get the metabolomics community to to be aware of, and get more involved in, and ongoing efforts in this area.

Workshop Objectives

In this workshop, participants will be able to learn about the current status of the development of a worldwide network of databases and data standards initiatives - such as COSMOS), HUPO-PSI the NIH Common Fund's Metabolomics Program, MassBank and MetabolomeXchange. All of these aim to provide metabolomics researchers with high quality metabolite data standards. These initiatives build on the earlier developments, and improve standardisation of reporting requirements for data and metadata, and to establish best practices and workflows for metabolomics data capture, deposition, and dissemination.

Learning Outcomes

To give an overview of the current state of the art in metabolomics standards and to get anyone interested in metabolomics data sharing and standards, ranging from PIs to PhD and graduate students to participate.

Schedule

- 5 min - **Data standards in metabolomics, current and future!** Reza Salek, EMBL-EBI, Cambridge, UK
- 10 min - **Why you should care about recording (and reporting) your experimental metadata.** Oliver Jones, RMIT University, Australia
- 10 Min - **Be FAIR: Publish experiment descriptors and data in ISA format, get indexed, get cited, get noticed.** Philippe Rocca-Serra, Oxford e-Research Centre (University of Oxford, UK) and Biocrates AG
- 10 min - **Complying with international data standards through data management software - an automated approach** Saravanan Dayalan, Metabolomics Australia, The University of Melbourne
- 15 min Short Discussion (meta-data): **Mutual Benefit for metabolomics community, instrument vendors, publishes and public repositories -gathering interest and suggestion**- Short survey using https://kahoot.it/#/
- 10 min **"Experiences to learn from the mass spectrometry proteomics field"** Juan Antonio Vizcaino, EMBL-EBI, Hinxton, Cambridge, UK
- 10 min - **"Data exchange formats - Why, how and a plea to the MS instrument vendors"** Steffen Neumann, Leibniz Institute of Plant Biochemistry (IPB Halle, Germany)
- 10 min - **"Complying with standards in a multi-user environment: the case of MassBank"** Masanori Arita (National Institute of Genetics, Japan)
- 15 min Discussion and questions

Workshop 3:

Metabolite Profiling in Population-Based Studies: Key Concepts, Pitfalls and Best Practices

Abstract

In recent years, the application of metabolite profiling in population-based studies has become possible due to technological advancements in the field. This is of particular interest due to the potential of metabolomics in evaluating the biological effects of exposures and identifying biomarkers for disease prediction and diagnosis using large-scale, well-designed epidemiological studies. Therefore, it is important for investigators

to be familiar with epidemiological and biostatistical approaches for applying metabolite profiling within population-based settings, which will be the focus of this workshop.

Workshop Objectives

The objectives of this workshop are to: 1) address fundamental epidemiological and biostatistical study design issues that must be considered for metabolomics research; 2) highlight key concepts, pitfalls and best practices for performing metabolite profiling in large, population-based studies; and 3) discuss current efforts to build capacity and infrastructure to support these types of studies, including the recently established International COnsortium of METabolomics Studies (COMETS). COMETS leverages resources and metabolomics data from 25 prospective cohorts and two consortia spanning the United States, Europe, Asia, and South America with cardiovascular, cancer, diabetes, and aging outcomes.

Learning Outcomes

By the end of this session, attendees will be able to:

- Identify key epidemiological study design issues that need consideration when performing metabolite profiling large-scale studies;
- Understand fundamental biostatical concepts for performing metabolite profiling in large-scale epidemiology studies;
- Recognize common pitfalls to performing metabolite profiling in these studies; and
- Become familiar with the COnsortium of METabolomics Studies (COMETS).

Schedule

Time	Speaker	Topic
00.00 00.05	Krista Zanetti	Introduction
00.05 00.35	**Marc Gunter, Ph.D.** Section and Group Head International Agency for Research on Cancer Nutritional Epidemiology Group Lyon, FR	Epidemiological Study Design
00.35 01.05	**Pietro Ferrari, Ph.D.** Statistician International Agency for Research on Cancer Nutritional Epidemiology Group Lyon, FR	Career Pathways in Industry
01.05 01.15	**Krista Zanetti** Program Director National Cancer Institute Division of Cancer Control and Population Sciences Rockville, Maryland, USA	Consortium of Metabolomics Studies (COMETS)
01.15 01.30	Panel Discussion with Speakers	

Workshop 4 :

EMN- The Importance of Experimental Design, Data Acquisition, Quality Assurance and Quality Control in Metabolomics

Organisers

Stacey Reinke (Karolinska Institutet), Fidele Tugizimana (University of Johannesburg)

Overview

Metabolomics is a powerful and exponentially growing field of science, continuously attracting new researchers from different scientific fields. This emerging 'omics' approach, being at the interface between biology, chemistry, statistics, and computer science requires multidisciplinary skill-sets. As such, metabolomics poses many challenges, which if

not considered lead to erroneous data and poor experimental outcomes. As shown in this workshop, a strong understanding of study design, sample preparation, analytical platforms, data processing and data analysis is essential for obtaining meaningful results in metabolomics.

Workshop Objective

This workshop will provide education on experimental design, data acquisition, and quality assurance/quality control in metabolomics experiments. Possible solutions for commonly encountered challenges in the abovementioned study aspects will be addressed.

Learning Outcomes

- Sources of experimental error and consequences of poor study design
- Experimental design strategies and how they can affect the outcome
- Data acquisition considerations and quality assurance measures
- Quality control assessment and data cleaning

Schedule

Time	Speaker	Topic
00.00 00.05	Stacey Reinke and Fidele Tugizimana	Introduction
00.06 00.30	**Prof. David Broadhurst** (Edith Cowen University, Australia)	#1,2
00.31 00.55	**Dr. Warwick Dunn** (University of Birmingham, UK)	#3
00.56 01.15	**Dr. Julia Kuligowski** (Health Research Institute La Fe, Spain)	#4
01.15 01.30	**Stacey Reinke** and **Fidele Tugizimana**	Open discussion and questions

Workshop 5:

metaRbolomics: The R toolbox for Metabolomics

Organisers

Jan Stanstrup (Steno Diabetes Center, Denmark) and Steffen Neumann (Leibniz Institute of Plant Biochemistry, Germany)

Abstract

R is a statistical and graphical environment, for which almost 10,000 add-on packages have been developed to extend the functionality of the core language. These include more than a thousand packages for the life sciences and bioinformatics area, and dozens (if not more) of packages applicable to metabolomics data processing and analysis. While the R language is not known for an easy learning curve, once the user have learned the basic syntax it is incredibly empowering and the possibilities become almost limitless.

Workshop Objectives

This workshop aims to highlight the tools available for metabolomics in the first part, and then proceed beyond the existing tools to emphasize the versatility of working in this environment, how existing packages can be combined and to envision future developments and synergies.

Target Audience

Biologists, Bioinformaticians, and Chemists interested in applying freely available high-throughput analyses to their metabolomics data to maximize efficiency, transparency, and reproducibility in data processing.

Schedule

- **Etienne A. Thévenot** <etienne.thevenot@cea.fr> and Philippe Rinaudo: (O)PLS(-DA) analysis and signature discovery with ropls and biosigner R/Bioconductor packages.
- **Michael Witting** <michael.witting@helmholtz-muenchen.de>, Michael Stravs, Emma Schymanski, Andrea Thum, Christoph Böttcher & Steffen Neumann: Semi-automated MS/MS database generation using the R packages MetShot and RMassBank
- **Augustin Luna** <aluna@jimmy.harvard.edu>, Ozgun Babur, Bulent Arman Aksoy, Emek Demir

and Chris Sander: paxtoolsr: Access Pathways from Multiple Databases through BioPAX and Pathway Commons

- **Tyler Backman** <tbackman@ucr.edu>, Thomas Girke: Analysis of Small Molecules and High-Throughput Screens with R/Bioconductor

Code examples from presenters will be available for own experiments. The workshop will also include room for discussions on challenges and opportunities for more metabolomics developments in R and Bioconductor.

Workshop 6:

Computational Workflows and Workflow Engines

Organisers

Mark Viant, Ralf Weber, Warwick Dunn, Pablo Moreno, Reza Salek, Christoph Steinbeck and the PhenoMeNal consortium

Abstract

Computational analysis of high-dimension and high-volume metabolomics data is a complex, time-consuming process including many steps, some of which still being the focus of intense research. Workflow management environments applied in metabolomics and cross-omics analyses are therefore an essential requirement to allow standardisation of bioinformatics analysis, provide access to the metabolomics community, and produce high-quality, reproducible results in a time-effective manner: on the one hand, experimenters should be able to easily select the tools via a graphical interface, choose the parameters, run the workflow and save/share the results; on the other hand, developers should be able to integrate new tools seamlessly into the environment. A few open-source workflows have recently been applied in different environments including Galaxy-M, Workflow4Metabolomics, MetaDB and MetaboAnalyst. There is a growing need for the international metabolomics community to understand the availability and capability of these workflow environments, and provide input into on-going development and interoperability.

Target Audience

The target audience will be metabolomics data producers interested in the post-wet lab phase of LC-MS, GC-MS, direct infusion MS and NMR data analysis as well as researchers involved in the computational aspects of metabolomics (data handling/analysis, tool developers).

List of speakers

Ralf Weber (University of Birmingham), Etienne Thevenot (CEA/ Yann Guitton, Laberca), Christoph Steinbeck (European Bioinformatics Institute (EMBL-EBI)), David Wishart (Edmonton, Canada), Reza Salek (European Bioinformatics Institute (EMBL-EBI)), Pietro Franceschi (Fondazione Edmund Mach), Theodore Alexandrov (EMBL)

Schedule

Short talks/demos (10 minutes) on the following platforms:

- Workflow4Metabolomics (MetaboHub - IFB Galaxy Metabolomics Workflow)
- MassCascade-KNIME (Steinbeck group, EMBL-EBI)
- Galaxy-M (Birmingham Galaxy Metabolomics Workflow)
- PhenoMeNal (PhenoMeNal-H2020 consortium)
- MetaboAnalyst (Wishart Group, Edmonton, Canada)
- MetaSpace(EMBL, Germany)

Round table discussion/QAs on:

- Current shortcomings and improvements that could help widen the adoption of these type of tools within the metabolomics community.

Interoperability between these technologies.

- General concerns from users.

Oral Abstracts

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Author: Sven Heiling, Emmanuel Gaquerel, Aiko Barsch, Heiko Neuweger, Ian Baldwin | **Oral Abstract N:** O-2002

A metabolomics approach to study the "war" between plants and insects - Identification of plant gene functions and their consequences in herbivory insects

17-hydroxygeranyllinallool diterpene glycosides (HGL-DTGs) are abundant secondary metabolites in aboveground tissue of Nicotiana attenuata which effectively defend valuable tissue against the herbivore Manduca sexta. Using a LC-QTOF-MS based metabolic profiling approach, we characterized the stably silenced lines IRrt1 (rhamnosyltransferase1), IRgt1 (glucosyltransferase1) and IRgt2 (glucosyltransferase2) which are impaired in the biosynthetic steps of glycosylation of HGL-DTGs. Using a software-based approach, we rapidly determined a complete loss of rhamnosylated HGL-DTGs in IRrt1 and the appearance of 12 novel intermediate products in IRgt1 and IRgt2. To elucidate the defensive capabilities of HGL-DTG, we performed feeding assays and screened the excreta of M. sexta. Hereby we found 55 novel formed HGL-DTG-like compounds with different decorations (like coumaryl and caffeoyl moieties) and further deglycosylation products. Interestingly the HGL-DTGs with caffeoyl moieties could only be detected in frass of caterpillars directly feeding on N. attenuata plants and not in frass of caterpillars feeding on detached leaves. This indicates that other systemically-induced defensive pathways play a crucial role in the process of detoxification or that HGL-DTGs are used to detoxify potential poisonous metabolites such as polyamine -hydroxycinnamic acid esters (phenolamides). To characterize the post-ingestive rearrangements of these different metabolic pathways responsible for defense, we analyzed the frass of caterpillars fed on IRmyb8, a line silenced for a transcription factor controlling the accumulation of phenolamides after herbivore attack and IRhqt, silenced for a hydroxycinnamoyl-CoA quinate transferase responsible for the synthesis of chlorogenic acid. The combination of experimental gene manipulation and our method guided by software-based metabolite identification proved to be extremely powerful for the characterization of glycosylation in the HGL-DTG pathway in tobacco and how these impact on chemical rearrangements with other pathways when ingested by the tobacco hornworm M. sexta.

Max Planck Institute for Chemical Ecology Department for Molecular Ecology Jena, Germany

Author: Franziska Hufsky, Kerstin Scheubert, Sebastian Böcker | **Oral Abstract N:** O-2023

Significance of metabolite identifications from searching mass spectral libraries

Untargeted metabolomics usually relies on tandem mass spectrometry and spectral reference library searching for identification of metabolites. When searching a spectral library, the best scoring hit is the most similar spectrum with respect to the scoring scheme. We cannot be sure whether this hit is correct or not, i.a. since the coverage of metabolites in spectral libraries is limited. Different from proteomics, no method to assign statistical significance to metabolite identifications is known. For interpretation of the results and downstream analysis, it is essential to develop automated methods for assessing the confidence of search results and estimating error rates. Two well-established measures of reliability are false discovery rates (FDRs) and q-values. To assess these measures, empirical Bayes or target-decoy approaches are commonly used. In proteomics, we can easily construct decoy databases by (pseudo-)reversing peptide sequences and predicting spectra from such artificial peptides. In contrast, predicting the fragmentation spectrum of a metabolite using its structure is challenging. Moreover, construction of decoy molecular structures which are plausible but non-existing in nature is challenging, if not impossible. We present empirical Bayes and target-decoy based methods to estimate FDRs and q-values in metabolomics experiments. In particular, we present methods to construct a decoy spectral library that avoid to construct "decoy metabolite structures". Using a reference target library and two reference query datasets with several thousand compounds in total, we show that these methods can estimate q-values with high accuracy. The presented methods are robust regarding different scoring schemes, query datasets and reference spectral libraries, even if they are measured on different MS instruments. Our methods allow the assessment of confidence in a match for metabolomics mass spectral library search and thus for an objective and sound statistical evaluation of search results in untargeted metabolomics.

Ernst-Abbe-Platz 2 , Jena 07745, Germany

Author: Ulf Sommer, Daniel Mayor, Kathryn Cook, Mark Viant | **Oral Abstract N:** O-2030

Responses in the metabolome & lipidome of marine copepods induced by climate-related food deprivation

Marine copepods dominate zooplankton biomass from the North Sea to the Arctic and are central to the productivity and biogeochemistry of marine ecosystems, but the effects of predicted climate change scenarios on their metabolic functioning remain poorly understood. In the current study [1], we examined how the physiology of Calanus spp. is affected by increased temperature and lower pH (ocean acidification) under conditions of food deprivation, another factor exacerbated by global warming. We analysed polar and lipid extracts by direct infusion FT-ICR nanoelectrospray mass spectrometry. We encountered a novel class of taurolipids that had not been previously described in literature but now has been published as copepodamides, which trigger a defense mechanism in algae [2]. The stresses associated with food deprivation clearly exceed those caused directly by seawater temperature or pH perturbations. Protein and lipid metabolism were upregulated in the food-deprived animals, as would be expected. However while most taurine-containing lipids and some phospholipid groups show significant relative increases, lipid species containing essential polyunsaturated fatty acids (PUFAs) decreased most substantially. Copepods do not synthesise these PUFAs themselves, but derive them by ingesting diatoms and flagellated microplankton respectively; preferential degradation of these compounds was therefore not expected. This strengthens our understanding that climate-driven changes in the composition of microplankton communities can influence the ability of copepods to survive starvation and other environmental stressors. [1] D.J. Mayor et al. (2015) Sci. Rep. 5:13690. [2] E. Selander et al. (2015) Proc. Natl. Acad. Sci. USA, 20, 6395–6400.

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Author: Ron Wehrens, Jos Hageman, Fred Van Eeuwijk, Robert Hall, Roland Mumm, Ric De Vos | **Oral Abstract N:** O-2035

Batch correction in the presence of non-detects

Introducing two novel quality criteria, the merits of several batch correction strategies are assessed using samples from three large and as yet unpublished LCMS and GCMS data sets. We aim to correct both between-batch and within-batch effects. The focus is on two different aspects: whether or not to use QC samples, and how to handle non-detects, i.e., values too low to be quantitated. For QC-based batch correction, explicitly taking into account batch label and sequence information (ANCOVA), this correction can be done for all metabolites present in the QC samples, which implies that there will also be some metabolites for which no correction is possible; alternatively, methods like RUV allow for a multivariate correction for all metabolites. The latter method needs more QC samples to be effective. The results show that also without QC samples a good batch correction is possible with ANOVA-based methods, provided that the injection order has been properly randomized. QC samples only included to counter batch effects could therefore be eliminated, resulting in shorter sequences. The influence of non-detects can be huge. Several strategies are compared here, including censored regression and imputation with single values. The main lesson is that imputation with too small numbers (zero, half the detection limit) leads to suboptimal results, whereas imputation with the detection limit (or simply the smallest value in the data set) works much better. ANCOVA methods work quite well with censored regression, or simply by ignoring the non-detects. The corresponding paper has just been accepted in Metabolomics, and the data and scripts are available in an R package demo, available from github.

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Author: Cynthia Marokane, Gerhard Prinsloo | **Oral Abstract N:** O-2040

Determination of the differences in metabolite profile in Sclerocarya birrea from different geographical origin and the effect on in-vitro glucose uptake activity

Determination of the differences in metabolite profile in Sclerocarya birrea from different geographical origin and the effect on in-vitro glucose uptake activity C.K. Marokane, G. Prinsloo Department of Agriculture and Animal Health, University of South Africa, Private Bag X6, Florida, 1710, South Africa cynthiakwena@yahoo.com Sclerocarya birrea (S. birrea) is a well-known traditional plant used as food and in the treatment of malaria, diarrhea, hypertension and diabetes. It is widespread in Africa from Ethiopia in the North to KwaZulu-Natal in the South, and its geographical origin can be determined by its biochemical composition. In this study the metabolic pattern in S. birrea from five regions within South Africa namely Limpopo, KwaZulu-Natal, North West, Gauteng and Mpumalanga was measured on 1H NMR, followed by multivariate data analysis. The samples clearly separated according to the sex of the trees as well as their geopgraphical origin. To investigate the effect of sex and origin on the chemical profile, plant samples were evaluated for their anti-diabetes activity screened against C2C12 myocytes. All the extracts were active in C2C12 myocytes with the male samples from Mpumalanga showing the highest activity, even better than insulin, the positive control. Metabolomics was used to compare the composition of the samples and several anti-diabetic compounds were identified. The results of this study indicate that aqueous extracts of S. birrea possesses hypoglycemic activity, and that it is affected by the sex of the trees as well as the geographical origin.

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Author: Peiyuan Yin, jun zeng, Aiguo Wang, Guowang Xu | **Oral Abstract N:** O-2041

Metabolomics study of early hepatocarcinogenesis from mice model: role of methylation and energy metabolism

Hepatocellular carcinoma (HCC) is a worldwide malignancy with high mortality especially in eastern countries. The fast development of HCC makes it difficult for early diagnosis and leads to serious clinical consequences. Thus, it is extremely important to define the molecular features of the cancer in its early stage. In this presentation, we shall introduce our work based on metabolomics studies of H-ras 12V transgenic male mice, which suffered from fatty degeneration of liver and progressed to HCC eventually. The occurrence and the feature of the tumor in the model mice are similar to those of the early stage of HCC. By using a CE-MS based metabolomics platform, we systemically measured the metabolic deregulations of early hepatocarcinogenesis. The current results delineate the abnormal metabolism of amino acids, amides, glycerolipids and nucleosides during the occurrence of HCC. We found that methyl donors, including S-adenosyl-L-methionine (SAM), betaine and choline play important roles in the early stage (e.g. fatty liver stage) of carcinogenesis. And the upregulation of nicotinamide n-methyltransferase (NNMT) in the metabolic pathway of NAD was also observed from our transcriptome data, which are related with methylation, energy metabolism and oxidative stress. Moreover, sulphur amino acids such as taurine and hypotaurine may take part in the regulation of the abnormal energy metabolism. Our current results indicated that the disorders of methylation may be a crucial metabolic events of early hepatocarcinogenesis. And a preliminary validation in patients has also proven the potential of betaine and choline used as biomarkers of HCC.

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Author: Jonathan Mosley, Drew Ekman, Tim Collette, Jenna Cavallin, Dan Villeneuve, Gerald Ankley | **Oral Abstract N:** O-2044

High Resolution Mass Spectrometry for Understanding Biochemical Impacts in Fish Exposed to Complex Mixtures of Environmental Contaminants

High Resolution Mass Spectrometry was used to analyze fish skin mucus collected from male and female fathead minnows (Pimephales promelas) exposed to a wastewater treatment plant (WWTP) effluent comprising a complex mixture of pharmaceuticals, industrial chemicals, and other anthropogenic contaminants. Breeding pairs of fish were exposed in real-time to the effluent at three concentrations for 21 days, after which skin mucus was collected for untargeted metabolomics analysis. Both sex-specific and non sex-specific responses were observed in the skin mucus metabolome, using partial least squares discriminant analysis (PLS-DA). Among these was a concentration-based response in females (concentration specific responses were not observed in males). Subsequent to PLS-DA, the Mummichog software package was used to enhance metabolite annotation and elucidate significantly impacted pathways. Impacts on pyrimidine metabolism, as well as pentose and glucuronate pathways were observed in both sexes. Relative expressions of select gene transcripts were also measured in liver tissues from the same fish. Partial least squares regression models using these gene expression data in combination with the metabolomics dataset revealed informative correlations between these two data types. Specifically, these models suggested that the fish are utilizing their metabolome to support phase I and II transformations of the contaminants in the effluent. The detection of a phase II transformation product for the nearly ubiquitous WWTP contaminant bisphenol A in the skin mucus suggests an additional role for skin mucus in fish for providing a non-lethal approach for monitoring and assessing exposures to complex mixtures of environmental contaminants.

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Integration of metabolomic and genome-wide transcriptomic networks in pregnant women reveals biological pathways associated with pre-eclampsia

Background: Preeclampsia is a leading cause of maternal and fetal mortality worldwide, yet its exact pathogenesis remains elusive. This study aimed to develop predictive metabolomics models of preeclampsia that could help elucidate its biological mechanisms. Methods: The study was nested within the Vitamin D Antenatal Asthma Reduction Trial. Metabolomic profiling was performed on first trimester plasma samples of 53 pregnant women who subsequently developed Preeclampsia and 62 controls with healthy pregnancies, using liquid-chromatography tandem mass-spectrometry. Predictive profiles were generated by identifying features associated ($p<0.01$) with Preeclampsia (adjusting for age, race, and gestational age). Partial least squares discriminant analysis and ROC curves were used to assess the profile's predictive ability. The profiles were validated using third trimester samples from the same women, and further refined through integration with a previously developed transcriptomic signature using network analysis. Results: In total 72 of 8095 (0.9%) metabolite features were associated with preeclampsia. These features had moderate to good predictive ability (R2: 0.36, Q2: 0.28, permuted p-value=0.007), and a summary score of these features displayed an AUC of 0.788 (95%CI 0.707, 0.869)). This profile retained the ability to distinguish preeclamptic from healthy pregnancies in the third trimester (AUC:0.692 (95% CI 0.593, 0.793)). Additionally, metabolite set enrichment analysis identified common pathways, including shingolipid and glycerophospholipid metabolism, at the two timepoints. Integration with the transcriptomic signature refined these results suggesting a particular role for antigen presentation and membrane maintenance. Conclusions: In one the largest prospective metabolomics and first integrative-omics studies of Preeclampsia, we identified and validated a predictive profile with a high discriminatory ability. The interrogation of this signature identified biologically relevant pathways, particularly relating to lipid imbalance. Integration with transcriptomic data confirmed and expanded upon these results and demonstrated an interplay between the transcriptome and metabolome in the development of preeclampsia, providing vital insights into pathogenesis.

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Author: Jessica Lasky-Su, Rachel Kelly, Yamini Virkud, Damien Croteau-Chonka, Amber Dahlin, Ann Wu, Michael McGeachie, juan Celedon, Scott Weiss | **Oral Abstract N:** O-2046

Integrating Metabolomics and Transcriptomics in the Study of Asthma Severity

AIM To integrate multiple hierarchical omics technologies to provide a systems biology overview of the biological pathways underlying asthma severity BACKGROUND Asthma represents a major global public health problem, but its pathogenesis is not fully understood. Metabolomics and integrated omic studies of asthma represent an exciting new approach to address this, however studies are currently limited. METHODS Metabolomic and transcriptomic profiling was performed on blood samples from 381 children (mean age: 9.3yrs (sd: 1.7)) with physician-diagnosed asthma, from a genetically isolated population living in Costa Rica that is enriched for allergic asthma. After QC and filtering four liquid chromatography tandem mass spectrometry (LC-MS) platforms and Whole genome Illumina sequencing provided information on 8600 endogenous metabolites and 25060 genes, respectively. Weighted correlation network analysis (WGCNA) was used to identify a metabolomic and transcriptomic networks comprised of co-regulation modules. The association between these modules and asthma severity, as measured by airway hyper-responsiveness (AHR) following methacholine challenge, was computed and network-level integration performed to elucidate pathways and mechanisms underlying severity RESULTS WGCNA identified 25 metabolite- and 26 gene-modules, summarized by their eigenvalue. Five metabolite- and six gene-modules were significantly associated with AHR after adjustment for age, gender and height. Interrogation of the significant modules revealed enrichment for different aspects of the asthma phenotype. Integration of the metabolite- and gene-modules further refined the findings and identified inflammation and oxidative stress as overall drivers of asthma severity.

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Author: David Rudell, Sara Serra, Nathanael Sullivan, James Mattheis, Stefano Musacchi | **Oral Abstract N:** O-2054

Fruit position within pear trees impacts ripening and associated metabolism after harvest

The characteristics of fruit ripening can contribute to the overall quality of the final product. Ripening of European pears (Pyrus communis) is impacted by a combination of cultural practices and postharvest storage conditions. Fruit position within a tree canopy can alter fruit development and ripening after harvest. Whether that tree position would, likewise, impact overall fruit metabolism associated with ripening and fruit flavor and quality was the subject of this research. 'd'Anjou' pear fruit harvested from internal and external portions of tree canopies of large, open vase trained trees were stored under a hypoxic controlled atmosphere at -0.5 ºC for up to 8 months. We employed multiple GC and LC-MS approaches, accounting for metabolites of a wide range of polarity and volatility, to track dynamic metabolic changes occurring alongside ripening under these conditions. PCA models indicated the estimated metabolomes of external and internal fruit were different at harvest and throughout storage. A PLS model was used to link a number of metabolites including those contributing to aroma and other flavor components with a particular tree position that would impact on-shelf fruit quality. Correlation networks indicated multiple potential areas of co-regulation of these and other metabolites indicating differential coordination of fruit quality-related metabolism. Pathways included phytosterol conjugation, lipid composition, aroma volatile production, sugar metabolism, and acid metabolism. Moreover, results indicate that tree position not only alters the rate at which fruit ripens, but also ripening characteristics, potentially impacting the consistency of the product throughout the commercial supply chain.

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Author: Silas Villas-Boas, Sergey Tumanov, Francesca Casu, Farhana Pinu, Marc Greven, Yuri Zubenko, David Greenwood | **Oral Abstract N:** O-2068

Wine and grape juice lipidomics: the impact of juice lipids on wine properties

In this study we presents a comprehensive lipidome analysis of Sauvignon blanc grape juice by combining GC–MS based fatty acid profiling with shotgun lipidomics strategy. We observed that despite grape juice being a water based matrix it contains a diverse range of lipid species, including common saturated and unsaturated free and intact fatty acids as well as odd-numbered and hydroxy fatty acids. We found that the total lipid content of grape juice can be as high as 2.80 g/L depending on the juice. The majority of lipids were present in the form of complex lipids with relatively small amount of free fatty acids (<15%). Using lab-based microvinification experiments, we demonstrated that several polyunsaturated fatty acids in Sauvignon blanc grape juice significantly affect the level of volatile thiols such as 3-mercaptohexanol (3MH) and 3-mercaptohexyl acetate (3MHA) and other important aroma compounds in the resulting wines. Apparently, these fatty acids affect the acetylation of different metabolites during wine fermentation. Through metabolomics, it was possible to conclude that the level of unsaturated fatty acids in the grape juice affect also the levels of amino acids and antioxidant molecules in the final wines independent of the yeast strain used for fermentation; but the effect on the production of 3MH seemed to be strain-specific. The wine yeast Saccharomyces cerevisiae cannot synthesise unsaturated fatty acids under anaerobic conditions, making them essential nutrients during wine making. Yet they are most unavailable for yeast cells in the form of complex lipids because S. cerevisiae does not produce extracellular lipases. Our study is the first to detail the lipid profile of Sauvignon blanc grape juice and we hypothesise that the potential liberation of intact fatty acids from grape juice medium may help improve fermentation performance and permit the development of new wine styles.

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Author: Ping-Chun Hsieh, Ching-Yu Lin, Hao-Jan Liang | **Oral Abstract N:** O-2069

Mass spectrometry-based lipidomics to study effects of naphthalene on various organs of mice

Naphthalene, the most common polycyclic aromatic hydrocarbons, is widely spread in the environment. Previous studies have demonstrated that naphthalene caused dose-dependent damage to airway epithelial cells and alteration of lipidome in mice. In this study, we intend to establish the dose-response relationship between naphthalene treatments and lipid perturbation in mice. Lipidomic approach is applied to study changes of lipidome in response to naphthalene exposure in mice. In this study, main lipid components of cell membrane, phosphorylcholine-containing lipids including phosphatidylcholine and sphingomyelin were profiled in various organs of mice treated with naphthalene. Phosphorylcholine-containing lipids which play important roles in cell energy storage, cell signaling, and fluidity modulation of cell membrane are likely involved in naphthalene-induced cell injury. In this study, seven-week male ICR mice were treated with naphthalene (0, 100 or 200 mg/kg, ip.). After 24h, the liver, lung and kidney were collected and extracted. Phosphorylcholine-containing lipids were analyzed by using ultra-performance liquid chromatography coupled with tandem mass spectrometry (UPLC-MS/MS) following partial least squares discriminant analysis (PLS-DA). After PLS-DA, the scores plots provide similarity of lipidome. The results demonstrated that control group could be clearly separated from the low and high dose groups. The lipid effects of high and low doses of naphthalene are different suggesting different mechanisms involved. Lipids contributing to grouping will be identified and interpreted in biological mechanism. We conclude that MS-based lipidomic approaches are an effective and powerful tool to understand changes of metabolic pathways and their possible biological impacts after toxicant exposure. Furthermore, the platform can be applied to disease prevention, drug development, and public health.

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Author: Roberto Fusetto, Elizabeth Gillam, Richard O'Hair, Philip Batterham | **Oral Abstract N:** O-2071

The role played by CYP6G1 in the metabolism of imidacloprid and its 5-hydroxy and olefin metabolites in Drosophila melanogaster

Agriculture is threatened by the ability of insect pests to develop resistance to different insecticides due to (1) target site mutations or (2) increased detoxification of xenobiotics. The latter mechanism, which typically involves the overexpression of metabolic genes, has evolved to counter most insecticidal chemicals, including the neonicotinoid insecticide imidacloprid. The controlled overexpression of the Cyp6g1 gene in D.melanogaster, in combination with the use of the mass spectrometric Twin-Ion Method (TIM), permitted us to study the ability of the CYP6G1 enzyme to metabolise imidacloprid in vivo. This allowed us to correlate in vivo enzyme activity, metabolism and insecticide resistance something which has not been achieved in any other system. The metabolism of imidacloprid was first analysed in vitro using CYP6G1 expressing E. coli membranes incubated with imidacloprid for 2 hours at 37°C. Then metabolism was investigated in vivo by exposing third instar larvae (200 for each of 3 replicates) overexpressing Cyp6g1 in digestive tissues or in the Central Nervous System (CNS) and a Cyp6g1 null mutant to a sublethal concentration (6ppm) of imidacloprid. In all experiments a 50:50 mixture of 12C6:13C6-imidacloprid was used. Metabolites were identified using the TIM. Metabolites extracted from the larval bodies and excreta were separated by high pressure liquid chromatography (HPLC) and analysed using a Quadrupole Time of Flight (QTOF) mass spectrometer. Using these methods, we showed that: 1. In vitro CYP6G1 metabolises imidacloprid predominantly forming the 5-hydroxy, 4,5-dihydroxy and olefin metabolites 2. In vivo CYP6G1 rapidly converts imidacloprid to 5-hydroxy and olefin with significant levels found 15-30 minutes after the initiation of exposure. 3. The 5-hydroxy and olefin metabolites are formed and excreted at different rates revealing a different insecticide-kinetic in the insect.

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Author: Marcus Ludwig, Kai Dührkop, Juho Rousu, Sebastian Böcker | **Oral Abstract N:** O-2077

Confidence score for metabolite identifications from structural library search

Untargeted metabolomics experiments based on mass spectrometry can detect thousands of compounds in a biological sample, but often, only few of them can be identified [da Silva et al., PNAS 2015]. Today, the vast majority of metabolites remain unknown. Identification is usually based on tandem mass spectrometry (MS/MS): Measured compounds are searched in spectral reference libraries e.g. GNPS (http://gnps.ucsd.edu). Unfortunately, spectral libraries are vastly incomplete: Available libraries of pure chemical standards cover only thousands of compounds. In contrast, molecular structure databases e.g. PubChem and ChemSpider contain millions of compounds. Recently, computational approaches for searching molecular structure databases using MS/MS data were introduced, which can overcome this bottleneck of spectral library search. Among these tools, CSI:FingerID showed best identification rates, outperforming its competitors by 2.5-fold when searching PubChem [Dührkop et.al, PNAS 2015]. But there is a second problem that is not addressed by any of the available tools for searching molecular structure databases: How to distinguish between true and false hits? It is understood that, given a sufficiently large structure database, any query MS/MS spectrum will result in some ``hit'' in the database. But in many cases, this hit is wrong. Discrimination between true and bogus hits is crucial for interpretation and downstream analysis of the results. Here, we present a method for separating CSI:FingerID hits into (presumably) true and false ones. The method uses information such as runner-up hits or the estimated quality of the predicted fingerprint. We use a linear Support Vector Machine to estimate confidence scores for the molecular structure hits. Using GNPS for training, we can predict true and false hits on an independent dataset (2100 compounds) with an accuracy of 88%. The classifier reaches AUC (area under receiver operating characteristic curve) of 0.88. This shows that our confidence scores can well separate true and false hits.

