

## In This Issue

Metabolomics Society  
News

Spotlight  
Environmental Molecular  
Sciences Laboratory

Recent Publications

Conferences & Events

Jobs

## Metabolomics Society News

### Members Corner

#### Board of Directors

Dear Colleagues,

I hope that you are all doing well as we continue to live in challenging times. I would like to highlight points in this issue of MetaboNews. First, in the past few months, the Precision Medicine Task Group has held two successful workshops in growing areas of metabolomics. We highlight the first of these two virtual workshops in this issue that was focused on single cell metabolomics. A comprehensive summary of the workshop is included, so please take some time to read the summary of that successful workshop.

There are now only 2 months until **Metabolomics 2021 Online**, and, on behalf of the Metabolomics Society, we would like to cordially invite you to Metabolomics 2021 Online, the 17<sup>th</sup> Annual Conference of the Metabolomics Society. The conference will run from Tuesday, June 22 to Thursday, June 24 and will have a fantastic program. A reminder that you can register now via the conference website, [metabolomics2021.org](http://metabolomics2021.org). Below are a few updated highlights that we would like to make you aware of.

On day one we will offer a series of exciting Workshops and Sponsor Studios. Workshops have been posted on the website. The scientific program will take place on days two and three and we have several exciting talks and updates to tell you about:

- The deadline for poster abstracts has been extended to **May 21**, and can be submitted via the conference website.
- We received an excellent variety of abstract submissions for oral presentations; selected oral talks will be announced this week.
- Workshops have been posted on the website. Due to the limited number of workshops in the conference schedule, we hope to have additional virtual workshops outside of the conference. Keep a lookout for these!

Metabolomics 2021 Online is your unique chance to connect to everyone virtually and learn about cutting-edge applications of metabolomics from friends and colleagues. Come join us!

For more updates on the conference stay tuned for the next issues for MetaboNews and the email announcements of the Metabolomics Society. Visit us at [metabolomics2021.org](http://metabolomics2021.org).

We are looking forward to seeing you all at Metabolomics 2021 Online.

All the best,



President of the Metabolomics Society

Ian Forsythe  
Editor

The Metabolomics Innovation Centre  
[metabolomics.innovation@gmail.com](mailto:metabolomics.innovation@gmail.com)



MetaboNews is a monthly newsletter published in a partnership between The Metabolomics Innovation Centre (TMIC) and 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](mailto:info@metabolomicssociety.org)

### Membership Enquiries

## Early-career Members Network (EMN)

### EMN Webinar Series

The EMN would like to thank again Dr. Maria Eugenia Monge and Nicolás Zabalegui, for their inspiring talks on a Python-based tool to read, process and visualize MS data generated in untargeted metabolomic studies as well as on strategies to improve the overall data quality. Find all our previous webinars [here](#).

The most recent Webinar organized by the EMN was held on May 20<sup>th</sup> 2021. The EMN welcomed Prof. Caroline Johnson and Ms. Ana Rosen Volmar, who presented their work on metabolic subphenotypes and colon cancer prognosis as well as on normalizing approaches of untargeted urine metabolomics data.

### New Expert Opinion

The new Expert Opinion is now published on the EMN wiki page, and it is a real pleasure to read the inspiring responses from Dr. Justine Bertrand-Michel. She shared with us her work and, of course, her experiences with lipidomics and the challenges related to human health applications. [Follow the link](#) to find out more.

## International Affiliates Corner

### Metabolomics Association of North America (MANA)

Visit <https://metabolomicsna.org>

The MANA WomiX Interest Group is looking for your input to shape the next Images of Success (IOS) Seminar Series. The next event in June will focus on Ph.D. students in metabolomics and is titled **“Ask anything from A to Z: Ph.D. students from metabolomics labs.”** Fill out this short survey [here](#) to let us know what you'd like! Check out their website for more information [here](#). The last IOS event in April featured Women in Metabolomics Cores and had 65 attendees at various career stages and from different sectors (academia, health and medical centers, industry, government, and for-profit/personal). Amanda Souza (Metabolomics Program Manager from Thermo Fisher Scientific) said, “I really enjoyed the last WomiX session ([April 2021 MetaboNews](#)). I was very encouraged to hear from my colleagues in the community.” Lastly, the WomiX Mentorship Program is planning their next workshop titled, “Let's Talk About: Soft Skills” coming up on May 20, 2021.

