MetaboNews

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In This Issue

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MetaboNews is a monthly newsletter published in a partnership between The Metabolomics Innovation Centre (TMIC) and Metabolomics Society.

Metabolomics Society News

Members Corner

Board of Directors

Dear Colleagues,

I hope that you have all had a good start to 2021. There are several exciting updates that I want to convey to you. As I mentioned in *MetaboNews* last month, plans for Metabolomics 2021, the second virtual conference that will take place from June 22-24, 2021, are well underway. While we will not be meeting in person, I am confident that the caliber of our program this year will push the boundaries of our understanding in multiple domains of metabolomics research and I encourage you to register. The conference website is now live and can be found at metabolomics2021.org. Like last year, the conference will take place in all time zones, enabling it to continue as a truly international event. Abstract submissions will open shortly, so be on the lookout and submit your latest cutting-edge work. We will also be announcing other conference details, such as the Keynote speakers, shortly. In other Society news, we are starting some new task groups to meet some growing demands and priorities within the Society. Importantly, we are starting a Diversity, Equity, and Inclusion (DEI) Task Group, to help the Society best identify and address the important issues in this area. If you have experience in this area and would like to contribute your expertise, please contact Natasa Giallourou (natasagiallourou@gmail.com), who is leading this effort. Also be on the lookout for other virtual workshops from the Society. Later this month, the Precision Medicine Task Group will host a virtual workshop on Single Cell Metabolomics on Friday, February 26 at 10 AM Eastern. Please contact Lisa Howerton (lisa.howerton@duke.edu) to register for free. We are looking forward to offering more virtual events throughout the year, with the hope of raising the quality of metabolomics research worldwide.

All the best,

Jessica Lasky-Su, *President, Metabolomics Society*

Metabolomics Society News

The Metabolomics Society is an independent non-profit organisation dedicated to promoting the growth, use and understanding of metabolomics in the life sciences.

General Enquiries
info@metabolomicssociety.org
Membership Enquiries

Early-career Members Network (EMN)

EMN Webinar Series

The EMN would again like to thank Dr. Gaud Dervilly and Dr. Luca Narduzzi for their inspiring talks on the intersection of chemical food safety and metabolomics. If you missed any of our latest webinars, the recordings are now available on the Metabolomics Society website.

Stay tuned for announcements sent over email and posted on our social media platforms for the next ones!

- Facebook
- Twitter

International Affiliates Corner

Metabolomics Association of North America (MANA)

Visit https://metabolomicsna.org

WomiX

MANA is happy to announce an exciting series of upcoming events from its Women in Metabolomics (WomiX) Interest Group. Additional details can be found on the recently launched WomiX website.

Images of Success: Women in Metabolomics is a regular bi-monthly workshop where we'll be hearing from women in metabolomics about their experience on different topics such as work/life balance, mentorship, career advancement strategies, etc. The first event in this series will be **Wednesday, Feb 17, 2021 from 12-1 PM PST/3-4 PM EST** with the topic of "Academia to Industry." **Register here**.

WomiX Mentorship Program will be launching in February. We have a great group of mentors and mentees. If you'd like to join at the last minute please email us, we still have spots available.

WomiX Women's Week (Mar 8 -12, 2021) - We are organizing a fun week to celebrate International Women's Day on March 8, 2021 and Women's History Month. We'll be engaging with our members via social media, highlighting women in STEM & metabolomics. **If you'd like to be featured submit your info here!** Then we'll wrap up the week with a fun networking event on **Friday, March 12, 2021 at 2 PM PST/5 PM EST. Register here.**

Webinar Series

The **MANA Microbiome Interest Group** is also excited to announce a new monthly seminar series. The first seminar in the series will be on **Tuesday, March 9, 2021 at 11 AM ET**, with **Dr. Stanley Hazen of the Lerner Research Institute at the Cleveland Clinic** presenting on "The Gut Microbiome as an Emerging Therapeutic Target for Cardiometabolic Disease". He will describe how use of untargeted metabolomics investigations of multiple large-scale clinical cohorts serves to help focus interest on which metabolic signatures show