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Comparative metabolite profiling from growth chamber, environmental simulation chamber or field trial experiments investigating cold acclimation of 49 natural accessions of Arabidopsis thaliana

Many plants of temperate regions, including Arabidopsis, are able to increase their freezing tolerance after an exposure to low, but non-freezing temperatures in a process called cold acclimation. Arabidopsis thaliana is a geographically widely spread species consisting of genetically and phenotypically different local accessions. A wide variation of freezing tolerance was shown before in a set of 54 accessions under controlled chamber conditions1. In the present study the effects of growth conditions on the complex cold response of primary metabolism were investigated. Experiments with 49 Arabidopsis accessions in common were conducted in growth chambers under controlled conditions, in environmental simulation chambers providing sun-like light spectra with UV-A and/or UV-B radiation and in the field during two consecutive winters. Metabolite composition of the rosettes were determined by GC-MS. Data were normalized to enable combination of these datasets measured over several years and 53 overlapping metabolites were included in the final comparison. Metabolite profiles from environmental simulation experiments showed higher similarity to data from field-grown plants than profiles from chamber experiments, identifying these conditions as a better approximation for natural growth conditions. Additional UV-A and/or UV-B radiation changed the metabolic responses to cold drastically. This work sheds new light on the environmental dependence of the metabolic response during cold acclimation and the metabolic determinants of plant freezing tolerance.

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Author: Doris Jacobs | **Oral Abstract N:** O-2088

The effect of plant sterols and different low doses of omega-3 fatty acids from fish oil on lipoprotein subclasses

Scope: Consumption of a low-fat spread enriched with plant sterols (PS) and different low doses (<2g/d) of eicosapentaenoic acid (EPA) and docosahexaenoic acid (DHA) from fish oil reduces serum triglycerides (TGs) and low-density-lipoprotein-cholesterol (LDL-Chol) and thus beneficially affects two blood lipid risk factors. Yet, their combined effects on TG and Chol in various lipoprotein (LP) subclasses have been investigated to a limited extent. Method: In a randomized, double-blind, placebo-controlled, parallel study, 282 hypercholesterolemic men and women consumed either a placebo spread or one of the four spreads containing PS (2.5g/d) and EPA+DHA (0.0, 0.9, 1.3 and 1.8 g/d) for 4 weeks. Diffusion-edited 1H NMR spectra were recorded on fasting serum samples collected before and after intervention. TG and Chol concentrations in various LP subclasses were predicted from partial least squares regression models calibrated on HPLC-derived data. Results: Statistically significant PLS models were obtained for total VLDL, LDL, and HDL lipoproteins, and for 13 LP subclasses, including 5 VLDLs (particle size 64-31.3 nm), 4 LDLs (particle size 28.6-20.7 nm) and 4 HDLs (particle size 13.5-9.8 nm). After PS treatment, total LDL-Chol was reduced, which was not further changed by EPA+DHA. No shift in the LDL-Chol particle distribution was observed. The addition of EPA+DHA dose-dependently reduced VLDL-Chol and VLDL-TG mainly in larger particles. Furthermore, the two highest doses of EPA+DHA increased Chol and TG in the larger HDL particles, while these concentrations were decreased in the smallest HDL particles. Conclusion: The consumption of PS- and EPA+DHA-enriched spreads shifted the LP distribution towards potential additional cardiovascular benefits over PS consumption alone.

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Metabolomics reveals the importance of the pre-conception metabolic state for pregnancy metabolism and programming offspring health

Obesity and its associated complications, e.g. diabetes and other non-communicable diseases, are major challenges for health, quality of life, and societal costs. The prenatal environment may program metabolic response and disease risk in offspring. For instance, exposure to elevated pre-pregnancy BMI (pBMI) and excess gestational weight gain (GWG) influence childhood growth and adiposity, but underlying mechanisms and potential targets for interventions remain unclear. To interrogate these mechanisms, this study investigated the influence of pBMI and the trimester specific variables GWG, maternal diet and insulin resistance on the metabolomic profile of 160 pregnant women in each trimester. A total of 254 plasma metabolites, known to be related to obesity and diabetes in non-pregnant populations, were analyzed by a targeted LC-MS/MS approach. Strong significant associations between pBMI and several metabolites were found, while GWG, maternal diet, and insulin resistance showed no or less effect on the maternal metabolome. 40 different metabolites were affected by pBMI. Non-esterified fatty acids (NEFA) showed a particularly strong positive association with pBMI in the second trimester, with specificity for mono-unsaturated and n-6 NEFA (20:3, 20:4, 22:4). Among the phospholipids, early pregnancy concentrations of sphingomyelins with two double bonds, containing mono-unsaturated fatty acids (FA), and phosphatidylcholines, containing FA 20:3 (PC 30:3, 32:3, 38:3), were positively associated with pBMI. Both, mono-unsaturated and n-6 FA can modulate fat storage in the mother and fetus and may “transfer” obesity risk across generations. Interestingly, branched-chain and aromatic amino acids as well as acylcarnitines were not associated with any parameter; despite being the most frequently mentioned metabolites in non-pregnancy investigations of diabetes and obesity. This study has clearly shown that the pre-conception state confers greatest influence in modulating maternal and consequently offspring metabolism. This study has identified that mono-unsaturated and omega-6 FA, predominantly those containing FA 20:3, represent potential targets for future interventions.

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New Approaches to NMR-Based Metabolite Identification

Metabolite identification is a bottleneck for metabonomics studies using either MS- or NMR-based detection technologies. In contrast to the 4 nucleotides in genomics and the 20 amino acids in proteomics studies, the chemical space of small molecule metabolites is huge and confident identification of these metabolites is challenging. Instructive guides for the use of both MS [1] and NMR-based [2] detection technologies for metabolite identification have appeared recently. However, a key issue is the confidence of metabolite identification. Metabolite identification is of two types: 1) the structure elucidation of novel metabolites, that require isolation or synthesis for rigorous identification and 2) the structure confirmation of known metabolites. The Metabolomics Standards Initiative recognizes 4 levels of metabolite identification [3] and proposed that a known metabolite cannot be classed as Identified unless compared with data from a reference standard of that metabolite in the laboratory. New proposals, including a method called metabolite identification carbon efficiency (MICE) [4] for NMR-based metabolite identification, have proposed that comparison with database or literature data is sufficient. We now describe the development of an improved MICE method incorporating metabolite topological analysis. 1. Watson DG. A rough guide to metabolite identification using high resolution liquid chromatography mass spectrometry in metabolomic profiling in metazoans. Computational and Structural Biotechnology Journal, 4(5), 1-10 (2013). 2. Dona AC et al. A guide to the identification of metabolites in NMR-based metabonomics/metabolomics experiments. Computational and Structural Biotechnology Journal, accepted doi:10.1016/j.csbj.2016.02.005 (2016). 3. Sumner LW et al. Proposed minimum reporting standards for chemical analysis. Metabolomics, 3(3), 211-221 (2007). 4. Everett JR. A new paradigm for known metabolite identification in metabonomics/metabolomics: metabolite identification efficiency. Computational and Structural Biotechnology Journal, 13, 131-144 (2015).

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Discovery of regulated metabolite families in untargeted metabolomics studies

The identification and quantification of thousands of signals acquired by liquid chromatography and high resolution tandem mass spectrometry is prerequisite to interpret metabolomics data. However, the identification of metabolites constitutes a major bottleneck in metabolomics studies. Here, we present a novel approach for the discovery of metabolite families from untargeted LC-HR-MS/MS measurements offering a bird's eye view on metabolic regulation. We explicitly group and annotate regulated MS1 features in comparative studies via hierarchical cluster analysis (HCA) on all MS/MS spectra. We consider characteristic fragments prevalent in these clusters to assign the corresponding MS1 features to distinct metabolite families. In order to facilitate the biochemical interpretation of the underlying biology, we combine the information on metabolite families obtained from HCA with principal component analysis (PCA). Exemplarily, we acquired metabolite profiles of glandular trichomes and trichome-free leaves from a wild tomato (Solanum habrochaites LA1777) using SWATH-UPLC-QToF-MS/MS in fully untargeted manner. Using MS-DIAL(1), we pre-processed all measurements resulting in a signal profile with 5823 MS1 features and a library with 2738 deconvoluted MS/MS spectra. Using this data set, we performed HCA on trichome-specific MS1 features and identified independent clades of similarity in the MS/MS spectra. By assignment of characteristic MS/MS fragments and exemplary structure confirmation by NMR we annotated two trichome-specific metabolite families, the acyl sucrose esters and sesquiterpene glucosides, both involved in the plant's herbivore defense. We demonstrate that this combination of statistical analysis of MS1 feature abundances and MS/MS structural annotations can not only speed-up the structure assignment to individual mass features, but allows to address novel questions, such as the discovery of group-discriminating metabolite families with biochemical relevance. We implemented the proposed methodology in the Open Source web application 'MetFamily' to make our approach freely available (accessible via http://msbi.ipb-halle.de/MetFamily/).

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Author: David Watson, Brian Walker, Roland Stimson, Ruth Andrew, Mohammed Al Washih | **Oral Abstract N:** O-2111

Metabolomic Profiling of Patients with Congenital Adrenal Hyperplasia Reveals Novel Biomarkers for Glucocorticoid Action.

Glucocorticoids have diverse physiological actions mediated by intracellular glucocorticoid receptors (GR) and mineralocorticoid receptors. GR are widely expressed in mammalian cells and affect energy metabolism, cardiovascular control, cellular proliferation, central nervous system function and innate immunity. Chronic excess of glucocorticoids results in Cushing's syndrome, characterised by obesity, type 2 diabetes, hypertension, impaired immunity, depression, cognitive dysfunction. Mass spectrometry based metabolomic profiling of serum from 132 patients with congenital adrenergic hyperplasia was carried out. The aim of the study was to use the sample set to uncover markers for glucocorticoid activity since the patients were all being treated with different doses of glucocorticoids. Initial modelling of the data did not reveal clear differences based on glucocorticoid dose. Multivariate analysis of the patients according to clinical tests and anthropometric data, revealed that they fell into three distinct groups based on these measures with glucocorticoid dose being only a minor contributor to the differences between the groups. Recognition of this lead to a re-designation of high and low dose GC groups so that steroid doses were significantly different while there were no differences between the groups with regard to anthropometric data or clinical tests. The metabolomic data were then re-assessed and it was found orthogonal partial least squares discriminant analysis based on eight metabolites including was able separate the high GC and low GC groups. The eight metabolites were combined to produce a receiver operator characteristic curve which had an area under the curve of 0.946 thus producing excellent classification according to dose with the variables being used for the classification being <10% of the number of observations. Seven out of the eight metabolites on the basis of prior literature have an association with glucocorticoid action and the combination of these eight metabolites was capable of producing a robust marker for glucocorticoid response.

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Serum metabolomic profiling of prostate cancer risk in the Prostate, Lung, Colorectal and Ovarian Cancer Screening (PLCO) Trial

Two recent studies conducted in the ATBC Study identified serum metabolites related to risk of aggressive prostate cancer up to 20 years prior to diagnosis, including particularly energy and lipid metabolites. The present study re-examines those associations in the PLCO cohort through a nested case-control study of 380 cases and 380 controls matched on age, race, study center, and date of blood collection. Median time from serum collection to diagnosis was 10 years. Sera were analyzed on an untargeted high-resolution accurate mass platform of ultrahigh performance liquid and gas chromatography/mass spectroscopy (Metabolon, Inc.) that identified 722 metabolites. Logistic regression estimated odds ratios (OR) and 95% confidence intervals of risk associated with an 80th percentile increase in metabolite concentration. Peptide metabolites were significantly associated with aggressive disease (p=0.02), and 27 metabolites were associated with overall prostate cancer at p<0.05. Pyroglutamine (pGLU), gamma-glutamylphenylalanine, phenylpyruvate, N-acetylcitrulline and stearoylcarnitine showed the strongest metabolite-prostate cancer risk signals (ORs =0.53, 0.51, 0.46, 0.58, and 1.74, respectively; 0.001= p =0.006). Findings were similar for aggressive disease. Interestingly, pGLU is a key amino acid residue in thyrotrophin-releasing hormone-like peptides present in the prostate. Our earlier findings of inverse associations with aggressive disease for energy and lipids metabolites were not replicated. The contrasting energy/lipid versus peptide metabolomic patterns for prostate cancer risk between the two cohorts is intriguing and may relate to aspects of study design, including fasting serum or smoking status, or the screening trial yielding low PSA cases versus more clinically advanced, higher PSA malignancies in ATBC. The two studies may therefore reflect metabolomic risk profiles of prostate cancers at developmentally different tumor metabolic states and requirements such that PLCO included smaller, earlier cases while ATBC included larger, more extensive primary tumors. The metabolite profiles identified here should be examined in additional prostate cancer studies.

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Oral Abstract N: O-2128

Human serum metabolites associate with severity and patient outcomes in traumatic brain injury

Traumatic brain injury (TBI) is a major cause of death and disability worldwide, especially in children and young adults. TBI is an example of a medical condition where there are still major lacks in diagnostics and outcome prediction. There is a substantial opportunity to employ metabolomics to allow the use of peripheral blood for characterizing pathophysiology and prognosis in TBI. Here we applied comprehensive metabolic profiling of serum samples and selected brain microdialysate samples using GCxGC-TOFMS analysis from TBI patients and controls in two independent cohorts. The discovery study included 144 TBI patients from Turku University Hospital (Finland). The samples were taken at the time of hospitalization, which was up to 12 h after the injury. The patients were diagnosed as severe (sTBI; n=22), moderate (moTBI; n=14) or mild TBI (mTBI; n=108) according to their lowest recorded pre-intubation Glasgow Coma Scale from the scene of accident or emergency department. The control group (n= 28) comprised of acute orthopaedic non-brain injuries. The validation study included sTBI (n=23), moTBI (n=7), mTBI (n=37) patients and controls (n=27) from Addenbrooke's Hospital (Cambridge, UK). We found that medium-chain fatty acids and sugar derivatives are strongly associated with severity of TBI, and most of them were also detected at high concentrations in brain microdialysates of sTBI patients. Based on metabolite concentrations from TBI patients at the time of hospitalization, an algorithm was developed that accurately predicted the patient outcomes (AUC = 0.84). Adding the metabolites to the established CRASH model, comprising clinical and CT data, significantly improved prediction of patient outcomes. The identified 'TBI metabotype' in serum, which is indicative of disrupted blood-brain barrier as well as of protective physiological response and altered metabolism due to head trauma, offers a new avenue for the development of diagnostic and prognostic markers of broad spectrum of TBIs.

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Oral Abstract N: O-2134

An integrated approach for the identification of predictive markers of type 2 diabetes.

The trajectory and underlying mechanisms of health are determined by a complex interplay between intrinsic and extrinsic factors. There is a need for more accurate assessment of the inputs and their consequences to health (Panagiotou, 2009). Therefore, our objective was to identify accurate and robust multidimensional markers, predictive of type 2 diabetes (T2D). A case-control approach was used within the French cohort GAZEL (n~20,000). Male overweight subjects (n=112, 25=BMI<30 kg/mÐ, 52-64 y.o.), free of T2D at baseline, were selected and compared for several parameters (clinical, biochemical parameters, and food habits) with Cases defined as having developed T2D at follow-up (5 years later; BMI, age, sex matched). Baseline serum samples were analyzed using mass spectrometry-based untargeted metabolomics. Data mining methods were used to select the best candidate for prediction. Models were built using linear logistic regressions on the reduced dataset and their performances were determined by calculating the area under the receiver operating characteristics curve (AUC) with their 95% confidence intervals (CI), sensitivity and specificity values. Metabolomic data were integrated with the different parameters from the database to determine whether multidimensional models improve prediction. Clinical data and consumption frequencies of vegetables and sugar showed significant differences between Cases and Controls. The metabolomics approach allowed the identification of 5 predictive biomarkers. The resulting metabolite-only model showed better performances than the one built with clinical data: a lower misclassification rate (18% vs 26%) and higher AUC (0.82 vs 0.74; CI=[0.748-0.892] vs [0.659-0.823]). Integration of metabolomic data with the available parameters allowed optimizing prediction performances (10.8% misclassification, AUC=0.89, CI=[0.833-0.950]). Correlation network analyses contributed to explore the links between metabolic, clinical parameters, and food habits. These results show the interest of an integrated approach including untargeted metabolomics in the discovery of predictive biomarkers 5 years before T2D occurrence to better stratify at-risk populations.

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Oral Abstract N: O-2138

What Makes a Peanut, a Peanut? Elucidating the Metabolome of the Raw Peanut Seed

Peanut production in the United States is a $1.12 billion industry. Of the four commonly produced market-types, runner and virginia-type peanuts account for 95% of U.S. production. Although the composition of the raw peanut seed has the potential to be improved through traditional breeding efforts, very little is known about the metabolome. The objective of this study was to elucidate a comprehensive metabolomic profile of raw runner and virginia-type peanuts. Runner (n=15) and virginia-type (n=15) peanut samples were each obtained from five independent lots (4.5 kg/lot) at three locations. Analytical platforms including (RP)/UPLC-MS/MS (positive and negative ion mode ESI) and HILIC/UPLC-MS/MS with negative ion mode ESI were utilized for generation of metabolomic profiles. Discriminant analysis of principal components and one-way ANOVA adjusted for multiple comparisons followed by hierarchical cluster analysis were performed to differentiate the samples. Clear clustering by market-type was not observed based upon overall metabolite profiles. A total of 355 metabolites primarily belonging to the amino acid, lipid, and carbohydrate super pathways were identified, many of which are being reported for the first time in peanut. Raw peanuts differed most in their content of oxylipins, aromatic amino acids, flavonoids, and gamma-glutamyl amino acids. Differences in levels of benzenoids and purine metabolism products also accounted for observed variability, although to a lesser extent. This study represents the most comprehensive analysis of the raw peanut seed to date, providing insight into the breadth of small molecules present in the peanut. The new information presented here will augment the toolbox for peanut quality improvement.

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Metabolite profiling of shoot extracts, root extracts, and root exudates of rice under nitrogen and phosphorus deficiency

Root exudates are derived from plant metabolites and the composition is affected by plant nutrient status. Deficiency of mineral nutrients such as nitrogen (N) and phosphorus (P) strongly affects the type and amount of plant metabolites. We applied a metabolite profiling technique to investigate root exudates of rice plants under N and P deficiency. Oryza sativa was grown in culture solution containing two N levels (0 and 60 mg N L-1) or two P levels (0 and 8 mg P L-1). Shoot extracts, root extracts, and root exudates were obtained from 5 and 15 day after transplanting and their metabolites were determined by capillary electrophoresis/time-of-flight mass spectrometry. Shoot N concentration and dry weight of rice plants grown at low N level were lower than that at high N level. Shoot P concentration and dry weight of rice plants grown at low P level were lower than that at high P level. One-hundred-thirty-two, 127, and 98 metabolites were identified in shoot extracts, root extracts, and root exudates, respectively at two N levels. One-hundred-thirty-two, 128, and 99 metabolites were identified in shoot extracts, root extracts, and root exudates, respectively at two P levels. Seventy-seven percent of the metabolites were exuded to the rhizosphere. Concentration of betaine, GABA and glutarate in root exudate is higher both at low N and low P levels than at high level. Concentration of spermidine in root exudate is lower both at low N and low P levels than at high level. Concentration of other metabolites in root exudate was affected differently by N or P status of plant. These results suggest that rice roots actively release many metabolites in response to N and P deficiency.

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Author: Dries Verdegem | **Oral Abstract N:** O-2153

TTFD: a metabolic network-based guidance tool for the setup and interpretation of stable isotope metabolomics experiments.

In classical metabolomics experiments, one deals with the measurement and identification of metabolites in biological samples using mass spectrometry (MS) or nuclear magnetic resonance (NMR) readouts. However, this information provides a foremost static view on the biological processes and gives little insight in underlying mechanisms. Stable isotope-based metabolomics can provide the additional understanding of metabolic pathway activities, as administered (heavier) tracer isotopes are only picked up by downstream metabolites if the upstream reactions are active. Any serious interpretation of the isotope incorporation data requires the use of computational methods. The current method of predilection is Metabolic Flux Analysis (MFA). However, it requires an inordinate amount of expert knowledge, resulting in limited application. To make the powerful potential of isotope-based metabolomics accessible to a larger public, we have developed a novel computational method called Theoretical Tracer Fate Detection (TTFD). TTFD is a model of whole-body metabolism comprising explicit knowledge on the metabolic network (reactions and pathways) and corresponding atom mappings. The model can be queried using specific tracer and/or gauge metabolites, isotopically labeled on user-defined positions and returns the paths (series of reactions) compatible with the specified labeling. Additional filters can be applied to include or exclude certain metabolites, reactions or pathways from the resulting paths. As such, the model is useful to guide experimental design and data interpretation. For instance, the answer to questions such as “Which specific tracers allow to distinguish between two modes of production of a metabolite of interest?” and “Which overseen path can explain (part of) an observed incorporation pattern?” can straightforwardly be obtained. TTFD is currently focused on human metabolism as it is built upon the curated databases MetaCyc and HumanCyc within the BioCyc database collection. However, extension to other models is envisioned. TTFD will be available as a freely accessible and easy-to-use web application.

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Metabolic profiling of total physical activity and sedentary behavior in community-dwelling men.

Objective: Physical activities are known as a preventive factor for various metabolic diseases. We aimed to investigate the relationship between daily physical activity levels with a targeted metabolomics approach in a population-based study. Methods: Cross-sectional associations of physical activity with 77 metabolites were assessed for 1193 Japanese men aged 35 to 74 who participated in a baseline survey of a cohort study from April to August 2012. Information on daily total physical activity, classified into four levels by quartile, and sedentary behavior, defined as hours of sitting/day, were collected through a self-administered questionnaire. Fasting plasma samples were collected and absolutely quantified by capillary electrophoresis mass spectrometry method. We applied linear regression models with multivariable adjustment and corrected p-values for multiple testing. Replication analysis was conducted to confirm the robustness of the results in a separate population created by random allocation. Results: Higher levels of total physical activity were associated with multivariate metabolic profiles, including lower concentrations of amino acids and their derivatives, and higher concentrations of pipecolate. The findings persisted after adjustments for age, body mass index, smoking, alcohol intake, and calorie intake. Short sitting time was also associated with lower concentrations of isoleucine, leucine, valine, alanine, proline, and 4-methyl-2-oxoisopentanoate in the mutually adjusted model. Conclusions: Physical activity is associated with multiple plasma metabolites, including known biomarkers for metabolic diseases. These metabolites may be the potential key role of the protective effects of higher physical activity and/or less sedentary behavior.

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Metabolic phenotyping to predict mortality and individualise treatment and transplant candidacy in patients with cirrhosis.

Metabolic phenotyping to predict mortality and individualise treatment and transplant candidacy in patients with cirrhosis. Rabiya Zia1, Vishal Patel2, Olivier Cloarec3, Julia A Wendon2, Mark JW McPhail2, Muireann Coen1 1 Computational and Systems Medicine, Department of Surgery and Cancer, Imperial College London 2 Institute of Liver Studies, Kings College Hospital, Denmark Hill, London 3 Korrigan Sciences The global incidence of cirrhosis is rising rapidly, owing to an increased prevalence of alcohol-related liver disease, non-alcoholic fatty liver disease, and viral hepatitis. Patients with cirrhosis are prone to sudden functional hepatic decompensation, requiring hospitalisation. Outcome prediction in decompensated cirrhosis is critical in decision making for liver transplantation and resource allocation. Multi-platform metabolic phenotyping was applied to profile blood plasma in a cohort encompassing healthy controls, stable cirrhotics, decompensated cirrhotics and acute-on-chronic liver failure patients (total n=350). The application of 1H NMR spectroscopy and both global and targeted ultra performance liquid chromatography coupled with mass spectrometry (UPLC-MS) enabled a broad coverage of the metabolome. Stratification of patients based on temporal metabolic phenotypes enabled the identification of a panel of biomarkers that provided mechanistic insight into the differential stages of decompensation and development of multiorgan failure. Multiple metabolic pathways were perturbed in cirrhosis including gluconeogenesis, the urea cycle, lipid and amino acid metabolism. In addition, gut microbial co-metabolites including short-chain fatty acids, were also identified as perturbed suggesting a role of the gut-liver axis in disease severity and outcome. The metabolic phenotype data was integrated with extensive clinical metadata and clinical scoring systems that predict survival (Model for end stage liver disease (MELD) and chronic liver failure sequential organ failure assessment (CLIF-SOFA)). A robust predictive model of outcome (90-day survival) was also computed from the multi-platform metabolic phenotype data which holds potential to enhance clinical management and to aid in transplant decision-making.

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Author: Simone Rochfort, Kioumars Ghamkhar, Myrna Deseo, Bidhyut Banik, Clinton Revell | **Oral Abstract N:** O-2168

Metabolomics and Methanogenic Potential - Reducing Agricultural Greenhouse Gases

Agriculture is a significant contributor to greenhouse gasses. Nearly 15% of Australia's greenhouse gas emissions come from agriculture, 67% of which is methane from ruminant animals such as sheep and cattle. One approach to improving the environmental footprint of animal production is to utilise pastures which have lower methanogenic potential compared to commonly used grasses. In this study we compared the in vitro methanogenic potential of the forage legumes red clover, subterranean clover and thirty accessions of biserrula (Biserrula pelecinus L.) sourced from eight Mediterranean/North African regions. Metabolomics analysis, both NMR and LCMS, were employed to investigate the relationship between the accessions. PCA and hierarchical clustering demonstrated that the accessions group by both methane content and geographical origin. A similar hierarchical cluster analysis using AFLP marker data showed no such clustering with the exception of accessions from Eritrea. Supervised analysis of the LCMS data allowed the identification of 47 putative markers that were associated with the methane lowering potential of certain accessions. These metabolites were highly upregulated in the accessions with low methanogenic potential (10 fold or greater, with $p < 0.005$). Initial NMR and LCMSn studies suggest that these molecules are triterpene saponins. Saponins possess diverse biological functions and this study suggests that a subset may contribute to methane reduction in ruminants. If confirmed in vivo, these metabolites will be attractive targets in biserrula breeding programs.

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Author: Ninna Granucci, Philip Harris, Silas G. Villas-Boas | **Oral Abstract N:** O-2173

Metabolomics to assess the potential of fermented fruit/vegetable by-products as a new source of functional foods

In a contemporary perspective fruit/vegetable by-products could be employed for developing new functional food through fermentation process.Therefore, the focus of this study is to use metabolomics tools to assess the potential of using fermentation process based on fruit by-products to produce novel food ingredients. We performed and compare a solid-state (SSF) and a liquid-state fermentation (LSF) using a food-grade non-Saccharomyces yeast species and three fruit/vegetable by-products. These by-products (apple, orange and carrot pomaces) were characterised before and after the fermentations to assess the capability of the yeast in bioconverting these substrates and preliminary metabolomics analysis were performed in order to determine the fine changes in biochemical composition. A fast alkylation reaction based on methyl chloroformate (MCF) and the traditional trimethyl silyl (TMS) derivatizations were used to characterise the composition of amino and non-amino organic acids, and soluble sugar and derivatives, respectively. After derivatizations, the samples were analysed by GC-MS. GC-MS analyses were able to detect over 400 compounds and metabolite identifications varied from 80-100 for the unfermented substrates and over 200 after fermentation using our in house MS library of standards. The fermented apple, orange and carrot pomaces presented higher levels of essential and non-essential amino acids after bioconversion as well as the levels of polyunsaturated fatty acids such as oleic acid and conjugated and gamma linoleic acid, increased. In the same way, various phenolic acids such as trans-cinnamic, caffeic, and vanillic acids were produced or had their levels increased through both SSF and LSF. We are now working in a more comprehensive characterisation of lipids, vitamins, and other phenolic acids in the substrates before and after fermentation. In conclusion, metabolomics showed that industrial fruit/vegetable by-products have the potential to become a promising substrate for bioconversion into (functional) food ingredients.

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Non-targeted and targeted metabolomic approaches reveal differences in legume chemistry before and after infestation with pea aphid host races.

The pea aphid (Acyrthosiphon pisum), a phloem-sucking insect, has undergone a rapid radiation together with the domestication and anthropogenic range expansion of several of its legume host plants. At present, the species is a complex of at least 15 genetically different host races. Each race is specialized on a particular plant species, such as alfalfa (Medicago sativa), red clover (Trifolium pratense), and pea (Pisum sativum), which makes it an attractive model insect for the study of ecological speciation. However, the role of host plant chemistry in this specialization has not been studied so far. We used a mass spectrometry-based non-targeted metabolomic approach to search for plant chemical compounds that could be involved in pea aphid-host plant specialization. Significant differences were found among the metabolic fingerprints of the host plants prior to aphid infestation, and the chemistry of each plant was altered by aphid feeding. The analysis resulted in a list of candidate chemical compounds that could be responsible for the specialization of pea aphid host races on the host plants. In addition, using a targeted metabolomic approach we collected information about the time course of plant hormone concentrations in response to pea aphid infestation by measuring the levels of jasmonates, salicylic acid, and abscisic acid. The results suggested that aphids were able to modulate the phytohormone levels on their native host plants to avoid defensive responses. Thus, we conclude that pea aphid host races use diverse feeding strategies to avoid the chemical defenses of their food plants. This information opens new opportunities to understand how plant chemistry can influence aphid performance and vice-versa, as well as how plant chemistry can be modified as a strategy to reduce the infestation of aphids on crop plants.

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Author: Robert Hall, Desalegn Etalo, Carmen Diezsimon, Matthieu Joosten, Ric De Vos | **Oral Abstract N:** O-2192

Metabolic mapping in plants: LAESI-MS imaging

Plant tissues are a tremendously rich source of highly diverse (secondary) metabolites, many of which are not evenly distributed throughout the plant but rather, have very strong organ, tissue or even cell-based localization. Unfortunately, when making a standard extract typical of a metabolomics analysis this spatial heterogeneity is generally lost. In situ metabolite imaging-based approaches have the potential to overcome this loss of spatial resolution and give us deeper insights into the location of metabolites within tissues. We have investigated the potential of applying Laser Ablated ESI (LAESI) – MS imaging for plant analyses. As LAESI does not require either a vacuum or an ectopically-applied chemical matrix it is possible to perform all analyses in situ and under ambient conditions with still-living tissue. Using visibly variegated (purple-white) Phalaenopsis petals and evenly yellow Bidens petals it proved possible to confirm the degree of spatial resolution by matching LAESI metabolic maps for specific metabolites with their known (visible / invisible) distribution across the petal surface. Maps made for e.g. invisible phenolic compounds also revealed extensive degrees of either co-localisation or co-exclusivity with other metabolites (such as anthocyanins). Knowledge of the pathway relationships between the metabolites concerned suggests that localisation of many metabolites is under strict cellular control. In this presentation next to presenting very promising results, attention shall also be drawn to some of the potential limitations and potential pitfalls, especially when using such an approach for comparative metabolomics.

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Exploring metabolomic data from designed experiments using ANOVA-Multiblock Orthogonal Partial Least Squares

Many experimental factors may have an impact on metabolic profiles. A thorough investigation of the potential effects and interactions between the factors is made possible by systematic procedures for rationally planning the trials, i.e. experimental design. However, assessing these influences remains often a challenging task, because high dimensional data with hundreds to thousands of correlated variables are generated, whereas only a limited number of samples is usually available. In that context, dedicated multivariate methods accounting for both the intrinsic characteristics of the data and the study design have been developed. However, most approaches rely on the separate analysis of ANOVA submatrices and remain somewhat limited for detecting and interpreting subtle metabolic perturbations hidden in complex datasets. In the present work, a supervised multiblock algorithm based on the Orthogonal Partial Least Squares (OPLS) framework, is proposed for the joint analysis of ANOVA submatrices. This strategy has several advantages: (i) the evaluation of a single multiblock model summarising all the data; (ii) the computation of a goodness of fit parameter for assessing the ANOVA decomposition reliability; (iii) an easy interpretation of the signals related to the different sources of variation in the dataset, and (iv) the investigation of an effect-to-residuals ratio to objectively evaluate the relative importance of each effect. A case study involving aggregating rat brain cells exposed to Paraquat herbicide is proposed to illustrate the ability of the method to extract relevant metabolomic information. Several biomarkers associated with neuronal differentiation and oxidative stress were highlighted in UHPLC-TOF/MS experiments with two factors, i.e. maturation and dose. The AMOPLS algorithm constitutes a potent approach in the context of explorative metabolomic data analysis with a simplified interpretation of signal variations related to main effects or interactions between experimental factors, using a single multiblock model.

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Dealing with sample dependency in metabolomics studies

In metabolomics studies sample dependency is common, for example characterization of the same subject at different time points, matched case and controls and combinations thereof. This dependency needs to be taken in to account both when preforming the analytical measurement and in the statistical evaluation of the study. In many cases the metabolic changes associated with a treatment effect or case-control difference are small in comparison to other systematic changes in the data such as instrumental drift and individual variation. Hence, it becomes a key step to minimize the influence of such variation so that small but true relevant changes can be detected and correctly interpreted. The presented strategy include constrained randomization of analytical run in order to minimize the influence of analytical drift and an extension of the previously presented OPLS-EP strategy [1] to cope with individual variation and provide a more detailed interpretation of relevant metabolite pattern change. We show that this will increase the sensitivity and lower the false discovery rate in biomarker detection. The full strategy will be explained and examples from clinical metabolomics studies will be given. 1 Jonsson, P. et al. Constrained randomization and multivariate effect projections improve information extraction and biomarker pattern discovery in metabolomics studies involving dependent samples. Metabolomics 11, 1667-1678, doi:10.1007/s11306-015-0818-3 (2015).