### Réseau Français de Métabolomique et Fluxomique (RFMF)

Visit <http://www.rfmf.fr/>

Save the date! Analyze your data with Galaxy and the Workflow4metabolomics e-infrastructure! The next Workflow4Experimenters international course (W4E2021) will take place in Toulouse, France (Monday 11<sup>th</sup> to Friday 15<sup>th</sup> October 2021). During this one-week course (entirely in English), you will learn how to use the W4M infrastructure and analyze your own LC-MS, GC-MS, or NMR data. Morning sessions will be dedicated to methodology and tools. Afternoon sessions will be devoted to tutoring.

## Metabolomics Society News

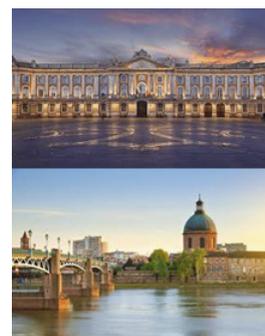


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### Agenda and preregistration:

<https://workflow4metabolomics.org/w4e2021>

(Deadline 15 May 2021)

Contact: [contact@workflow4metabolomics.org](mailto:contact@workflow4metabolomics.org)

### Sponsor:

W4M is jointly developed and maintained by the French Institute of Bioinformatics (IFB, Elixir node) and the Infrastructure for Metabolomics and Fluxomics (MetaboHUB).



### Financial support:

This course receives support from the Francophone Network of Metabolomics and Fluxomics (RFMF) and Genotoul (Toulouse technology platforms in life sciences).



See you soon in Toulouse!

## Other News

The Precision Medicine Task Group of the Metabolomics Society and MANA held a successful virtual Workshop on Single Cell Metabolomics on Friday, February 26, 2021.

Please find the final report on the successful **Single Cell Metabolomics Workshop** [[PDF](#)].

### Invited speakers:

L. Mervant (Ph.D. student), D. Touboul (CR, CNRS), F. Jourdan (DR INRAE)

### Scientific committee:

C. Delporte (ULB, Brussels), Y. Guitton (Laberca, Nantes), C. Dalle (U.DAB IRBA, Brétigny-sur-Orge), M. Pétéra, F. Giacomoni (PFEM INRA, Clermont-Ferrand), G. Le Corguillé, (Abims, Roscoff), B. Diémé (PFEM Université Clermont Auvergne), F. Souard (ULB, Brussels & Université de Grenoble), C. Canlet, J.F. Martin, M. Tremblay-Franco (Toxalim INRA, Toulouse), Ralf Weber (University of Birmingham)

# SpOtlight



## Comprehensive Metabolomics at EMSL

Spotlight article contributed by Sarah Wong, PNNL, in collaboration with Kristin Burnum-Johnson, EMSL, Yuri Corilo, EMSL, Mary Lipton, EMSL, and Thomas Metz, PNNL

### About EMSL

The [Environmental Molecular Sciences Laboratory](#) (EMSL) located at Pacific Northwest National Laboratory (PNNL) is a United States Department of Energy-funded user facility focused on gaining a predictive understanding of the molecular processes that control continuous changes underpinning biological and ecosystem functions. EMSL advances and integrates process-level understanding of complex systems, across wide temporal and spatial scales.

Scientists around the world are invited to access EMSL's world-class experts and state-of-the-art equipment—for free—to accelerate their research. The only requirement is that project data is open and non-proprietary. Access to EMSL, and other federally funded user facilities, is determined through a competitive peer-reviewed proposal call process. For more information about EMSL's proposals process visit: <https://www.emsl.pnnl.gov/user-program>.

Enabling new science insights means cross-disciplinary expertise and collaboration. EMSL's seven [Integrated Research Platforms](#) provide the atmosphere needed for tackling our greatest energy and environmental challenges. As an intrinsically transdisciplinary topic, metabolomics at EMSL encompasses expertise across many of these platforms.

