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

Conference Corner

Metabolomics 2021 Online

Save the Date! - 22-24 June 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.

Members Corner

Board of Directors

Dear Society Members,

After the year 2020, I think that we are all happy to welcome in 2021 with a fresh beginning and the Society has several exciting things planned for the upcoming year. First, we are excited about Metabolomics 2021, the virtual conference that will take place from June 22-24, 2021. The conference will follow the general format that we instituted this past year for a virtual conference, with the conference taking place in all time zones, enabling it to continue as a truly international event. We will open the conference with focused workshops on special interest topics, which has now become a tradition of our conference format. While not all of the details are decided, we want you to know that careful thought and consideration has been taken to think of creative ways that we may expand the virtual conference in terms of attendee interaction, scientific content, and networking opportunities. Development of the conference website is underway and abstract submissions will open by the end of the month.

In other Society news, we have been working to revamp the Society website and expect it to be completed in the early part of this year. I think we all can agree that the year 2020 transitioned us to become comfortable with remote learning and virtual interactions. We are hoping to capitalize on this throughout the year by increasing opportunities for virtual education and interaction during the year and not just at the annual conference. So please be on the lookout for virtual events as they arise, which we hope to highlight in this newsletter among other places. Through these efforts, we hope to expand the scientific knowledge and scope of Society members while also increasing interactions outside of the Society conference.

As we look back at 2020, my hope is that we take advantage of the lessons learned, innovations developed, and change in perspective to make 2021 a truly spectacular

Metabolomics Society News

year. As always, I look forward to hearing any of your ideas that may make this society continue to serve the metabolomics community.

All the best,

Jessica Lasky-Su, *President, Metabolomics Society*

Early-career Members Network (EMN)

New Expert Opinion

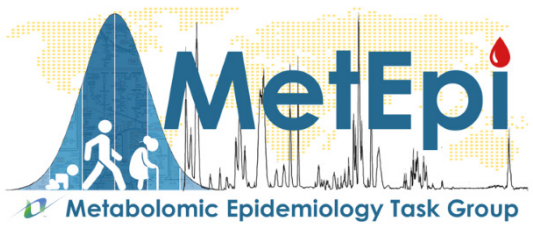
Our new Expert Opinion is out! Dr. Augustin Scalbert has kindly shared with us his work and career experiences, including valuable tips for early-career researchers! Follow the link to find out more.

EMN Webinar Series

The EMN would like to thank once again Dr. Fabien Jourdan and Dr. Pablo Rodríguez-Mier for their great presentations on metabolomics networks, and Prof. Daniel Raftery and Dr. Fausto Carnevale for their inspiring talks on new biostatistical methods for metabolomics. If you missed 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!

Metabolomic Epidemiology Task Group



Contact: Jessica Lasky-Su (jessica.su@channing.harvard.edu)

The Metabolomic Epidemiology Task Group was established approximately one year ago with the mission to promote the growth and understanding of metabolomic epidemiology as an independent research discipline. The supporting pillars of that mission are to:

a. Establish a network of collaborations to enable the development of the required infrastructure, resources, and funding opportunities that will ensure the sustained growth of metabolomic epidemiology in the 21st century.
b. Accelerate scientific discovery by addressing the unique challenges faced by metabolomic epidemiology researchers.
c. Promote education to enable epidemiologists to work effectively with metabolomics data, and for fundamental metabolomics researchers to collaborate with epidemiologists.
d. Provide a unified voice for the views and concerns of the metabolomic epidemiology community, assuring that they help drive the future direction of the Metabolomics Society.

One of the primary actions that we accomplished this year was a presentation of the workshop entitled "Metabolomic Epidemiology Matters: Perspectives on the impact of population-based studies on the future of metabolomics research" at Metabolomics 2020. Using a discussion-oriented framework with moderation, important topics in the field of metabolomic epidemiology were reviewed with representation from a diverse range of viewpoints incorporating the multi-disciplinary scientific expertise that encompass the Metabolomics Society. The workshop was a tremendous success and was the most attended event at the 2020 virtual conference. Throughout 2021, we are hoping to build on this momentum and identify additional creative ways to meet our objectives, even in the midst of a virtual environment.

