

Scottish Metabolomics Network Annual Meeting 2019

Technology and Innovation Centre, University of Strathclyde, Glasgow, 13th - 15th November

PROGRAMME

Day one / Wednesday 13th November 2019

Workshop on modelling of metabolomics data | Gavin Blackburn, Nik Rattray, Tim Ebbels

SMN Workshop Schedule

10:00 - 10:45 Registration with Tea/Coffee

10:45 - 11:00 **Gavin Blackburn:** Introductory Lecture on Experimental Design

11:00 - 12:00 **Nik Rattray with room help from Gav Blackburn and PhDs:**
Workshop #1 – MetaboAnalyst overview, data formatting, upload and preprocessing

12:00 - 13:00 Lunch

13:00 - 14:00 **Dr Tim Ebbels with room help from Gav, Nik and PhDs:**
Workshop #2 – Univariate Analysis

14:00 - 14:30 **Nik Rattray with room help from Gav Blackburn and PhDs:**
Workshop #1 Part 1 – Multivariate analysis covering PCA, PLS-DA and oPLS-DA

14:30 - 15:00 Tea/Coffee Break

15:00 - 16:00 **Dr Tim Ebbels with room help from Gav, Nik and PhDs:**
Workshop #3 Part 2 – Multivariate analysis covering PCA, PLS-DA and oPLS-DA

- 16:00 - 16:30 Open house for questions to panel
- 17:00 - 18:00 **Opening Key Note Lecture delivered by Dr Tim Ebbels (Imperial)**
Computational Metabolomics: the key to the future?
- 18:00 onwards Drinks Reception sponsored by Shimadzu then a meal out for those interested.

Day two / Thursday 14th November 2019

10:00 - 10:30 Registration with Tea/Coffee

10:30 - 10:45 **Karl Burgess:** Welcome from the SMN board

Scientific Session One - Metabolomics and Biomarker Discovery (Chair - Dave Watson)

10:45 - 11:10 **Ruth Andrew (University of Edinburgh):** Mass Spectrometry Imaging of Small Molecules – an Update from Edinburgh.

11:10 - 11:35 **Mike Barrett (University of Glasgow):** Untargeted Metabolomics for Patient Stratification: Delivering Precision Medicine.

11:35 - 12:00 **Sponsor 1 Bruker Ltd – Lucy Woods (Bruker Ltd):** High Speed Untargeted 4D-Lipidomics LC-MS/MS Workflows with Parallel Accumulation Serial Fragmentation (PASEF).

12:00 - 12:25 **Sponsor 2 Waters Ltd – Ian Wilson (Imperial College):** Smaller, Better, Faster: Rapid Methods for the Analysis of Biofluids *via* Microbore UPLC/IM/MS.

12:25 - 13:25 Lunch, Networking, Sponsor Exhibitions

Scientific Session Two – Cell Based Metabolomics (Chair – Oliver Maddocks)

13:25 - 13:50 **Giovanny Rodriguez Blanco (Beatson Laboratories):** Comprehensive Evaluation of a One-Step Sample Preparation for Global LC-MS Lipidomics of Cancer Cell Cultures.

- 13:50 - 14:15 **Andy Finch (University of Edinburgh):** Energetic Stress in MYC-Induced Apoptosis.
- 14:15 - 14:40 **Sponsor 3 Anatune Ltd – Nathan Hawkins (Anatune Ltd):** Automated Thermal Desorption (TD)-SIFT-MS: A New Paradigm for Breath Analysis.
- 14:40 - 15:05 **Sponsor 4 Sciex Ltd – Gina Eagle (Sciex Ltd):** SWATH Acquisition for Untargeted Metabolomics and Comprehensive Metabolite Quantitation.