### Comprehensive Metabolomics at EMSL

EMSL houses a unique and integrated suite of approaches and instrumentation that provide comprehensive measurement of the metabolome, including state-of-the-art and advanced mass spectrometry and nuclear magnetic resonance (NMR) platforms. Users leverage the lab's cross-disciplinary expertise and breadth of capabilities to perform a full range of metabolomics studies, including conventional targeted and untargeted metabolomics and lipidomics, as well as advanced measurements, such as spatially-resolved imaging, and ultra-high mass resolution mass spectrometry.

Users of EMSL's facilities receive support from experts in all stages of the analysis pipeline: from sample prep to data analysis, including the one-pot biomolecule extraction method, [MPLEx](#) ([Figure 1](#)). Users who would like to focus on a limited number of analytes can take a targeted metabolomics approach. This is a hypothesis-driven approach to address a specific scientific question. Researchers at EMSL are well equipped to answer these questions using various

instrumentation and methods, including a suite of triple quadrupole mass spectrometers and NMR instrumentation that are implemented in highly sensitive and specific assays to quantify specific molecules of interest or in metabolic flux measurements.

Those who desire to perform a comprehensive analysis of their sample, including measurement of both known and unknown metabolites and lipids, can use an untargeted metabolomics or lipidomics approach. Over 25 instruments are available to comprehensively measure metabolites and lipids with no intended bias including GC-MS, Orbitrap, NMR, and FT-ICR MS instrumentation.

Not only does EMSL boast an impressive array of world-class instrumentation, it also produces cutting-edge software that connects the user to the instrument to automate data acquisition, processing, analysis and interpretation. With this software, EMSL is a one-stop-shop for metabolomics research projects, providing support for all stages of the experiment pipeline. This includes standardization of conventional data processing, analysis and curation pipelines, and the centralization of *in silico* and standards-based molecular reference libraries leading to reproducible, consistent results across studies and projects. These are further enhanced by EMSL's High Performance Computing (Tahoma Cluster) and Cloud computing (RZR cluster) capabilities, and the seamless orchestration of data and metadata management (NEXUS), data processing ([CoreMS](#)), data curation, integration, interpretation (iMAP) services.

EMSL's status as a National User Facility means that EMSL researchers contribute to many important research projects with a broad range of collaborators. Select contributions are outlined below.

### Agile Biofoundry

[Agile Biofoundry](#) is a collaborative project among the U.S. Department of Energy national laboratories aiming to engineer biological systems to produce biofuels and other biomolecules at relatively low cost and high efficiency. This involves the genetic engineering of a host organism, usually a bacterium or fungus, to produce a specific molecule, then testing the metabolome of said organism to see if the target molecule is being produced and if other metabolic pathways were affected by the genetic engineering. The EMSL team is investigating the metabolic products of the engineered mi-

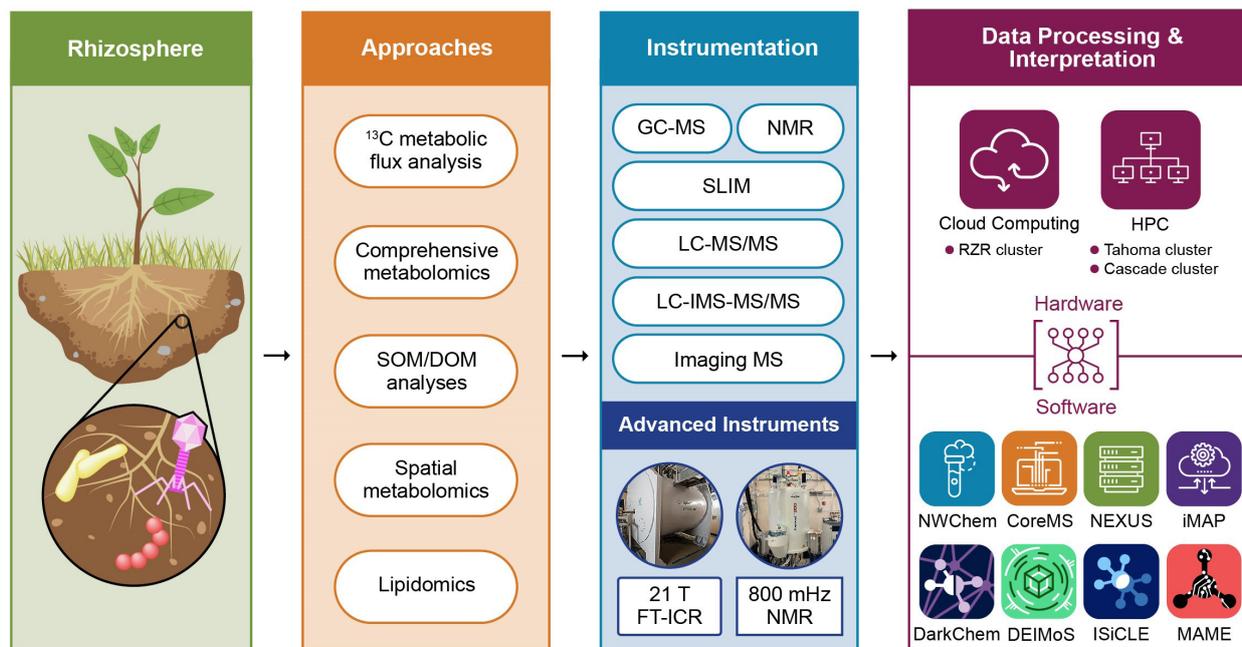
## Spotlight | Environmental Molecular Sciences Laboratory