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Author: Jelena Sostare, Jennifer Kirwan, Riccardo Di Guida, Karnpreet Chalal, Warwick Dunn, Mark Viant | **Oral Abstract N:** O-2203

Towards a fully-automated extraction of polar and apolar metabolites from low mass tissue samples

In the last decade metabolomics has experienced significant advances in the throughput and robustness of analytical methodologies. Yet the preparation of biofluids and low-mass (<10mg) tissue samples remains a laborious and potentially inconsistent manual process, and a significant bottleneck for high-throughput metabolomics. To address this, we are developing an automated extraction process that features an optimised set of solvents, with the aim to deliver high-throughput and reproducibility. First, we have investigated and re-optimised the solvent ratios in the recently introduced methyl tert-butyl ether (MTBE)/methanol/water solvent system (here termed modified-MTBE; 2.6:2.0:2.4, v/v/v) and compared it to the original MTBE method (10:3:2.5, v/v/v) and the conventional chloroform/methanol/water (modified Bligh and Dyer, 2.0:2.0:1.8, v/v/v) using four sample types (Daphnia, liver, serum and urine). The modified-MTBE method yielded more metabolites than both the original MTBE method and the Bligh and Dyer method. The reproducibility of the modified-MTBE method was also higher, based upon the observation of a lower median relative standard deviation. In addition, the extraction process has been automated by employing a novel integration of a robotic liquid handler (Biomek NXp Span8; Beckman Coulter), bead-based homogeniser (GenoGrinder2020; SPEX) and robotic arm (Precise SCARA). Extracted samples were then analysed by direct infusion MS (Thermo Scientific Q Exactive) or LC-MS (Thermo Scientific Ultimate3000 UHPLC Q Exactive). The preliminary automation results revealed that the Biomek NXp proved to be an effective approach for increasing sample throughput in particular for laborious preparation of tissue samples. Compared to the traditional Bligh and Dyer method (in which cellular debris collects at the solvent-solvent interface), the original and modified-MTBE methods benefited from the cellular debris collecting at the bottom of the tubes; this enabled the automated collection of each solvent phase. In conclusion, the modified-MTBE method is automation-friendly and provides a higher yield and reproducibility than traditional methods.

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Real time detection of fish fraud using rapid evaporative ionisation mass spectrometry (REIMS)

The increasing number of reports regarding global food fraud scandals has brought food authenticity and safety to the attention of regulators, industry and consumers worldwide. Ambient ionization mass spectrometry (AMS) methods have overcome a number of intrinsic constraints of traditional mass spectrometric analysis schemes, allowing in situ, real-time analysis of a wide variety of samples. Rapid evaporative ionisation mass spectrometry (REIMS) has been used for the analysis of human tissue during surgery and has shown to be capable of the identification of different tissue types based on lipid fingerprinting. In this study, we present for the first time an effective, near real time method to identify fish product speciation methods using REIMS. Over 2000 spectra were acquired from five different authenticated species of fish; cod, coley, haddock, pollock and whiting. The resulting data was subjected to preprocessing and multivariate analysis such as principal component analysis (PCA) followed by a linear discriminant analysis (LDA) using a non-commercial prototype software developed by Waters. Both PCA and LDA score plots, built using m/z 600-1200, identified clear signs of fish speciation, albeit there was some overlap between cod and haddock. Leave 20% out cross validation of the PCA- LDA models resulted in a 95.90% correct classification rate independent from the sampling site and instrument. The multivariate model created from the fish database was then tested real-time on novel fish samples at two different sites, Belfast and Budapest. 10 authentic samples from all different species were sampled and subjected to real-time analysis during sampling using the same prototype software. All samples were correctly classified by our method at both sites. REIMS technology could provide a paradygm shift across authenticity applications by providing real-time, reliable, and simple method for the analysis of food products.

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Stable isotope-labeled yeast extracts as internal standard for LC-MS/MS based amino acid quantification in samples of human origin

Mass spectrometry, is an established technology in almost all research fields of the life-sciences, furthermore it is on the point to become a cutting edge technology in the field of clinical diagnostics. Nowadays issues in personalized medicine continuously require new approaches in research and diagnostics and therefore the importance of mass spectrometry is constantly increasing. A key application is the quantification and/or assessment of fold changes of molecules derived from the primary and secondary metabolism. Samples derived from human origin have a wide variety in metabolites and concentration range, additionally the matrix (e.g. blood) is often very complex. Therefore quantification and quality control via mass spectrometry of metabolite concentrations in analysis for biomedical research is often laborious and inefficient. Through unintentional variations in sample preparation and measurement the repeatability of analytical results is often compromised. A method to overcome those problems is the addition of stable isotope-labelled internal standards. In the presented approach we used internal standards produced by in-vivo labelling. By this method cells are grown on an isotopically enriched (e.g. 13C, 34S) growth media. These cells can be harvested and extracted to obtain an isotopically enriched extract of the metabolome that can be exploited as internal standard for a plethora of metabolites. To prove the applicability of in-vivo synthesized internal standard extracts for real life human samples we investigated on SRM (Standard Reference Material) 1950 (metabolites in frozen human plasma). SRM 1950 provides certified concentration values for a variety of metabolites. In this example we covered 14 certified amino acids. We defined the values in the certificate as our target values and evaluated calibrations with and without addition of internal standard on their applicability and figures of merit. The application of in-vivo labelled standards resulted in a significant improvement of trueness and precision.

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Crosstalk between astrocytes and motor neurons: a metabolomics study

No consensus exists about the most suitable cell model to assess the pathophysiology of neurodegenerative diseases. The metabolism alteration in the brain and the associated crosstalk between astrocytes and motor neurons are largely contributor of cell death but a comprehensive understanding of this crosstalk remain elusive. The main aim of this study was to assess the effects of a co-culture system on the metabolism of astrocytes and motor neurons, using a metabolomics approach. We investigated for the first time, the metabolism of astrocytes and motor neurons by LC-HRMS-based metabolomics approach completed by a 1H-NMR study of extracellular medium. We used primary astrocytes and motor neurons in mono- and co-culture systems. The metabolic pattern showed a clear discrimination between motor neurons and astrocytes in mono- versus co-cultured system. Pathway analysis of discriminating metabolites revealed interactive partners, involving metabolic dysregulation in both cell types. Astrocytes induced dysfunction of arginine and proline metabolism, alanine, aspartate and glutamate metabolism, glutathione metabolism, aminoacyl-tRNA biosynthesis, tryptophan metabolism, and purine metabolism pathways in motor neurons-astrocytes co-culture. Motor neuron interactions in co-cultures induced dysfunction of lysine degradation, arginine and proline metabolism, tyrosine metabolism, purine metabolism, and pyrimidine metabolism pathways in astrocytes. Our study indicated that co-culture induced dramatic metabolic changes. Thus we suggest that crosstalk between astrocytes and motor neurons is crucial to evaluate the mechanisms of motor neuron death. These findings demonstrate that it would be more relevant to use co-culture system instead of monotypic cultures for in vitro pathophysiology studies in the context of neurodegenerative and neurologic diseases.

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Author: Andrew Palmer, Eric Weaver, Katherine Kellersberger, Amanda Hummon, Theodore Alexandrov | **Oral Abstract N:** O-2237

Spatio-temporal metabolomics of tumor organoids treated with chloroquine.

3D tumor organoids cultured from the HCT116 human colorectal cancer cell line are a model for poorly vascularised tumours that goes beyond simple cell-culture systems. It provides heterogeneous cell phenotypes in structured layers due to the gradients of nutrient penetration and oxygenation, similar to that found in vivo. Bulk analysis of these models neglects heterogeneity, inaccurately assigning metabolic activity and phenotype. High Resolution imaging Mass Spectrometry can detect hundreds of metabolites whilst localizing them across a sample. After 3D cell culture, the organoids were perturbation with an antimalarial drug with posited tumor suppressant properties and spatio-temporal metabolomics changes were studied using HR imaging MS in combination with our recently developed false-discovery-rate controlled spatial metabolomics annotation (see abstract by Theodore Alexandrov). 3D tumor organoids were cultured from HCT116 human colorectal cancer cells, and assigned to control and 12h, and 24h treatment with chloroquine (n=16, 8, 10) Sections were acquired and imaged with MALDI-FTICR Imaging MS (Solarix 7T, Bruker). Each of the datasets was translated from raw spectral data into putative metabolite annotation (median of 145 annotations per dataset, total of 415 unique annotations). Following annotation, statistical analysis was performed using only the biologically relevant information, in contrast to previous approaches which include arbitrary sets of peaks from the spectra. Specific metabolites were discovered colocalized within individual layers potentially associated with the altered metabolism seen between varying environmental conditions. We also characterized metabolic changes associated with the drug treatment. Using discriminant analysis, we discovered metabolites showing increased penetration into an organoid over time that could be associated with the drug penetration. Finally, we mapped metabolites potentially associated with the drug treatment onto the known metabolic pathways in order to provide insight into potential pathways associated with with the chloroquine treatment, and how these are associated with the spatially distribution of cell phenotypes.

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Oral Abstract N: O-2238

Optimus + `ili: software for LC-MS based untargeted spatial metabolomics in 2D and 3D

A widely used method for unveiling metabolic profiles of biological samples is liquid chromatography-mass spectrometry (LC-MS). However, currently no computational tools exist for LC-MS based metabolomics of samples collected in spatially-resolved manner. We developed Optimus, a software workflow enabling such analysis, and `ili, a web-application for visualization of produced spatial maps. Optimus is an open-source workflow for signal processing of untargeted LC-MS data (https://github.com/alexandrovteam/Optimus). Optimus includes feature detection, alignment and quantification, using algorithms provided by OpenMS library, complemented by filtering, mz-RT matching, and heatmap visualization. Ultimately, the workflow produces data for spatial mapping that can be browsed in `ili, an open-source application for visualization of spatial surface maps in 2D and 3D (https://github.com/ili-toolbox/ili). `ili employs, in addition to a conventional on-screen mode, cutting-edge virtual reality (VR) technologies to deliver more realistic impression. The VR mode supports Oculus Rift, Google Cardboard and Samsung Gear VR devices. For the interaction between a user and virtual environment, a voice control system was implemented. We evaluated Optimus and `ili in several studies, including, but not limited to those described in abstracts by Prasad Phapale and Luca Rappez. In addition, we developed a module for optimization of feature detection sensitivity by training on samples with standards, if available. Moreover, Optimus provides several feature filters, including removal of features from blank samples, minimal observation rate across samples, and presence of MS/MS spectra. The latter one proved to be useful for skipping those features that cannot be later identified. Afterwards, the features can be matched with a list of known ions by their m/z and, if provided, retention time. The matching is interoperable with the Global Natural Product Social molecular networking service by accepting metabolite identifications obtained from it. This procedure revealed a few tens of putative molecular annotations in each of the considered studies.

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Oral Abstract N: O-2246

MetFish: A suite of chemoselective tags combined with tandem mass spectrometry for quantitative and comprehensive metabolomics analyses in extreme environments

Extreme environments or matrices typically prohibit metabolomics measurements. For example, microbial communities often reside in extreme ecosystems consisting of high mineral content or salinity, making the assessment of the role of metabolic exchange among community members difficult when using mass spectrometry (MS)-based approaches. Commonly used sample preparation techniques (e.g., solid phase extraction) are inadequate for isolating polar metabolites from these matrices, resulting in an incomplete or biased metabolite profile. We developed a workflow (MetFish) based on chemoselective enrichment as a viable solution for metabolomics analyses in hypersaline and other highly complicated environments or matrices. MetFish is elegant in its simplicity and enables metabolites to be “fished out” of the sample both in vitro and in situ. The workflow currently consists of four chemical tagging approaches for quantification of metabolites with amine, carboxyl, carbonyl, and hydroxyl functional groups using dansylchloride, dansylcadaverine, dansylhydrazine, and 4-(dimethylamino)benzoyl chloride, respectively. After chemical tagging of metabolites, a simple liquid-liquid extraction is performed, followed by analysis using online SPE-nanocapillary LC coupled with selected reaction monitoring MS. The MetFish workflow provides sensitive and specific quantification of metabolites, with limits of quantification at low nM levels in sample matrices containing up to 2 M total dissolved salts. The chemistry of the probes also allows for the discovery of unknown metabolites in an untargeted approach based on the generation of distinct fragment ions specific to each probe. We have applied MetFish in analyses of model microbial consortia in hypersaline media and in situ analyses of soil and fracking fluid. For soil metabolomics, MetFish in combination with a high salt wash (0.5M K2SO4) provided higher recovery (2-10 fold) of extracellular metabolites in comparison to water and low salt extractions, allowing for more precise quantification of extracellular metabolites while imparting minimal to no effects on microbial intracellular metabolite profiles.

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Oral Abstract N: O-2284

Metabolomic profiles in different models of hepatocytes proliferation: partial hepatectomy and mitogen-induced hyperplasia

A relevant characteristic of the liver, a part from its implication in metabolic functions, is its high regenerative capacity. Hepatocyte proliferation has been largely studied in experimental animal models. In particular, its proliferative capacity has been examined in rats subjected to two/third partial hepatectomy (PH) or by exposing the animals to mitogenic agents such as lead nitrate (LN). As a consequence of an inflammatory response and cellular loss, PH-induced proliferation is associated with activation of signaling pathways elicited bygrowth factors, cytokines and matrix remodeling. Opposite, lead nitrate administration induces liver cell proliferation without cell loss and only a minor degree of inflammation. However, metabolic changes associated with these different models of proliferation and their effects on hepatocytes are still unknown. In this contest, the aim of this study was to elucidate the metabolic alterations in compensatory regeneration after PH and direct hyperplasia induced by LN. The metabolic profile was elucidated by nuclear magnetic resonance, liquid chromatography-mass spectrometry and gas chromatography-mass spectrometry analysis followed by multivariate statistics. In order to define possible changes during the proliferation process, different time points (24, 48, 72 hours, and 10 days) following PH and LN administration (100Qmol/kg) were analyzed. Significant metabolic changes and associated pathways were found, such as energy, amino acid and pyrimidine metabolisms. In conclusion, we believe this approach might help to better define common or specific metabolic changes during different models of liver cell proliferation and to identify possible targets in the control of cell division.

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Oral Abstract N: O-2285

The metabolic signature of stored red blood cells can be used for assessing the quality of red cell concentrate units during the storage

Transfusion of red blood cells (RBCs) is an integral part of modern healthcare and relies on blood banking technologies for extended storage of RBC units over time. Red blood cells (RBCs) are routinely stored up to 46 days. During storage, however, the quality of RBC unit is affected by the development of a set of complex biochemical and physiological changes known as "storage lesion". In this study, we used mass spectrometry based metabolomics approaches to profile 20 RBC units over 42 days of storage with a very fine time resolution (14 time points). At each time point, we tracked 135 parameters including intracellular and extracellular metabolites, and more traditional measurements of RBC physiology. Using multivariate statistics, we then identified a non-linear decay process that can be split into three distinct metabolic stages (Days 0-10, 10-17, 17-42). Surprisingly, hematological parameters traditionally measured in the transfusion setting do not distinguish these three stages. Using systems biology modeling, we then determined systemic changes in metabolic pathway usage between the three stages, finding that key pathways change in both magnitude and direction. We then used receiving operating characteristic curves to define a set of biomarkers that are able to distinguish between the three metabolic stages described. Finally, we perturbed the metabolic network by changing the concentration of main substrates of RBCs in the storage solution and by using metabolomics and stable isotope labeling analysis we gained a deep understanding of adenine and glutathione metabolism in RBCs during extended storage.

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Oral Abstract N: O-2286

Batch correction strategies to reduce non-biological variation in large-scale metabolic profiling

Background: Batch correction is essential in high-dimensional data analysis to reduce variability due to laboratory batches. However, empirical evidence of the importance of batch correction is sparse. Methods: We evaluated fasting-blood measures from 10,683 participants in the Fenland Study in the United Kingdom. Targeted metabolic profiling was performed for 185 molecules by using liquid-chromatography electrospray-ionization and flow-injection-analysis tandem mass-spectroscopy using the Biocrates kit (138 batches). After Box-Cox normalization, we conducted four different batch corrections: location correction, location-scale (LS) correction, parametric empirical Bayes (pEB) correction, and non-parametric EB (nEB) correction (Location correction adjusts for batch-specific means, and the others adjust for batch-specific means and standard deviations). We evaluated two sets of correlations of the un-corrected and corrected metabolomics variables with comparable variables assessed independently, (i) comparing LC-MS/MS creatinine with serum creatinine based on a Jaffe-reaction assay and (ii) FIA-MS/MS hexose, comprised of >90% glucose in normal adults, with plasma glucose based on a hexokinase assay. Additionally, to examine the role of batch correction in a small-scale setting, we repeated the same analysis using 5, 25 or 50 batches randomly selected from the available dataset. Results: Pearson correlation coefficients of LC-MS/MS creatinine with Jaffe-reaction assay creatinine were 0.71 when uncorrected for batch effects; 0.76, location correction; 0.77, LS correction; 0.77, pEB correction; and 0.77, nEB correction. Correlations of FIA-MS/MS hexose with glucose were 0.53, 0.64, 0.67, 0.68, and 0.68, respectively. In analyses using smaller datasets, higher correlations were observed in batch-corrected variables than uncorrected variables. For example, in the 5-batch dataset (n=399), correlations for creatinine measures were 0.58 when uncorrected; 0.65, LS correction; and 0.65, nEB correction. Conclusions: In metabolomics analysis, correction for batch effects benefits further biological analysis by reducing non-biological variation. This work supports the use of LS, pEB, or nEB correction for both batch-specific means and standard deviations.

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Oral Abstract N: O-2287

Brain tumour: Can LC-MS-based metabolomics reveal the tumour invasive margin?

Glioblastoma (GBM) is an incurable adult brain cancer with a median survival of 14 months and approximately 5000 UK deaths annually despite aggressive surgery, chemotherapy and radiotherapy. Distinct molecular biology underlies different regions of a single GBM indicating that there are multiple tumour sub-populations termed 'intra-tumour heterogeneity' (ITH) likely leading to therapy failure as treatments typically target one molecular pathway. Therefore, next-generation GBM chemotherapy must account for ITH and effectively remove invasive residual sub-populations that persist beyond the surgical resection margin. For this reason, quantitative characterisation of GBM metabolic changes is required to understand GBM recurrence post-surgery and resistance to therapy, which can be performed by liquid chromatography (LC)-mass spectrometry (MS)-based metabolomics. Here we present the first global metabolite profiling of multi-region brain tumour biopsies for the investigation of intra-tumour metabolic heterogeneity and description of the invasive margin. Multi-region brain tumour tissues including core, enhancing and invasive margin regions were resected during surgery. Metabolites extracted from the tumour fragments were then assessed by LC-MS-based metabolite profiling whilst cellular ITH was confirmed by immunohistochemistry and qPCR arrays. Clustering analyses showed a clear separation between invasive and non-invasive tumour regions and metabolic network analysis revealed that metabolites associated with purine and pyridine metabolism were altered significantly. Furthermore, lipidomics demonstrated that sphingolipids and lysophosphatidyl lipids are more prominent towards the tumour margin whilst the level of shorter chained free fatty acids increased in the tumour core. This innovative approach with multi-region biopsies is the first to address ITH using LC-MS-based metabolite profiling and the results showed that the invasive region was biologically distinct compared to tumour core, which revealed potential drug targets. Additionally, integration of transcriptomic and metabolomic data sets to investigate metabolite associations with metabolic enzymes in the context of GBM subtypes will be discussed.

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Author: Linda Oude Griep, Elena Checkmeneva, Jeremiah Stamler, Linda Van Horn, Queenie Chan, Elaine Holmes, Gary Frost, Paul Elliott, Timothy Ebbels **Oral Abstract N:** O-2298

A Metabolome Wide Association Study of fruit intakes

Recent application of metabolomics in small-, well-controlled dietary intervention studies identified potential markers of fruit intake. To our knowledge, no previous study comprehensively evaluated the urinary metabolome of fruit intake in free-living populations with diverse lifestyles. In a metabolome-wide approach, urinary signatures of fruit intake, total and by processing were characterised in participants from the US (N=2,032) and UK (N=449) of the INTERMAP (International Study of Macro- and Micronutrients and Blood Pressure) study. Univariate linear regression analyses was used to calculate associations of fruit intakes from four 24-hour dietary recalls with 7,100 individual chemical shifts of two 24-hour urine collections measured by 600 MHz proton nuclear magnetic resonance (NMR) spectroscopy. Adjustments were made for demographic and lifestyle variables, and body mass index. False Discovery Rate thresholds of 1% for US and 5% for UK were applied to account for multiple testing. Urinary metabolic profiles showed consistent, reproducible patterns of metabolite excretions associated with total, raw, and juiced fruit. Metabolites significantly and consistently positively related to higher total fruit intake in the US, UK, and both visits were fructose, hippurate, proline betaine, and scyllo-inositol. STOCSY (statistical total correlation spectroscopy) and untargeted urinary analyses of direct injection mass spectrometry data of top 10% versus non-fruit consumers confirmed hippurate (gut-microbial metabolite of polyphenol metabolism), proline betaine (direct marker of citrus fruit) and its metabolites, but not fructose and scyllo-inositol. Proline betaine was significantly associated with raw fruit (r=0.20-0.30) and fruit juice (r=0.48-0.62); hippurate with raw fruit (r=0.12-0.25). No chemical shifts were consistently significantly related to processed and dried fruit. Exploration of the urinary fruit-NMR metabolome confirmed hippurate and proline betaine as consistent markers of total, raw, and juiced fruit intakes across two free-living populations. Assessment of objective markers of fruit intake can improve reliability of diet-disease associations in large-scale epidemiological studies.

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Author: Roland Mumm, Jos Hageman, Mariafe Calingacion, Ric de Vos, Melissa Fitzgerald, Robert Hall **Oral Abstract N:** O-2300

Multi-platform metabolomics analyses of a broad collection of fragrant and non-fragrant rice varieties reveals the high complexity of grain quality characteristics

Rice is the most important food crop in the world. It is the staple of almost half of the world's population. The quality of rice in terms of its aroma and flavour is becoming increasingly important in modern rice breeding where global targets are focused on both yield stability and grain quality. Important rice flavours are often associated with the fragrant basmati and jasmine style rices. We have exploited multi-platform metabolomics approaches to elucidate the biochemical differences and similarities in 31 rice varieties with diverse genetic backgrounds and countries. All varieties were 100 % pure and were grown under the specific local conditions for which they have been bred for. Analyses using 6 analytical platforms have revealed the extent of biochemical differences between the chosen rice varieties. Comparison of fragrant jasmine and basmati rice varieties showed clear differences in the metabolic profiles, however with no consistent separation of the germplasm class. The storage of grains had a significant effect on the metabolome of both basmati and jasmine rice varieties but changes were different for the two rice types. This shows how a causal relationship with developing good quality in basmati rice or incurring quality loss in jasmine rice in aged grains may be proven by metabolic changes. Such metabolomics approaches are leading to hypotheses on the potential links between grain quality attributes, biochemical composition and genotype in the context of breeding for improvement.

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Author: Katharina Johnston, Dong-Hyun Kim, Michael Barrett, Fiona Achcar **Oral Abstract N:** O-2304

Mapping metabolism in the parasite Trypanosoma brucei using U-13C-labelled amino acids and LC-MS.

Trypanosoma brucei is the causative agent of Human and Animal African Trypanosomiasis. The metabolism of this extracellular parasite has several unique features when compared to other eukaryotes. For example, it relies on a partly compartmentalised glycolytic pathway as its only energy supply. Gaining a more detailed knowledge of the parasite's metabolism can help design new drugs and understand the mechanisms of action and resistance of current drugs. LC-MS-based metabolomics using uniformly (U)-13C-labelled glucose enabled Creek et al (PMID: 25775470) to explore T. brucei metabolism more extensively; they found that more pathways use glucose derived carbon than previously thought, including pathways essential to the parasite survival. This study also raised many new questions. In order to answer them and complete our map of bloodstream form T. brucei metabolism, we used 5 U-13C-labelled amino acids: cysteine, glutamine, methionine, arginine and proline. Parasites were grown in the presence of these labelled amino acids for 48 hours, prior to analysing their intracellular extracts using LC-MS to trace the fate of individual carbon atoms derived from these precursors inside the cells. The results show the presence of metabolic pathways previously thought to be absent or present only in the insect stage of the parasite. We could also detect the presence of unexpected novel metabolites, likely to be inadvertent products of promiscuous enzymes.

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Oral Abstract N: O-2311

Lipid mediator profiling for identifying sub-phenotypes of respiratory disease

Respiratory diseases are among the leading causes of death worldwide, collectively accounting for 9.5 million deaths worldwide during 2008, one-sixth of the global total. WHO estimates that 235 million people suffer from asthma alone, which is the most common chronic disease among children. Chronic obstructive pulmonary disease (COPD) is a leading cause of global mortality. However, despite extensive study, the pathogenesis of many chronic respiratory diseases is still incompletely understood and effective therapeutics are lacking. Lipid mediators (e.g., eicosanoids) are known to play a vital role in the pro-inflammatory component of respiratory disease. We have therefore extensively investigated the use of lipid mediator-profiling to identify sub-phenotypes of respiratory diseases. We will present two examples of these efforts. The first study is a pan-European study on severe asthmatics in which urinary eicosanoid levels were quantified in baseline and longitudinal samples (n=597 and n=305, respectively) in the U-BIOPRED cohort (Shaw et al., European Respiratory Journal, 46(5):1308-21, 2015) by UPLC-MS/MS. Clustering of urinary eicosanoid profiles identified five distinct asthma sub-phenotypes, including: 1) a Th2-like sub-group with high urinary cysteinyl leukotriene E4 and, 2) a female/obese sub-group with high isoprostanes and prostaglandin D2. The second study investigated the effects of smoking, in relation to COPD, on lipid mediators in the bronchoalveolar compartment and serum (n=114). A subset of lipid mediators created a highly significant model for classifying female non-symptomatic smokers from female smokers with COPD (p=6Ð10-6). No differences were observed for the corresponding male population (p=1.0). These findings were replicated in an independent cohort with 92% accuracy (p=0.005). These alterations may play a role in the gender-specific etiology of the disease and have consequences for ongoing efforts to develop therapeutics to treat COPD. Taken together, our efforts demonstrate the utility of a targeted lipid mediator profiling approach to perform molecular phenotyping in respiratory disease.

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Oral Abstract N: O-2313

Childhood obesity and insulin resistance, metabolomics strategies unveil early onset metabolic alteration and the influence of sex

In obese children, hyperinsulinemia usually occurs much earlier than the rise in glycaemia, suggesting the existence of predisposing factors for obesity-associated insulin resistance (IR) that remains unclear to date. Potentially deranged metabolic pathways in obese children with and without IR have been investigated by an MS-based multiplatform metabolomics approach. Plasma samples from 60 prepubertal (tanner I) obese children (30 girls/30 boys, 30 IR/30 non-IR) were analyzed by LC-ESI-QTOF-MS, GC-EI-Q-MS and CE-ESI-QTOF-MS (Agilent Technologies) following an untargeted approach. The results were validated in a second cohort of 100 children with the same characteristics, by using LC-ESI QqQ-MS and GC-EI-Q-MS. 47 metabolites showed statistically significant differences ($p<0.05$ after FDR) between groups. Bile acids exhibit the greatest changes indicating the magnified contribution of the microbiome in case of IR and obesity. Moreover, several lysophospholipids (15) and amino acids (17) were found altered, suggesting inflammation and central carbon metabolism as the most altered processes in IR. ROC curve and correlation analyses were then performed (Metaboanalyst and SPSS) to investigate the potential biomarkers arisen from the validation study. Concerning the ROC curve, the best biomarker was Alanine (AUC=0.81) for males, and a metabolite cluster (alanine-C3carnitine-5-oxoproline) for the whole cohort (AUC=0.86) and females (AUC=0.88). Clinical parameters (i.e. HOMA, lipid profile, adiponectin and leptin serum levels) were further correlated to the metabolites; 25 out of the 84 metabolites correlated to them ($R=0.4$, $p<0.005$), showed differences in the strength and in the direction of the correlation in a sex-specific fashion, highlighting differences related to sex despite the prepubertal status of the children. In conclusion, this study reveals the great potential of metabolomics to provide valuable information capable of depicting the metabolic signature of two highly correlated conditions (obesity and IR), by suggesting biomarkers for the early identification of high-risk individuals for whom the prevention plays its essential role.

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Oral Abstract N: O-2324

Addition of drift-tube ion mobility to liquid chromatography-mass spectrometry workflows: examining the potential for cellular metabolomics

The combination of liquid chromatography with low-field drift-tube ion mobility spectrometry and high-resolution mass spectrometry (IM-QTOFMS) can provide a powerful addition to existing LC-MS workflows aimed at metabolome assessment. We are currently investigating this strategy to improve cellular metabolome studies as the comprehensive sampling of chromatographic peaks and subsequent low-field drift-tube IM separation prior to measurement by a high-resolution QTOF-MS adds a valuable and precise identification parameter (collisional cross section, CCS) to support the non-trivial task of correct metabolite annotation. Underpinned by an ongoing international interlaboratory study focusing on stepped- and single-field CCS determinations, specific focus is placed on the use of precise and reproducible CCS values for metabolite identity confirmation, resolution of co-eluted isobaric ions, and the potential of more confident library matching for low abundance metabolites using drift time-filtered mass spectra. Various instrumental parameters affecting the measurement of small primary metabolites are also discussed including the influence of IM trapping conditions, data quality considerations, and the potential of using IM multiplexing functionality in the pursuit of improved dynamic range and analytical limits of detection. Our current LCÐIM-MS workflows exhibit high repeatability of analysis with average drift time precision of <0.50%, sub-2 ppm mass accuracy, and average abundance repeatability precision of <10% for extracted features using a full analytical workflow. Finally, the addition of IM multiplexing functionality for the analysis of cell factory extracts is shown to provide improvements in the signal intensities and detection of small metabolites within a complex background in comparison to non-multiplexed measurements.

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Author: Tytus Mak, Maryam Goudarzi, Stephen Stein | **Oral Abstract N:** O-2326

IFrID: A Novel In-Source Fragmentation Detection and Deconvolution Algorithm for LC-MS Metabolomics Data

In recent years, LC-MS metabolomics has emerged to become one of the most promising platforms for high-throughput characterization of metabolic processes and small molecule identification in biological systems. However, as with any burgeoning field, there are still many aspects that are inadequately understood. In-source fragmentation (ISF), which refers to the typically undesired fragmentation of ions during electrospray ionization, is both poorly characterized with respect to complex biological matrices, and often unaccounted for during chromatogram deconvolution. ISF may account for a significant fraction of the thousands of "unknown features" that are observed in metabolomics datasets, and potentially a major contributor to the perceived noisiness of the data. As such, we have developed a novel algorithm, called In-Source Fragmentation Inferenced Deconvolution (IFrID), which attempts to identify and minimize the potentially deleterious impact of in-source fragments during the MS1 deconvolution stage in metabolomics. IFrID utilizes the NIST Tandem Mass Spectral Library for inferencing potential in-source fragments of over 8,000 compounds. Candidate parent ions are initially identified in the experimental chromatographic data via exact mass matching to the NIST library. Ions with similar retention times to the candidate parent ion are compared to its associated fragments, which in effect utilizes the NIST library's MS/MS derived fragmentation data as a means for detecting ISF. This ISF-aware approach enables IFrID to produce deconvoluted MS1 datasets that have reduced confounding features. Data from a previous human urine metabolomics study consisting of 304 urine samples collected from 95 patients undergoing total body irradiation was deconvoluted via IFrID. Out of an initial 484,168 raw peaks identified across all samples which in 20,330 first-pass peak groups, 18.84% of peaks were eliminated, producing 18,342 final peak groups, a 9.78% reduction. IFrID represents one of the first attempts at creating a database dependent in-source fragmentation aware approach to metabolomics data deconvolution.

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Author: Shama Naz, Johan Kolmert, Mingxing Yang, Magnus Sköld, Åsa Wheelock, Craig Wheelock | **Oral Abstract N:** O-2328

Metabolomics profiling identifies gender-enhanced upregulation of oxidative stress in COPD

Chronic obstructive pulmonary disease (COPD) is an umbrella diagnosis, characterized by vigorous airflow obstruction and irreversible reduction of the forced expiratory volume. COPD evidences gender dependency, with higher mortality in women, even after correction for smoking. We hypothesized that metabolomics-based profiling of individuals with COPD would identify gender-based mechanisms in the pathobiology of COPD. Serum was obtained from healthy never-smokers (n=38), smokers with normal lung function (n=40), and COPD patients (GOLD I-II/A-B, n=37). A non-targeted metabolomics platform was applied using LC-HRMS. Significantly altered metabolites were confirmed using three different targeted LC-MS/MS platforms. Multivariate modeling was employed to examine the relationship between observed metabolites and disease. Gender-based multivariate models revealed significant metabolic shifts in healthy smokers vs. COPD smokers, which were primarily driven by females (p=2.4Ð10-7) relative to males (p=4.0Ð10-4). Of the 68 MS/MS-confirmed metabolites, phospholipase D-derived lysophosphatidic acid evidenced the strongest correlation with lung function (%FEV1; r=0.77; p<0.0001) in individuals with COPD. CD4+T-cells positively correlated with the oxidative stress marker hypoxanthine (r=0.72, p=0.009) in females with COPD, while the correlation was weaker in the corresponding male population (r=0.52, p=0.05). Pathway analysis of the COPD-associated metabolic perturbations highlighted a strong oxidative stress state in COPD, which was primarily upregulated in women. These findings were confirmed via targeted LC-MS/MS methods, substantiating the observed gender differences and upregulation of oxidative stress in COPD. These findings suggest that phospholipase D, together with phospholipase A2, influences the pathobiology of COPD, further highlighting phospholipase D for therapeutic intervention in COPD. In addition, results identified the gender-enhanced dysregulation of oxidative stress in COPD, which agrees with previous findings that female sex hormones affect smoking-related shifts in oxidative stress pathways. These findings further emphasize the molecular differences between the presentation of COPD in male and female populations, stressing the need to consider gender when evaluating treatment for COPD.