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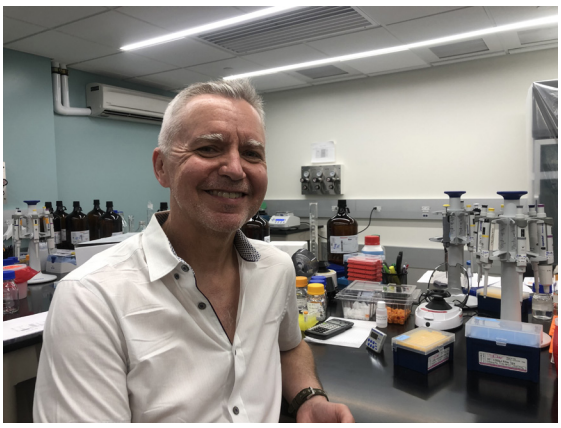
reproducible clinical associations independent of traditional risk factors, comorbidities, and medications.

The MANA Microbiome Interest Group aims to facilitate microbiome-focused metabolomics research by providing general guidance on the gold standards in the field and by fostering new networking opportunities for our members across the multidisciplinary scientific communities. If you are interested in joining the Microbiome Interest Group to focus on and develop topics related to application of metabolomics in microbiome research, and for information on how to register for Dr. Hazen's seminar, please contact us at mana.microbiome@metabolomicsna.org.

METABOINTERVIEW

Dr. Dave Goodlett



Don and Eleanor Rix BC Leadership Chair in Biomedical & Environmental Proteomics at University of Victoria

Short Biography

David R. Goodlett has spent his 30-year career using mass spectrometry to solve biomedical problems via novel technology and software developments. His Ph.D. training was with Richard B. van Breemen on protein adducts and postdoctoral work with Richard D. Smith on Native MS, CE-MS and ESI fundamentals. His current research interests lie in developing a better understanding of the lipid A structure-activity relationship in order to elucidate the molecular basis by which lipid A can act as agonist or antagonist on binding to MD2/TLR4. He currently holds the Don and Eleanor Rix BC Leadership Chair in Biomedical & Environmental Proteomics as Professor at the University of Victoria where he is also Director of the UVic-Genome BC Proteomics Centre. He is a co-organizer of the MSBM.ORG mass spectrometry summer school held annually in Dubrovnik and for the last decade has been an Editor at Rapid Communications in Mass Spectrometry.

Interview Q&A

How did you get involved in metabolomics?

Firstly, through structure analysis of microbial lipids like cardiolipin and lipopolysaccharide. However, now at the UVic-Genome BC Proteomics Centre we have access to hundreds of targeted assays developed by Dr Jun Han who is our technical lead for metabolomics. I'm very impressed with Dr. Han's efforts, which are of the highest quality. His experience will be useful in my own work to understand the structures of lipids from bacteria and fungi that I am excited about doing at UVic.

What are some of the most exciting aspects of your work in metabolomics?

While we began our work on structure analysis of microbial lipids with Robert "Bob" Ernst in Seattle and continued it at the University of Maryland-Baltimore, this structure project has morphed into two interesting research directions. The first involves use of microbial lipids as diagnostic molecules much in the same way that the Bruker Biotyper uses protein mass spectra, but unlike that method we can identify microbes direct from specimens like urine or blood bottles or bronchoalveolar lavage fluid (BALF). Secondly, we are working with Bob and Alison Scott to define the structure-activity relationship for lipid A in order to better understand the molecular basis by which lipid A can act as agonist or antagonist on binding to MD2/TLR4. This latter research has implications for therapeutics such as vaccine adjuvants and anti-septic prophylactics.

You recently moved from the United States to the Universiry of Victoria. What changes have you noticed since moving from the US to Canada?

It's quiet here! We lived in downtown Baltimore which was alive with urban activities. No day went by without the sound of police helicopters overhead with spotlights at night, gunshots, sirens, road noise and some occasional chaos from groups like the Twelve O'Clock Boys. So, we are learning to adapt to the peaceful suburban life here in Victoria. Of course, we also moved across the continent during a pandemic and spent our first two weeks here in quarantine. On the science front, life is pretty similar here except perhaps with the size of funding awards that are smaller here, but the quality of science at UVic is at the highest international standards, which I expected but now see up close.