International Affiliates Corner

Metabolomics Association of North America (MANA)

Visit https://metabolomicsna.org

MANA is excited to announce the election of a new President, Vice President and three members to its Board of Directors:

- Tom Metz, Pacific Northwest National Laboratory; President (2021-2023)
- Tracey Schock, National Institute of Standards and Technology; Vice President (2021-2023)
- Tim Garrett, University of Florida; Board Member (2021-2023)

- Mark Styczynski, Georgia Institute of Technology; Board Member (2021-2023)
- Dajana Vuckovic, Concordia University; Board Member (2021-2023)

The Board has also exercised its option from the bylaws to extend the term of Maryam Goudarzi (Cleveland Clinic) for one year, through 2021.

MANA would also like to thank the following Board members who finished their terms; we appreciate your service and support for the community as part of the first Board, helping to get things off the ground!

- Art Edison, University of Georgia
- Rima Kaddurah-Daouk, Duke University
- Susan Murch, University of British Columbia

Lastly, MANA is excited to announce the establishment of a virtual journal club, organized by Art Edison. The new MANA virtual journal club will promote awareness and discussion of key issues in the field of metabolomics and provide opportunities for MANA members to build networks with other members. Weekly meetings will be on Wednesdays for one hour at 3 pm Eastern time, beginning January 27. If you are interested in participating in this virtual journal club and for more details about the scope, schedule, and format, send an email with your name and position (student, postdoc, staff, faculty, other) to Karen Howard (khoward@ccrc.uga.edu). She will add you to the list and will send you a schedule, signup list, and zoom link after January 4. We encourage you to participate.

METABOINTERVIEW

Dr. Jan Krumsiek

Assistant Professor of Weill Cornell Medicine

Short Biography

Jan Krumsiek, MSc, PhD, is currently an Assistant Professor of Computational Genomics at Weill Cornell Medicine (2018 - present). In this role, Dr. Krumsiek develops and applies novel data analysis methods for metabolomics and multi-omics datasets. These include pathway-based methods, network approaches, machine learning techniques, and deep learning models. One of his latest specializations is the development of data-driven approaches to pinpoint drug effects and discover novel drug targets. Dr. Krumsiek has analyzed metabolic datasets in the fields of diabetes, cancer research and Alzheimer's Disease, and has published extensively on the topic of etiology and risk prediction. Prior to his work at Cornell, he was a Team Leader (2016 - 2018) and Researcher (2009 - 2016) at Helmholtz Zentrum München, which is part of the Helmholtz Association of German Research Centers. Dr. Krumsiek obtained his Master of Science in Bioinformatics and his Doctor of Philosophy from the Technical University of Munich.

Interview Q&A

How did you get involved in metabolomics?

I'm a trained computational biologist and my PhD project was on systems biological analysis methods. This was in 2009, when metabolomics was just starting to become mainstream.

What are some of the most exciting aspects of your work in metabolomics? What key metabolomics initiatives are you pursuing at your research centre or institute?

While working on algorithms, machine learning methods, network tools, etc. is exciting and fun, what really matters to me are the biomedical applications of metabolomics. My work is heading in two directions there: First, we are working on Alzheimer's Disease, a devastating disease for which there is currently no cure. Using metabolomics measurements, we are looking for early biomarkers to detect the disease, but also for the pathological changes in the brain after death. Second, we are working on cancer-related projects, where we also look for biomarkers, for example for treatment outcome and survival. The latest direction here is to use metabolomics to find escape mechanisms of a tumor that will tell us how to kill it. This can, for example, be done in patient-derived organoids, a lab-model of a cancer that we can manipulate in a way that we obviously could not do in patients.