crobes using mass spectrometry.

### Decrypting Bacterial Metabolism

Maintaining a healthy soil microbiome is important for both agriculture and the environment at large. Polyphenols are secondary metabolites produced by bacteria that were thought to be metabolized only under aerobic conditions.

In a collaboration with scientists from Colorado State University and other institutions, EMSL investigators performed Fourier Transform Ion Cyclotron resonance mass spectrometry (FT-ICR MS) to analyze polyphenol metabolism in bacteria under anoxic conditions. These findings have implications on the regulation of soil organic matter content.



**Figure 1: EMSL researchers can perform the full range of metabolomics experiments, from sample prep to data analysis using a variety of techniques, advanced instrumentation, high performance computing and software workflows.** Abbreviations are as follows: SOM, soil organic matter; DOM, dissolved organic matter; LC-MS/MS, liquid chromatography-tandem mass spectrometry; LC-IMS-MS/MS, liquid chromatography-ion mobility spectrometry-tandem mass spectrometry; SLIM, Structures for Lossless Ion Manipulations; NMR, nuclear magnetic resonance spectroscopy; GC-MS, gas chromatography-mass spectrometry; HPC, high performance computing; DEIMoS, data extraction for integrated multidimensional spectrometry; ISiCLE, *in silico* chemical library engine; MAME, multi-attribute matching engine; RZR, (Razor) Kubernetes cloud native cluster; [NWChem](#), Northwest Chemistry ab initio computational chemistry software; NEXUS, Network for Execution of User Science; iMAP, multi-omics analysis portal; [CoreMS](#), mass spectrum software framework and data processing portal.

### National Microbiome Data Collaborative

In July 2019, the [National Microbiome Data Collaborative \(NMDC\)](#) was initiated as a joint project between Lawrence Berkeley National Laboratory, Los Alamos National Laboratory, Oak Ridge National Laboratory and PNNL. As part of this project, EMSL developed bioinformatics tools to process large-scale multi-omics data. These tools will be publicly available as open-source tools for standardized workflows.

### EMSL and Beyond

Proper identification of unknown metabolites is challenging. To face this challenge, EMSL collaborates with [PNNL researchers](#) who are creating a variety of tools for standards-free identification of small molecules in complex systems. As only a small percentage of molecules are available as

pure standards, PNNL scientists built, leveraging EMSL's computational chemistry NWChem software and EMSL HPC infrastructure, comprehensive metabolite reference libraries through *in silico* calculations or predictions using the quantum chemistry-based [ISiCLE workflow](#) and the AI/ML-based [DarkChem tool](#); DEIMoS, a data extraction tool for multidimensional spectrometry; and [MAME](#), a chemical property matching software.

