Programme

Clinical Metabolomics
Copenhagen 2021

Thursday 26 August - Friday 27 August

Clinical Metabolomics Copenhagen 2021

Thursday 26 August

8:20	Registration

Session 1: Health - Chaired by Karolina Sulek

8:50	Welcome by Niels Henrik von Holstein-Rathlou, SCO, Novo Nordisk Foundation
9:00	Jennifer Kirwan. Metabolomics enables precision medicine: improving health by understanding disease.
9:30	Cristina Legido Quigley. Metabolomics in the Diabetes Clinic, current and future perspectives
10:00	Mette Christensen. Metabolomic screen for inborn errors of metabolism in the (Danish) biochemical genetic laboratory – present and future perspectives.
10:25	Coffee Break

Session 2: System biology - Chaired by Mette Christensen

10:45	Maria Fedorova. From analysis to data integration: lipidomics signatures of human metabolism
11:15	Maria Klapa. Metabolomics in Psychiatric Research: Profiling antenatal and postpartum depression
11:45	Gabi Kastenmüller. From associations to insights: Building an integrated molecular atlas of Alzheimer's Disease
12:15	Douglas McCloskey. SmartPeak Automates Metabolomics, Fluxomic, and Lipidomic Data Processing
12:45	Lunch

Session 3: Nutrition - Chaired by Madeleine Ernst

13:45	Lorraine Brennan. Metabolomic based insights for Nutrition Research
14:15	Hanne Christine S. Bertram. Food of animal origin: the good, the bad or the evil?
14:45	Sofia Moco. The NAD+ metabolome from mechanistic to clinical applications – a window towards assessing NAD+ biosynthesis and breakdown.
15:15	Justin J.J. van der Hooft. The urine and fecal metabolome decomposed into food, drug, host, and microbiome-related components through substructure-based approaches
15:40	Coffee Break

Session 4: Personalised Medicine - Chaired by Markus Herrgård

16:00	Nicola Zamboni. Democratization of untargeted methods in clinical research
16:30	Alice Limonciel. Metabolomics in the context of the gut-brain axis
17:00	David Wishart. Making Metabolomics More Personal
18:30	Social event KU for local attendees and speakers

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Friday 27 August	
8:30	Registration
Session 1: Lipidomics - Chaired by Cristina Legido Quigley	
9:00	Craig Wheelock. Lipid Mediator Metabolic Profiling for Identifying Sub-Phenotypes of Respiratory Disease: a case of the right needle in the right haystack
9:30	Anne Bendt. Human Plasma Lipidomics & Clinical Applications
10:00	Sven Meyer. Advancing clinical research with 4D-OMICS approaches
10:30	Panagiotis A. Vorkas. A comprehensive metabolic atlas of atherosclerosis reveals a novel sphingolipid pathway of foam cell apoptosis.
10:55	Coffee Break
Session 2: Computational Metabolomics - Chaired by Douglas McCloskey	
11:15	Alberto Santos. Connecting Knowledge to Improve Interpretation of Omics Clinical Experiments
11:45	Madeleine Ernst. Developing the next generation metabolomics tools for personalised diagnostics in early life
12:15	Lunch
Session 3: Health - Chaired by Thomas Moritz	
13:45	Marta Cascante. Integration of transcriptomics and metabolomics into genome-scale metabolic models reveals cysteine and folate
14:15	Peter Spégel. The Magic of Gastric Bypass Surgery - What does metabolomics tell us?
14:45	Jin Xu. Multi-omics application and plasma biomarker discovery in Alzheimer's Disease
15:10	Adam Kennedy. Clinical Metabolomics of Rare Diseases Using Untargeted Mass Spectrometry
15:40	Coffee Break
Session 4: Future Perspectives - Chaired by Julie Courraud	
16:00	Jules Griffin
16:30	Thomas Moritz. It is not just to measure the metabolome
17:00	Karolina Sulek. Directed metabolomics for reproduciable results in large clinical studies
17:30	Douglas McCloskey. Closing remarks

Speakers

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Speakers

Alberto Santos, **PhD.** Research group leader at the Center for Health Data Science and the University of Copenhagen and at the Big Data Institute (BDI) at the University of Oxford. He started his own research focusing on network biology to understand the complexity of disease and health. The Multi-omics analytics group works on the integration and analysis of clinical multi-omics data, mainly proteomics and metabolomics, to identify markers of disease, prognosis, and treatment.

Alice Limonciel, **PhD.** Scientist specializing in data analytics and metabolomic data interpretation at Biocrates life sciences ag, Austria. With a background in molecular biology and toxicology, she has applied integrated omics to investigate the effects of xenobiotics on human renal cells. Her work at biocrates now combines data analysis and out-of-the-box thinking to uncover new mechanisms relevant to health and disease using metabolomics.

Anne Bendt, PhD. Singapore Lipidomics Incubator at the National University of Singapore. Principal Investigator and Deputy Director at SLING, the Singapore Lipidomics Incubator at the National University of Singapore. She focusses on translation of mass spectrometry-based technologies into clinical applications, primarily for lipids and small molecules. Early 2019 Anne co-founded the global initiative 'Females in Mass Spectrometry' (FeMS), serving as co-chair on the Board.