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Author: Benjamin Blaise, Goncalo Correia, Adrienne Tin, Hunter Young, Anne-Claire Vergnaud, Matthew Lewis, Jake Pearce, Paul Elliott, Jeremy Nicholson, Elaine Holmes, Timothy Ebbels | **Oral Abstract N:** O-2330

A Novel Method for Power Analysis and Sample Size Determination in Metabolic Phenotyping

Estimation of statistical power and sample size is a key aspect of experimental design. However, in metabolic phenotyping, there is currently no accepted approach for these tasks, in large part due to the unknown nature of the expected effect. In such hypothesis free science, neither the number or class of important analytes, nor the effect size are known a priori. We introduce a new approach, based on multivariate simulation, which deals effectively with the highly correlated structure and high-dimensionality of metabolic phenotyping data. First, a large data set is simulated based on the characteristics of a pilot study investigating a given biomedical problem. An effect of a given size, corresponding either to a discrete (classification) or continuous (regression) outcome is then added. Different sample sizes are modeled by randomly selecting data sets of various sizes from the simulated data. We investigate different methods for effect detection, including univariate and multivariate techniques. Our framework allows us to investigate the complex relationship between sample size, power and effect size for real multivariate data sets. For instance, we demonstrate for an example pilot data set, that certain features achieve a power of 0.8 for a sample size of 20 samples, or that a cross-validated predictivity Q2Y of 0.8 is reached with an effect size of 0.2 and 200 samples. We exemplify the approach for both Nuclear Magnetic Resonance and Liquid Chromatography – Mass Spectrometry data from humans and the model organism C. elegans.

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Oral Abstract N: O-2338

Metabolomics and proteomics analysis of vitreous humor from healthy, non-proliferative and proliferative diabetic retinopathy patients

Diabetic retinopathy (DR) is one of the leading causes of visual loss in working age population. DR is normally detected in advanced stage of the disease when microcirculatory abnormalities occur. However, retinal neurodegeneration is an early event in the pathogenesis, therefore, the study of the mechanisms leading to neurodegeneration is necessary to identify new therapeutic targets in the early stages of DR. Factors released from the retina can diffuse into the vitreous, and components within the vitreous can affect retinal function, suggesting that the vitreous may play an integral role in retinal physiology. Here, we have implemented for the first time an untargeted metabolomics and label-free quantitative proteomics approach based on NMR, LC-qTOF and LC-Orbitrap MS to study the progression of DR using human vitreous humor from 12 control, 4 non-proliferative diabetic retinopathy (NPDR) and 12 proliferative diabetic retinopathy (PDR) patients. Gene Ontology (GO) analysis of the vitreous proteome revealed overrepresented pathways, biological processes and molecular functions. We investigated the expression trend of proteins overrepresenting GO categories from healthy patients to the last stage of the pathology. From this analysis we observed a novel downregulation of proteins in PDR involved in cell adhesion in the neural system. We also found a downregulation of proteins involved in the oxidative stress response in PDR combined with lower levels of ascorbic acid. Since DR is characterized as a multifactorial disease encompassing vascular, inflammatory and neuronal complications, the integration of metabolome and proteome provides the study of metabolic pathway interactions and biological mechanisms of disease development and progression.

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Oral Abstract N: O-2343

Brain metabolomics identifies involvement of unsaturated fatty acid metabolism in "asymptomatic Alzheimer's disease"

Amyloid plaques and neurofibrillary tangles are well-characterized hallmarks of Alzheimer's disease (AD) pathology. The metabolic basis of AD pathology is poorly understood. It is hoped that a better understanding the role of metabolism and its relationship with these two mainstays of pathology will provide insights to symptom onset and disease progression. A combined UHPLC-qToF-MS and GC-MS method was applied to maximise coverage of the brain metabolome from a single split phase in-vial dual extraction. The aqueous phase was analysed using hydrophilic liquid interaction chromatography, the non-aqueous phase was analysed by reversed phase chromatography with both phases analysed by GC-MS. Samples were taken from three brain regions; cerebellum (CB) a low pathology control, inferior temporal gyrus (ITG) with high tau pathology and the middle frontal gyrus (MFG) with high amyloid pathology. Samples from 44 participants were stratified as controls, AD and asymptomatic AD (i.e. participants with significant AD pathology at death but without cognitive impairment during life). Six poly-unsaturated fatty acids (UFA) were shown to be strongly associated with Alzheimer's disease ($p< 0.05$) as well as measures of tau and Aß pathology. Shifts in the ITG of asymptomatic patients were comparable to those observed in demented patients, whilst in the MFG levels of these metabolites in asymptomatic individuals were more similar to controls than demented subjects. Our findings implicate UFA metabolism in the Alzheimer's pathogenesis. The difference in the abundance of these 6 UFAs in the MFG of asymptomatic patients would suggest that these metabolites are conferring resilience to the asymptomatic AD patients.

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Oral Abstract N: O-2345

Isotope tracer-based metabolomics applied to non-steady state circadian systems

A genetic basis for our endogenous circadian rhythms is well-established through genomics and transcriptomics studies. These rhythms are critical for both anticipating environmental changes, as well as adapting to new surroundings. Recently, the specific impact of the clock on metabolism has been better elucidated through metabolomics profiling across cells, tissues, and whole organisms, including humans. Stable isotope-assisted metabolic flux analysis provides a definitive metabolic phenotype for the system of study. However, appreciable time resolution and metabolic inference from these studies typically comes from simplified systems, such as in vitro models. Experimental designs for circadian rhythms research include short sampling intervals over periods of 24 to 48 hours in order to fit curves to the oscillations in metabolomic output, which is not tractable to typical steady-state labeling experiments and both difficult and costly in in vivo settings. Here we aim to address these concerns by developing an isotope-assisted metabolomics platform for in vivo studies which require short labeling times and provide throughput commensurate with time-resolution requirements of circadian rhythm detection. We perform metabolomics in both targeted and untargeted analyses using triple quadrupole and quadrupole time-of-flight instruments, respectively. Differential labeling analysis from the untargeted metabolomics is processed and analyzed for time-dependent metabolic patterns, and corroborated using traditionally targeted 13C-flux analysis. We are able to analyze labeling patterns from 30 compounds downstream of glucose tracers, providing valuable insight into the kinetics of central energy, lipid, and amino acid metabolism. We present a novel workflow for assimilating multiple isotope-assisted metabolomics analyses for sensitive and specific analysis of changes in circadian metabolism at high time resolution. We expect to find concerted changes in metabolism which are under control of our endogenous genetic clocks.

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Evidence for a chemically enabled non-enzymatic origin of the Krebs cycle

The metabolic network is essential for providing building blocks for the synthesis macromolecules such as proteins, lipids and DNA. However, the evolutionary origin of the tricarboxylic acid (TCA), which represents a core module of cellular metabolism, is still only barely understood. Hypotheses exist that suggest this metabolic cycle to have emerged from non-enzymatic chemical reactions, facilitated by inorganic ions or molecules available to early world organisms, while others explain the TCA cycle pathway structure to result from evolutionary optimization. We addressed this central question by using combinatorial, quantitative metabolomics enabling to systematically process thousands of samples, and measured specific reactivities of TCA intermediates in a series of iron and sulfate reaction milieus that orient on Archean sediment constituents. We found that many intermediates were stable in many tested conditions. However, a chemical environment containing peroxydisulfate and ferrous sulfide enabled 24 mutually compatible non-enzymatic reactions interconverting TCA intermediates. A detailed characterisation of these reactions unravelled their dependency on sulfate radicals and demonstrated their high efficiency. Analysed in a network graph the observed sulphate and iron reactivity closely replicated the chemical topology of the modern enzymatic Krebs cycle, along with the co-occurring glyoxylate and succinic semialdehyde pathways. These results suggest that a non-enzymatic origin Krebs cycle is plausible and does not require complex catalysts but can be facilitated by an aqueous iron-sulfate environment rich in sulfate radicals. This chemical reaction network hence represents an optimal template to allow a first biological system to take over catalytic control in an evolution-driven process and to facilitate autotroph life. An additional aspect of these results is that non-enzymatic reactions can still contribute to modern metabolism and therewith contribute to the metabolic network structure, representing so far often overlooked constrains for drug design strategies and biotechnological applications.

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Plasma Metabolomics for Prognostic Biomarker Development in Pancreatic Cancer

Early detection and diagnosis of pre-neoplastic lesions and tumors have the potential to improve treatment and clinical outcomes in pancreatic cancer (PC). However, there is no reliable screening test that can be used non-invasively and accurately for early detection of PC. The development of anticipatory biomarkers is important since the disease is often diagnosed in advanced or metastatic setting when curative treatment options are severely limited. We performed comparative plasma metabolomics using targeted mass spectrometry based approach on 79 newly diagnosed PC patients, 66 non-cancer controls (NC) and 79 newly diagnosed colon cancer (CC) disease controls. The “at-diagnosis” cohort was divided into discovery and validation sets; the discovery cohort comprised of 40 randomly selected PC patients and 30 normal controls while the validation cohort was comprised of the remaining 39 PC patients and 33 normal controls. The selection of putative metabolite biomarkers was carried out using the regularized logistic regression approach. To avoid overfitting of the model and reduce inter-correlation of metabolites, 10-fold cross-validation was used to determine tuning parameters and calibrate the prediction model in the discovery set. Metabolites that were significantly dysregulated in PC patients (compared to NC and CC) were included for biomarker evaluation. We used logistic regression to create a classifier model and evaluated the performance using ROC analysis. The optimal classification panel was comprised of eight metabolites including taurocholic acid, ornithine and tryptophan and yielded a ROC AUC = 0.93 and the panel were adjusted for age, gender and Type 2 diabetes status. In summary, we demonstrate the development of a biomarker development pipeline for PC diagnosis using metabolomics approaches that can be easily translated to an anticipatory biomarker panel in future studies. The dysregulation of these specific metabolites provides insights into biochemical perturbations that define the molecular basis of PC disease progression.

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Identification of serum metabolites associated with risk of type 2 diabetes by untargeted metabolomics approach: A nested case control study

Type 2 diabetes (T2D) is a chronic metabolic disease which is characterized by impaired insulin action and/or secretion. The exact metabolic pathways underlying diabetes development and progression are incompletely understood. It is important to analysis the early alteration of metabolites for the research of diabetes. The metabolomics technology developments make it possible to get the whole metabolites in biological samples. In this study, we applied untargeted metabolomics approach to obtained metabolites profiling in serum samples of subjects from the CVDFACTS. Total 50 subjects who developed T2D within a 3 years follow-up and 50 subjects who had no diabetes were included in this study. UPLC-MS was used to profile the metabolites in baseline serum. After univariate analysis to select metabolites with the strongest contribution to disease classification, multivariable logistic regression was used to assess the association of these metabolites with T2D. A total of 39 compounds were found to have association with the risk of diabetes. Then by the forward stepwise selection, 5 candidate metabolites in combination with 2 traditional risk factors (BMI and serum glucose) were selected into the T2D risk prediction panel. With the comparison to traditional risk factors mode (AUCs= 0.77, 95%CI=0.67-0.87), our model performed the significantly better ROC result (AUCs= 0.99, 95%CI=0.98-1.00) for T2D prediction (p-value <0.0001).

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Oral Abstract N: O-2365

Large-scale metabolomics to assess pharmacokinetics of conjugated black tea catabolites in human plasma

Black tea polyphenols have been proposed to exert beneficial cardiovascular bioactivity, mostly through the gut microbial catabolites derived from them. This hypothesis is difficult to verify because the conjugation patterns and pharmacokinetics of the conjugated tea compounds and their catabolites are largely unknown. Here we aimed to identify, quantify, and assess the pharmacokinetics of conjugated black tea metabolites in plasma of healthy humans by means of an a priori untargeted LCMS-based metabolomics approach. Plasma was collected at 14 time points from 12 healthy men, after each had consumed a single dose of black tea extract or a placebo in a randomized crossover study . All study samples and quality controls were analyzed in a single series using a UPLC-LTQ-Orbitrap FTMS platform and raw data were preprocessed in an untargeted manner. From the total of about 600 metabolites accordingly deduced per volunteer, 131 could be readily annotated as conjugated black tea-derived compounds, based on the accurate masses of both their molecular and fragment ions and by comparison with tea-catabolites previously identified in urine using MSn and NMR. For 59 of these compounds a kinetic response in plasma was observed upon black tea extract consumption, for 11 of these in a quantitative manner by using tea-catabolites purified from urine as authentic standards. Our results indicate distinctive pharmacokinetics for directly-absorbed tea metabolites (e.g. catechins, kaempferol, gallic acid) and gut microbial catabolites (e.g. valerolactones, valeric acids, pyrogallol). The inter-individual variation was larger for the gut catabolites then for the directly absorbed tea compounds, likely reflecting the differences in the gut microbiome of the volunteers. The rapid and sustained circulation of conjugated catabolites, of which some were present in plasma at physiologically relevant concentrations, suggests that these compounds may be particularly relevant to the proposed health benefits of black tea.

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Oral Abstract N: O-2366

High quality metabolomics Mass Spectrometry Imaging using sputtered gold nanolayers

Mass spectrometry imaging (MSI) is a molecular histology technique by mapping the distribution of molecules on biological tissues with high spatial resolution. The extraordinary development on the analytical instrumentation and strategies in the last decade makes MSI a key tool in clinical research. Here, we present a novel MSI matrix-free methodology for laser desorption/ionization mass spectrometry (LDI-MS) based on sputtered gold nanolayers deposited straight over tissue sections. Gold is a highly stable material and neither degradation nor oxidation occurs after sample preparation and during the LDI-MS acquisition. The sputtered deposition method is fast (ca. 5 min), fully automated and highly reproducible. This dry deposition method avoids the delocalization of the metabolites in the biological tissues allowing the acquirement of ultra-high resolution images (<10 Qm), only limited by the laser spot of the instrument. Furthermore, the peaks coming from the gold nanolayer are easily identifiable, have minimal interference on metabolite detection, and are useful for the reliable spectrum alignment and mass calibration between pixels. Other innovative feature is that the discontinuous structure of the gold nanolayer permits the acquirement of histological images of the same section analyzed by MSI, making this technology extremely useful to define regions of interest and to correlate the histological images with the MSI ones. The viability of the gold-based MSI method was checked by acquiring MS images of different mice tissue sections, including brain and kidney. The mass spectra obtained from the different tissues were very rich in the m/z range under 1000 Da. Dozens of endogenous metabolites have been putative identified with a mass accuracy under 5 ppm for most of them, including different kind of lipids (fatty acyls, glycerolipids, glycerophospholipids, sphingolipids, sterol lipids), as well as aminoacids and other smaller metabolites. These results make gold-based MSI a valuable alternative for high-throughput clinical diagnosis.

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Oral Abstract N: O-2368

Novel indicators of severe acute malnutrition in a cohort of Nigerian children identified through untargeted metabolomics

Background: Severe acute malnutrition (SAM) is a major cause of child mortality worldwide, however studies investigating the metabolic characteristics of SAM in humans are limited. As recent studies have revealed associations between the gut microbiome and malnutrition, biomarkers of SAM may have microbial origins. Objectives: To identify metabolites in stool and plasma that discriminate children with SAM from controls, and their association with changes in the gut microbiota. Methods: We applied an untargeted multi-platform metabolomics approach (Q-Exactive Orbitrap LC-MS and Agilent 7890A GC-MS) to stool and plasma samples from 47 Nigerian children with SAM and 11 control children. Metabolites were identified by library comparison, as well as de novo compound identification from MS/MS spectra, and confirmed by authentic standards when available. The composition of the stool microbiota was also assessed by 16S rRNA gene sequencing. Results: Univariate and multivariate analyses demonstrated that the plasma metabolome discriminates SAM from controls, while no significant differences were observed in the microbial or small molecule composition of stool. A total of 585 features in plasma were significantly altered in SAM (Wilcox test, FDR corrected $P < 0.1$), representing approximately 15% of the metabolome. As expected, children with SAM exhibited a marked reduction in many essential nutrients, including amino acids/dipeptides and phospholipids. We also observed a significant decrease in bioactive lipids belonging to the eicosanoid and docosanoid family. Metabolites elevated in SAM were indicative of increased intestinal permeability and a catabolic state, and included disaccharides, two forms of truncated fibrinopeptide A, angiotensin I, acylcarnitines, lactate, and heme. Conclusions: This work provides a deeper understanding of the metabolic changes that occur during malnutrition, and identifies novel biomarkers of SAM in humans. Monitoring of such biomarkers may allow better identification of high-risk individuals and provide a more quantitative measure of response to treatment.

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Oral Abstract N: O-2375

GC-MS metabolomics towards a putative urinary biosignature for Tuberculous Meningitis in children

Tuberculous meningitis (TBM) is the most severe manifestation of tuberculosis, presenting with high morbidity and mortality in children. Existing diagnostic methods for TBM are invasive and time-consuming, often causing complications due to delayed treatment. The need for highly sensitive and selective diagnosis thus remains high on the TBM agenda. Our aim was to use the 'gold standard' of metabolomics — gas chromatography-mass spectrometry (GC-MS), to generate data that could identify metabolites with characteristics to define a potential diagnostic biosignature for children with TBM through a noninvasive means. The crux of this aim was unravelling new information on the vast range of excreted metabolites in the urinary profile as a result of the perturbation caused by this neuroinflammatory disease. Urine samples were selected for this study, using three paediatric groups: patients with confirmed TBM (12 cases), patients clinically suspected with meningitis but later confirmed to be negative (18 cases), and an age-matched control group (30 cases). GC-MS metabolomics data were generated and through sophisticated statistical analyses it was revealed that six groups of metabolites characterized TBM — three groups reflected the host response and three groups apparently related to a host-microbial response. We proposed a global metabolite profile reflecting the potential diagnostic host-microbial metabolites and identified a sum total of the concentrations of methylcitric, 2-ketoglutaric, quinolinic and 4-hydroxyhippuric acids — designated as SUM-4 — as a Mtb–host biosignature. This study is the first to illustrate holistically the metabolic complexity of TBM-confirmed cases and acts as a proof-of-concept that a biosignature of urinary metabolites can be used in the diagnosis and assessment of prognosis of our specific TBM population. It is our hope that SUM-4 could be developed and validated through future studies to generate a urinary medical algorithm with potential for diagnosis and monitoring of TBM everywhere.

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Oral Abstract N: O-2383

Novel pathways, metabolites and bioactivity – A fresh look at salicinoid biosynthesis through NMR-MS metabolomics

Novel pathways, metabolites and bioactivity – A fresh look at salicinoid biosynthesis through NMR-MS metabolomics Jane L. Ward, Yanqi Wu, Claudia Harflett, Charlotte Lomax, Delia Irina Corol, Michael H. Beale Rothamsted Research, Harpenden, Herts, AL5 2JQ, UK Email: Jane.ward@rothamsted.ac.uk The relatively simple, and hugely successful, drug aspirin (acetylsalicylic acid) was developed by Bayer in 1897, from a lead compound (salicin) identified by the study of salicyl glycosides in Salix alba bark. It is however surprising that despite over 100 years of natural product chemistry research, the biosynthesis of salicin and related salicinoids remains largely unknown. Rothamsted Research maintains The UK National Willow Collection (Salix sp.) as well as large genetic mapping populations that contribute to the breeding of new varieties of biomass crops. Many thousands of Salix genotypes are growing in field plots, offering a huge chemical diversity, and thus are available for screening, not only in relation to biomass traits, but also for the identification of novel metabolites for pharmaceutical applications. We will demonstrate how the use of an NMR/LC-MS metabolomics approach has allowed us to structurally identify many new entities, some of which are suggestive of the true biosynthetic route to these famous compounds. Profiling of mapping populations has also enabled us to add insight into the genes responsible. Our studies have allowed us, for the first time, to suggest a complete metabolic grid explaining the biogenesis of the majority of the known salicinoids. The presentation will demonstrate the use of multiple unbiased metabolomics experiments, each yielding new information, on salicinoid formation and putative pathway intermediates. We will also demonstrate novel analytical approaches to reveal new, unusual, salicinoid derivatives in the datasets and also show how high-throughput NMR/LC-MS screening data can be combined with pharmacological testing to deliver novel bioactivity, from previously un-described compounds.

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Oral Abstract N: O-2384

Early serum biomarkers to predict risk of third trimester placental abruption

Non-invasive biomarkers are needed for the early prediction of placental abruption (PA). PA is an ischemic placental disorder that occurs for 1 in 100 pregnancies and has a major association with maternal and perinatal morbidity and mortality worldwide. We conducted a metabolomics analysis of serum that was collected in early pregnancy (~16 weeks gestation) from women who, in the 3rd trimester of pregnancy, either had a normal delivery or a placental abruption (51 PA cases, and 51 normal delivery). Quantitative targeted metabolic profiles of the 2nd trimester serum were acquired using the Absolute IDQ® p180 kit and electrospray ionization liquid chromatography-mass spectrometry (ESI-LC-MS/MS). Logistic regression models incorporating maternal sociodemographic characteristics and reproductive history were developed to evaluate the potential for metabolites in the 2nd trimester serum to predict abruption alone, or in combination with the current clinical standard - vaginal bleeding. The AUC for early pregnancy vaginal bleeding alone was 0.65, and significantly (P=0.003) improved to 0.75 with the addition of quantitative metabolite data for phosphatidylcholine acyl-alkyl C 38:1 (PC ae C38:1) and dodecanoylcarnitine/ dodecenoylcarnitine (C12 / C12:1). While larger studies are needed to validate these results, and discover additional metabolites for improving the prediction value, this study has demonstrated that metabolomics is a useful tool for improving our ability to predict PA early in pregnancy. The metabolomics analysis was funded by the NIH Common Fund Metabolomics Program (1U24DK097193), and the human subject investigation was funded by NIH (R01-HD059827).

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Application of LC - Data independent acquisition (DIA) - digital archiving (DA) mass spectrometry for mycotoxin and metabolite profiling of silage

Introduction: Yearlong feeding of silage to farm animals in North America and Europe provides important digestible nutrients and proteins. Penicillium species can grow and produce toxins in this environment but with advances in mass spectrometry (MS) and next generation sequencing (NGS) we wanted to determine all of the fungi and mycotoxins present on ensiled corn, haylage and barley. Silage samples were obtained from 26 farms in Canada, where either dairy goats or cows were experiencing a number of health issues ranging from reduced milk production to neurological problems and death. Methods: Predominant filamentous fungi were isolated from silage samples and DNA from both fungi and bacteria present were profiled using NGS. Silage was extracted and analyzed using our untargeted liquid chromatography data independent acquisition mass spectrometry (LC-DIA-MS) method developed for mycotoxins in corn. All LC-MS and MS/MS data were stored in our digital archive for retrospective 'data mining' and mycotoxins were identified based on comparison to our in-house standard spectral library. Results: Fifteen fungal species, half of which were Penicillium, were isolated from the infected silage and an additional 103 fungal species and 343 bacterial species were detected by NGS. Metabolomic profiling of the infected silage has revealed the presence of 46 mycotoxins and fungal secondary metabolites, these included both toxins from the field and toxins produced during storage. Statistical analysis of the data including Principal Component Analysis (PCA) has allowed for comparison of fungi and toxins between sites and revealed that fungal species and toxins tend to be farm and substrate specific. Conclusions: The combination of LC-DIA-MS metabolite profiling with NGS sequencing data has provided important new insights in the mycotoxins and fungi present in silage, this will help farmers prevent future health issues in their dairy herds.

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Medium-throughput metabolomics screening identifies modes of action for novel antimalarials

Malaria is a deadly disease caused by the protozoan parasite, Plasmodium falciparum, and threatens over 40% of the world's population. Drug-resistance has emerged to all current antimalarials, and new drugs are urgently required for the treatment of malaria. Recent drug discovery programs based on high-throughput phenotypic screens have identified thousands of small molecules that have antiparasitic activity against P. falciparum in vitro. A representative subset of these novel antimalarials, known as the 'Malaria Box', has been released openly to the research community to facilitate drug discovery. However, little is known about the mechanism of action of these compounds, restricting further development of these promising leads. Metabolomics offers an ideal platform to investigate mechanisms of drug action in a hypothesis-free manner. Specifically, metabolomics provides a snapshot of the metabolic state of the parasite after drug treatment, and can reveal the direct impact of a test compound on metabolism. LCMS-based untargeted metabolomics methods for P. falciparum cultures were optimised for 96-well plate format, allowing analysis of the metabolic phenotype induced by 100 known and novel antimalarials. Many of the novel compounds induced metabolic phenotypes that clustered with the known antimalarials, atovaquone, chloroquine and artemisinin. In particular, inhibition of pyrimidine biosynthesis was a common mechanism of antimalarial action, as indicated by accumulation of dihydroorotate and N-carbamoyl aspartate. Furthermore, depletion of unique parasite peptides and lipids for specific test compounds indicated selective inhibition of parasite pathways that may facilitate further development of these hit compounds. This study demonstrates the successful scaling of untargeted metabolomics to a medium-throughput screen, which revealed biochemical impacts and potential drug targets associated with many of these novel antimalarial compounds.

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The placental mitochondrial metabolome suggests the importance of lipid metabolism in pre-eclampsia

Background: Pre-eclampsia is a pregnancy complication characterised by the new onset of hypertension and proteinuria. The aetiology of pre-eclampsia remains unclear, but growing evidence suggests that mitochondrial dysfunction contributes to the pathogenesis. We hypothesised that metabolic dysfunction of the mitochondria in pre-eclampsia would be reflected in the placental mitochondrial metabolome. Methods: We isolated mitochondria from human placental trophoblasts. The mitochondrial metabolome in pre-eclampsia (n=16) and normal pregnant (n=17) placentae were compared using Gas Chromatography-Mass Spectrometry (GC-MS). Metabolite peaks were deconvoluted, identified, and extracted by AMDIS and our in-house R package. Student's t-test, false discovery rate, receiver operating characteristic (ROC) were applied to determine which mitochondrial metabolites differed significantly between pre-eclampsia and normal pregnant placentae. Pathway Activity Profiling (PAPi) R package was used to predict which metabolic were pathways affected. Results: The mitochondrial metabolome was significantly different between pre-eclampsia and normal pregnant placentae; higher levels of 7 amino acids, 13 fatty acids, and 14 other metabolites were observed in pre-eclampsia while lower levels of 2 metabolites were found in pre-eclampsia (p-value <0.05 and $q<0.05$). Five fatty acids had an area under the ROC curve above 90%. These fatty acids were involved in aspects of lipid metabolism including fatty acid elongation, fatty acid oxidation, biosynthesis of unsaturated fatty acids, linoleic acid metabolism, and arachidonic acid metabolism. Conclusion: Metabolic dysfunction of the mitochondria in pre-eclampsia was reflected in the placental mitochondrial metabolome. Our findings suggest that lipid metabolism is dysregulated in pre-eclampsia. Future research is needed to validate the results of our pilot study.

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Author: Theodore Alexandrov, Andrew Palmer, Michael Becker, Dominik Fay, Artem Tarasov, Jens Fuchser, Vitaly Kovalev, Sergey Nikolenko | **Oral Abstract N:** O-2397

FDR-controlled metabolite annotation for high-resolution imaging mass spectrometry

Metabolites play central roles in biological processes of health and disease. High-resolution imaging Mass Spectrometry (HR imaging MS) promises to localize hundreds of metabolites directly from tissues, cell cultures, and agar plates with cellular resolution, but is hampered by the lack of bioinformatics for metabolite identification. We have bridged this gap by developing the first bioinformatics framework for False Discovery Rate (FDR)-controlled metabolite annotation introducing a Metabolite-Signal Match (MSM) score and a target-decoy-based FDR estimator. Our open-source framework is based on the following principles: database-driven annotation, use of a novel MSM score combining conventional spectral (e.g. isotopic fine structure) and novel spatial measures (e.g. measure of spatial chaos, colocalization between signals), generation of a decoy database by considering implausible adducts, and target-decoy-based direct estimation of FDR. We proposed a strategy for evaluating the proposed metabolite annotation framework and the FDR estimator based on the following principles: comparison of the decoy and target signals, calculation of the error of the FDR estimator on a simulated dataset with known ground truth, and a negative control experiment. We evaluated the developed FDR-controlled molecular annotation on selected HR imaging MS datasets from wild-type mouse brain specimens (snap-frozen, cryosections, matrix sublimation). Datasets were of 50-500 GB in size. The evaluation demonstrated the relevance of the proposed approach for creating decoy signals, good approximation of the true FDR by our proposed FDR estimator, and overall positive results of the negative control experiment. Metabolites from various molecular classes were detected, showing high levels of biological and technical reproducibility. We could compare imaging MS datasets of different mass resolutions and determine minimal acceptable mass resolution for a desired level of FDR. Our framework enables automated high-throughput untargeted metabolic imaging based on HR imaging MS.

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Author: Albert Koulman, Georgia Billing, Animesh Acharjee, Philippa Prentice, Gail Goldberg | **Oral Abstract N:** O-2398

The application of lipid profiling to understand dietary fat metabolism in breast-fed infants.

Different studies showed that formula feeding can lead to too rapid growth and catch up growth predisposing the infant to obesity in later life. Lipid metabolism of breast-fed infants is significantly different to that of formula fed infants. Breast-fed infants have lower levels of specific phospholipids such as PC(34:1), which has a positive association with weight at 3 months and higher levels of specific such as sphingomyelins SM(36:2), which has a negative association with weight gain from 3 to 12 months. We want to understand which components in the diet are driving these differences in lipid metabolism that are associated with growth and development. Breast-milk samples and infant plasma samples from 30 mother-infant pairs were obtained 12 weeks post-partum in rural Gambia. Samples were extracted with an organic solvent and profiled by direct infusion mass spectrometry, using chip based nanospray and high-resolution mass spectrometry. Breast-milk lipids showed strong associations with specific plasma lipids, from different classes. Smaller triglycerides and diglycerides in breast-milk correlated with sphingomyelins e.g. SM(36:2) but not with plasma triglycerides. Higher levels of the breast-milk sphingomyelin SM(34:2) associated with higher levels of plasma triglycerides e.g. TG(54:2). These results suggest that the lipid composition of the infant's diet has a profound influence on which pathways are activated, to metabolise and repackage the dietary fatty acids. It is well-documented that changes to fatty acid composition of milk affect infant development. Our study shows for the first time that intact dietary lipids in breast-milk determine how dietary fat is metabolised.

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Stability of human plasma "metabotypes" in response to dietary challenges

Introduction and Objective – Metabolic phenotyping in humans is usually done in fasting state not taking into account that metabolism is highly dynamic with major changes in space (organs) and time. To assess this flexibility of the human metabolic system we performed standardized challenge tests combined with metabolite profiling of plasma and tissues as part of the NutriTech project. Methods – 72 volunteers (men and women, age = 6033 yrs., BMI = 3032 kg/mÐ) were recruited, submitted to whole body MRI and underwent an oral glucose tolerance test (OGTT) and a mixed meal tolerance test (MMTT). The two tests were repeated after 13 weeks with 40 volunteers on a diet providing 20 % less calories, while 32 followed a standardized diet without energy restriction. Metabolite profiling was performed in plasma samples using LC-MS/MS, GC-MS and NMR platforms with around 260 entities covered. Results – Despite a mean weight loss of 4.530.2 kg, caloric restriction did not induce major changes in plasma metabolite concentration profiles during the challenge tests. Assessed by ANOVA, the overall contribution of the caloric restriction to the observed variations of metabolite concentrations was negligible, ranging from 0.25% for lyso PC C18:2, to about 2.3% for Alanine. This indicates the individual responses to the challenges were highly reproducible on the two occasions, identifying "robust metabotypes". Despite little effect of the intervention, inter-individual variability is extremely high. Taking all metabolites analyzed into consideration, on average inter-individual differences account for more than 50% of the observed variability; ranging from 10% for non-esterified fatty acids to more than 80% for cholesterol in VLDL particles. Conclusion – The results demonstrate that on a time axis of three months, metabolic phenotypes derived from challenge experiments such as OGTT or MMTT are highly reproducible despite large inter-individual differences.

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Carbon Flux Signatures of Mycobacterium tuberculosis

Tuberculosis (TB) remains a major problem worldwide being responsible for 1.5 million deaths and 9.0 million developed clinical diseases each year. Being the causative agent of TB, Mycobacterium tuberculosis is the target for development of anti-TB drugs. M. tuberculosis lives in human macrophages and has evolved the ability to adapt its metabolism to harsh environments. Studies indicate that M. tuberculosis evolved its metabolic network to cope with these conditions. Despite of more than a century of intensive research, the knowledge about the intracellular metabolic processes acting in M. tuberculosis is still limited. By means of carbon labeling experiments, isotopomer analysis and modeling, we investigated which carbon sources are eaten by M. tuberculosis and how the microbe metabolizes them. M. tuberculosis was grown on 13C-labeled glycerol in chemostats to generate detailed insights into the central metabolic fluxes. With mass isotopomers of proteinogenic amino acids and extracellular rates, ex vivo flux modes of the pathogen were quantified by rigorous 13C metabolic flux analysis. A large scale host-pathogen network model was built that covered cofactor usage, biosynthesis and degradation of metabolic compounds for both, the macrophage and the tuberculosis bacillus. With the integrated model the diversity of nutrient uptake scenarios and emerging flux distributions was explored in silico. To delineate the in vivo flux signatures of M. tuberculosis, infected macrophages were fed with 13C-labeled glucose. With a technique, called 13C-flux spectral analysis (13C-FSA), a mix of amino acid, C1 and C2 carbon sources for M. tuberculosis was identified. Disruption of the associated flux routes may provide a new avenue for anti-TB drug design and therapeutical strategies. We discuss the challenges of 13C-FSA and its potential to investigate carbon flows in host-pathogen systems.