These tools can be utilized to identify unknown metabolites via multiple analytical pipelines and based on multiple experimental data types, including NMR (e.g., chemical shifts), as well as liquid chromatography coupled with ion mobility spectrometry and tandem mass spectrometry (LC-IMS-MS/MS) where retention times, collision cross sections, accurate masses, isotopic distributions, and tandem mass

## Spotlight | Environmental Molecular Sciences Laboratory

spectra are measured. Next generation ion mobility separations based on Structures for Lossless Ion Manipulations (SLIM) are also possible. Metabolites are identified by comparing experimental data with the appropriate *in silico* library without the need for a reference standard.

### Training the Next Generation

EMSL places a strong emphasis on supporting the next generation of scientists through a variety of education and training opportunities. Graduate students and postdoctoral researchers whose mentors have user projects are frequently hosted at the laboratory. Graduate students in the Office of Science Graduate Student Research (SCGSR) Program may pursue some of their thesis research at EMSL facilities. The lab also participates in the DOE Science Undergraduate Laboratory Internship (SULI) program, which allows STEM and science policy undergraduates to gain valuable research experience.

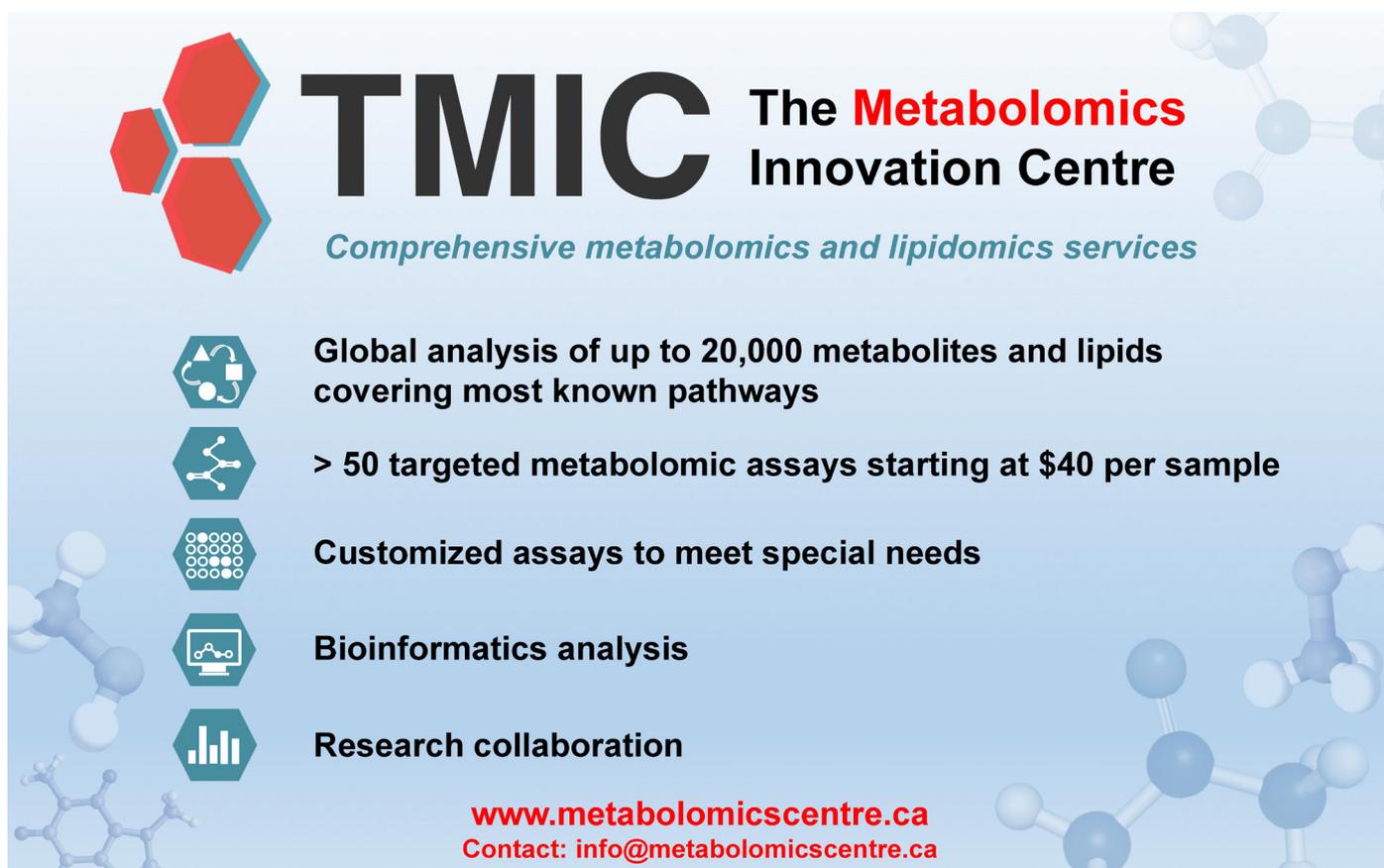
Additionally, EMSL hosts an annual summer school for