What benefit do you see in being part of a pan-Canadian research centre like The Metabolomics Innovation Centre?

TMIC, as it is known, provides immediate visibility for our metabolomic efforts at the Proteomics Centre, which is misnamed because we do at least as much metabolomics work as proteomics. For years before moving to UVic I was of course aware of and impressed by Dave Wishart's efforts. So, it has been great to finally get to know him professionally via TMIC. To answer your question though, being part of TMIC gives us visibility in the metabolomics world, which is helpful in part because of our name, but also because of the years of work by the Wishart laboratory to lay the groundwork for TMIC.

How do you see your work in metabolomics being applied today or in the future?

Prior to my move to UVic, our work has been mostly in the microbial lipidomics space. In this space we have developed a diagnostic capable of identifying microbes directly from specimens: i.e., specifically in a clinical setting we can provide identifications directly from urine or BALF or a blood bottle. This approach cuts up to one day off methods that require a pure colony be picked from a Petri dish, which in turn aids antibiotic stewardship. In our work on developing the lipid A SAR we are developing a better understanding of the host-immune system interaction with microbes, which – thanks to the large number of targeted, quantitative assays available from Dr. Jun Han – we will leverage to understand more about how infections affect the host metabolome and microbiome, e.g., his targeted bile acids assays are looking to be quite useful to investigate the interplay between the host immune system and pathogens or symbiotes. To this end we are working with Dr. Han and Dr. Julian Lum of BC Cancer on pathway specific assays.

As you see it, what are metabolomics' greatest strengths?

The direct connection to what is going on biochemically. For example, in most discovery-style proteomic workflows the identity of a given protein detected in a sample is one step removed from reality because of the necessity to match a peptide tandem mass spectrum to a sequence in a database at a defined false-discovery rate. With metabolomics there is no such fungible step, but rather the metabolite is either identified by old-school pen and paper to divine the structure or if it is known already then often a standard is added in providing even more certainty in the identification. Of course, one can use standards in proteomics to do discovery work but far and away most discovery-based proteomics is done by label-free quantitation without standards.

What do you see as the greatest barriers for metabolomics?

Here it is the same as with any science using mass spectrometry: throughput. Mass spectrometers are not designed originally to be used as we use them today in proteomics and metabolomics, but rather for structure analysis or simple molecular weight measurements. While the industry has made great gains to improve throughput, neither proteomics nor metabolomics can compete with genomics. OK. Some will argue about the newer, faster mass spectrometry methods coming out making metabolomics more competitive, but we still are stuck with LC (or related methods) to introduce a sample, which limits throughput. Innovation is needed in this space to improve throughput and this will likely come sooner than later. Remember that in the mid-80s and even into the late 90s, Edman chemistry was used to *de novo* sequence proteins. This industry almost vanished in favor of better throughout even though the MS-based methods had more uncertainty.

How does the future look in terms of funding for metabolomics?

Hard to say, of course. However, at the "Proteomics Centre" we are doing more metabolomics than proteomics. While this could be due to the lag created by COVID19, the general trend was already in place prior to the pandemic hitting. I think this will continue because of the reasons mentioned above about uncertainties in protein identifications versus the more direct nature of metabolomics. And of course, also because the metabolites are the outcomes of protein biochemical pathways that change as the host changes. Thanks to the work of folk like Wishart and Fiehn, to name a couple of Fathers in the field, metabolomics is now more approachable than ever.

What role can metabolomics standards play?

They are one of the keys to success. While traditional discovery-based metabolomics, which like discovery-based

proteomics is used to generate hypotheses that are tested by other methods, one can get by without a standard for every compound. Eventually, though there is a high likelihood they will be needed and certainly so if the mass spectrometry data is a means to an end. With metabolomics this need for standards is more important than proteomics because of the likely existence of isomers and stereochemistry. DNA, RNA and proteins are rather simple polymers compared to metabolites. Just think about the simple case of butene which can be in either the cis or trans form and now multiple the complexity of the overall molecule as you begin to add more moieties. From an analytical perspective this complexity can quickly get out of hand. So where available standards are very important and more so where one isomer may have biological activity over another.

Do you have any other comments that you wish to share about metabolomics?