Craig Wheelock. Karolinska Institutet, Sweden Craig Wheelock is an Associate Professor at the Karolinska Institute, where he founded the Integrative Molecular Phenotyping Laboratory. He is also a Visiting Professor in metabolomics at Gunma University, Japan. Research in his group focuses on molecular phenotyping of respiratory disease. A particular area of interest is investigating the role of eicosanoids and other lipid mediators in disease.

Cristina Legido Quigley, MSci, PhD, DIC. Steno Diabetes Center Copenhagen, Denmark Heads Systems Medicine (Steno, Copenhagen) & is an Assoc. Prof. in Chemical Biology –King's College London. She works in the interface between analytical chemistry, data science & medicine. She has worked with Metabolomics since 2006. She wants to understand the molecular crosstalk between the liver & the brain during disease and healthy aging.

David Wishart, PhD. University of Alberta, Canada, is a Professor in the Departments of Biological Sciences and Computing Science at the University of Alberta. His research interests are very wide ranging, covering nanotechnology, molecular biology, analytical chemistry, nutritional science and bioinformatics. He currently directs The Metabolomics Innovation Centre (TMIC), Canada's national metabolomics laboratory.

Douglas McCloskey, PhD. Novo Nordisk Foundation Center for Biosustainability, Technical University of Denmark, Kongens Lyngby. Currently at The Novo Nordisk Foundation Center for Biosustainability as Group Leader, where his group focuses on developing automated workflows for "Big Data" generation and analysis. Douglas completed a PhD in Bioengineering Engineering from the University of California (UC), San Diego, in 2017; and received a BA in Biomedical Engineering from the UC, Irvine, in 2010

Emma Schymanski. Associate Professor Luxembourg Centre for Systems Biomedicine, University of Luxembourg. Head of the Environmental Cheminformatics (ECI) group at the Luxembourg Centre for Systems Biomedicine (LCSB), University of Luxembourg. Her research combines cheminformatics and computational (high resolution) mass spectrometry approaches to elucidate the unknowns in complex samples, primarily with non-target screening, and relating these to environmental causes of disease.

Gabi Kastenmüller. IBIS Institute of Bioinformatics and Systems Biology, Helmholtz Zentrum München, Germany. Heading a research group at the Helmholtz Zentrum München, Germany, focusing on the bioinformatic analysis of large metabolomics datasets in the context of health and disease. To elucidate the role of metabolites and their changes in progression to disease at a systems-level, her group develops new strategies to integrate and visualize results from metabolome- and genome-wide association analyses within easy-to-use frameworks.

Hanne Christine S. Bertram. Aarhus University, Denmark. Professor at Aarhus University, Department of Food Science. She works with NMR applications in food science and has been pioneering in the introduction of NMR-based metabolomics in nutrition research. Her recent research focuses on the use of metabolomics to gain mechanistic insight into nutritional aspects of animal-derived foods.

Jennifer Kirwan, PhD. Berlin Institute of Health Metabolomics Platform at the Charité, Germany. Head of the Berlin Institute of Health Metabolomics Platform at the Charite, Germany. Educated as clinical veterinarian, she worked at the University of Birmingham before moving to Germany 5 years ago to head the BIH Metabolomics Platform. Her research focuses on the gut-brain-heart health triad and how the metabolome and microbiome influence each other.

Jin Xu. Institute of Pharmaceutical Science, King's College London, United Kingdom Dr Jin Xu is a Research Associate at King's College London. Her research focuses on the application of metabolomics and lipidomics to understand the underlying biology in Alzheimer's disease (AD). With the integration of multi-omics and clinical data, she is interested in establishing early diagnostic metabolite panels in the general population as well as finding female-specific AD biomarkers.

Julian Griffin. Imperial College London, United Kingdom. Prof. Jules Griffin is the Professor of Biological Chemistry at Imperial College London and head of the Section of Biomolecular Medicine, part of the Department of Metabolism, Digestion and Reproduction. He is the current President of the Metabolomics Society, an Agilent Thought Leader, a Fellow of King's College Cambridge and a Fellow of the Royal Society of Chemistry.

Justin J.J. van der Hooft. Wageningen University, Netherlands. Dr Justin van der Hooft is an Assistant Professor in Computational Metabolomics at Wageningen University, Wageningen, the Netherlands and an author of over 60 peer-reviewed articles in the metabolomics field. His group in the Bioinformatics Chair Group develops computational metabolomics methodologies to decompose complex metabolite mixtures into their (sub)structures and chemical compound classes, inspired by text-mining algorithms and machine learning approaches.

Karolina Sulek, PhD. Steno Diabetes Center Copenhagen, Denmark. Assistant Professor at the Centre for Protein Research, University of Copenhagen. After many years of research focused around clinical metabolomics, she is currently developing mass-spectrometry based approaches for robust and reproducible multi-omics analysis in large-scale applications, such as hospital settings.