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Global Untargeted Metabolomics Approach to Reveal Metabolic Shifts during Postharvest Cold Storage of 'Kinnow' Mandarin.

Fruit metabolism continues at an inhibited rate during postharvest cold storage, leading to significant changes in fruit quality attributes generally measured as quantification of a few metabolites having nutritional and flavour importance. Mass-spectrometry based global untargeted metabolomics is an approach to gain comprehensive coverage and insight into the fate of thousands of metabolites in a biological system. To study the metabolic shifts during cold storage of 'Kinnow' mandarin, commercially mature fruit were stored at low temperature (5°C) for 8 weeks and sampling was conducted at weekly intervals. Methanolic (80%) extracts of juice were injected into an UHPLC-QTOF mass spectrometer operated in an independent data acquisition mode enabling generation of TOF-MS and MS/MS data. Mass spectral output analysis involved peak alignment, normalization against an internal standard, and then unsupervised and supervised multivariate analyses using Analyst™, PeakView™ and MarkerView™ software. About 8000 features for each data set were detected in the mass range of 100-1000 m/z. Following data pre-processing, multivariate statistical analyses reflected significant metabolic shifts during cold storage for 8 weeks. Clustering of fruits into three major groups was possible: early-(0-2 weeks), mid- (3-5 weeks) and late- (6-8 weeks) stages of cold storage. Multivariate analyses coupled with metabolite annotation using databases such as Metlin and MassBank revealed putative identification of discriminant metabolites linked to different stages of cold storage of 'Kinnow' mandarin. In conclusion, LC-QTOF based metabolomics can be a powerful tool to unravel the mechanisms underlying the postharvest cold storage-induced metabolite changes ultimately leading to fruit quality.

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Metabolomic based identification of clusters that reflect dietary patterns

The use of metabolomics in dietary biomarker discovery has predominantly focused on single foods. A novel approach, nutritypes (metabolic profiles that reflect dietary intake) has emerged facilitating a more comprehensive relationship between nutrition and disease-risk while also addressing issues of nutrient-interactions. The aim of this study is to use metabolic profiles to define dietary intake patterns and link these dietary patterns with nutrient and biochemical data. Urinary data, analysed by 1H NMR spectroscopy and dietary data from the Irish National Adult Nutrition Survey (NANS)(www.iuna.net) was used in the analysis (n=600). K-means cluster analysis was applied to the metabolomic data to identify clusters. Discriminatory metabolites responsible for cluster separation were identified. Foodgroup, nutrient and biochemical data were compared across the clusters. Participants from the NutriTech food intake study (n=40) were used to investigate the ability of this model to classify people into different dietary patterns. Two clusters; cluster 1 (C1), the "healthy" cluster and cluster 2 (C2) the "unhealthy" cluster were identified. C1 had a significantly higher mean percentage intake of nutritionally desirable foodgroups; breakfast cereals and porridge, low fat/skimmed milks and poultry compared to C2 ($P<0.05$). Nutrients; carbohydrates, protein, fibre, calcium, folate and vitamin C and biochemical measurements; red cell folate, serum folate and 25-hydroxyvitamin D were also significantly higher in C1 compared to C2 ($P<0.05$). Validation of this model in an independent group revealed that 95% of subjects were placed into the correct dietary pattern. The current analysis identified two distinct clusters that were reflective of a healthy and unhealthy dietary pattern intake and this was further validated using an external cohort. Future applications of this approach could be developed for rapid and objective assignment of subjects to a dietary pattern and incorporated into the delivery of precision medicine.

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Author: Christoph Bueschl, Bernhard Kluger, Maria Doppler, Alexandra Simader, Marc Lemmens, Hermann Buerstmayr, Gerhard Adam, Rudolf Krska, Rainer Schuhmacher | **Oral Abstract N:** O-2416

Towards enhanced plant metabolomics by combining 13C-labeling assisted workflows to study the metabolic defense of wheat against Fusarium

Introduction Fungi of the genus Fusarium infect crop plants thereby causing plant diseases and contamination of food with mycotoxins. Crop plants have various defense mechanisms including the formation of different secondary metabolites, some of which are derived from the amino acid phenylalanine (Phe). A novel metabolomics workflow combining global 13C-labeling with untargeted 13C-Phe tracer metabolism was used to investigate and characterize known and unknown defense related metabolites in wheat. Methods Wheat was grown in 99% 13CO2-atmosphere to achieve a global 13C-labeling. Additionally, native wheat was treated with 13C-labeled Phe to investigate its biotransformation. Both experimental setups were performed with the mycotoxin deoxynivalenol and control treatment and samples were subsequently measured on an LC- Orbitrap-HRMS. The datasets were independently processed with the in-house developed software MetExtract II, which is designed for detecting corresponding MS signals of native and U-13C-labeled metabolites or native and partly 13C-labeled biotransformation products. The two datasets were then merged with a custom script using the detected ion's retention times and m/z values. Thus, each detected metabolite was annotated with its total number of carbon atoms and that derived solely from the Phe-tracer. Results About 3.000 ions of 400 metabolites were detected, of which about 25% were annotated with Phe-derived carbon atoms identifying them as Phe-derived secondary metabolites. A database search showed that some of the Phe-containing metabolites were known to be involved during plant pathogen response. Moreover, the deoxynivalenol and control samples were clearly separated in statistical analysis of the Phe-containing metabolites with many metabolites showing increased abundances in the mycotoxin treated samples. By combining the two labeling-assisted workflows we were for the first time able to classify many of the secondary metabolites to be derived from Phe. These unknown Phe-derived metabolites are promising targets for further investigation of the metabolic response of wheat to Fusarium infection.

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Author: Nicolas Di Giovanni, Marie-Alice Meuwis, Edouard Louis, Jean-François Focant | **Oral Abstract N:** O-2424

In the quest of robust biomarkers for inflammatory bowel disease phenotypes using GCÐGC-HRTOFMS

We developed, validated, and implemented a strict QA/QC system for a GCÐGC-HRTOFMS method for the metabolic profiling of human serum. We were able to highlight sets of biomarkers capable to discriminate between various inflammation phenotypes representative of inflammatory bowel diseases. During this study, two of the main challenges of untargeted metabolomics were especially considered. First, the issue of data handling –large datasets and low number of samples compared to variables- was considered by the definition of a workflow of data preprocessing and processing, including the creation of a study template, the rigorous selection of good chromatographic quality features, and the multiplication of statistic techniques to be combined before test validation. In practice, 94 injections were made over 4 weeks, consisting of 70 study samples along with 16 QC samples and 8 reinjections due to QC system rejection. The chromatogram template included 524 verified features that were then reduced to less than two hundreds after selection of the ones having an analytical variation under 30%, based on the QC samples. This resulted in the finding of robust biomarkers that positively discriminated between the different phenotypes of inflammation, including high and low inflammation, remission, and healthy statutes. Second, the identification of unknown compounds was enhanced by using state-of-the-art high-resolution (HR) time-of-flight mass spectrometry and allowed to name and characterize putative biomarkers with higher degree of confidence. This is a mandatory step for integration of the results obtained in biological pathways interpretation, as well as their possible use at the clinical level. In conclusion, this study, through the use of optimized and fully controlled GCÐGC and high resolution mass spectrometry, highlighted inflammation biomarkers able to discriminate between and better understand different phenotypes of inflammatory bowel diseases.

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Origin of plasma acylcarnitines in humans during fasting and exercise

Acylcarnitines are potential biomarkers of impaired fatty acid oxidation and insulin resistance. Circulating acylcarnitines are also elevated during two physiological conditions, fasting and exercise. However, little is known about the fluxes of these acylcarnitines. We aimed to evaluate the contribution of liver and skeletal muscle to the plasma acylcarnitine pool in fasting and exercising humans. Using liquid chromatography/mass spectrometry, acylcarnitines were investigated in young healthy males after an overnight fast and during physical exercise. In one study, we assessed acylcarnitine levels in skeletal muscle biopsies and arterial-to-venous plasma differences over the exercising and resting leg. In a second study, we analyzed acylcarnitine fluxes over the hepato-splanchnic bed. After an overnight fast, pronounced amounts of C2- and C3-carnitine were released from the hepato-splanchnic bed and absorbed by the legs. Exercise caused an increase of most acylcarnitines in plasma and in the exercising muscle. In the recovery phase, circulating acylcarnitines rapidly declined to pre-exercise values. Free carnitine levels, in contrast, decreased in the exercising muscle and returned to baseline levels thereafter. Only C6-, C8-, C10- and C10:1-carnitine were released from the exercising leg and these species were taken up by the hepato-splanchnic bed. In contrast, C2- and C3-carnitine were continuously released from the hepato-splanchnic bed during exercise, and the uptake of C2-carnitine into the exercising leg tended to be increased. To conclude, we could show that the liver is a major contributor to systemic C2- and C3-carnitine levels during fasting and exercise. While most circulating acylcarnitines are elevated during exercise, the contracting muscle only contributes to the increase in medium-chain acylcarnitines. The increase of several other acylcarnitines in plasma is neither caused by the skeletal muscle nor by the hepato-splanchnic bed.

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Metabolomics and inverse modelling of the AMPK-TOR crosstalk in plants and animals

Genome sequencing and systems biology are revolutionizing life sciences. In the last decade transcriptomics and RNAseq techniques revealed that dynamics of mRNA represent only a small part of a complex regulatory biochemical network which is yet unpredictable from genome sequences [1]. Here, an integrated metabolomics/proteomics/phosphoproteomics platform suited for functional genomics and systems biology is presented [2]. This platform serves also as the basis for a recently established Vienna Metabolomics Center (VIME) (http://metabolomics.univie.ac.at/). A convenient workflow for data processing, integration, multivariate statistical analysis and genome-scale inverse metabolic modelling will be presented based on the data mining toolbox COVAIN (COVAriance INverse)[3, 4]. The complex integration of phosphoproteomics using single and tandem MOAC (metal-oxide affinity chromatography [5-7]), metabolomics and genome-scale inverse metabolic modelling is demonstrated for the analysis of central energy-signaling networks in plants and animals. Energy signalling networks involve the AMPK-TOR pathways. These two evolutionary highly conserved key players of energy signalling in any eukaryotic cell from plants to animals are involved in human diseases (T2D, Cancer, autoimmune disease etc.), nutritional physiology but also in plant growth and stress defense. Therefore our aim is a comparative and evolutionary analysis of those key signalling pathways in different systems (human, animals, plants, fungi,).

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mzCloud: An online substructural database of spectral trees for the identification of metabolites.

Traditionally, a spectra library search technique using reference mass spectra is one of the most straight forward methods of compound identification in metabolomics. However, existing spectral libraries cover only a small fraction of the compounds found in biological samples and even if they contained those compounds, the inherent spectra reproducibility problems in high resolution LC/MSn experiments hinders the identification further. To address the problems of reliable compound identification that plague metabolomics applications, we have developed a freely accessible mass spectral database that combines experimental mass spectral data with high-quality fragment annotations derived from quantum-chemical (QC) calculations, to provide the essential means for the identification of unknown metabolites when traditional library search methods are unsuccessful, and the analyst is left with absolutely no structural pointers whatsoever. To date, the mzCloud database features over 1 000 000 processed spectral records covering a wide range of collision energies up to MS8 in 4 400 human endogenous metabolites, plant secondary metabolites, food additives, pharmaceuticals and other compounds relevant for metabolomics, and new records are accumulating rapidly. More than 400 000 molecular structures and 6 000 000 formulas annotating individual spectral peaks are predicted by heuristic methods. The QC processing pipeline for precursor ion prediction contains over 500 000 unique 3D structures with calculated thermochemical properties in semi-empirical and DFT levels of theory. The mzCloud database provides both high-quality spectral collections, and carefully selected peak annotations employing advanced QC methods, supplementing experimental data with independent theoretical predictions exploiting a fundamentally different, and thus unbiased, apparatus. As such, it is a first-of-its-kind spectrometric tool extending its appliance well beyond traditional library searches. Such tools are urgently needed in metabolomics to keep pace with state-of-the-art analytical instrumentation that generates far more features than we are currently able to interpret.

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Author: Sony Tuteja, H. Shanker Rao, John Millar, Stephanie DerOhannessian, Richard Dunbar, Daniel Rader | **Oral Abstract N:** O-2453

Serine, threonine metabolic pathways associated with HDL-C response to niacin treatment

Background: Niacin has been used for decades to modulate plasma lipids, but its mechanism of high-density lipoprotein cholesterol (HDL-C) raising is still unclear. We conducted metabolomic profiling in two human cohorts of niacin treatment to characterize metabolomics signatures associated with HDL-C response to niacin. Methods: The discovery cohort consisted of n=70 healthy subjects (50 European and 20 African ancestry) receiving an inpatient 1 gram immediate-release niacin challenge. Samples were assayed at time 0,2,5,8 hours surrounding the niacin dose. The validation cohort included n=28 metabolic syndrome patients receiving 12 weeks of extended-release niacin. HDL-C was quantified before/after treatment for both cohorts. An untargeted GC-MS based platform identified 180 primary metabolites (UC Davis). A time-series anova was performed on normalized metabolite concentrations, adjusting for sex, in each ancestry group separately. For metabolic pathways showing enrichment, linear regression was performed with post-niacin HDL-C as the outcome and age, sex, race, pre-treatment HDL-C, and baseline metabolite levels as predictors. Results: Niacin significantly altered the concentrations of 64 metabolites in the healthy European subjects (FDR <5%), with 27 metabolites replicated in the African individuals. Pathway enrichment revealed linoleic acid metabolism and glycine, serine, threonine metabolism as pathways most impacted by niacin. Regression analysis showed that baseline levels of serine (p=0.005) and threonine (p=0.004) were independently associated with post niacin HDL-C levels. Baseline serine (p=0.009) and threonine (p=0.02) levels were also correlated delta HDL-C levels in the metabolic syndrome cohort receiving chronic niacin treatment. Conclusions: Using an unbiased metabolomics approach, we provide important insight into mechanisms underlying niacin's HDL-C raising response that involves serine-threonine metabolism.

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When NMR spectroscopy is not such a DOSY alternative – using NMR to model complex formation and the origins of metabolism

One central question concerning metabolism is how metabolic pathways evolved during the early stages of evolution, or whether the structure of extant metabolic systems is a consequence of their chemical origins. While many of the individual reactions of metabolic pathways have low standard Gibbs Free Energy Changes and operate at close to equilibrium, meaning they can readily go forwards or backwards dependent on the environment, these reactions occur kinetically slowly under non-enzymatic conditions. One likely candidate as a catalyst in the early Archean world is Fe(II), the most abundant transition metal ion found in the Archean sediment, and a catalyst or co-substrate for metabolism-like non-enzymatic reactions. Fe(II) ions could form a point for metabolites to complex around increasing reaction rates as well as providing electrons for redox reactions. However, it is a real analytical challenge to model transient complex formation, especially in a composite mixtures such as used for in vitro reconstructions of metabolic pathways. While NMR spectroscopy is used less in metabolomics in favour of more sensitive approaches based on mass spectrometry, the technique has a number of inherent advantages including being non-destructive, capable of being performed readily in vitro, in situ and in vivo, relatively cheap on a per sample basis and excellent for studying the chemical environment of molecules. We have used a combination of diffusion ordered spectroscopy (DOSY) and relaxation weighted spectroscopy (using T1 spin-lattice measurements) to examine complex formation of metabolites in glycolysis and the pentose phosphate pathway (PPP) with Fe(II) to understand how catalysis may have arisen over 4000 million years ago. We show that pH dependency determines whether a PPP-like or glycolytic-like pathway emerge to form a metabolic network in vitro. Chemical networks that obtain structure and catalysis on the basis of transition metals are hence plausible direct precursors of cellular metabolic networks.

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Spatial Metabolomics: MALDI Mass Spectrometry Imaging of Plant Metabolites

Mass spectrometry imaging (MSI) is a developing technique to measure the spatio-temporal distribution of many biomolecules in tissues at once. Over the preceding decade, MSI has been adopted by plant biologists and applied in a broad range of areas, including primary metabolism, natural products, plant defense, plant responses to abiotic and biotic stress, plant lipids and the developing field of spatial metabolomics. Of the MSI techniques employed to examine plant metabolism, Matrix Assisted Laser Desorption Ionisation (MALDI) is the most common. In contrast to mammalian tissues, preparation of plant tissues for MALDI-MSI has some special considerations to enable generation of sections suitable for imaging. The development of suitable methods and results of imaging the distribution of specific plant lipids, secondary metabolites and defense molecules, including cyanogenic glycosides and saponins in a variety of systems and different tissues will be presented. Novelty: Development of sample preparation methods to measure the distribution of lipids and labile plant secondary metabolites in tissues.

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The dynamic range of the human metabolome revealed by challenges: a non-target view

Metabolic challenge protocols, such as the oral glucose tolerance test, can uncover early alterations in metabolism preceding chronic diseases. Nevertheless, most metabolomics data accessible today are derived from blood or urine samples collected in the fasting state. To analyze the dynamics of the human metabolome in response to environmental stimuli, we submitted 15 young healthy male volunteers to a highly controlled 4 d challenge protocol, including 36 h fasting, oral glucose and lipid tests, liquid test meals, physical exercise, and cold stress (Humet study). Blood, urine, exhaled air, and breath condensate samples were analyzed on up to 56 time points by MS- and NMR-based methods, yielding 275 metabolic traits with a focus on lipids and amino acids. The results of the Humet study were reported previously by Krug et al. (FASEB, 26:2607-2619, 2012). We now extended substantially the coverage of metabolites in the Humet study based on a non-targeted MS-based approach. Blood and urine samples were analyzed on 56 (plasma) and 16 time points (urine), respectively, at Metabolon Inc., yielding 575 blood and 619 urinary metabolic traits for each time point. The data set reveals a rich and complex signature of many biochemical pathways, accessing for the first time human metabolism at such a high level of metabolic comprehensiveness and temporal coverage. Here we present a global overview of the Humet 2.0 study. Two companion papers in this session by Mohney et al. and Kastenmüller et al. shall provide a detailed description of analyzed metabolites and a data resource that we are currently developing to provide broad and easy access to the data. We intend to initiate a shared analysis of this data set at the Metabolomics Conference and invite all members of the science community to participate in the discussion that is planned after the talks of this session.

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Myc linked to aberrant lipid metabolism in lung cancer by mass spectrometry imaging

Myc expression is frequently increased in human cancers. Whilst Myc is responsible for controlling a wide variety of functions in healthy cells, its oncogenic activation results in aberrations of these processes, leading to uncontrolled cell proliferation. The detailed molecular mechanisms underpinning Myc-dependent tumorigenesis are not fully understood, in particular the role of Myc in driving lipid metabolism and biosynthesis. Here we use a novel transgenic mouse model of K-Ras driven lung adenocarcinoma with reversible activation of Myc, to study the changes in the lipid profile of lung tumours with high Myc activity, and following deactivation of Myc. We characterised the spatial and temporal changes in lipid composition in lung tissue using advanced mass spectrometry imaging and surface analysis techniques. We found that normal lung tissue was characterised predominantly by saturated phosphatidylcholines and phosphatidylglycerols - major lipid components of pulmonary surfactant. In contrast, tumour regions had increased phosphatidylinositols and arachidonate-containing phospholipids that can serve as signalling precursors. Deactivating Myc resulted in a dramatic decrease in arachidonic acid and its eicosanoid metabolites. This corresponded to a decrease in cytosolic phospholipase A2 (cPLA2) activity over time with Myc deactivation. Interestingly, phospho-cPLA2 positive-staining was associated with tumour cells undergoing mitosis. Using gene expression data and immunohistochemistry, we propose that high Myc leads to increased activity of cPLA2, through phosphorylation via the mitogen activated protein kinase pathway, which is in turn amplified by Angiogenin (Ang) and secretory PLA2 (Pla2g1b), in addition to K-Ras. cPLA2 preferentially releases arachidonic acid from the phospholipid membrane and initiates the lipoxygenase and cyclooxygenase pathways. These pathways produce specific eicosanoids, implicated in angiogenesis, proliferation and migration, and highlight new targets in cancer therapies.

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Author: Kate Bennett, Jan Kehr, Fu-Hua Wang, Thomas Moritz, Katrin Lundstedt-Enkel, Johan Trygg, Torbjörn Lundstedt **Oral Abstract N:** O-2503

How humanisation of the liver affects metabolism in the mouse brain

The metabolic differences between humans and mice, present a major drawback in the use of conventional mouse models to study human metabolic diseases. The generation of mice with 'humanised' livers provides an alternative and innovative approach to overcome these limitations. The liver is a key metabolic organ able to control metabolism via the poorly understood liver-brain axis. Dysfunction in the liver is a major cause of many metabolic disorders, which emphasises the great potential of humanised liver mice models, for the discovery and evaluation of reliable diagnostic and therapeutic targets in human metabolic diseases. In this study, we investigated the downstream effects of the humanised liver on metabolic processes in different areas of the brain and in the plasma of humanised mice. Metabolic profiling was performed on five different regions of brain tissue (cerebellum, cortex, hippocampus, hypothalamus and striatum) and plasma taken from humanised liver mice models and untransplanted controls. All samples were analysed by gas chromatography mass spectrometry. In order to identify any changes to the metabolic profiles of the humanised mice multivariate data analyses were performed. Distinct differences in the metabolite composition were observed in all five areas of the brain and in the plasma of the humanised mice, with each brain region displaying a unique metabolic profile. The levels of several metabolites were found to be altered in the plasma and all five brain sections, whereas variations in other metabolites were restricted to specific brain areas or plasma only. Changes in the metabolite composition indicated the disturbance of several biochemical pathways in different regions of the brain and in the plasma of the humanised mice. The metabolic differences and their relation to the liver-brain axis, following humanisation of the mouse liver, will be discussed.

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Evolution of Gut Microbiota:Host co-metabolic processes determined both by term and mode of birth in the INFANTMET Cohort

The aim of this study was to characterise the gut microbiome development and its impact on host metabolome in a cohort of breast-fed infants (n = 199) between 1 and 4 weeks of age, using both culture-independent 16S rRNA amplicon sequencing and untargeted urinary LC-HRMS Orbitrap metabolite profiling. Full-Term (FT), Spontaneous Vaginally Delivered (SVD) infants' microbiota remained stable at both phylum and genus levels during the 4 week period. FT Caesarean section (CS) infants displayed an increased faecal abundance of Firmicutes ($p < 0.01$) and lower Actinobacteria ($p < 0.001$) abundance after the first week of life compared to FT-SVD infants. FT-CS infants gradually progressed to a microbiota more closely resembling that of FT-SVD infants at week 4. The gut microbiota of preterm (PT) infants displayed a significantly greater abundance of Proteobacteria compared to full-term infants ($p < 0.001$) at week 1. By 4 weeks of age, Actinobacteria abundance had significantly increased ($p < 0.001$) and Proteobacteria and Firmicutes abundance both significantly decreased ($p < 0.001$ and $p < 0.01$ respectively) in PT-CS infants. Metabolomic analysis of urine at week 4 indicated that PT-CS infants have a functionally different metabolite profile to FT (both CS and SVD) infants. Nearly 5000 statistically significant metabolic features were found to distinguish PT from FT infants. Co-inertia analysis showed co-variation between the urine metabolome and the faecal microbiota of the infants illustrating the considerable contribution of co-metabolic processing between microbiome and host in determining urinary metabolite profiles. These findings confirm that mode of delivery and gestational age have significant effects on early neonatal microbiota composition and their metabolic output.

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Oral Abstract N: O-2524

Stable isotope assisted evaluation of different extraction solvents for metabolomics of cereals using LC-HRMS

Proper evaluation of analytical workflows for untargeted LC-HRMS based metabolomics research is still a major challenge. The high number of non-specific MS signals and features can be successfully tackled by stable-isotope-assisted methods. These recently developed approaches allow the direct consideration of every analytical feature detected in individual biological samples. In this work, the efficiency and complementarity of commonly used extraction solvents were compared at the example of wheat. 1:3 (v/v) mixtures of water and selected organic solvents such as methanol, acetonitrile and methanol/acetonitrile 1:1 (v/v), each of those with and without 0.1% (v/v) formic acid were used for extraction of four different wheat organs ear, leaf, stem and root. Samples were extracted and analysed by reversed phase (C18) LC-HRMS and subsequent data evaluation was performed with the in-house developed MetExtract II software and R. In total about 1000 metabolites were detected across the different wheat organs. 871 metabolites were found in ear samples, 785 in stem, 733 in leaf and 517 in root. Surprisingly, for each organ, the total number of metabolites was similar across the different solvents (ear: 650-730-, stem: 530-610, leaf: 520-580, root: 350-400). While the total number of extracted metabolites in a particular organ did not depend on the extraction solvent, the metabolic composition of the resulting extracts differed substantially. Only about 50% of the metabolites of the respective organ were consistently found with all solvents. Interestingly, numerous metabolites were preferentially extracted by either methanol or acetonitrile and the corresponding metabolite ions also showed clearly different retention times. Moreover for each organ / extraction mixture combination, the precision of metabolite abundances was investigated. Our study showed that for untargeted LC-HRMS based metabolomics, the complementary behaviour of methanol and acetonitrile can be balanced by the use of a methanol / acetonitrile / water mixtures as extraction solvent.

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Oral Abstract N: O-2532

Metabolite profiling of plasma and tissues from mouse models of diabetes at different stages of disease development

Metabolomics approaches have identified changes in plasma metabolite concentrations associated with obesity, insulin resistance as well as type I and type II diabetes. Although each stage of disease progression is characterized by distinct changes in subsets of metabolites, the origins of these alterations remain largely unknown. To assess metabolite changes in tissues and in plasma along the progression from obesity to ß-cell failure, we studied three mouse models. Leptin-deficient ob/ob mice served as a model for early obesity-induced insulin resistance. Leptin-resistant db/db mice - which are more susceptible for diabetes due to their C57BLKs genetic background - were employed to study a more advanced stage of obesity-induced insulin resistance with hyperglycemia. The third was the streptozotocin-induced insulin deficiency as a type 1 diabetes or an end-stage of type 2 diabetes model. Plasma and tissues (liver, muscle, kidney, adipose tissue) were collected and metabolite profiles were obtained using different LC-MS/MS and GC-MS approaches. Next to a broad metabolite profiling comprising a large spectrum of lipids, fatty acids, sugars and other organic solutes, targeted LC-MS/MS was applied derive a comprehensive profile of amino acids and acylcarnitines. Specific sets of metabolites were found to mark individual stages of disease related to the degree of hyperinsulinemia and hyperglycemia. These sets included known markers such as 3-hydroxybutyric acid, glyoxylate and 1,5-anhydrosorbitol, as well as new metabolites such as odd-numbered and branched-chain fatty acids and acylcarnitines. Obese hyperinsulinemic models were characterized by increases in lipids from various classes and this was related to hepatic de novo lipogenesis. Diabetes models showed signatures of increased catabolism. A branched-chain amino acid-related metabolite signature could be observed in all three models. While this was related mainly to adipose tissue changes in ob/ob and db/db mice, skeletal muscle seemed to play a more dominant role in streptozotocin-treated mice.

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Oral Abstract N: O-2548

NMR spectroscopy detects metabolite differences between culture media of hepatitis C virus negative and positive cells after harvest

Introduction: Chronic infection with hepatitis C virus (HCV) is one of the main causes of hepatocellular carcinoma. Given the importance of glutamine in carcinogenesis, we investigated the role of glutaminolysis in HCV infection. Here we report on a NMR sub-study investigating metabolite differences between cell culture supernatants of hepatitis C virus negative (HCV-) and positive (HCV+) cells after harvest. Methods: HCV infected and uninfected cells were cultured in conditioned Dulbecco's Modified Eagle's Medium complemented with (1) additional Glucose and Glutamine, (2) void of Glutamine or (3) void of Glucose. Cells and supernatants were collected at days 3, 4, and 5 after addition of conditioned cell media. For each medium composition and time point, three HCV positive and three HCV negative cell cultures were harvested. Water-suppressed 1D-NOESY spectra of 54 cell supernatants were acquired on a 400MHz Bruker Avance-II spectrometer at 298K. Spectra were bucketed and buckets from control culture media were subtracted from those of the supernatant spectra, and scaled to the number of cells at the harvest point. Results: A complete separation in PLS-DA was obtained between cell media in contact with either HCV+ or HCV- cells for all three media types. Moreover, the media separated further with increasing time post incubation. Two media separated also well between those in contact with HCV+ or HCV- cells in unsupervised PCA. Loading plots demonstrated contributions from numerous metabolites responsible for the separation including glutamine and glutamate. Discussion: HCV infected cells appear to have different nutrition and excretion pathways compared to non-infected cells. Most importantly glutamine was reduced, while glutamate was increased in HCV+. These NMR results support complementary measurements demonstrating that HCV modulates the transcript levels of key enzymes of the glutamine metabolism in vitro and in liver biopsies of chronic HCV patients. Consistently, HCV infection increased glutamine utilization and dependence.

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Author: Reza Salek, Kenneth Haug, Mark Viant, Christoph Steinbeck | **Oral Abstract N:** O-2551

The Time is Right to Focus on a Model Organism Database

The study of model organisms as a cornerstone of biological and medical research hopes to yield insights into biological processes from one species, which are transferrable to other species, including and in particular, humans (Edison et al. 2016). Different areas of biomedical sciences, including the omics sciences, focus on the same or similar sets of model organisms at different time points in history. The systematic study of model organisms through genomic methods, for instance, has led to unprecedented insights into the evolution of model organisms and related species(Hedges and Blair Hedges 2002). Apart from the experimental and community efforts that are needed for deep metabolome annotation of model organisms and which are discussed in (Edison et al. 2016) we would like to highlight the role that central submission databases such as the MetaboLights database (Salek et al. 2013; Haug et al. 2013) are playing in the assembly of model organism metabolomes. MetaboLights has now been established as one of the central repositories for metabolomics studies and submissions to MetaboLights are recommended by major journals such as the Nature Journals, PLOS, the EMBO journal, the Metabolomics Journal and others. Studies deposited in MetaboLights are annotated with a rich set of meta-data, including study factors, assay description, and of course species information. This is complemented with lists of identified metabolites. As a result, MetaboLights is effectively building a collection of community annotated (model-) species metabolomes. In this presentation, we will advocate that the time is right for model species deep annotation and describe the mechanism by which wide-spread community submissions to MetaboLights are, right now, building a rich collection of knowledge about model species metabolomes.

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Linking the gut microbiome, blood metabolites and Volatile Organic Compounds in breath

Analysis of volatiles organic compounds (VOCs) in exhaled air enables rapid diagnoses. VOCS analysis easily adapts to long term monitoring and screening. Many VOCs are produced by intestinal microbiota. Understanding microbiome activity is essential to the development of personalized medicine. Gut microbiota are linked with essential and numerous biological functions in humans through a “network” of microbial-host co-metabolism. The microbiome in the gastrointestinal tract generates a number of compounds during the metabolism. Some of these compounds are excreted into feces while others enter the systemic circulation where they can be further modified by the host. 194 fecal, blood and breath samples were collected from Crohn’s disease (CD) patients visiting an outpatient clinic. Blood, fecal and breath samples were collected. Patients were assigned into 2 groups: active disease (n=97) and inactive disease (n=97). The microbial composition of fecal samples was assessed by 454 pyrosequencing (16S rRNA). Blood content was analyzed by NMR. Breath samples were analyzed by GC-tof-MS. Sophisticated machine learning approaches were necessary to extract clinically relevant patterns and to find correlation between VOCs and microbial communities. Data fusion and Canonical Correlation Analysis allow for the discovery of significant correlations between VOCs in exhaled air, fecal microbiome and blood metabolites. The influence of CD diseases activity on the VOCs-microbionme relation is further investigated. Using CD as a case study, we will present that the VOCs profile in exhaled air fluctuates in relation to the gut’s bacteria. The metabolomics analysis of blood allows us to explain the interface between microbiome and VOCs. Oxidative stress and bacteria-metabolites appears to be associated with the active CD active phase are reflected in both microbiome and VOCs. Moreover, some evidence points at the possible involvement of a subset of bacteria as a cause of the disease flares and thus as a potential therapeutic target.

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Metformin metabolomic profiles to inform pharmacogenomic discovery

Millions of individuals are diagnosed with type 2 diabetes mellitus(T2D), which increases the risk for a multitude of acquired health outcomes including cardiovascular events and kidney disease. While metformin is the most widely prescribed medication for T2D treatment, its mechanism is not fully understood and individuals vary in their response to this therapy. We aimed to: 1) develop metformin amino acid metabolite response profiles from human plasma samples in an electronic health record-linked biobank, and 2) utilize metabolite profiles as proxy biomarkers to inform pharmacogenomic genome wide association (GWA) discovery analyses. We measured 42 metabolites using an LC-MS/MS platform in a cohort of 548 Caucasian age and gender matched cases and controls enrolled in the Mayo Clinic Biobank. An independent cell culture system was utilized to gain insights about drug mechanism of action.
Out of 14 metabolites not associated with T2D(Nat Med 2011;17(4):448-53), 4 metabolites were statistically associated with metformin-induced change. Increased lysine(t=4.62,p<.001,d=0.54) and glutamic acid(t=4.65,p<.001), and decreased arginine(t=-4.91,p<.001,d=.31) and citrulline(t=-7.09,p<.001,d=1.11) were observed. Naïve metabolite-informed GWA were generated for these metabolites; key pharmacogenomic insights will be discussed in detail. Further research is needed to validate the biomarkers of metformin exposure and response identified in this study, and to understand the mechanistic implications of metformin.