I think the community is awakening to the benefits of using metabolomics to investigate everything from how cancer develops and metastasizes to climate change. The origins of metabolomics go back to the generations of scientists who defined metabolic pathways in the 1900s. We stand ready to further their groundbreaking efforts that have remained somewhat fallow for many years. However, now I think the recent rise in the utility of metabolomics will provide for great discoveries and I'm delighted to be part of that effort here at UVic and with TMIC.

Recent Publications

Recently published papers in metabolomics

- Isoform-specific Activities of Androgen Receptor and its Splice Variants in Prostate Cancer Cells
- Biomarkers of Major Depressive Disorder: Knowing is Half the Battle
- Diabetes mellitus: a primary metabolic disturbance. Metabolomics underlying vascular responses to stress and ischemia?
- Charged metabolite biomarkers of food intake assessed via plasma metabolomics in a population-based observational study in Japan
- Altered lung metabolism and mitochondrial DAMPs in lung injury due to acute kidney injury
- Metabolomic approach to characterize the metabolic phenotypes and varied response to ouabain of diffuse large B-cell lymphoma cells
- Colorectal cancer screening and diagnosis: omics-based technologies for development of a non-invasive blood-based method
- LC-MS based plant metabolic profiles of thirteen grassland species grown in diverse neighbourhoods
- Transcriptomic, Protein-DNA Interaction, and Metabolomic Studies of VosA, VelB, and WetA in Aspergillus nidulans Asexual Spores
- Sulfur Metabolites Play Key System-Level Roles in Modulating Denitrification
- Endogenous Metabolites Released by Sanitized Sprouting Alfalfa Seed Inhibit the Growth of Salmonella enterica
- Human Milk-Fed Piglets Have a Distinct Small Intestine and Circulatory Metabolome Profile Relative to That of Milk Formula-Fed Piglets
- Virgin Olive Oil Phenolic Compounds Modulate the HDL Lipidome in Hypercholesterolaemic Subjects: A Lipidomic Analysis of the VOHF Study

Metabolomics Events

Postponed Until 2021

The Third Annual Canadian Metabolomics Conference

Venue
Edmonton, Alberta, Canada

Overview
The Third Annual Canadian Metabolomics Conference has been postponed until 2021. The conference will highlight work by leading researchers, including new technologies and approaches for metabolomics research, and applications in various fields. The conference will feature networking opportunities and a poster session designed for trainees to present their work. Our goal is to highlight the exceptional metabolomics science that is being done in Canada and abroad, and foster Canada's leadership role in the global research community.

We look forward to seeing you in 2021!

Conference Link
https://www.canmetcon.ca/

1-26 Feb 2021

Metabolomics Data Processing & Data Analysis

Venue
Online, Birmingham Metabolomics Training Centre, University of Birmingham, UK

Overview
This online course explores the tools and approaches that are used to process and analyse metabolomics data. You will investigate the challenges that are typically encountered in the analysis of metabolomics data, and provide solutions to overcome these problems. The materials in this course are delivered via the FutureLearn platform over a four week period, with an estimated learning time of four hours per week. Each week you will work through a number of steps to complete the learning material. A step may include a short video, an article, an exercise with step-by-step instructions, a test or a discussion to interact with your peer or the educators. All of the course material is uploaded to the FutureLearn platform so that you can complete the steps at a convenient time for you.

Metabolomics Events

Topics Covered

- An introduction to metabolomics
- An overview of the untargeted metabolomics workflow
- The influence of experimental design and data acquisition on data analysis and data quality
- An overview of processing NMR data
- Processing direct infusion mass spectrometry data with a hands-on exercise
- Processing liquid chromatography-mass spectrometry data with hands-on exercises
- Reporting standards and data repositories
- Data analysis, detecting outliers and drift, and pre-treatment methods
- Univariate data analysis with a hands-on exercise
- Multivariate data analysis (including unsupervised and supervised approaches) with hands-on exercises
- The importance of statistical validation of results
- Computational approaches for metabolite identification and translation of results into biological knowledge with hands-on exercises
- What are the future challenges for data processing and analysis in metabolomics

Course Link

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26 Feb 2021

Single Cell Metabolomics Workshop

Online Workshop

The Precision Medicine Task Group of the Metabolomics Society in partnership with other organizations and interest groups is organizing a virtual workshop on Single Cell Metabolomics, to be held on **Friday, February 26, 2021 10 AM - 1:00 PM EST**.