15:05 - 15:30 Refreshments, Networking, Sponsor Exhibitions

Scientific Session Three - Lipidomics and Steroids (Chair – Ruth Andrew)

- 15:30 - 15:55 **Phil Whitfield – (UHI Inverness):** A Walk Through the World of Weird and Wonderful Lipids.
- 15:55 - 16:20 **Terry Smith (University of Saint Andrews):** The Choline Cycle: its Quantification and Inhibition.

Keynote Lecture

- 16:20 - 16:55 **Julian Griffin (Imperial College):** Fatty Liver Disease: from MALDI Imaging to Population Studies Using Lipidomics.

16:55 - 18:00 Posters Drinks Reception Sponsored by LECO

19:00 - 20:30 Conference Meal at Drygate Brewery

20:30 - 12:00 Ceilidh (The Jiggers Ceilidh Band)

Day three / Friday 15th November 2019

Scientific Session Four - Metabolomics Technologies I (Chair – Natalie Homer)

- 09:15 - 09:40 **Gavin Blackburn (University of Glasgow):** Quality Control in Metabolomics, What Do We Do and How Can We Improve it?
- 09:40 - 10:05 **Emily Dickie (University of Glasgow):** Lipidomic Analysis of *Trypanosoma congolense*.

10:05 - 10:30 **Sponsor 5 Leco Ltd – Rachel Hand (De Montfort University):** Working Towards Comprehensive Steroid Detection in Urine *via* Targeted MIPs Clean-up and Fully Automated GCxGC-MS Analysis.

10:30 – 10:55 **Sponsor 6 Shimadzu – Emily Armitage (Shimadzu Ltd):** A High Speed DIA-MS/MS Untargeted Metabolic Profiling Approach to Study Ethanol Toxicity in Mouse Cerebral Tissue.

10:55 - 11:20 Refreshments, Networking, Sponsor Exhibitions

Scientific Session Five - Metabolomics, Food Nutrition, Natural Products and Health (Chair – Wendy Russell)

11:20 - 11:45 **Elena Conti (Rowett Institute):** Discovery of novel antimicrobial metabolites from the human gut microbiota.

11:45 - 12:10 **Will Allwood (James Hutton Institute):** Investigating the Effects of Future Climate Scenarios in Soft Fruit: Application of HPLC-PDA-MS Metabolite Profiling in Blackcurrant Cultivated Under Increased Temperature and Altered Light Regimes.

12:10 - 12:35 **RuAngelie Edrada Ebel (University of Strathclyde):** Secondary Metabolomics: Targeting the Bioactives from a Haystack.

12:35 - 13:00 **Sponsor 7 Thermo Fisher Scientific – Lena Becciolini (Thermo Fisher Scientific):** AcquireX...A Deep Dive into the Sea of Metabolic Features

13:00 - 14:00 Lunch, Networking, Sponsor Exhibitions

Scientific Session Six - Metabolomics Technologies II (Chair - Gavin Blackburn)

14:00 - 14:25 **Hannah Lawther (University of St Andrews):** Marine Organisms, Viruses and Pollen: Wild (Type) Approaches to Addressing AMR.

14:25 - 14:50 **Karl Burgess (University of Edinburgh):** Metabolomics in Industrial Biotechnology.

14:50 - 15:15 **Elena Kuzmanova (University of Dundee):** Improving Imprecision in Stable Isotope Dilution LC-MS/MS Analysis.

15:15 - 15:40 **Sponsor 8 Agilent Ltd – Hannah Florance (Agilent Ltd):** Addressing Analytical Challenges in Lipidomics Using Retention Time, Accurate Mass, Fragmentation and CCS.

15:40 - 16:00 Refreshments, Networking, Sponsor Exhibitions

Plenary Lecture (Chair - Karl Burgess)

16:00 - 16:50 **Roy Goodacre (University of Liverpool):** Metabolomics by Numbers: Lessons from Large-Scale Phenotyping.

16:50 - 17:10 Prizes and Announcement of SMN 2020

Wi-fi Access

There will be free Wi-Fi (NETWORK: TIC Conferences PASSWORD: GlasgowGreen).



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