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Oral Abstract N: O-2565

Direct from Sample Microbial Metabolomics using Rapid Evaporative Ionisation Mass Spectrometry (REIMS)

Rapid evaporative ionisation mass spectrometry (REIMS) has seen a number of successful applications in direct from sample metabolomics; initially as a real-time, intra-operative tissue identification platform. REIMS works via the generation of a radiofrequency electrical current through a biomass, causing it to rapidly heat and generate a vapour containing gas phase ions of metabolites and structural lipids. This is then transferred to a mass spectrometer using the instrument's vacuum system; allowing for mass spectral data to be generated within a second of sample heating. For microbial metabolomics, our recent work has focussed on direct from colony analysis using either a handheld bipolar probe or a high-throughput monopolar probe platform, both connected to a Q-ToF instrument (Waters). The latter is capable of analysing between 4,000 and 5,000 microbial colonies a day, with mass spectral data generated within the 50 to 2500 m/z range of the instrument. We are currently exploring optimisation of the high-throughput monopolar probe platform with a view to developing a diverse range of probes, suited to the analysis of different sample types. To date, we have utilised REIMS analysis for microbial identification to species level, with classification accuracy above 94%, but it is also well suited to the metabolomic study of microorganisms. To support this, we are developing a microbial metabolite library which will ultimately consist of 50,000 isolates from 4,000 species; isolated from both clinical and environmental samples. Through utilisation of this library, we are currently exploring the application of REIMS analysis to microbial metabolism including the study of secondary metabolite production, antimicrobial resistance pathways, and virulence profiles; which will be covered in this presentation. Furthermore, we have conducted direct from sample analysis of a range of samples, including human stool and blood, which shows both metabolomic biomarkers of microbial communities, and indicators of microbial metabolism.

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Oral Abstract N: O-2583

Visualizing and exploring the dynamics of the human metabolome: the Humet 2.0 data repository

In the Humet study, we previously investigated the dynamic range of the "normal" (male) human metabolome by submitting fifteen young, healthy men to a series of challenges over four days (Krug et al., FASEB, 2012). We monitored the individual metabolic response to these challenges by analyzing metabolite abundances in blood, urine, breath air and breath air condensate samples taken at different time points. As outlined in companion papers of this session by Suhre et al. and by Mohney et al., we recently extended the set of quantified metabolites substantially by applying Metabolon's non-targeted mass spectrometry based metabolomics approach. Incorporating these new data, we are now able to span a four-dimensional description of the normal metabolome regarding individual variation (15 subjects) at different time points (56) or challenges (6) in different fluids/media (4) for a large set of different metabolites (>800) covering a broad range of biochemical pathways. To facilitate the exploration of the >945,000 data points collected in Humet 2.0, we here introduce an interactive data repository that provides customizable visualizations and different entry points to access the high-dimensional data from various perspectives. Typical questions arising in many metabolomics studies across various disciplines can readily be answered within our repository, for example: How robust is the metabolite that I identified as disease biomarker against fasting versus non-fasting conditions? How long does it take to wash out a specific dietary metabolite after ingestion? Can this metabolite be observed in urine after a certain delay? How individual is metabolic response to physical activity among healthy subjects? Which metabolites exhibit the same longitudinal patterns over a challenge or the complete study duration? Besides such questions, which can be answered through data visualization and interactive exploration alone, the extended dataset of Humet 2.0 forms a valuable resource for a plethora of future systematic analyses.

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Oral Abstract N: O-2589

Dynamic Response of the Human Metabolome to Environmental Stimuli through Comprehensive Metabolomic Profiling – the Humet 2.0 Study

The human body has evolved a complex set of interactive mechanisms designed to maintain a homeostatic balance. Perturbations to homeostasis, such as that induced by disease or metabolic challenges, result in measurable changes in physiology, oftentimes manifest by alterations in the metabolome. We examined the metabolic plasticity that occurs on an individual basis by characterizing plasma and urinary biochemical changes in response to a diverse set of environmental stimuli. Fifteen young healthy male volunteers were subjected to a highly controlled metabolic challenges designed to stimulate catabolic or anabolic states, including 36h fasting, standard liquid test meals, oral glucose and lipid tolerance tests, physical exercise, and cold stress (Humet study). Using a non-targeted global metabolomics platform (Waters ACQUITY UPLC coupled to a Thermo Scientific Q-Exactive high resolution accurate mass spectrometer), a time-course of blood plasma and urine biochemical profiles were analyzed for each individual, and structurally identified metabolites in each matrix were mapped to diverse metabolic pathways. A subset of plasma samples were separately analyzed using a novel lipidomics platform (LC-DMS-QTRAP® System) that generated fully quantitative data, including complex lipid class concentration, individual lipid molecular species concentration, and fatty acid composition of each complex lipid class. Data were analyzed to identify metabolic pathways and lipid class changes associated with individual metabolic responses. By utilizing a comprehensive metabolomic profiling approach, we have enabled a broader understanding of the plasticity of the human metabolome in response to diverse metabolic challenges. Companion papers in this session by Suhre et al. and Kastenmüller et al. outline the complexity and biological implications of these data.

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Author: Rima Kaddurah-Daouk, Richard Weinshilboum | **Oral Abstract N:** O-2591

Pharmacometabolomics: Enabling Tool for Precision Medicine

Precision Medicine initiatives such as the One Million Cohort in the United States are emerging as an approach for disease treatment and prevention that takes into account individual variability in genome, metabolome, gut microbiome, exposome, environment, and lifestyle for each individual. Through a partnership with the pharmacogenomics community we have applied metabolomics tools to the study of commonly used drugs that include statins, antidepressants, antihypertensives and antiplatelet therapies. We will exemplify how inclusion of metabolomics data informs about treatment outcomes and disease heterogeneity. We will share data to support how metabolic profiles inform about gender differences in response to aspirin, ethnic differences in response to antihypertensives and a role for the gut microbiome on PK and PD profiles of many therapies. Using treatment with antidepressants SSRIs we will exemplify how the metabolome informs the genome and together they enable highlighting of pathways implicated in variation in response. Majorly depressed patients (306) were treated with escitalopram blood was drawn at baseline, 4 and 8 weeks for blood drug levels, genome-wide single nucleotide polymorphism (SNP) genotyping and metabolomic analyses. SSRI treatment decreased plasma serotonin concentrations ($P<0.0001$). Baseline and plasma serotonin concentration changes were associated with clinical outcomes ($P<0.05$). Therefore, baseline and serotonin concentration changes were used as phenotypes for genome-wide association studies (GWAS). GWAS for baseline plasma serotonin concentrations revealed a genome-wide significant ($P=7.84E-09$) SNP cluster on chromosome four 5' of TSPAN5 and a cluster across ERICH3 on chromosome one ($P=9.28E-08$) that were also observed during GWAS for change in serotonin at 4 ($P=5.6E-08$ and $P=7.54E-07$, respectively) and 8 weeks ($P=1.25E-06$ and $P=3.99E-07$, respectively). Knockdown (KD) and overexpression (OE) of TSPAN5 in a neuroblastoma cell line significantly altered the expression of serotonin pathway genes and response exemplify how pharmacometabolomics and pharmacogenomic present powerful enabling tools for precision medicine.

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DESI-Imaging of inflammatory markers for cancer

Desorption Electrospray Ionisation (DESI) is an ambient ionisation technique that uses a charged-solvent guided by nitrogen gas to desorb molecules of interest from sample surfaces generating secondary ions, analysed by mass spectrometry.For the past decade DESI-MSI has extensively been used as an imaging mass spectrometry technique (DESI-MSI), allowing the spatial distribution of particular molecules to be determined. This technique has been of particular interest in the field of diagnosis, in particular cancer. As a diagnosis tool, DESI-MSI allows cancer diagnosis to be quicker, more precise, and more accurately compared to routinely used methodologies in histo-pathology laboratories. That is instead of taking approximately 10 working days it would only take approximately 3 working days and most-importantly it would be based in sample's biochemical information and user-independently preventing miss-diagnosis. With DESI-MSI it is possible to obtain phospholipid profiles, where differences could suffice for the identification of different types of tissues, type status (healthy or cancer) and even different types of cancer. One important aspect of cancer, is to understand tumour microenvironment. One particular aspect of this topic is to try and understand the role of eicosanoids in cancer. It has been know that this reactive lipid species is involved in inflammation and cancer. Fresh frozen colorectal, ovarian tissue samples, healthy and cancerous, were analysed by DESI-MSI using a QToF (Xevo G2-XS, Waters), with 1.5Ql/min 95:5 v/v methanol: water as ionisation solvent and scan rate of 4 scans per second. The spatial distribution of eicosanoids was determined using an in-house toolbox and statistical analysis were performed between the different types of samples. The presence of eicosanoids was as expected more abundant and more homogenous in cancerous tissue than in healthy tissue. In conclusion, DESI-MSI can be utilised for the spatial determination of eicosanoids in tissue samples, hence

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New classification and validation system for intake biomarkers to improve assessment of food intake and nutritional status – A FoodBAll project goal

The measurement of dietary exposure is one of the main issues in nutritional science, as it is of crucial importance for the discovery of true associations between dietary intake and effects on health. By far, the most commonly applied tools for estimating dietary exposure are based on self-reporting (e.g. food frequency questionnaires) that may often be biased. In this context, biomarkers of food exposure, measured in biological samples, may provide an objective estimate of actual intake, representing a promising supplement to the actual self-reporting tools. Anyway, only a limited number of foods are covered by validated exposure markers and a general validation system is still missing. Therefore, common criteria for biomarker validation are required. One of the main goals of the FoodBAll (Food Biomarkers Alliance) project (http://www.foodmetabolome.org) is to provide a new biomarker classification system and an overview of current food intake markers, as well as a new biomarker scoring system. For this purpose, a list of food groups has been held in order to get a good coverage of the food intake in different population groups within Europe. Nine main food groups have been identified: i) alcoholic beverages, ii) food of animal origin, iii) fruit and vegetables, iv) cereals and wholegrain, v) fats and oils, vi) legumes, vii) non-alcoholic beverages, viii) confectionary, ix) spices and herbs. For each group a systematic review on the status of current intake markers has been carried out and each marker identified has been scored for analytical validity, biokinetics/metabolism, robustness and consistency. Based on the quality of existing markers a plan for metabolomics-based investigations has been elaborated with an aim to cover all major food groups with validated biomarkers of intake. Funding: JPI HDHL FoodBAll project (2014-2017)

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MoOD – Our novel Metabolomics Outlier Detector for R-Shiny

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Quantification of bioactive N-acylethanolamines and in human plasma

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Metabolic changes in prefrontal cortex of humans, chimpanzees and macaques during postnatal development.

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Statistical considerations in handling unwanted variation in large-scale metabolomics studies

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Novel metabolite biomarkers of Huntington's disease (HD) as detected by high resolution mass spectrometry

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A metabolomics approach for identification of novel biomarkers of chicken consumption

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PeakForest: a spectral database and its toolbox, dedicated to the Metabolomics' community

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Don't reinvent the wheel! Re-using standards and software from computational proteomics

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Dept. of Medical Sci., CARAMBA, Uppsala University, Akademiska sjukhuset, Ing. 61, 3tr, Uppsala 751 85
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EMBL-EBI, European Molecular Biology Laboratory, European Bioinformatics Institute (EMBL-EBI), Wellcome Trust Genome Campus Hinxton, Cambridge Cambridgeshire CB10 1SD
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Bruker Daltonik GmbH, Fahrenheitstr. 4, Bremen
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Korea Institute of Radiological & Medical Sciences, 75 Nowon-ro, Nowon-gu, Seoul 01812
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Sung Hee Hong
Korea Institute of Radiological & Medical Sciences, 75 Nowon-ro, Nowon-gu, Seoul 01812
Application 2D-NMR Spectroscopy on Radiation Exposed Human Primary Cells

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Abstract number: 2087
chi-hung Chen, Ching-Yu Lin, Charlene Wu, Kuen-Yuh Wu
national taiwan university, Rm. 905, No.16-3, Siyuan St., Zhongzheng Dist., Taipei City 100, Taiwan (R.O.C.), Taipei
Effects of Repeated Exposure to Maleic Acid in Rats by 1H NMR-based Metabolomics

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Abstract number: 2086
Michael Gerlich, Frederik Walter, Marcus Persicke, Aiko Barsch, Heiko Neuweger, Matthias Szesny, Nikolas Kessler, Klaus Meyer, Jörn Kalinowski
Bruker Daltonik GmbH, Fahrenheitstraße 4, Bremen 28211
Applying an untargeted Metabolomics workflow linking HRAM QTOF data to biology enabled to increase arginine production in C. glutamicum by rational strain design

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Abstract number: 2301

Florence Vinson, Ludovic Cottret, Yoann Gloaguen, Benjamin Merlet, Florence Maurier, Floréal Cabanettes, Maxime Chazalviel, Sanu Shameer, Clément Frainay, Nathalie Poupin, Fabien Jourdan

INRA, 180 Chemin de Tournefeuille, Toulouse 31027

MetExplore: handling genome scale metabolic networks online

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Abstract number: 2501

Mei Chong, Anusha Jayaraman, Silvia Marin, Vitaly Selivanov, Pedro de Atauri Carulla, Daniel Tennant, Marta Cascante Serratosa, Ulrich Günther, Christian Ludwig

Kings College London

Model-free analysis of NMR and MS spectra for metabolic tracer experiments

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Abstract number: 2131

Thomas Naegele, Lisa Fuertauer, Matthias Nagler, Jakob Weiszmann, Wolfram Weckwerth

Dept. Ecogenomics and Systems Biology, University, Althanstr. 14, Vienna 1090

Deriving strategies of metabolic network regulation from metabolomic time series data

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Abstract number: 2392

Mi-Ri GWON, Bo Kyung Kim, Boram Ohk, Ji-Won Lee, Sook Jin Seong, Young-Ran Yoon

Kyungpook National University, 303 Bio-Medical Research Institute, 135 Dongdeok-ro, JUNG-GU, DAEGU

Metabolomic Analysis of Plasma on Alternate Day Fasting in Metabolic Syndrome Patients by UHPLC-QTOF/MS

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Abstract number: 2445

David Wishart, Yannick Djoumbou Feunang, Craig Knox, Tanvir Sajed, Felicity Allen, Yifeng Liu, Zheng Shi, Zachary Budinski, Russell Greiner

The Metabolomics Innovation Centre, Departments of Biological Sciences and Computing Science University of Alberta, Edmonton AB T6G 2E9

New bioinformatic tools for metabolomics

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Abstract number: 2602

Chris Beecher, Felice de Jong, Tim Garrett, Rick Yost

UF, SECIM, 1510 SW 25th place Apt 6, Gainesville FL 32608

IROA Fluxomic analyses: a non-targeted, all-encompassing protocol using IROA (Isotopic Ratio Outlier Analysis)

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Abstract number: 2364

Nathalie Poupin, Anne Corlu, Nicolas Cabaton, Hélène Dubois-Pot-Schneider, Cécile Canlet, Clément Frainay, Florence Vinson, Marie-Anne Robin, Daniel Zalko, Fabien Jourdan

UMR1331, TOXALIM (Research Center in Food Toxicolo, 180 chemin de Tournefeuille, Toulouse N/A = Not Applicable 31027

A combined multi-omics and in silico approach to decipher metabolic network shifts during the differentiation of human hepatocyte

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Abstract number: 2307

Maxime Chazalviel, Florence Vinson, Clement Frainay, Benjamin Merlet, Yoann Gloaguen, Floréal Cabanettes, Ludovic Cottret, Nathalie Poupin, Fabien Jourdan

INRA - ToxAlim, 59, 59 rue de Belbèze Midi Pyrennee 31170

Visualization of metabolic networks and pathways with MetExploreViz

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Abstract number: 2318

Clément Frainay, Nicolas Weiss, Benoit Colsch, Frédéric Sedel, Dominique Thabut, Christophe Junot, Fabien Jourdan

Toxalim, Université de Toulouse, INRA, Toulouse, INRA UMR1331 TOXALIM-MeX 180 Chemin de Tournefeuille, Toulouse

Inferring missing compounds from metabolic profile using network topology analysis

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Abstract number: 2502

Venkata Nainala, Benjamin Merlet, Florence Vinson, Maxime Chazalviel, Fabien Jourdan, Egon Willighagen, Reza Salek, Kenneth Haug, Christoph Steinbeck

EMBL-EBI, EMBL-EBI, Wellcome Trust Genome Campus, Hinxton Cambridgeshire CB10 1SD

Metabolic Pathways and Networks Integration with MetaboLights: Visualisation and Analysis

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Abstract number: 2600

Michelle Reid, Irwin Kurland, Yunping Qiu, Timothy Garrett, Richard Yost

University of Florida, Department of Chemistry PO BOX 117200, Gainesville FL 32611

Imaging of Muscle and Adipose Tissue by MALDI-MS for Exercise Metabolomics

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Abstract number: 2223

Catherine Deborde, Patricia Ballias, Camille Bénard, Stéphane Bernillon, Thierry Berton, Cécile Cabasson, Virginie Cocureau, Salimata Diarrassouba, Yves Gibon, Daniel Jacob, Marie Lefebvre, Mickaël Maucourt, Dominique Rolin, Simon Roques, Laetitia Fouillen, Sébastien Mongrand, Frédéric Domergue, Jean-Jacques Bessoule, Marina Le Guédard, Eric Testet, Annick Moing

INRA PMB-MetaboHUB, 71 av E. Bourlaux, Villenave d'Ornon 33140

Plant Metabolomics at Bordeaux Metabolome Facility, a member of MetaboHUB and PHENOME IA projects. Tools and Applications

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Abstract number: 2297

Kimberly Colson, K. Brian Killday, Christian Fischer

Bruker BioSpin, 15 Fortune Drive, Billerica MA 01821

Cell Culture Media: NMR Approaches to Evaluating Quality and Nutrient Consumption

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Abstract number: 2009

Wiebke Timm, Jens Decker, Sven Brehmer, Sandra Groscurth, Peter-Réne Steiner, Till Kühn, Jens Fuchser

Fahrenheitstrasse 4, Bremen 28359

Fully automated structure verification of organic compounds by combining accurate MS with NMR data analysis

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Abstract number: 2060

Jun Han, Georgia Mitsa, Lin Karen, Christoph Borchers

UVic-Genome British Columbia Proteomics Centre

Comprehensive profiling of bile acids in human and mouse

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Abstract number: 2174

Tairo Ogura, Takeshi Bamba, Akihiro Tai, Eiichiro Fukusaki

Shimadzu Scientific Instruments, Inc., 7102 Riverwood Drive, Columbia MD 21046

The development of compound annotation technique extended for conjugates.

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Abstract number: 2070

Soeun Kang

Seoul National University, Seoul National Univ. 1 Gwanak-ro, Gwanak-gu, Seoul, Korea, Seoul 08826

Monitoring Glutathione Redox Reaction in Living Human Cells by Heteronuclear NMR and Its Application to Anticancer Drug Resistance

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Abstract number: 2215

Johannes Hartl, Patrick Kiefer, Julia Vorholt

ETH Zürich, Vladimir-Prelog-Weg 1-5/10, Zürich 8093

Targeted and untargeted strategies for analysis of dynamic labeling experiments using LC-HRMS

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Abstract number: 2276

Christian Fischer, Kimberly Colson

Bruker BioSpin GmbH, Silberstreifen 4, Rheinstetten

New Strategies for Identification of Metabolites in NMR Spectra using Databases, e.g. HMDB

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Abstract number: 2188

Anna Weiser, Pieter Giesbertz, Hannelore Daniel, Britta Spanier

TU München, Ernährungsphysiologie Gregor-Mendel-Str. 2, Freising Bavaria 85354

Acylcarnitine profiling in plasma and tissues of NZO mice as model for obesity-induced T2 diabetes

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Abstract number: 2407

Alexandra Simader, Alexandra Parich, Manuel Hofer, Michael Sulyok, Maria Doppler, Christoph Bueschl, Barbara Steiner, Marc Lemmens, Hermann Buerstmayr, Gerhard Adam, Justyna Rechthaler, Rudolf Krska, Rainer Schuhmacher

BOKU University Vienna, IFA-Tulln, AZ, Konrad Lorenz Straße 20, Tulln 3430

Metabolomic analysis of Fusarium head blight on wheat – elucidation of fungal attack

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Abstract number: 2412

Matthieu Schoumacher, Vincent Lambert, Sylvain Hansen, Justine Leenders, bernadette Govaerts, Bernard Pirotte, Jean-Marie Rakic, Agnes Noël, Pascal de Tullio

Ulg (CIRM), Quartier Hôpital, Avenue Hippocrate 15, Liege 4000

New Insight into exudative Age-related Macular Degeneration (AMD): A Metabolomics Approach

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Tyler Backman, Thomas Girke

University of California Riverside, 1170 Greene Terrace, Davis CA 95618

Bioactive molecule discovery with large screening data

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Tiago Jorge, Maria Florêncio, Ana Ribeiro-Barros, CARLA ANTONIO

Plant Metabolomics Laboratory, ITQB NOVA, Avenida da República, Oeiras 2780-157

LC-MS analysis of raffinose family oligosaccharides in salt tolerant Casuarina glauca tissues

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Abstract number: 2310

Carolina Gonzalez-Riaño, Silvia Tapia, Fernanda Rey-Stolle, Alberto Muñoz, Gonzalo Leon, Laura Ravanetti, Antonia Garcia, Javier de Felipe, Coral Barbas

University CEU San Pablo, CEMBIO (Centre for Metabolomics and Bioanalysis), Facultad de Farmacia, Universidad San Pablo CEU, 28668 Madrid, Spain, Madrid

MULTIPLATFORM NON-TARGETED METABOLOMIC STUDY OF BRAIN TISSUE AT DIFFERENT POST MORTEM TIME POINTS

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Abstract number: 2042

Laurie Favre, Annick Ortalo-Magné, Clément Coclet, Jean-François Briand, Jean-Charles Martin, Benjamin Misson, Cédric Garnier, Gérald Culioli

Université de Toulon CS 60584, TOULON (83041)

LC-MS-based metabolomics analysis of marine biofilm-forming bacteria: Impact of culture parameters and copper contamination

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Abstract number: 2085

Fidele Tugizimana, Ian Dubery, Paul Steenkamp, Lizelle Piater

University of Johannesburg, Auckland Park, Johannesburg Gauteng 2006

Maximizing the value of metabolomics data: exploring the influence of data analysis parameters on model classification and feature selection

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Abstract number: 2159

Alex Lee, Simon Swift, Silas Villas-Boas

School of Biological Sciences, University of Auckl, 3A Symonds street, Auckland 1010

The mechanism of action of biocides: Epicoccum derived antimicrobials

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Abstract number: 2527

Rabiya Zia, Nicola Gray, Vishal Patel, Ian Wilson, Julia Wendon, Mark McPhail, Muireann Coen

Imperial College London, Computational and Systems Medicine, Department of Surgery and Cancer, Imperial College London, London UK SW7 2AZ

The plasma metabolic phenotype of patients with Acute Liver Failure characterised using 1H NMR and targeted UPLC-MS

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Abstract number: 2425

Álvaro Fernández Ochoa, isabel Borras Linares, Amudena Perez Sánchez, Enrique Barrajón Catalán, David Arráez Román, Vicente Micol, Antonio Segura Carretero

Universidad de Granada, Avda. del Hospicio, S/N, Granada 18010

In-situ perfusion absorption study of rosemary compounds.

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Abstract number: 2507

Cristian Gómez-Canela

IDAEA-CSIC, Jordi Girona, 18-26, Barcelona 08034

Targeted metabolomics of Gammarus pulex following controlled exposures to selected pharmaceuticals in water

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Abstract number: 2572

Christelle Andre, Lena Fragner, Sonja Tischler, Marc Behr, Sophie Charton, Jenny Renaut, Wolfram Weckwerth, Jean-Francois Hausman

Department of Environmental Research and Innovatio

Primary and secondary metabolome associated with bast fibre development in hemp

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Abstract number: 2371

Pim Leonards, Sara Tufi, Marja Lamoree, Juliette Legler, Jessica Legradi

VU University, De Boelelaan 1087, Amsterdam 1081HV

Alternative animal and cell models for testing (developmental) neurotoxicity of chemicals using a metabolomic approach

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Abstract number: 2599

Sastia Putri, Toshiyuki Yamashita, Walter Lavina, Sammy Pontrelli, James Liao, Eiichiro Fukusaki

Osaka University, 2-1 Yamadaoka Laboratory of Bioresource Engineering, C2-222, Suita 5650871

Strain improvement of 1-butanol producing Escherichia coli: A metabolomics approach

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Abstract number: 2434

Luis Valledor, Jesús Pascual, Mónica Escandón, Wolfram Weckwerth, María Jesús Cañal, Mónica Meijón

University of Oviedo, Catedrático Rodrigo Uria s/n, Oviedo Asturias E-33006

The integration of physiological, proteomic, and metabolomic levels reveals new adaptive and stress-responsive mechanisms in Pinus.

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Abstract number: 2078

Thomas Kursar, Natasha Wiggins, Dale Forrister, Maria-Jose Endara, Phyllis Coley, James Nicholls, R. Pennington, Kyle Dexter, Graham Stone, Catherine Kidner

University of Utah, 257 South 1400 East Dept Biology, U of Utah, Salt Lake City UT 84112-0840

Chemocoding as an identification tool where morphological- and DNA-based taxonomic methods fall short: Inga as a case study

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Abstract number: 2438

Tom Walker, Lena Fragner, Luca Bragazza, Constant Signarbieux, Susan Ward, Nicholas Ostle, Brian Forde, Richard Bardgett, Wolfram Weckwerth

Faculty of Life Sciences, Michael Smith Building,

Contrasting plastic and evolutionary responses of Eriophorum vaginatum to climate warming cascade from molecular to ecosystem levels

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Abstract number: 2211

Donggu Oh, Sarah Lee, Sunmin Lee, Ga Ryun Kim, Jong Seok Lee, Hee-sun Yang, Joohong Yeo, Choong Hwan Lee

Konkuk University, 5029, Seoul

Mass Spectrometry-Based Metabolite Profiling of 62 Indigenous Plant Species and Their Correlation with Bioactivities

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McGill University, 21111 Lakeshore Road, Ste-Anne-de-Bellevue QC H9X 3V9

Data Integration & Systems Biology for Metabolomics

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Sunmin Lee, Ga Ryun Kim, Donggu Oh, Jong Seok Lee, Hee-sun Yang, Joohong Yeo, Sarah Lee, Choong Hwan Lee

Konkuk university, Neungdong-ro 120, Seoul

Comparative parts(leaf, twig, and fruit) of Alnus firma based on metabolite profiling and bioactivity

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Joao Mokochinski, Paulo Mazzafera, Alexandra Sawaya, Ric de Vos, Robert Hall

Wageningen University and Research, Zeemanstraat, 12, Wageningen Gelderland 6706 KB

Metabolic responses of Eucalyptus ssp to changes in different regimes of temperature

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Francisco de Abreu e Lima, Matthias Westhues, Lothar Willmitzer, Albrecht Melchinger, Zoran Nikoloski

Max-Planck Institute of Molecular Plant Physiology, Am Mühlenberg 1, Potsdam 14476

Metabolic robustness underpins a predictive mechanism of maize hybrid performance in the field

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Abstract number: 2047

Noluyolo Nogemane

UNISA, cnr Christian de Wet and Pioneer Ave, Florida P/Bag x06, Unisa, Florida,, Roodepoort Gauteng 1709

1H-NMR-based metabolomics approach to understanding the influence of seasons on the metabolomic profile of Greyia radlkoferi

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Stefan Schaebler

German, Julius-von-Sachs Platz 2, Wuerzburg 97082

Towards the Circadian Drosophia Metabolome

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Abstract number: 2545

Ebru Yilmaz, Kerem Kaya, Bahar Sogutmaz Ozdemir, emrah nikerel

Yeditepe University, Department of Genetics and Bioengineering, Istanbul

Effect of drought stress on amino acid metabolism of model plant Brachypodium distachyon

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Abstract number: 2271

María Tortosa, Pablo Velasco, Elena Cartea, Víctor Rodríguez

Misión Biológica de Galicia (CSIC), Carballeira, 8 - Salcedo, Pontevedra 36143

Effector-triggered immunity (ETI) of Brassica oleracea to the infection of Xanthomonas campestris pv. campestris

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Mpho Makola

University of Johannesburg, C2 LAB 322 Biochemistry Department University of Johannesburg, Johannesburg Other 2006

New Insights on Metabolite Identification: MS fragmentation, adduct formation and quantum chemistry

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Alexandra Sawaya, Alexandre Borghi

UNICAMP, Institute of Biology, Department of Plant Biology, bloco J subsolo,IB, UNICAMP, Cidade Universitária Zeferino Vax. Distr. Barão Geraldo, Campinas 13083-862

UHPLC-MS analysis of extracts of guaco (Mikania glomerata Spreng. and Mikania laevigata Schultz Bip. ex Baker) submitted to different drying procedures

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Noam Reshef, Aaron Fait, Nurit Agam, Natasha Walbaum

Ben Gurion University, Midershet ben gurion, Beer sheva -- Please Select -- 84990

Integrating metabolomics and micrometeorology to assess the regulation of cluster sunlight exposure as a tool to improve wine quality in arid to semi-arid regions

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Abstract number: 2553

Cheol-ho Jang

kookmin University, 77, Jeongneung-ro Seongbuk-gu, Seoul

Dose-dependent and time-dependent metabolic dynamics of Chlamydomonas reinhardtii under phosphate-deprivation

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Maria Urrutia, Stephane Bernillon, Nadia Lamari, Mickaël Maucourt, Patricia Ballias, Hélène Sellier, Yves Gibon, Catherine Giauffret, Annick Moing

INRA - UMR1332 Fruit Biology and Pathology

Combining LCMS data from two years for plant performance biomarkers discovery

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María Tortosa, Marta Francisco, Pilar Soengas, Pablo Velasco

Misión Biológica de Galicia (CSIC), Carballeira, 8 - Salcedo, Pontevedra 36143

Early metabolomic response of Brassica oleracea plants against Xanthomonas campestris pv. campestris

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Juan Carreño, Mónica Cala, Julián Sánchez, José Guio, Wolfram Baumann, Roland Meesters

Universidad de los Andes, Cra 1 Nº 18A- 12, Bogotá, D.C. Cundinamarca 111711

Amino Acid-Profiling of Breast Cancer Test Subject Samples by GC-MS

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Abstract number: 2225

Julian Aldana, Mónica Cala, Julián Sánchez, Ismael Guio, Roland Meesters, Wolfram Baumann

Los Andes University, Cra 1 Nº 18A- 12, Bogotá, D.C. Cundinamarca 111711

Alterations in Plasma Lipid Profiles from Breast cancer Patients

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Dorna Varshavi, Dorsa Varshavi, Nicola McCarthy, Jeremy Everett

University of Greenwich, Central Ave, Chatham Maritime, Chatham Kent ME4 4TB

Metabolic Reprogramming in Mutant KRAS Colorectal Cancer Cells

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Reiko Kiyonami, Elena Sokol, David Peak, Ken Miller

Thermo Fisher Scientific, 355 River Oaks Parkway, San Jose CA 95134

Discovering Diabetic Lipid Biomarker Using HRAM LC-MS-MS Approach on a High Field Hybrid Quadrupole-Orbitrap Mass Spectrometer

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Reiko Kiyonami, Sergei Snovida, Devin Drew, David Peak, Julian Saba, Andreas Huhmer, Ken Miller

Thermo Fisher Scientific, 355 River Oaks Parkway, San Jose CA 95134

Facilitate Biomarker Discovery Using Integrated Omics Differential Analysis with High Resolution Accurate LC/MS Approach

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Pawel Derezinski, Agnieszka Klupczynska, Timothy Garrett, Vanessa Rubio, Wojciech Dyszkiewicz, Zenon Kokot

Poznan University of Medical Sciences, 6 Grunwaldzka Street, Poznan 60-780

Serum global metabolomics approach to examine non-small cell lung cancer

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Hannah Johnston

Joseph Black Building David Brewster Road, Edinburgh EH9 3FJ

A Snapshot into a Cancer Cell

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Filippos Michopoulos, Emma Davies, Hannah Brown, Alwin Schuller, Richard Woessner, Susan Critchlow

Senior scientist, Oncology, iMED, Alderley Park, Macclesfield SK10 4TG

Metabolite measurements enhance our understanding of the immunooncology portfolio

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Abstract number: 2062

Sehyun Oh

Seoul National University, College of Pharmacy, Seoul National University, 1 Gwanak-Ro, Gwanak-gu, Seoul, Korea, 151-742, Seoul

Metformin Targets PHGDH And Lowers 2-HG In Inhibiting Breast Cancer Cell Proliferation

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Abstract number: 2099

Laura Brunelli, Elisa Caiola, Mirko Marabese, Massimo Broggini, Monica Lupi, Roberta Pastorelli

IRCCS-Istituto di Ricerche Farmacologiche Mario Ne, via La Masa 19, Milano 20156

Mutants KRAS exhibit different metabolic responses to PI3K inhibition in non-small lung cancer cells: implication for therapeutic susceptibility

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José Pérez, Caridad Díaz-Navarro, Ana Laura Ortega-Granados, Sergio Granados-Principal, Maria Ruiz, Mónica Fernández, Nuri El Azem, Francisca Vicente, Olga Genilloud, Pedro Sánchez-Rovira

Fundación MEDINA, Centro de Excelencia en Investig, Av. del Conocimiento, 34, Granada

Untargeted LC-TOFMS -based metabolomics for breast cancer biomarkers: A pilot study

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Abstract number: 2578

Maike Aurich, Ronan MT Fleming, Ines Thiele

Luxembourg Centre for Systems Biomedicine, 7, avenue des Hauts-Fourneaux, Esch-sur-alzette L-4362

MetaboTools: Analysis of extracellular metabolomic data in the context of the metabolic model

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Abstract number: 2011

Paola Marignani

Faculty of Medicine Sir Charles Tupper Medical Building, Rm 9F1, 5850 College St, Halifax NS B3H 1X5

Combination therapies targeting metabolic processes inhibits tumourigenesis.