Omics at single cell resolution have expanded very rapidly, most obviously in genomics/transcriptomics. However, this approach lacks direct analysis of function, such as cellular metabolism. Most tissues are fundamentally heterogeneous at the cellular level, and heterogeneity is a hallmark of several pathologies including cancer.

The Workshop will comprise invited talks and a general open discussion forum.

AREAS OF INTEREST INCLUDE:

- Intrinsic technical problems and current status
- Coverage
- Imaging based methods (MS, microdissection, optical, other)
- Prospects for stable isotope tracing at single cell resolution
- Emerging approaches and applications

PARTICIPANTS ARE WELCOME TO REGISTER FOR FREE.
To register, please email Lisa Howerton at lisa.howerton@duke.edu

For more information, please check out the event flyer.

Metabolomics Events

8-26 March 2021

Quality Assurance & Quality Control in Metabolomics

Venue
Online, Birmingham Metabolomics Training Centre, University of Birmingham, UK

Overview
The application of quality assurance and quality control in the metabolomics field is vital to ensure the collection of high quality data. In this course you will explore the importance of quality assurance and quality control in both untargeted and targeted metabolomics studies. We will explain the difference between quality control and quality assurance and how to apply in your studies and laboratories. You will evaluate the types of quality control samples that can be applied in metabolomics, what is the most appropriate quality control sample to use in your research, and how to apply the data in your quality assurance procedure to produce robust and reproducible data.

Topics Covered

- What are quality assurance and quality control and how do they differ
- What is the importance of quality assurance in metabolomics
- The types of quality assurance and quality control in untargeted and targeted metabolomics
- The importance of quality control samples
- The types of quality control samples applied in untargeted and targeted metabolomics
- Preparation of quality control samples in untargeted and targeted metabolomics
- Analytical studies including untargeted and targeted metabolomics
- Processing data in untargeted and targeted metabolomics
- Recommended quality assurance procedures in untargeted and targeted metabolomics
- Reporting quality assurance procedures in untargeted and targeted metabolomics

Course Link

1 April 2021

Introduction to Bayesian Statistics in Metabolomics

Venue
Online

Institution: University of California, Davis, Davis, California
Instructor: Dr. Christopher Brydges, UC Davis
Registration: Link

Required software:

- JASP (can be downloaded for free from https://jasp-stats.org). The current version is 0.14, but it may well be updated between now and April.

Participant prerequisites: Basic knowledge of statistics (e.g., know what a t-test and a correlation are). No coding experience needed, and there is no coding taught in this session.

Short description of the course: Bayesian statistics are a useful method for estimating effect sizes and testing the strength of evidence in favor one hypothesis over another—things that p-values and traditional statistics can't do. However, they are under-utilized in metabolomics research. This short course will provide a brief refresher on traditional statistics, teach the basic principles behind Bayesian statistics, learn how to conduct basic Bayesian analyses in JASP (free, open-source software

available from https://jasp-stats.org/) and learn how to report the results in the style of a journal article.

For more information, please visit the Bits & Bites: Short Course Series 2021 website.

6-7 April 2021

Targeting CNS Tumor Metabolism Symposium

Venue
NIH Campus, Bethesda, Maryland

Overview
This is the first conference that focuses on the tumor metabolism and it is expected to be a didactic and collegial learning environment. Metabolic investigations for these tumors have been conducted in isolation and the goal of this meeting is to bring together the clinicians with the experts in metabolism to increase the utilization of metabolic investigations in the clinical settings. This will, in turn, enhance partnerships and advance the treatment for patients.

In addition to oral and poster presentations selected from the submitted abstracts, the conference will feature invited lectures from an internationally recognized faculty, including keynote talks from Craig Thompson, MD (President and CEO of Memorial Sloan Kettering Cancer Center) and Paul Mischel, MD (Distinguished Professor, University of California San Diego).