graduate students and early career researchers to strengthen their knowledge and technical skills in a particular topic. This year's topic is "[Multi-omics Modeling of Biochemical Pathways](#)". Attendance at this virtual event is free and open to anyone.

### Connect With Us

As a user facility, EMSL thrives on collaboration. Researchers from all career levels, from graduate students to senior researchers, and welcome to submit proposals under any of our scientific areas of expertise. Interested users can view our calls for proposals here: <https://www.emsl.pnnl.gov/proposals>

Those interested in connecting with our metabolomics researchers directly may contact [Dr. Mary Lipton \(mary.lipton@pnnl.gov\)](mailto:mary.lipton@pnnl.gov) or [Dr. Kristin Burnum-Johnson \(kristin.burnum-johnson@pnnl.gov\)](mailto:kristin.burnum-johnson@pnnl.gov) for targeted metabolomics studies, [Dr. Tom Metz \(thomas.metz@pnnl.gov\)](mailto:thomas.metz@pnnl.gov) for untargeted metabolomics, and [Dr. Yuri Corilo \(corilo@pnnl.gov\)](mailto:corilo@pnnl.gov) for data processing.



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 Contact: [info@metabolomicscentre.ca](mailto:info@metabolomicscentre.ca)

# Recent Publications

## Recently published papers in metabolomics

- [CpG-ODN induced antimicrobial immunity in neonatal chicks involves a substantial shift in serum metabolic profiles](#)
- [Urinary Metabolites Enable Differential Diagnosis and Therapeutic Monitoring of Pediatric Inflammatory Bowel Disease](#)
- [The maternal serum metabolome by multisegment injection-capillary electrophoresis-mass spectrometry: a high-throughput platform and standardized data workflow for large-scale epidemiological studies](#)
- [Quantum Chemistry Calculations for Metabolomics](#)
- [Unveiling metabolic changes in marsupialized odontogenic keratocyst: A pilot study](#)
- [Metabolomic Changes are Predictive of Aging in Laying Hens](#)
- [Biomarkers and Fatty Fish Intake: A Randomized Controlled Trial in Norwegian Preschool Children](#)
- [Effect of D-allulose feeding on the hepatic metabolomics profile in male Wistar rats](#)
- [A multi-omics approach for understanding the effects of moderate wine consumption on human intestinal health](#)
- [Circadian misalignment disturbs the skeletal muscle lipidome in healthy young men](#)
- [Comparative Metabolomics Revealing the Metabolic Responses of Pathogenic Bacteria to Different Antibiotics](#)
- [New software tools, databases, and resources in metabolomics: updates from 2020](#)
- [Integration of machine learning and genome-scale metabolic modeling identifies multi-omics biomarkers for radiation resistance](#)



# 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/>

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## 27 May 2021

### Metabolomics and Life Sciences Series

#### Venue

Online

*Find out how metabolomics can move your discoveries towards translation*

**May 27, 2:00 - 3:00 PM MDT - [Metabolomics and the Environment](#)**

Monitoring soil, water and air is becoming increasingly important as the human footprint on our planet grows. In this presentation Dr. David Wishart will explain how metabolomics can be used to make environmental monitoring both easier and more comprehensive, including examples of how metabolomics is being used to track water contamination, to assess soils and to identify chemicals in the air. Learn how metabolomics is being widely used to identify and quantify herbicides, pesticides and other toxic compounds in our food, water and environment and how

## Metabolomics Events

TMIC (The Metabolomics Innovation Centre) is developing many cutting-edge techniques and resources for this area.