What is happening in your country in terms of metabolomics?

First, as of a couple of years ago, we are past the point of having to justify the use of metabolomics in the first place. It is now an established technology due to technological advancements, and due to scientific success stories. This has been recognized by the big funding agencies, for

example through substantial funding in the NIH Common Fund Metabolomics program. There are now hundreds of labs in the US working both on the measurement and analysis side of metabolomics.

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

Actual clinical applications of metabolomics are an exciting and ambitious goal. If we could reliably and quickly measure metabolomics in the blood of patients, we could guide clinical decision making in the same way that classical clinical lab parameters or nowadays mutation profiling in cancer do. Various initiatives and companies are working on ways to figure out the technological hurdles of collecting and analyzing metabolomics samples in a fast-paced setting in the clinics or even at home.

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

One of the biggest strengths, the well-known and widely discussed feature of metabolomics, is that it integrates all signals of the other omics in the molecular dogma of biology. You can hardly do anything to a biological system without leaving a signal in the metabolome. Another major advantage of metabolomics is that it is very informative in blood. While other omics layers either occur to different compartments in the blood (such as the transcriptome of circulating immune cells) or are usually informative for specific diseases (such as circulating tumor DNA), blood metabolites inform us about processes from all organs across the body.

What do you see as the greatest barriers for metabolomics?

First, I personally believe we need more dedicated funding specifically for the statistical and computational analysis of metabolomics data. This is slowly being recognized by the field and the funding agencies but requires even more momentum. Second, especially for clinical research we need established biobanking procedures to make sure that samples are in a state that is suitable for metabolomics. Third, we need cheaper technology. On some platforms, we still pay up to $500 for a single sample, which prevents us from doing metabolomics in large numbers on a daily basis.

What improvements, technological or otherwise, need to take place for metabolomics to really take off?

As mentioned above, I believe metabolomics needs to be cheaper and needs to be applicable in a fast setting for example during a doctor's visit or at home. How to achieve this is slightly beyond my field of expertise.

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

I would highly encourage everyone in the metabolomics field to push reproducible research and open-source codes forward. For every published paper, we should have an online supplement that reproduces the entire analysis from the beginning to the end.

Recent Publications

Recently published papers in metabolomics

- Serum Metabolite Biomarkers for Predicting Residual Feed Intake (RFI) of Young Angus Bulls
- Deep dive to the secrets of the PREDIMED trial
- Metabolomic analysis coupled with extreme phenotype sampling identified that lysophosphatidylcholines are associated with multisite musculoskeletal pain
- Metabolomic Profiling for Diagnosis and Prognostication in Surgery: A Scoping Review
- A case of personalized and precision medicine: Pharmacometabolomic applications to rare cancer, microbiological investigation, and therapy
- Electrospray ionization and heterogeneous matrix effects in liquid chromatography/mass spectrometry based meta-metabolomics: A biomarker or a suppressed ion?
- Exploring the metabolic phenotypes associated with different host inflammation of acute respiratory distress syndrome (ARDS) from lung metabolomics in mice
- Global Changes to HepG2 Cell Metabolism in Response to Galactose Treatment
- Metabolomic Profiling and Neuroprotective Effects of Purslane Seeds Extract Against Acrylamide Toxicity in Rat's Brain
- Urinary metabolome of infants with colic treated with Lactobacillus reuteri DSM 17938: a pilot randomized trial
- Radiotherapy and the gut microbiome: facts and fiction
- Metabolomics analysis reveals altered metabolites in lean compared with obese adolescents and additional metabolic shifts associated with hyperinsulinaemia and insulin resistance in obese adolescents: a cross-sectional 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/

25-29 Jan 2021

Hands-on LC-MS Data processing and Statistics 2021 (Online)

Where: Online, course starts at 8:30 AM Pacific Standard Time
Registration: Link
Pay by Credit Card: Link
Email: Jeannette Martins, jmartins@ucdavis.edu
Phone: +1-530-754-5357

The course is completely redesigned for an online format and will also be recorded for the participants to view at a later time. All software training has transitioned to a virtual machine environment so training can be done from any location. Virtual machines are hosted by Amazon Web Services and can be accessed using either a PC or a Mac computer. To guarantee the same hands-on quality that you would experience in our face-to-face course, every unit is taught using interactive tools such as polling, using the annotation tool, utilizing non-verbal feedback, live questions, chat, and group work in breakout rooms.