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Abstract number: 2048

Kyoung-Soon Jang

Korea Basic Science Institute, 162 Yeongu Danji-ro, Ochang-eup, Cheongwon-gu, Cheongju

High-resolution metabolic profiling unveils the differences between glio- and neuroblastoma

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Sei Harada, Ayako Kurihara, Kota Fukai, Ayano Takeuchi, Tomonori Okamura, Akiyoshi Hirayama, Masahiro Sugimoto, Tomoyoshi Soga, Masaru Tomita, Toru Takebayashi

Keio University, 35 Shinanomachi Shinjuku-ku, Tokyo

Plasma metabolome associated with chronic kidney disease in general population

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Lukasz Boguszewicz

Maria Sklodowska-Curie Memorial Cancer Center and, Wybrzeze AK 15, Gliwice 44-101

Metabolomics based on J-resolved NMR spectroscopy in monitoring of anticancer treatment toxicity

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Wang Zhichao, Jun Zeng, Guowang Xu, Hailong Piao

DICP, CAS, 457, Zhongshan Road, Dalian

13C6-Glucose labeling metabolomics reveals effects of PTEN mutation on prostate cancer metabolism

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Noriyuki Ojima, Shuichi Kawana, Yumi Unno, Yukihiko Kudo, Takero Sakai, Takashi Kobayashi, Shin Nishiumi, Masaru Yoshida

Shimadzu Coporation, 1, Kuwabara-cho, Nishino-kyo Nakagyo-ku, Kyoto 604-8511

Evaluation of gas-chromatography tandem mass spectrometry system with automated TMS derivatization in analysis of plasma metabolites

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Abstract number: 2169

Majda Haznadar

Laboratory of Human Carcinogenesis, NCI, NIH, 37 Convent Drive Building 37/Room 3060, Bethesda MD 20892

Urinary Metabolite Risk Biomarkers of Lung Cancer: A Prospective Cohort Study

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Renata Bujak, Wiktoria Struck-Lewicka, Malgorzata Patejko, Marta Kordalewska, Tomáš Kovalczuk, Agnieszka Ulanowska, Grzegorz Straczynski, Roman Kaliszan, Michal Markuszewski

Medical University of Gdansk, ul. Sklodowskiej-Curie 3A, 80-210 Gdansk, Poland

The external and intra-laboratory validation of potential biomarker candidates for prostate cancer

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Marta Kordalewska, Renata Bujak, Karolina Siedlecka, Wiktoria Struck-Lewicka, Arlette Yumba Mpanga, Marcin Markuszewski, Marcin Matuszewski, Roman Kaliszan, Michal Markuszewski

Department of Biopharmaceutics and Pharmacodynamic, Al. Gen. J. Hallera 107, Gdansk 80-416

Urine metabolic fingerprinting in renal cell carcinoma for proper classification of cancer patients and healthy volunteers

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second military medical university, No. 325 Guohe Road, Shanghai Shanghai 200433

Metabolic alterations and the effect of sophocarpine and matrine therapy in an experimental cancer cachexia murine model

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Abstract number: 2546

Aryo Pamungkas

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Biomarker discovery using high resolution metabolomics of Korean male lung cancer patient serum in association with alcohol consumption

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XUEJIAO YIN

National University of Singapore, 3 Science Drive 3 Department of Chemistry, S5-02-05/13, Singapore Singapore 117543

Metabolomic analysis of Nicotinamide phosphoribosyltransferase (NAMPT) inhibition on human cancer cell line

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Nour Madhoun, Samah Gadhoum, Abdul-Hamid Emwas, Jasmeen Merzaban

King Abdullah University of Science and Technology, Thuwal, Thuwal

Effects of anti-CD44 Monoclonal Antibodies on Metabolic Profiles of Acute Myeloid Leukemia

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Henry Oppermann, Jeevan Pharma, Mandy Berndt-Paetz, Frank Gaunitz, Claudia Birkemeyer

University Hospital Leipzig Neurosurgery, University Hospital Leipzig Research Facilities Neurosurgery Liebigstraße 19, Leipzig 04103

Metabolite Profiling of Brain Tumor Cells under different nutritional conditions using GC-MS

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James Alexander, Louise Gildea, Simon Cameron, James McKenzie, Frances Bolt, Nicole Strittmatter, Adele Savage, Julian Teare, James Kinross, Zoltan Takats

Imperial College London, 10th Floor, Surgical Unit QEQM Building, St Mary's Hospital, Praed Street, London London W2 1NY

Rapid Evaporative Ionisation Mass Spectrometry of Human Faecal Samples

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Abstract number: 2167

Mónica Cala, Jose A. Lopez-Martin, M. Teresa Agullo Ortuno, Carolina Gonzalez-Riano, Antonia Garcia, Coral Barbas

Los Andes University, Cra 1 Nº 18A- 12, Bogotá, D.C. Cundinamarca 111711

Multiplatform Plasma Fingerprinting in Cancer Cachexia: A Pilot Study

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Wilson Gonsalves, Tumpa Dutta, Shaji Kumar, Taro Hitosugi, S. Vincent Rajkumar, K. Sreekumaran Nair

Mayo Clinic, 200 First Street SW, Rochester MN 55905

Utilizing large scale metabolomics profiling to identify patients with high risk smoldering myeloma

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Abstract number: 2278

San-Yuan Wang, Yufeng Tseng, Te-Hsuen Tzeng, Chun-Yen Kuo, Po-Kai Huang, Yen-Ming Huang, Wei-Che Hsieh, Yu-Jie Huang, Po-Hung Kuo, Shih-An Yu, Si-Chen Lee, Wei-Cheng Tian, Shey-Shi Lu

National Taiwan University, R403, CSIE, NTU, No. 1, Sec. 4, Roosevelt Road, Taipei 10617

Lung Cancer Associated Volatile Organic Compounds Detection Using a Novel Portable Gas Chromatographic Device Integrated MEMS and CMOS Technology

P-126

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Marta Cascante Serratosa, Carles Foguet, Pedro de Atauri, Vitaly Selivanov

Faculty of Biology, Department of Biochemistry and, Avda. Diagonal, 643, Edifici Nou, pl -2, Barcelona 08028

Iso2Flux: A new software for 13C fluxomics developed in the framework of PheNomeNal

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Abstract number: 2292

Ibrahim Halil Polat, Vitaly Selivanov, Miriam Tarrado-Castellarnau, Silvia Marin, Marta Cascante Serratosa

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13C Metabolic Flux Analysis of MCF7 cells with impaired mitochondria

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Alexsandro Silva, Josiane Steluti, Aline Carvalho, Andreia Miranda, Antonio Augusto Carioca, Ismael da Silva, Regina Fisberg, Dirce Marchioni

University of São Paulo, Lord Cockrane, 26 ap.82, São Paulo São Paulo 04213000

Amino acids profiling as biomarkers to identify healthy individuals: a targeted metabolomic approach

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Abstract number: 2322

Ed Reznik, Augustin Luna, Arman Aksoy, Eric Minwei Liu, Chris Sander

Memorial Sloan-Kettering Cancer Center

The Landscape of Metabolic Changes Across Tumor Types

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metanomics GmbH, Berlin, Tegeler Weg 33, Berlin 10589

A novel plasma based assay for the differentiation of pancreatic cancer from chronic pancreatitis

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Leitat Technological Center, Avenida Fernando Abril Martorell, 106 Torre A, Planta 0, Valencia 46026

Metabolomic analysis of gastric cancer progression within the Correa's cascade using UPLC-MS

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Comprehensive LC/MS, GC/MS and 1H NMR urine metabolic fingerprinting in bladder cancer

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Daniel Crooks, Teresa W.-M. Fan, Andrew Lane, W. Marston Linehan

National Institutes of Health, 10CRC, Room 1-5888 10 Center Drive, Bethesda MD 20892

Exploration of Tumor Metabolism in Hereditary Kidney Cancer Syndromes Using Stable Isotope-Resolved Metabolomics

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Shuichi Shimma, Satoko Osawa, Yasushi Kojima, Masahiro Aoki, Tomoyoshi Soga

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Microscopic MALDI-imaging mass spectrometry in intestinal tumors of Apc mutant mice using two-step matrix application

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Ilona Dudka, Elin Thysell, Henrik Antti, Anders Bergh, Pernilla Wikström, Gerhard Gröbner

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Comparative tissue metabolomic and proteomic analysis of Prostate Cancer subtypes

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Facundo Fernandez, Martin Paine, Danning Huang, Jingbo Liu, Shane Ellis, Ron Heeren, Tobey MacDonald

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Three-dimensional MALDI Imaging to Understand Metastasis in Pediatric Medulloblastomas

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Metabolomic Changes Associated with Postmenopausal Hormone Therapy

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Multi-omic data integration via constraint-based modeling to unveil metabolic alterations in prostate cancer associated to a chronic exposure to endocrine disruptors

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Role of 9-cis Retinoic Acid in Inducing Epithelial to Mesenchymal Transition in Human Pancreatic Ductal Adenocarcinoma Cell Lines

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Runhan Yan, Xiaowei Fang, Zhenglong Bi, Huanwen Chen

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Differential analysis of lung cancer patients' and healthy volunteer's serum samples using ICP-MS

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Metabolomic profiling of blood plasma from pre-diabetic and healthy subjects at the Taiwan Biobank

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Jin Seong Hyeon, Hunjoo Ha, Geum-Sook Hwang

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1H NMR-based global metabolomic analysis in diabetic nephropathy mice

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Janina Tokarz, Gabriele Moeller, Martin Hrabe de Angelis, Jerzy Adamski

Helmholtz Zentrum Muenchen, Institute of Experimen, Ingolstaedter Landstrasse 1 Genome Analysis Center, Neuherberg Bavaria 85764

Metabolomic analyses of the effects of statins on healthy human cell lines reveal an impaired amino acid metabolism

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Metabolic profiling of human heart affected by dilated cardiomyopathy

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Jeongae Lee

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Urinary metabolomics approaches in metabolic syndrome based liquid chromatography-electrospray ionization/ mass spectrometry

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Adel Alghamdi, Ali Tohari, Xinhua.Shu@gcu.ac.uk Shu, David Watson

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Metabolomics Profiling of Adult Retinal Pigment Epithelial (ARPE-19) cells After Adding Vitamin D.

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Caroline Muschet, Cornelia Prehn, Anna Artati, Gabriele Möller, Martin Hrabe de Angelis, Jerzy Adamski

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Impact of metformin and glucose on the hepatocellular metabolism

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Plasma metabolites profile in Inuit adults from Nunavik (northern Quebec) with metabolic syndrome

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Association of age and sex with plasma and urine metabolite profiles from healthy humans

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Jacquelyn Walejko

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Diabetes during Pregnancy Produces Placental Metabolic Alterations at Term

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Novel insights from a metabolomics study of heart failure in a mouse model

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Metabolomic signatures of bean-to-rice ratio in the Costa Rica Study

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Antonis Myridakis, Leanne Nye, Ian Wilson, Marc-Emmanuel Dumas

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UPLC-MS targeted profiling of aromatic phenolic compounds, related with cardiometabolic diseases

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NEW INSIGHT ON OBESITY AND ADIPOSE-DERIVED STEM CELLS BY COMPREHENSIVE METABOLOMICS

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Michal Markuszewski

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Non-targeted metabolomics in early vascular ageing syndrome

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Jeeyoun Jung

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A CE-MS based metabolomics study reveals the therapeutic mechanism of Shaofu Zhuyu decoction in a diet-induced obesity mouse model

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ZIEL – Institute for Food and Health. Technical Un, Gregor Mendel Strasse 2, Freising Bavaria 85354

Diversity of plasma bile acid profiles in response to dietary challenges

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Circulating 1H NMR based metabolomic profiling associated to proteinuria in diabetic patients

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Nami Kim

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Curcumin derivative induces energy metabolism and increases intracellular lactate production through AMPK signaling pathway in muscle cells

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Coupling Urinary Trihalomethanes and Metabolic Profiles of Type II Diabetes Mellitus: a Case-Control Study

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Lipotype, Tatzberg 47, Dresden 01307

Lipidomic parameters associated with obesity

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Sex Differences in the Association of Phospholipids and Sphingolipids with the Metabolic Syndrome in young adults

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Korea University, College of Pharmacy

Metabolomic analysis on the three stages of diabetes acquisition

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Metabolomics for new colchicine treatment of experimental atherosclerosis

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Ryan Gil,

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Inter-Sample Chemical shift variations in 1H NMR: An Improved Workflow for Measurement of Urine Metabolome and Biomarker Discovery

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Red blood cells metabolomics for the stratification of diabetic patients

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Lee Gethings, Johannes Vissers, Jose Castro-Perez, Yvonne Woolerton, Lynn McLean, Robert Beynon, James Langridge

Stamford Avenue, Wilmslow

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Helmholtz Zentrum München, Deutsches Forschungszen, Ingolstädter Landstraße 1, 85764 Neuherberg

Metabolic profiling of bile acids in intestine and feces samples of diabetic mice using UPLC-MS

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Application of capillary electrophoresis mass spectrometry for unravelling changes associated with gestational diabetes mellitus

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Sunhee Jung, Miso Nam, Do Hyun Ryu, Geum-Sook Hwang

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Metabolic profiling of human aorta with atherosclerotic plaques using liquid chromatography/mass spectrometry.

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1H NMR-based metabolomic profiling reveals potential biomarkers of renal function in non-diabetic and diabetic populations

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Atul Rawat, Dinesh Kumar

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Serum metabolic disturbances associated with acute myocardial infarction elucidated by NMR-based metabolomics

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Cord blood metabolome is associated with birth weight, but not predictive for weight gain and later BMI

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Indolepropionic acid and certain lipid metabolites are related to decreased risk of developing type 2 diabetes in the Finnish Diabetes Prevention Study

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NMR-based assessment of liraglutide therapy effectiveness

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INSELSPITAL - University Hospital Bern, University, Freiburgstr. 15 INO-F, Clinical Chemistry, Bern 3010

HRMS and MRM based screening - where to start in Clinical Metabolomics

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MedDay Pharmaceuticals, 96 avenue Haussmann, 75008 Paris

Lipid metabolism in hypothalamic neuron treated with saturated fatty acid using high resolution mass spectrometry

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Susan McRitchie, Susan Sumner, Andrea Richardson, Wimal Pathmasiri, Frederica Perera

RTI International, 3040 E Cornwallis, Research Triangle Park NC 27709

Structural equation modeling: Linking exposure to birth- and early life-health outcomes via the metabotype of cord blood

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Profiling of plasma metabolites in postmenopausal women with metabolic syndrome

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Metabolic flexibility in the insulin resistant heart and skeletal muscle: a dynamic 13C labelling approach

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Riccardo Di Guida, Warwick Dunn, Jonathan Hazlehurst, Jeremy Tomlinson

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Effects of glucocorticoids administration and their interaction with insulin: an untargeted metabolomics investigation

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GC/MS based steroid profiling method for rat serum with large volume injection

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Workflow methodology for rodent brain metabolome exploration using NMR, LC-HRMS and GC-MS analytical platforms

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Application of mass spectrometry-based lipidomics in the study of bipolar disorder

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Serum metabolomics study for identification of potential biomarkers of long-term survival in renal transplantation patients based on liquid chromatography-tandem mass spectrometry

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Gaëlle Diserens, Damian Hertig, Balazs Legeza, Sandra Eggimann, Martina Vermathen, Julien Furrer, Christa Flück, Jean-Marc Nuoffer, Peter Vermathen

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Improving the metabolic stability of cultured cells during extended HR-MAS NMR measurements by prior heating

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Non-targeted metabolite profiling reveals metabolic alterations in dogs with behavioral abnormalities

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Phospholipid ratios in Zellweger Spectrum disorder patients

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Mette Kristensen, Scott Harrison, Hao Luo, Konstantin Schneider, Rebecca Lennen, Markus Herrgard, Hanne Bjerre Christensen

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Application of a targeted metabolomics approach to investigate regulation of the biosynthetic pathway of melatonin in Escherichia coli

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The metabolic state in newborns and infants is linked to inflammasome activity and respiratory diseases

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SHIRISH YAKKUNDI, Lee Gethings, Aude-Claire Morillon, James Langridge, Louise Kenny

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An untargeted metabolomics approach for to identify potential biomarkers in spontaneous pre-term birth (sP-PTB) delivery, using a label-free LC-DIA-MS approach

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Mitochondrial DNA Replication Defects Disturb Cellular dNTP Pools and Remodel One-Carbon Metabolism

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David Peake, Mandy Bowman, Reiko Kiyonami

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Innovations and Applications of Quantitative Metabolomics in Human Health

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University Institute of Clinical Chemistry

Routine plasma preparation protocols and their influence on the metabolome

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Volker Behrends

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Opportunity looms: metabolic regulation of an opportunistic pathogen

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Sampling Methods for Profiling Plant Volatiles Profiling by GCxGC-TOFMS

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Yasuyo Sekiyama, Kazuyuki Okazaki, Seishi Ikeda, Jun Kikuchi

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NMR-based metabolic profiling of field-grown leaves from sugar beet plants harbouring different resistance levels to Cercospora leaf spot disease

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Snehil Srivastava

Ben-Gurion University, Jacob Blaustein Institute for Desert Research, Albert Katz Department of Dryland Biotechnologies, Ben-Gurion University of th, Beer Sheva 84990

Effect of the rootstock-scion grafting combination on stress tolerance and fruit quality of mandarin (Citrus reticulata)

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Varietal characteristics of apple aroma associated with sensory attributes

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Anna Kårlund, Marko Lehtonen, Reijo Karjalainen, Kati Hanhineva

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The effects of genetic background and cultivation methods on the phytochemical profile of strawberries

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LC-MS METABOLOMICS SHOWS A SMART WAY TO REDUCE SULFITES IN WINE

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Laura Millan, Alicia Sanchez, Ramon Barrio, Maria Aranzazu Goicolea, Carmen Sampedro

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UNTARGETED METABOLOMIC STUDY FOR IDENTIFICATION OF BIOACTIVE METABOLITES AS POTENTIAL HEALTH PROMOTING AGENTS IN GRAPE TISSUES

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A METABOLOMICS APPROACH TO CHARACTERIZE RAW, PASTEURIZED AND ULTRA-HIGH TEMPERATURE MILK USING UPLC-QTOF-MS and MULTIVARIATE DATA ANALYSIS

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Istituto Zooprofilattico Sperimentale delle Venezi, Viale dell'Università, 10, Legnaro Padova 35020

Metabolomics analysis of liver to reveal profiles disruption in bovines upon steroid treatment

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Sunmin Lee, Sarah Lee, Ji Young Oh, Eun Jung Jeon, Dong Wan Lee, Beom Seok Kim, Choong Hwan Lee

Konkuk university, Hwayang-dong, Seoul

Correlation with microbial diversity and MS-based metabolite profiling of doenjang, a fermented soybean paste during industrial process

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Milena Lussu, Tania Camboni, Francesco Del Carratore, Corrado Serra, Aldo Manzin, Luigi Atzori

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1H NMR-based metabolomic analysis for diagnosis of uncomplicated urinary tract infection (UTI)

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iDiv - German Centre for Integrative Biodiversity, Deutscher Platz 5e, Leipzig

Plant-soil feedbacks introduce changes in the metabolome of common grassland species

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Different metabolism of Aspergillus oryzae and Bacillus amyloliquefaciens on rice koji fermentation

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Benita Percival, Sarah Moumtaz, Kerry Grootveld, Devki Parmar, Richard Odhurogu, Kavita Desai, Pim Jansson, Martin Grootveld

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Explorations of the generation of aldehydic lipid oxidation products in thermally-stressed culinary oils and fats: A 1H NMR-linked PCR modelling strategy

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HyeRyun Kim

Korea Food Research Institute, 1201-62, Anyangpangyo-ro, Seongnam-si, Gyeonggi-do

Metabolomic approach for antioxidative activity of the makgeolli brewed with Korean traditional nuruk

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University of Calcutta, Department of Botany, 35 Ballygunge Circular Road, Kolkata 700019

Metabolomics and chemometric study of Nymphaea pubescens flower extract to identify metabolite(s) contributory to the acetylcholinesterase inhibition

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Murielle Gaugain

Anses-Laboratoire de Fougères, 10 B rue Claude Bourgelat - Javené - CS 40608, Fougères 35306

ASSESSMENT OF METABOLOMIC APPROACH FOR THE SCREENING OF ILLEGAL ADMINISTRATION OF CEPHALOSPORINS IN LAYING HENS

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Shuichi Kawana, Takero Sakai, Yusuke Takemori, Daichi Yukihira, Tsuyoshi Nakanishi

Shimadzu Corporation, Hankyu Terminal Bldg. 14F, 1-1-4, Shibata, Kita-ku, Osaka

Mass spectrometry-based metabolomics to differentiate beer types

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Jang Eun Lee, Jae Ho Kim

Korea Food Research Institute, 1201-62 Anyangpangyo-ro Bundang gu, Seongnam city Gyeonggi-do 13539

Foodomics research on the traditional Korean Nuruk and alcoholic beverages

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Jimmy Yuk, Maged Sharaf, Giorgis Isaac, Mark Wrona, Kate Yu

Waters Corporation, 34 Maple Street, Milford MA 01757

Chemical Profiling of Actaea (Black Cohosh) Species Using UPLC-QTof-MS

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Anas Kamleh

Thermo Fisher Scientific, Telefonvägen 30, Hägersten 12626

Systematic Integration of Omics Data to Improve Innovation in Beer Crafting

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Lisa M. Røst, Zdenka Bartosova, Kåre A. Kristiansen, Truls C. Rasmussen, Per Bruheim

Department of Biotechnology, Norwegian University, Stadsing Dahls gate 2, Trondheim 7015

Classification of Beer by Mass Spectrometric Metabolite Profiling

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Magdalena Buszewska-Forajta, Lukasz Kubik, Roman Kaliszan

Medical University of Gdansk, M. Curie Sklodowskiej 3a 584-09-55-985, Gdansk 80-210

Quantitative structure-retention relationships study in lipidomic analysis of grasshopper abdominal secretion (Chorthippus spp.)

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Yann GUITTON, Anne-Lise ROYER, Christelle Destoits-Lethimonier, Séverine Mazaud-Guittot, Bernard Jegou, Bruno Le Bizec, Jean-Philippe Antignac

LABERCA, Route de Gachet, Nantes 44307

Integrated metabolomic, lipidomic and steroidomic profiling for revealing signatures and markers of effect induced by bisphenols exposure on human testicular function

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Rosa Vázquez-Fresno, Shima Borzouie, Rupasri Mandal, David Wishart

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Application of Multi-platform Metabolomics for Characterization of the Chemical Composition of Food

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Koel Chaudhury, Mainak Dutta, Mamata Joshi, Sudha Srivastava, Swagata Dasgupta, Baidyanath Chakravarty

School of Medical Science and Technology, Indian I, School of Medical Science and Technology, Indian Institute of Technology, Kharagpur

Metabolomics reveals perturbations in the metabolome of endometriosis women

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Abstract number: 2380

Michael Judge, Ricardo Borges, James Griffith, Jonathan Arnold, Art Edison

University of Georgia, 410 Springdale St. Apt. 2, Athens GA 30606

Systems biology of circadian clock signaling in Neurospora crassa

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Kwang-Hyeon Liu, Jong-Cheol Shon, Yunhi Cho, Choong Hwan Lee

80 Daehakro, Bukgu, Daegu, 41566, Korea, Daegu 41566

Skin and plasma lipid profiling for the evaluation of the nutricosmetical effect of borage oil diet in healthy human subjects

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What Are We Eating? Differential Metabolomic Profiles Reveal an Insight into our Dietary Habits

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Mee Youn Lee, Yu Kyung Jang, Digar Singh, Hyang Yeon Kim, Soo Hwan Yeo, Seong Yeol Baek, Yoo Kyoung Park, Choong Hwan Lee

Konkuk University, Konkuk Univ., Hwayang-dong, Gwangjin-gu, Seoul, Korea, Seoul

MS-based metabolomic evaluation of traditional Rubus coreanus vinegar and its antiosteoporotic prophylactics in ovariectomized rat models

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Giorgis Isaac, Bharathi Avula, Yanhong Wang, Jimmy Yuk, Mark Wrona, Kate Yu, Ikhlas Khan

Waters Corporation, 34 Maple Street, Milford MA 01757

Metabolomics Approach for the Authentication of Various Botanicals and Dietary Supplements Using UPLC/QTof-MS

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Tim Stratton, Romain Huguet, Mark Berhow, Chad Weisbrod

Thermo Fisher Scientific, 355 River Oaks Parkway, San Jose CA 95134

The ETD-Like Fragmentation for Small Molecules

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Rachel Spicer, Larissa Richardson, Jules Griffin, Reza Salek, Christoph Steinbeck

EMBL-EBI, 10 Chesterford House Southacre Drive, Cambridge CB2 7TZ

The Lipidome in Weight Loss

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Po-Sheng Wang, Wen-Harn Pan

National Taiwan University, IBMS, No.128, Sec. 2, Academia Rd., Nangang Dist., Taipei

Using metabolomics approaches to explore the potential disease-causing mechanism of cooking oils: a short-term human feeding study

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Lee Gethings, David Charles, Peter Burney, Vanessa Garcia-Larsen

Stamford Avenue, Wilmslow

Nutritional metabolomics: A serum based metabolomics strategy for determining dietary flavanoid intake in human adults

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Kab Tae Park

College of Pharmacy and Research Institute of Phar, College of Pharmacy and Research Institute of Pharmaceutical Sciences, Kyungpook National University, Daegu 41566, Korea, Daegu

Lipidomics Analysis Reveals the Pharmacological Effects of Platycodon grandiflorum extracts in High-Fat Diet Induced Obese Mice

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Millie Rådjursöga, Göran Karlsson, Helen Lindqvist, Anders Pedersen, Cecilia Persson, Rui Pinto, Lars Ellegård, Anna Winkvist

Department of Internal Medicine and Clinical Nutri, Medicinaregatan 13 C, Box 459, Gothenburg 40530

Metabolic profiles from two different breakfast meals characterized by 1H NMR-based metabolomics

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Marie Tremblay-Franco, Cécile CANLET, Aurélien AMIEL, Isabelle SAVARY-AUZELOUX, Didier REMOND, Sergio POLAKOF

INRA ToxAlim, 180 chemin de Tournefeuille BP93173, TOULOUSE Midi Pyrénées 31027

Comparison of statistical methods to analyze longitudinal metabolomics data

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Matthew Teegarden, Morgan Cichon, Jessica Cooperstone, Jennifer Ahn-Jarvis, Christopher Weghorst, Yael Vodovotz, Steven Schwartz

The Ohio State University, 2015 Fyffe Court, Columbus OH 43210

Strawberry consumption alters the urinary metabolome of smokers and nonsmokers

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Olimpio Montero

Spanish Council for Scientific Research (CSIC), Francisco Vallés 8, Boecillo Valladolid 47151

Plasma biomarkers in Parkinson's disease

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Drupad Trivedi, Katherine Hollywood, Nicholas Rattray, Holli Ward, Dakshat Trivedi, Joseph Greenwood, David Ellis, Roy Goodacre

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Meat, the metabolites: an integrated metabolomics and lipidomics approach for the detection of meat adulteration

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Abstract number: 2221

Ying Wang

Novartis Institutes for Biomedical Research, Novartis Campus, Basel CH-4002

Precise Molecular-Feature Analysis (PMA) of UHPLC/Q-TOF MS for Metabolite Profiling in Synthetic Biology

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Annelaure Damont, Sophie Feuillastre, Grégory Pieters, Christophe Junot, François Fenaille

CEA Saclay, DRF/IBITEC-S/SPI/LEMM, Gif-sur-Yvette 91191

Investigation of metal-catalyzed regioselective H/D exchange as an efficient and flexible tool to produce stable isotope labelled compounds for quantitative metabolomics

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Jan Schripsema, Sonia Maria da Silva, Jaine Luiz, Anelique Almeida, Denise Dagnino

Universidade Estadual do Norte Fluminense, Grupo Metabolômica Av. Alberto Lamego, 2000, Campos dos Goytacazes 28013-602

Obtaining component NMR spectra through calculation – Isolation not required

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Nayumi Akimoto, Kunihiro Suda, Chiaki Ikeda, Daisuke Nakajima, Hideyuki Suzuki, Daisuke Shibata, Nozomu Sakurai

Kazusa DNA Research Institute, 2-6-7 Kazusa-kamatari Kazusa DNA Research Institute, Kisarazu Chiba 292-0818

FlavonoidSearch for high-throughput detection of flavonoids

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WENJUN XU

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Real-time monitoring of p53's effects on pyruvate metabolism in live mitochondria using in-organelle NMR metabolomics

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Serge Rudaz, Giuseppe Marco Randazzo, Julien Boccard, Fabienne Jeanneret, David Tonoli, Davy Guillarme, Alessandra Nurisso, Laura Goracci, Stephanie Hambye

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Dynamic LC retention times prediction for marker candidate's identification: steroidomics as a case study.

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yasumune nakayama, Takeshi Bamba, Eiichiro Fukusaki

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Avoiding compound miss-annotation caused by MS in-source decay using data-independent acquisition

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Prasad Phapale, Theodore Alexandrov, Maria Elena Diaz-Rubio, Andrew Palmer, Dominik Fay, Ivan Protsyuk

EMBL, Meyerhofstraße 1, HEIDELBERG Baden-Wuerttemberg 69117

Developing sample-specific workflows for broad and sensitive metabolomics

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Miriam Navarro, Oriol Senan, Xavier Domingo-Almenara, Jordi Capellades, Antoni Aguilar-Mogas, Jesus Brezmes, Marta Sales-Pardo, Roger Guimera, Oscar Yanes

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From 'peakomics' to metabolomics in LC-MS global profiling of human plasma

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Hector Gallart-Ayala, Shama Naz, Stacey Reinke, Caroline Mathon, Richard Blankley, Craig E. Wheelock

Karolinska Institutet, Scheeles väg 2, Stockholm

IMPROVING CONFIDENCE IN METABOLITE IDENTIFICATION IN NON-TARGETED LC-HRMS METABOLOMICS

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Hendrik Treutler

Leibniz Institute of Plant Biochemistry, Weinberg 3, Halle (Saale) D-06120

MetFamily – a novel tool to coin data into information

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Heike Bähre, Roland Seifert, Volkhard Kaever

Institute of Pharmacology, Hannover Medical School, Carl-Neuberg-Straße 1, Hannover 30625

Identification and quantitation of 2´,3´-cyclic nucleotides in murine tissues

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Felice de Jong, Chris Beecher

IROA Technologies, LLC, 184 Century Mill Rd, Bolton MA 01740

Identification of LC-MS metabolite fragments using IROA (Isotopic Ratio Outlier Analysis)

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Yong Jin An

Seoul National University, Seoul National Univ., Daehak-dong, Gwanak-gu, Seoul

13C-labeled dimethyl-a-ketoglutarate as a new tracer for real time metabolomic monitoring of TCA cycle in live cells.

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Michael Witting, Nina Sillner, Dany Spaggiari, Serge Rudaz, Jutta Lintelmann, Jörg-Peter Schnitzler, Olga Begou, Georgios Theodoridis, Helen Gika, Philippe Schmitt-Kopplin, Michael Quilliam

Helmholtz Zentrum München, Ingolstädter Landstraße 1, Neuherberg 85764

Retention time indexing in RP-LC-MS based metabolomics for enhancing metabolite identification: A cross-lab trial

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M. Elena Diaz-Rubio, Prasad Phapale, Andrew Palmer, Dominik Fay, Theodore Alexandrov

EMBL, Meyerhofstraße 1, Heidelberg Baden-Wurttemberg 69117

Open LC-OrbitraP-MS/MS spectral library facilitated by Curatr, a webapp for library curation, browsing and sharing

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Abstract number: 2542

Gavin Blackburn, Fiona Achcar, Karl Burgess

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Biological inference of metabolite identity from isotope labelled experiments.

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Tung Ting Sham, Chi On Chan, Na Ge, Hui Li Sun, Daniel Kam Wah Mok

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UPLC-QTOF-MS based serum metabolomic effect of diabetic kidney disease in Chinese patients

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Justin van Der Hooft, Joe Wandy, Sandosh Padmanabhan, Ronan Daly, Michael Barrett, Karl Burgess, Simon Rogers

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Exploring the fragmentome with unsupervised clustering and topic models

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Matthew Lewis, Jake Pearce, Konstantina Spagou, Simon Lovestone, Paul Elliott, Zoltan Takats, Elaine Holmes, Jeremy Nicholson

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Optimized UPLC-MS for High Precision Large Scale Metabolic Phenotyping of Human Urine

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Michael Groessl

TOFWERK, Uttigenstr. 22, Thun

Separation of isomers in lipidomics and metabolomics experiments by high resolution ion mobility-mass spectrometry

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Mark Sartain, Amy Caudy, Adam Rosebrock

Agilent Technologies, Inc., 5301 Stevens Creek Boulevard, Santa Clara CA 95051

A Targeted LC-MS/MS Method and Acquisition Database Optimized for Central Carbon Pathway Metabolites

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Abstract number: 2249

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Agilent Technologies, 5301 Stevens Creek Boulevard, Santa Clara CA 95051

High Performance Ion Pair-Reverse Phase LC/Q-TOF Method for Profiling Diverse Classes of Endogenous Metabolites with Separation of Important Isomers

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Jun Han, Georgia Mitsa, Karen Lin, Juncong Yang, Christoph H. Borchers

UVic-Genome BC Proteomics Centre, 3101-4464 Markham St, Victoria BC V8Z 7X8

Development of a chemical derivatization - UPLC-MRM/MS method for quantitation of bile acids in dried blood spots

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Stephen Ayris

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Evaluation of High Speed, High Resolution Data Independent Acquisition for the Analysis of Metabolomic Flux, Kinetics and Pathway Mapping

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Akiyoshi Hirayama, Masaru Tomita, Tomoyoshi Soga

Keio University, 246-2 Kakuganji, Mizukami, Tsuruoka Yamagata 997-0052

Development of anionic metabolome analytical platform using ion chromatography-mass spectrometry (IC-MS)

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Andrew Chetwynd, Riccardo Di Guida, Elliott Palmer, Giovanny Rodriguez-Blanco, AnnMarie Withanage, Warwick Dunn

University of Birmingham, School of BioSciences, Birmingham

Mammalian Tissue Metabolomes: A Qualitative Comparison

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Katrice Lippa, Bruce Benner, Jr., Nik Blonder, Werickson Rocha, David Sheen, Yamil Simon, Dan Bearden

National Institute of Standards and Technology, 100 Bureau Drive MS 8390, Gaithersburg MD 20899

A Quality Assurance Program for Metabolomics: Can NIST Help?