Course Link

15-16 Apr 2021

Data Analysis for Metabolomics

Venue
Wageningen Campus, The Netherlands

Overview
Event postponed from June 4-5, 2020 to now April 15-16, 2021

Metabolomics experiments based on mass spectrometry (MS) or nuclear magnetic resonance (NMR) produce large and complex data sets. This course will introduce approaches to process and analyze data and design high-quality experiments. Through hands-on workshops and lectures highlighting the different concepts you will get a thorough basis for tackling the challenges in metabolomics data analysis.

For information and registration click here.

Metabolomics Events

3 June 2021

Using MSDIAL to Generate Accurate Comprehensive LC-MS/MS Metabolomics Datasets

Venue
Online, University of California, Davis, Davis, California

Instructor
Jake Folz, University of California, Davis

Registration

Required software:
MS-DIAL vs. 4.0 for PCs. This software does not run on Mac or Linux environments.

Participant prerequisites: Basic understanding of LC-MS and understanding of how MS/MS spectra are used in metabolite identification.

Short description of the course: This short course will focus on how to perform fine tuned curation of processed LC-MS/MS data generated through MS-DIAL including compound identification, data quality analysis, and unknown feature reduction. Data from rat blood plasma analyzed using LC-MS/MS with MS/MS data collected in a data-dependent manner will be used to generate an example dataset, but the methods and techniques are applicable to many different sample types.

For more information, please visit the Bits & Bites: Short Course Series 2021 website.

22-24 June 2021

Metabolomics 2021 Online

Save the Date! June 22-24, 2021

The 17th International Conference of the Metabolomics Society will be online again this year. Information will be available on the website soon; abstracts and registration are scheduled to open at the end of January.

METABOLOMICS SOCIETY

Metabolomics Jobs

If you have a job you would like posted, please email Ian Forsythe (metabolomics.innovation@gmail.com).

Jobs Offered

Job Title	Employer	Location	Posted	Closes	Source
Various Positions			18-Feb-21		Metabolomics Association of North America Jobs
Research Technician I	Cold Spring Harbor Laboratory	Cold Spring Harbor, NY, USA	17-Jan-21	Until Filled	Cold Spring Harbor Laboratory
Post-doctoral Fellow / Staff Scientist – Metabolomics	Oklahoma Medical Research Foundation	Oklahoma City, Oklahoma, USA	17-Dec-20	Until Filled	Metabolomics Society Jobs
PhD Research Project Opportunities, Centre for Integrative Metabolomics and Computational Biology	Edith Cowan University	Joondalup, Australia	13-Dec-20	28-Feb-21	Edith Cowan University
Postdoctoral Scholarship - Metabolomics in Diabetes Research	Lund University	Lund, Sweden	24-Nov-20	Until Filled	Lund University
Postdoctoral Position	NIH	Rockville, Maryland, USA	20-Nov-20	Until Filled	Metabolomics Society Jobs
Post-Doctoral Position with influence of multiple 'omics' datatypes on the development of respiratory and/or neurological disease	Brigham and Women's Hospital	Boston, MA, USA	20-Nov-20	31-May-21	Metabolomics Society Jobs
Postdoctoral Fellow – Biosensors Device Development	University of Alberta	Edmonton, Canada	23-Oct-20	Until Filled	Wishart Research Group
Postdoctoral Position in Nuclear Magnetic Resonance (NMR) Spectroscopy	University of Alberta	Edmonton, Canada	23-Oct-20	Until Filled	Wishart Research Group
Laboratory Assistant/ Technician – Biosensors Device Development	University of Alberta	Edmonton, Canada	23-Oct-20	Until Filled	Wishart Research Group
Senior Bioinformatician/ Cheminformatician Position	University of Alberta	Edmonton, Canada	23-Oct-20	Until Filled	Wishart Research Group

Jobs Wanted

This section is intended for very highly qualified individuals (e.g., lab managers, professors, directors, executives with extensive experience) who are seeking employment in metabolomics.

We encourage these individuals to submit their position requests to Ian Forsythe (metabolomics.innovation@gmail.com). Upon review, a limited number of job submissions will be selected for publication in the Jobs Wanted section.

- Dr. Nara Consolo - Seeking a position involving the application of NMR-based metabolomics in animals/animal production; it could be a Researcher position or an Assistant Professorship