Lorraine Brennan. University College Dublin, Ireland. Lorraine Brennan is a Full Professor of Human Nutrition in University College Dublin, Ireland, where she is running the Nutrition, Biomarkers, and Health research group. Recent funding includes a European Research Council (ERC) Consolidator Award and US-Ireland tripartite grant. She was a member of the EU Food2030 Expert group which assisted the European Commission with the development of FOOD2030.

Madeleine Ernst, PhD. Danish Center for Neonatal Screening, Statens Serum Institut, Copenhagen, Denmark, Head of the Clinical Metabolomics Research Group at the Danish Center for Neonatal Screening, Statens Serum Institut, Copenhagen, Denmark. Our group's research aims at developing predictive and personalized diagnostics in early life using metabolomics methods and the massive population-based sample resource available at the Danish National Biobank.

Maria Fedorova. PhD. Center for Membrane Biochemistry and Lipid Research, University Hospital and Faculty of Medicine Carl Gustav Carus of TU Dresden. Studied Biochemistry at Saint-Petersburg State University and obtained her PhD at Faculty of Chemistry and Mineralogy, Leipzig University. Now she is a group leader at the Center for Membrane Biochemistry and Lipid Research, TU Dresden. Her research is focused on implementation of LC-MS methods in discovery lipidomics targeting human lipidome in variety of metabolic disorders.

Maria Klapa, PhD. Metabolic Engineering and Systems Biology Lab, FORTH/ICE-HT, Patras, Greece. Principal Researcher, Head, Metabolic Eng & Systems Biology Lab, Inst of Chem Eng Sciences, Foundation for Research & Technology–Hellas, Patras Greece & Adjunct Prof, Chem & Biomolecular Eng Dpt, U.

Maryland College-Park USA. She works on experimental & computational metabolomics, protein interactomics & multi-omics in systems biology & leads the 2019-21 ELIXIR fluxomics implementation study.

Marta Cascante. Institute of Biomedicine, University of Barcelona, Spain
Marta Cascante is Full Professor at the Dept. of Biochemistry and Institute of Biomedicine (IBUB) at Universitat de Barcelona. She has large experience in supporting the international biomedical community in Stable-Isotope-Resolved-Metabolomics and targeted metabolomics profiling for a wide range of sample types. Her research team has achieved outstanding recognition for the study of metabolic flux reprogramming in multifactorial diseases.

Mette Christensen. Metabolic Laboratory, Department of Clinical Genetics, Copenhagen University Hospital (Rigshospitalet), Denmark MSc, Senior Specialist and Clinical Laboratory Geneticist at Metabolic Laboratory, Department of Clinical Genetics, Copenhagen University Hospital (Rigshospitalet). Specialized in metabolic pathways, analysis of small molecules and interpretation of data for biochemical diagnosis of inborn errors of metabolism. Metabolic Laboratory is the only laboratory in Denmark conducting complex biochemical screening for diagnosis of inborn errors of metabolism.

Nicola Zamboni. Institute of Systems Biology, ETH Zurich, Switzerland
Faculty member of the Institute of Systems Biology of ETH Zurich, Switzerland and head of the Center of Clinical Metabolomics of the federal Personalized Health and Related Technology initiative. His team focuses on the development and application of methods to investigate metabolism and its regulation, with a particular emphasis in high-throughput mass spectrometry.

Panagiotis Vorkas. Institute of Applied Biosciences, Centre for Research & Technology, Hellas, Thessaloniki, Greece
Researcher at the Institute of Applied Biosciences (INAB), Centre for

Research & Technology, Hellas (CERTH), Greece. His research mainly focuses on cardiovascular disease and particularly atherosclerosis, with special interest in atherosclerotic plaque formation and instability. Furthermore, his work is oriented towards developing metabolomics and multi-omics workflows for expanding metabolome coverage in combination with trans-level interactions.

Peter Spégel, PhD. Lund University Diabetes Centre, Sweden. Associate Professor at the Centre for Analysis and Synthesis and Lund University Diabetes Centre. His research focuses on the mechanisms controlling endocrine hormone secretion, translation of biomarkers into metabolic mechanisms and metabolic consequences of bariatric surgery.

Sofia Moco, PhD. Amsterdam Institute for Molecular and Life Sciences, Netherlands
Chemical Engineer, PhD in Biochemistry, Assistant Professor at VU Amsterdam, the Netherlands. Her research focuses on making use of LC-MS and NMR-based metabolomics to address biological questions related to human metabolism and metabolic diseases, from cellular systems to clinics. Over the past years, she has developed strategies to study the influence of natural bioactives in modulating mitochondrial and redox biology, namely in NAD+ and glutathione biosynthesis.

Sven Meyer. Bruker Daltonics, Bremen, Germany. Sven Meyer holds a doctoral degree in chemistry with a background in structural elucidation of novel natural products based on NMR and Mass Spectrometry. He is with Bruker for 11 years, and is working in the small molecule applications development team, with a focus on the timsTOF platform.