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Mohamed Salem

Max Planck Institute of Molecular Plant Physiology, Am Mühlenberg 1 Golm, Potsdam Brandenburg 14476

A triphasic single-step method for rapid, comprehensive and simultaneous extraction of lipids, metabolites and proteins from a single plant sample.

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Mark Haid, Marina Rudisch, Caroline Muschet, Jerzy Adamski

Helmholtz Zentrum Muenchen, Ingolstaedter Landstr. 1, Neuherberg/Muenchen Non US/ Canada 80637

Target metabolomics assay for absolute quantification of omega-3 and omega-6 oxylipins in human plasma

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Xue Li, Lei Huang, Zhen Zhou

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Real-time measurement of chemical composition of exhaled human breath by ambient ultrahigh resolution mass spectrometry

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hanna eriksson röhnsich, Elisabeth Mullner, Jan Eriksson, Peter Agback, Ali Moazzami

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Automated high-throughput profiling of human plasma NMR-metabolites

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Oliver Jones, Michelle Spencer

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Computational chemistry in metabolomics: The design and application of novel fluorescent tags for the detection of fatty acids by HPLC

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Carl Brunius, Lin Shi, Rikard Landberg

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Strategies for within and between batch data correction for large-scale LC-MS metabolomics data

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Rick Reisdorph, Nichole Reisdorph, Scott Walmsley, Samantha Bokatzian, Kevin Quinn, Roger Powell

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Effective, standardized metabolomics workflow applied to 3 studies of cell toxicity

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DIRCE MARCHIONI, Augusto Carioca, Josiane Steluti, Andreia Miranda, Aline Carvalho, Ismael Silva, Alexsandro Silva, Regina Fisberg

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Association between obesity and amino acids: a metabolomics approach

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Nan Wang, Xiaoling Su, Jingjing Lu, Derrick Blackmore, Zaeem Siddiqi, Liang Li

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Comprehensive and Quantitative Metabolomic Analysis Using Chemical Isotope Labeling LC-MS for Disease Biomarker Discovery

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Christopher Hughes, Lee Gethings, Johannes Vissers, Keith Richardson, Jason Wildgoose

Waters Corporation, Stamford Avenue Altrincham Road, Wilmslow UK SK9 4AX

Advances in Targeted Omics Quantitation Using a Novel Scanning Quadrupole DIA Method

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Guowang Xu, Ping Luo, Yanni Zhao, Yang Ouyang, Xinjie Zhao, Peiyuan Yin, Xin Lu

Dalian Institute of Chemical Physics, CAS, 457 Zhongshan Road, Dalian 116023

How to carry out large-scale metabolomics studies based on GC-MS or LC-MS

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Karl Burgess, Stefan Weidt, Jennifer Haggarty, Cristian Cojocariu, Paul Silcock, Gordon Ramage

University of Glasgow, Wolfson Wohl CRC, Garscube Campus University of Glasgow, Glasgow

Application of GC - QExactive to explore fungal/bacterial interactions

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Shinobu Kudoh, Ippei Takeuchi

Shimadzu Techno-Research, Inc, 3-19-2 minami-Rokugoh, Ohta-ku Tokyo 144-0045

Introduction of a quantitative microsampling device

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Reiko Kiyonami, Claire Dauly, Ralf Tautenhahn, David Peake, Ken Miller

Thermo Fisher Scientific

Increased Metabolome Identification Coverage Using Optimized LC-MS-MS Conditions on a Tribrid Orbitrap Mass Spectrometer

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SU JIN LEE

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Multiple isotopomer analysis with Non-uniform sampled NMR for cellular metabolomic studies.

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Huanwen Chen, Hua Zhang, Liang Zhu, Haiyan Lu

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Internal Extractive Electrospray Ionization Mass Spectrometry for Metabolomics Studies

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Arturas Grauslys, Ralf Weber, Warwick Dunn, Andrew Jones, Mark Viant

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Galaxy workflows for mass spectrometry and NMR spectroscopy-based metabolomics

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Richard Yost, Christopher Chouinard, Michael Costanzo, Michael Wei, Robin Kemperman, Nicholas Oranzi, Timothy Garrett

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Ion Mobility/Mass Spectrometry for Metabolomics and Clinical Analysis: Progress and Prospects

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Shao Thing Teoh, Sastia Putri, Yukio Mukai, Eiichiro Fukusaki

Osaka University, C2-211, Graduate School of Engineering, Osaka University Yamada-oka 2-1, Suita Osaka 565-0871

A data mining algorithm based on Random Sample Consensus (RANSAC) for the selection of metabolites relevant to strain improvement

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Yutaka KONYA

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Novel high-throughput and widely-targeted LC-TOFMS method for D-amino acids Metabolomics

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Single sample analysis for proteomics and metabolomics

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Daniel Raftery, Haiwei Gu

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Globally Optimized Targeted Mass Spectrometry (GOT-MS): Reliable Metabolomics Analysis with Broad Coverage

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Fedor Kryuchkov, Mathias Ziegler, Frank Kjeldsen

UiB, Thormølens gate 55, 5th floor, Bergen Hordaland 5008

Segmenting of mass range improves metabolite identification for Exactive type mass spectrometers

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Dajana Vuckovic, Dmitri Sitnikov, Hanieh Peyman, Parsram Ramrup

Concordia University, 7141 Sherbrooke Street West, Montreal QC H4B1R6

Doubling metabolite coverage in untargeted metabolomics of human plasma

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Abstract number: 2355

Garth Maker, Alicia Manning, Ian Mullaney, Robert Trengove

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Biochemical changes associated with retinoic acid-induced differentiation of SH-SY5Y human neuroblastoma cells

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Padma Maruvada, David Balshaw, Arthur Castle, Danthi Simhan, Leslie Derr, Chanda Dutta, Yih-Woei Fridell, Katrnia Gwinn, Conrad Mallia, Aaron Marquitz, Gary Murray, Andrew Maynard, Laurie Nadler, Richard Okita, Steven Oversby, Lita Proctor, John Satterlee, Daniel Shaughnessy, Lillian Shum, Pothur Srinivas, Danilo Tagle, Hung Tseng, Jose Velázquez, Mukesh Verma, Keren Witkin, Krista Zanetti, Oliver Fiehn, Charles Burant, Susan Sumner, Richard Yost, Richard Higashi, Sree Nair, Shankar Subramaniam

National Institute of Diabetes, and Digestive and, 6707 Democracy Blvd #663, Bethesda MD 20892

National Institutes of Health Common Fund-Metabolomics Community Resources

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Abstract number: 2374

Aoife O'Gorman, Mary Cannon, Lorraine Brennan, UCDDavid Cotter, Matej Oresic, Tuulia Hyotylainen, Tommi Suvitaival, Stanley Zammit

Royal College of Surgeons in Ireland, Beaumont Hospital Beaumont, Dublin 9 na

Identification of biomarkers associated with early psychotic disorder (ages 12 and 18) in the Avon Longitudinal Study of Parents and Children (ALSPAC) cohort using a lipidomic approach.

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Abstract number: 2558

Michaela Schwaiger, Karin Ortmayr, Gerrit Hermann, Kristaps Klavins, Evelyn Rampler, Walter Miklos, Walter Berger, Gunda Koellensperger

University of Vienna, Analytical Chemistry, Waehringer Str. 38, Vienna 1090

Comparison of different analytical platforms for non-targeted metabolomics of cancer cells

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Abstract number: 2485

Haiyan Lu, Hua Zhang, Wei Zhou, Yiping Wei, Huanwen Chen

East China University of Technology, No.418, Guanglan Avenue, Nanchang

Sequential Detection of Metabolites, Lipids and Proteins in a Bulk Tissue Using Internal Extractive Electrospray Ionization Mass Spectrometry

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Abstract number: 2554

Cyrus Papan, Joerg Dojahn, Hartmut Michel, Julian Langer

AB Sciex Germany, Landwehrstrasse 54, Darmstadt 64293

Selexion-based removal of detergent interference for shotgun-lipidomics

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Terri christison, Junhua Wang, Ken Cook, Ryo Komatsuzaki, Linda Lopez, David Peake

Thermo Fisher Scientific, 1214 Oakmead Parkway, Sunnyvale CA 94088

Determining polar metabolites using high throughput ion chromatography (IC) coupled with high resolution accurate mass spectrometry (HRAM)

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Clémence de Jaham

INRA Bordeaux, UMR 1332 Fruit Biology and Pathology CS 20032, Villenave d'Ornon Aquitaine 33882

Carbon metabolism in sugar beet leaves experiencing heat stress

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Abstract number: 2219

Thierry BERTON, Stephane BERNILLON, Mickael MAUCOURT, Catherine DEBORDE, Natalia FALAGAN, Marine SAUX, Hayat BOUTEAU, Christophe BAILLY, Annick MOING

INRA Bordeaux, UMR1332 Fruit Biology and Pathology 71 avenue Edouard Bourlaux, Villenave-d'Ornon F-33140

Metabolomic study of tolerance to water limitation for sunflower germination

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Abstract number: 2387

Amal Surrati, Rober Linforth, Ian Fisk, Virginie Sottile, Dong-Hyun Kim

Wolfson Centre for Stem Cells, Tissue, Engineering, Wolfson Centre for Stem Cells, Tissue, Engineering and Modelling (STEM), School of Medicine, University of Nottingham, Nottingham

LC-MS-based metabolite footprinting: Application to the characterisation of mesenchymal stem cell differentiation

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Abstract number: 2414

Christine Sambles, Hannah Florance, Deborah Salmon, Thomas Howard, Nicholas Smirnoff, Lene Rostgaard Nielsen, Erik Dahl Kjær, David Studholme, Murray Grant

University of Exeter, Geoffrey Pope Building, University of Exeter Stocker Road, Exeter Devon EX4 4QD

Metabolomic profiling of Fraxinus excelsior genotypes tolerant or susceptible to ash dieback disease reveals changes in specific glycosides.

P-310

Abstract number: 2012

Martin Schafer, Christoph Brutting, Mario Kallenbach, Gordon van 't Slot, Magdalene Kutyniok, Ian Baldwin

MPI for Chemical Ecology, Jena, Germany, Max Planck Institute for Chemical Ecology, Department for Molecular Ecology

Targeted analysis of primary- and secondary-metabolites, and phytohormones from a single plant extract – a method accounting for complexity in plant metabolomics

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Abstract number: 2207

Annick Moing, Maria Urrutia, Olivier Fernandez, Vanessa Zhendre, Nadia Lamari, Stephane Bernillon, Mickael Maucourt, Catherine Deborde, Daniel Jacob, Patricia Ballias, Helene Sellier, Isabelle Quillere, Bertrand Hirel, Nicolas Langlade, Catherine Giauffret, Yves Gibon

INRA Bordeaux, UMR1332 Fruit Biology and Pathology Bordeaux Metabolome Facility, 71 av. E. Bourleaux, Villenave d'Ornon F-33140

Searching for marker metabolites of crop performance

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Abstract number: 2139

Jan Hazebroek, James Janni, April Agee Carroll, Roland Welle, Richard Fox, Teresa Harp, Chris Vlahakis, Jian Jin

DuPont Pioneer, 8325 NW 62nd Ave. P.O. Box 7062, Johnston IA 50131-7062

High throughput metabolomics and hyperspectral imaging of greenhouse grown maize plants reveal response to nitrogen treatments and predict field yield

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Yasuhiro Higashi, Yozo Okazaki, Fumiyoshi Myouga, Kazuo Shinozaki, Kazuki Saito

RIKEN CSRS, 1-7-22 Suehiro, Tsurumi, Yokohama Kanagawa 230-0045

Landscape of the lipidome and transcriptome under heat stress in Arabidopsis thaliana

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Fidele Tugizimana, Ian Dubery

University of Johannesburg, Auckland Park, Johannesburg Gauteng 2006

Metabolic reprogramming in Sorghum bicolor in response to Colletotrichum sublinoelum infection.

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CARLA ANTONIO, Carola Päpke, Marcio Rocha, Houssein Diab, Anis Limami, Toshihiro Obata, Alisdair Fernie, Joost van Dongen

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Regulation of respiratory metabolism in response to flooding stress as revealed by 13C-stable isotope redistribution

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Si Wu, Lothar Willmitzer

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Metabolomics-based genome wide association study combining with network analysis provides insights into Arabidopsis secondary metabolism

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Matthias Szesny, Dirk Wunderlich, Jens Fuchser, Stephanie Grond, Florian Zubeil, Dorothee Weisbrod

Bruker Daltonik, Fahrenheitstr. 4, Bremen

Interaction between pathogenic bacteria and higher organisms -MALDI-Imaging based study reveals novel secondary metabolites

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Hayashi G, Junko S, Kubo A, Imanaka T, Agrawal GK, Shioda S, Fukumoto M, Oros G, Rakwal R, Deepak SA, Seetaramanjaneyulu Gundimeda, Upendra Simha, Arunkumar Padmanaban

Tohoku University

A multi-omic approach to reveal the effect of low-level gamma radiation in rice seeds

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Chuan-Ho Tang, Shu-Han Shi, Shu-Hui Lee, Wei-Hsien Wang

National Museum of Marine Biology and Aquarium, 2 Houwan Rd., Checheng, Pingtung

Glycerophosphocholine profiling of the coral symbiotic algae in response to slight copper contamination

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Roderquita Moore, Michael Leitch, Erick Arellano-Ruiz, Doreen Mann

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Mountain beetle pine infestation: Acetone extractives polar fraction of Lodge pole (pinus contorta) pine

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Ralf Tautenhahn, Tim Stratton, Dipankar Ghosh

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Cloud-based analysis of complex sample systems for outlier and trend analysis in the context of water monitoring

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24 avenue Blaise Pascal, Clermont-Ferrand F-63171

Meta-metabolomics, what did you expect ?

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Alexander Weinhold, Onno Calf, Michael Singer, Camille Parmesan, Nicole van Dam

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Ecometabolomics – Understanding biodiversity on a chemical level

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Christina Jones, John Bowden, Russell Day, Tracey Schock

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Environmental Metabolomics Using a Sentinel Species: Methodological Considerations

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Morteza Gholami

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Stereoselective regulation of metabolism of tobacco cells under salinity stress by means of ornithine enantiomers

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Rahul Kapoore, Maria Huete-Ortega, Katarzyna Okurowska, Seetharaman Vaidyanathan

The University of Sheffield, Sir Robert Hadfield Building Mappin street, SHEFFIELD South Yorkshire S1 3JD

Influence of enhanced CO2 concentration and light/dark cycles on growth, biochemical composition and metabolic profile of Chlorella vulgaris (CCAP 211/21A)

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Gregory Ellis

4555 Overlook Ave. SW, Washington DC 20375

Eavesdropping on Marine Microbial Communication: Influence of Quorum Sensing on the Vibrio campbellii Metabolome

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Vera Kovacevic, André Simpson, Myrna Simpson

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1H NMR-based metabolomics reveals that dissolved organic matter alters the toxicity of organic contaminants to Daphnia magna.

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A multiscale modeling approach including metabolomics reveals the differential impact of dairy fats on the development of atherosclerosis in hamsters

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Nicole van Dam, Alexander Weinhold, Katharina Grosser, Stan Harpole

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Ecometabolomics for Biodiversity: Tapping into chemical communication in the wild

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Núria Dalmau

IDAEA-CSIC, Jordi Girona 18-26, Barcelona 08034

Untargeted lipidomic study of UV radiation effects in human skin cells

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Zhi-Yi Du, Guang-Wen Lien, Pau-Chung Chen, Ching-Yu Lin

Institute of Environmental Health, College of Publ, No. 16-5, Siyuan Street, Zhongzheng Dist., Taipei City 100 Building C, Floor 14 Rm No. 28, Taipei

Metabolomic Study of Environmental Exposure: Effects of Perfluoroalkyl Substances and Phthalates on Children

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Dae-Yong Yun, Young-Gyu Kang, Myoyeon Kim, Jun Seong Park, John Hwan Lee, Young-Shick HONG

Chonnam National University

Metabolomic Unveiling of Distinctive Metabolism between Semi-wild and Wild Soybean

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Meritxell Navarro-Reig, Joaquim Jaumot, Gabriel Vivo-Truyols, Peter Schoenmakers, Romà Tauler

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UNTARGETED LCxLC-HRMS APPLIED TO THE METABOLOMIC STUDY OF CIRCADIAN RHYTHM IN JAPANESE RICE

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Carl Angelo Medriano, Ryan De Sotto, Sungpyo Kim, Youngja Park

Korea University, College of Pharmacy, Korea University Sejong Campus, Sejong-ro, Sejong City 30019

Zebrafish response to low concentration perfluorinated compounds PFOA and PFOS: Metabolomic perspective

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Community Metabolomics for Analysing Stress Responses in Environmental Biofilms

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Sophie Dietz, Katharina Herz, Karin Gorzolka, Nadine Strehmel, Ute Jandt, Helge Bruelheide, Dierk Scheel

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Effects of biodiversity on exuded and inner root metabolites in grassland communities

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Isma Belouah, Thierry Balliau, Camille Bénard, Bertrand Beauvoit, Sophie Colombie, Stéphane Bernillon, Patricia Ballias, Cécile Cabasson, Mickäel Maucourt, Catherine Deborde, Annick Moing, Benoit Biais, Dominique Rolin, Michel Zivy, Yves Gibon, Mark Hooks

INRA -- University of Bordeaux, INRA -- University of Bordeaux, UMR 1332 Fruit Biology and Pathology, 71 Ave E. Bourlaux, BP 81, Villenave d'Ornon 33882

The timing of shifts in the transcriptome and proteome in relation to metabolic state during tomato fruit development

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Hilal Taymaz-Nikerel, Serpil Eraslan, Betul Kirdar

Bogazici University, Department of Chemical Engineering, Bebek, Istanbul 34342

Metabolomic analysis of Saccharomyces cerevisiae in the presence of imatinib

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Alexey Shavarda, Ekaterina Kotlova, Gregory Pozhvanov, Katerina Sazanova, Svetlana Senik

Komarov Botanical Institute, prof.Popov Str. 2, St.-Petersburg

EXISTENTIAL METABOLOMICS: VISUALIZATION OF GROWTH AND DEVELOPMENT PROCESSES THROUGH METABOLITE PROFILING

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Marit Stafsnes, Truls Rasmussen, Per Bruheim

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Metabolite profiling of Saccharomyces cerevisiae grown on different carbon sources

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Francesca Casu, Sergey Tumanov, Eliezer Stefanello, Farhana Pinu, Silas Villas-Boas

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The metabolic response of Saccharomyces cerevisiae to linoleic and conjugated linoleic acids

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Olli Kärkkäinen, Jouni Ihalainen, Katja Savolainen, Kati Hanhineva, Markus Forsberg

University of Eastern Finland, Yliopistonranta 1, Kuopio 70211

Phencyclidine-induced changes in the metabolic activity of the rat brain

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Michael Muelleder, Markus Ralser

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A genome-scale map of amino acid metabolism by metabolic profiling of a prototrophic gene deletion collection of Saccharomyces cerevisiae

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Clare Scott Chialvo, Fariba Tayyari, Thomas Werner, Arthur Edison, Laura Reed

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Characterizing the metabolism of the deadly mushroom toxin a-amanitin in mushroom-feeding Drosophila

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Robin Wördenweber, Jan Mussgnug, Olaf Kruse

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Metabolic analyses of the calcification process in the marine microalgae Emiliania huxleyi

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Isabel Orf, Stefan Timm, Hermann Bauwe, Alisdair Fernie, Martin Hagemann, Joachim Kopka, Zoran Nikoloski

MPI of Molecular Plant Physiology, Am Mühlenberg 1, Potsdam OT Golm 14476

Meta-data analysis of metabolite profiles reveals potential usability of cyanobacteria as models of plant photorespiration

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Vishal Oza

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Untargeted metabolomics elucidates the role of diet and triglyceride storage in Drosophila melanogaster larvae

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Anders Honoré, Henrik Jensen, Niels Christensen, Panagiotis Chanos, Helle Jackson, Joseph Kozole, Jana Fischer

DuPont Nutrition Biosciences ApS, Edwin Rahrs vej 38, Brabrand DK-8220

Forced degradation and LC/MS profiling in search of bioactive metabolites in Bacillus amyloliquiefaciens fermentates

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Yunping Qiu, Michelle Reid, Robyn Moir, Ian Willis, Chris Beecher, Richard Yost, Timothy Garrett, Irwin Kurland

Albert Einstein College of Medicine, 1301 Morris Park Ave, Bronx NY 10461

Improved Global identifiability with orthogonal platforms of LC/Orbitrap-MS and GC/TOF-MS using IROA

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Martin Jones, Tom Lawson, Ralf Weber, Clement Heude, Andrew Chetwynd, Warwick Dunn, Mark Viant

University of Birmingham

Multi-platform non-targeted deep metabolome annotation of the ecotoxicological and NIH model organism, Daphnia magna

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Federico Torta

National University of Singapore, 28 Medical Drive, Singapore

A murine sphingolipids atlas and its use in translational research

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Danuta Chamot, Lu Deng, Rupasri Mandal, Trent Bjorndahl, Siamak Ravanbakhsh, Jason Grant, Michael Wilson, Beomsoo Han, Arnau Serra-Cayuela, Ying (Edison) Dong, Russell Greiner, David Wishart

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Automated kits and software for quantitative metabolomics

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Noelia Ramirez, Sara Samino, Sonia torres, Neema Adhami, Manuala Martins-Green, Xavier Correig

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Multiplatform MS metabolomics reveals metabolic disorders in mice exposed to thirdhand tobacco smoke

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Ákos Kenéz, Sven Dänicke, Martin von Bergen, Korinna Huber

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Characterisation of the blood metabolome of dairy cows as affected by adaptation to lactation

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Michael Witting, Marianna Lucio, Romé Voulhoux, Steve Garvis, Reto Ossola, Andrea Amantonico, Cassandra Wigmore, Philippe Schmitt-Kopplin

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A metabolomics approach to study bacterial virulence in Caenorhabditis elegans

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Karin Gorzolka, Hendrik Treutler, Gerd Balcke, Steffen Neumann, Dierk Scheel

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13CO2 Isotope labelling for the elucidation of carbon fixation, metabolite transport and exudation processes in Arabidopsis thaliana

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Software: Nexus Point of a Targeted Lipid Analyzer

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Abstract number: 2176

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Global metabolomics reveals hydroxyacylcarnitine as a novel endogenous metabolic marker for CYP3A activity

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Kumsun Cho

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Combined untargeted and targeted metabolomic profiling reveals urinary biomarkers for discriminating obese from normal weight adolescents

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Luca Rappez, Andrew Palmer, Ivan Protsyuk, Prasad Phapale, Bachir El Debs, Joel Selkrig, Nassos Typass, Theodore Alexandrov

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Metabolic factors involved in Salmonella pathogenicity

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Baldur Sigurdsson, Giuseppe Paglia, Sigurdur Smárason

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Chemometric optimization of an LC-MS/MS method for the quantification of 70 selected metabolites related to mitochondrial health

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Isabel Borrás Linares, Álvaro Fernández Ochoa, Rosa Quirantes Piné, David Arráez Román, Marta Alarcón Riquelme, Ángel De la Torre Vega, Antonio Segura Carretero

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Fingerprinting metabolomic approach by HPLC-ESI-QTOF-MS to find biomarkers of Mixed Connective Tissue Disease (MCTD): A preliminary study.

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Ali Yilmaz, Stewart Graham, Ray Bahado-Singh

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Metabolomic biomarkers in saliva for the diagnosis of Alzheimer's disease

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Lars Ridder, Lonneke Duijghuijsen, Richard Bas, Martie Verschuren, Jaap Keijer, Harry Wichers, Renger Witkamp, Klaske Van Norren

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Distinct urinary metabolite profiles after strenuous exercise combined with casein intake

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alicia sanchez, Sandra Benito, nora unceta, ramon barrio, maria aranzazu goicolea, J.J. Jansen, G Postma, L.M.C. Buydens, fernando andrade, L Aldámiz-Echevarria

University of the Basque Country (UPV/EHU), miguel de unamuno 3, vitoria-gasteiz

IDENTIFICATION OF POTENTIAL BIOMARKERS IN PLASMA FROM PEDIATRICS WITH CHRONIC KIDNEY DISEASE BY MEANS OF MULTIVARIATE CHEMOMETRIC APPROACHES APPLIED TO LC-QTOF-MS BASED TARGETED METABOLOMICS DATA

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Metabolic characterization of internet addiction disorder and discovery of integrative biomarker coupled to clinical parameters.

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Dorsa Varshavi, Ian Phillips, Flora Scott, Elizabeth Shephard, Kirill Veselkov, Jeremy Everett

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Biomarkers of Ageing in wild type and flavin monooxygenase 5 knockout mice

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Metabomatching: A tool for untargeted identification of genetically determined metabolites

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Enara Arretxe, Raul Jimenez-Agüero, Marta Iruarrizaga-Lejarreta, Luis Bujanda, David Balgoma, Maria J Perugorria, Emma Eizaguirre, Marcin Krawczyk, Frank Lammert, Jesus M Banales, Cristina Alonso

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A NOVEL LIPIDOMIC MODEL IN SERUM CORRELATES WITH THE BIOCHEMICAL AND MAGNETIC RESONANCE IMAGING RESULTS IN NAFLD DIAGNOSIS

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ERHAN SIMSEK, Sam Fong Yau Li

Chemistry Dept, NUS, Blk 236 Bt Panjang Ring Road # 05-53, SINGAPORE SINGAPORE 670236

LC-MS based untargeted metabolomics approach to explore biomarkers of aging in rat serum

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Shachi Saluja, Dietrich Merkel, Ujjaini Dasgupta, Dipankar Malakar, Manoj Pillai, Avinash Baja

RCB, Faridabad, India

Sphingolipid Profiling using Robust and Sensitive LC-MS-MS Method

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Nilanjana Ghosh, Elavarasan Subramani, Mamta Joshi, Saumya Samanta, Parthasarathi Bhattacharyya, Rintu Banerjee, Koel Chaudhury

Indian Institute of Technology, Kharagpur, School of Medical Science and Technology, Kharagpur West Bengal 721302

NMR based metabolomics of exhaled breath condensate to differentiate between asthma, chronic obstructive pulmonary disease and asthma-chronic obstructive pulmonary disease overlap syndrome

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David Alonso, Xiaoli Wei, Ming Song, Xinmin Yin, Biyun Shi, Joe Binkley, Michelle Page, Craig McClain, Xiang Zhang

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Increased fructose consumption and inadquate copper intake on the pathogenesis of nonalcoholic fatty liver disease (NAFLD): A feces and liver metabolomics study

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Olga Begou, Anastasia Chrysovalantou Chatziioannou, Kosmas Sarafidis, Agathi Thomaidou, Helen Gika, Aggeliki Kontou, Elisavet Diamanti, Charalambos Agakidis, Vasiliki Drossou, Nikolaos Raikos, Georgios Theodoridis

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Urine targeted LC-MS/MS profiling of hydrophilic metabolites in neonates with late onset sepsis

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Spyros Vernardis, Athanasios Mantalaris

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ROCK inhibition affects the metabolic physiology of human pluripotent stem cells

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Lea Johnsen, Morten Danielsen

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PARADISe a novel allinone software for automated chromatographic peak deconvolution, identification, and quantification

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Alexandra Parich, Benedikt Warth, Christoph Bueschl, Denise Schoefbeck, Bernhard Kluger, Rudolf Krska, Marc Lemmens, Gerhard Adam, Rainer Schuhmacher

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GC-MS based metabolomics of Fusarium head blight using near-isogenic lines of wheat

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Johannes Hertel, Nele Friedrich, Maik Pietzner, Katharina Wittfeld, Kathrin Budde, Sandra Van der Auwera, Alexander Teumer, Lara Strobel, Robin Winkelmann, Hans Liebscher, Thomas Kocher, Matthias Nauck, Hans Grabe

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Statistical Criteria for Testing Metabolites and Prediction Rules on Stability over Time in One-Time Urinary Metabolomic Measurements

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Abstract number: 2429

Daniel Wilkinson, Matthew Swift, Philip Atherton, Ken Smith

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Targeted metabolomics to identify links between ageing and musculoskeletal health in humans – A pilot study

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Martin Grootveld, Victor Ruiz-Rodado, Danielle te Vruchte, Daniel Sillence, Fay Probert, David Elizondo, Robin Lachmann, Frances Platt

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Seeking Biomarkers for Niemann-Pick Type C1 Disease: A 1H NMR-Linked Metabolomics Study

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Maria Laura Santoru, Cristina Piras, Antonio Murgia, Sonia Liggi, Pierluigi Caboni, Paolo Usai, Aldo Manzin, Tonina Lai, Luigi Atzori

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GC/MS and 1H-NMR metabolomic approach for the study of IBD patients

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Julian Avila, Amanda Souza, Shuba Gopal, Sarah Jeanfavre, Ralf Tautenhahn, Tim Stratton, Nathan Shappiro, Clary Clish

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Identification of plasma metabolic indicators of sepsis and sepsis severity using high-resolution accurate-mass and fragmentation profiles

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Maik Pietzner, Beatrice Engelmann, Tim Kacprowski, Janine Golchert, Anna-Luise Dirk, Georg Homuth, Elke Hammer, Matthias Nauck, Henri Wallaschofski, Thomas Münte, Nele Friedrich, Uwe Völker, Georg Brabant

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Complementary fingerprinting of a human thyrotoxicosis model using proteomics and metabolomics

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GLYCOSPHINGOLIPID ANALYSIS BY UHPLC-MS IN FIBROBLASTS – A FEASIBILITY STUDY

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Abstract number: 2351

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Metabolite identification using Orbitrap based spectral library matching: challenges and insights

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Abstract number: 2404

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Institute of Microbiology ASCR, Vídenská 1083, Prague

Spontaneously hypertensive rats on high-fat diet as a model of metabolic syndrome and impact of antiobesity treatment

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Abstract number: 2539

Barbara Rindlisbacher, Carina Strebel, Sabina Guler, Thomas Geiser, Cédric Bovet, Manuela Funke

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Metabolic profiling of exhaled breath condensates as potential diagnostic tool for patients with idiopathic pulmonary fibrosis – a pilot study

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Utility of lung-related biofluids in metabolomics-based lung disease research

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Caroline Mathon, Hector Gallart Ayala, Shama Naz, Stacey Reinke, Kameran Daham, Sven-Erik Dahlen, Barbro Dahlen, Craig Wheelock

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Non-targeted metabolomics approach to evaluate the effects of a selective COX-2 inhibitor in asthma

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SCOTT HARRISON, Andrew Chetwynd, Donna O'Neil, Giovanny Rodriguez Blanco

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The analysis of extremely polar compounds

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Abstract number: 2584

Marc Gunter, Steven Moore, Cornelia Ulrich, Rachael Stolzenberg-Solomon, Elizabeth Poole, Marinella Temprosa, Mukesh Verma, Demetrius Albanes, Eric Boerwinkle, Juan Casas, Clary Clish, Robert Gerszten, Bing Yu, Tamara Harris, David Herrington, Claudia Langenberg, Luca Lotta, Loic Le Marchand, Charles Matthews, Cristina Menni, Alexandre Pereira, Kathryn Rexrode, Svati Shah, Xiao Ou Shu, Victoria Stevens, Krista Zanetti

International Agency for Reserach on Cancer

COnsortium for METabolomics Studies (COMETS): Leveraging Resources to Accelerate Scientific Discovery

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Staphylococcus aureus Mediated Cell Death in Keratinocytes

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UPLC-MS/MS Analysis of Glucosylceramide and Galactosylceramide Isoforms in Parkinson's Disease Brain Tissues

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Investigation of the Stability of Dried Blood and Urine Spots for Untargeted Metabolomic Applications of Healthy Ageing

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Abstract number: 2121

Giovanny Rodriguez Blanco, Riccardo Di Guida, Elliott Palmer, Andrew Chetwynd, Emily Bailey, Matthew Soden, Scott Harrison, Sarah Aldred, Warwick Dunn

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Metabolic perturbations associated with exercise to exhaustion and the influence of cherry juice to reduce oxidative stress during exercise

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LYSOPHOSPHATIDYLCHOLINES TO PHOSPHATIDYLCHOLINES RATIO PREDICTS ADVANCED KNEE OSTEOARTHRITIS

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Abstract number: 2182

Anna Artati, Anja Wilmes, Alexander Cecil, Paul Jennings, Jerzy Adamski

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Metabolome changes during differentiation of induced pluripotent stem (iPS) cell into renal lineages

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Abstract number: 2255

Andrew Kim, Jaeseong Oh, Bora Kim, Jieon Lee, SeungHwan Lee, Kyung-Sang Yu, In-Jin Jang, Joo-Youn Cho

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CYP3A ACTIVITY AMONG SUBJECTS WITH DIFFERENT CYP2C19 GENOTYPES: GC-MS BASED QUANTITATION OF ENDOGENOUS METABOLIC MARKERS

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Abstract number: 2277

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A simple method for the diagnosis of bile acids malabsorption: quantification of 7a-hydroxy-4-cholesten-3-one

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