For details, visit the course website.

Metabolomics Events

1-4 Feb 2021

5th HBP Student Conference on Interdisciplinary Brain Research

Venue
Virtual

Registration will open from September 2020 free of charge.

Call for Submissions
We invite original high-quality submissions describing innovative research in all disciplines addressed in the HBP. These contributions can emphasize theoretical or empirical works relating to a wide spectrum of fields including but not limited to: neuroscience, computer science, robotics, medicine, psychology, cognitive science or philosophy. We particularly encourage submissions with a potential to inspire collaboration in the research community by introducing new and relevant problems, concepts, and ideas, even if the work is at an early stage of development.

Registration deadline: 14 January 2021.
View announcement here.
Further information on abstract submission and the conference.
For any further questions, please contact education@humanbrainproject.eu.

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.

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

Metabolomics Events

- 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

2 Feb 2021

Pan-Cohort Metabolomics – The Future of Population Health

Virtual event

Join a panel of world-leading experts in discussing the power of metabolomics in large scale studies.

Date: Feb 2, 2021
Time: 9:00 am - 1:00 pm CET

Registration **(Note: There is no cost to attend this event)**

4 Feb 2021

Network inference, visualization, and module detection in metabolomics data

Venue
Online

Institution: University of California, Davis, Davis, California
Instructor: Dr. Jan Krumsiek, Cornell University
Registration: Link

Required software:
- R, version 3.6.3 or higher
- GeneNet package
- igraph package
- RCy3 package
- Modentify package + dependencies: https://github.com/krumsieklab/MoDentify

Participant prerequisites: Basic knowledge of data analysis in R is required for this course,

since we will directly start by reading a metabolomics data matrix and applying statistical models to it.

Short description of the course: In this short course, we will implement typical steps of network analysis in metabolomics data. We will start from a metabolomics data matrix and walk through every step of the process, all the way to network visualizations and the identification of regulated network modules. For this, we will use Gaussian Graphical Models, a correlation-based statistical model which has been widely used in metabolomics datasets. The networks will be visualized using the igraph package and the RCy3 Cytoscape interface. A simple version of a module identification algorithm will be implemented from scratch. At the end of the course, the participants will be able to reproduce the major steps of network analysis contained in several publications from the Krumsiek lab.

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

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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

22-24 June 2021

Metabolomics 2021 Online

Save the Date! 22-24 June 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 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
Scientist – Metabolomics and Proteomics	KeyGene USA	Rockville, Maryland, USA	21-Jan-21		KeyGene
Various Positions			20-Jan-21		Metabolomics Association of North America Jobs
Postdoctoral Research Associate in Paper-Based Biosensors for Mass Spectrometry	University of Liverpool	Liverpool, UK	7-Jan-21	3-Feb-21	University of Liverpool
Postdoctoral researcher in Computational Metabolomics and Exposomics	Örebro University	Örebro, Sweden	7-Jan-21	31-Jan-21	Örebro University
Postdoctoral researcher in Chemistry	Örebro University	Örebro, Sweden	7-Jan-21	31-Jan-21	Örebro University
NMR and MS based spatial Metabolomics	The Leibniz-Institut für Analytische Wissenschaften - ISAS	Dortmund, Germany	7-Jan-21	31-Jan-21	Metabolomics Society Jobs
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
Postdoctoral Position	Brigham and Women's Hospital	Boston, MA, USA	20-Nov-20	31-May-21	Metabolomics Society Jobs

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