Following the presentation, join the panel discussion and Q&A moderated by Dr. Wishart.

### Speaker

Dr. David Wishart, Director, The Metabolomics Innovation Center

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## 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](#).

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## 14-18 June 2021

### CliMetabolomics

#### Venue

Versailles and Bordeaux, France

#### Overview

CliMetabolomics aims to better understand the plasticity of plants and to develop sustainable plants adapted to climate change. The event consists of seminars, discussions and many practical courses. The workshop is aimed at doctoral students, post-docs and young researchers working in France or Germany. It is funded by INRAE, Science Campus and the Franco-German University.

#### Event Link

## Metabolomics Events

### 15-18 June 2021

#### Hands-on Data Analysis for Metabolic Profiling

##### Venue

Online, Imperial College London, London, United Kingdom

##### Overview

This course will be run online, with Live lectures and tutorials using MS Teams.

We offer a comprehensive, hands-on training in processing and analysing metabolomics data from LC-MS and NMR technologies.

##### Attendees will have the opportunity to:

- Learn directly from internationally recognised leaders in the field
- Benefit from practical training in computational techniques and statistical methods

##### Course Aims

This 3.5 day online course provides a comprehensive overview of data analysis for metabolic profiling studies focussing on data from NMR spectroscopy and Liquid Chromatography-Mass Spectrometry. It combines lectures and tutorial sessions using open source software to ensure a thorough understanding of the theory and practical applications.

##### [Course Link](#)

### 16-18 June 2021

#### Canadian Bioinformatics Workshops: Metabolomics Analysis

##### Venue

Online

##### Course Objectives

High-throughput sequencing of RNA libraries (RNA-seq) has become increasingly common and largely supplanted gene microarrays for transcriptome profiling. When processed appropriately, RNA-seq data has the potential to provide a considerably more detailed view of the transcriptome. The CBW has developed a 3-day course providing an introduction to RNA-seq data analysis followed by integrated tutorials demonstrating the use of popular RNA-seq analysis packages. The tutorials are designed as self-contained units that include example data (Illumina paired-end RNA-seq data) and detailed instructions for installation of all required bioinformatics tools (HISAT, StringTie, etc.).

Participants will gain practical experience and skills to be able to:

- Perform command-line Linux based analysis on the cloud
- Assess quality of RNA-seq data
- Align RNA-seq data to a reference genome
- Estimate known gene and transcript expression
- Perform differential expression analysis
- Discover novel isoforms
- Visualize and summarize the output of RNA-seq analyses in R
- Assemble transcripts from RNA-Seq data

##### [Workshop Link](#)

## Metabolomics Events

# 22-24 June 2021

### Metabolomics 2021 Online

**Save the Date!** Metabolomics 2021 Online will take place June 22-24, 2021. Registration is now open!

We are excited to introduce **Metabolomics 2021 Online**, the second virtual conference that will take place from June 22-24, 2021. 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.

The conference will follow the general format that we instituted for Metabolomics 2020 Online, with the conference taking place in all time zones, enabling it to continue as a truly international event. We will open the conference with day 1 offering workshops on special interest topics, which has now become a tradition of our conference format. Days 2 and 3 will feature scientific sessions that will begin with a keynote speaker followed by talks selected from submitted abstracts and the ability for viewers to ask questions, in order to maximize member interactions. For each of us, some talks will be at more convenient times than others because the conference will take place through many time zones. Fortunately, recorded talks will be available to access and watch later during the virtual event, so don't worry about staying up all night to attend a talk you wanted to hear at 3 AM!

We will also host virtual poster sessions, networking opportunities, and special interest sessions that will include a town hall and early career member network meetings, among others. One thing that we can say is the plethora of virtual meetings over the last year has taught us much on how to effectively engage through virtual events and we will use this to our advantage. So get excited about Metabolomics 2021 Online! Registration fees for the meeting will be greatly reduced for all registered members of the Society.

Now is a great time to become a member of the Society! If you are already a member, then please go ahead and register for the meeting. I would also encourage you to submit an abstract to present your work at the conference, as we depend on each of you to hear about the latest in cutting-edge research. We look forward to seeing you virtually at Metabolomics 2021 Online.

### [Conference Link](#)



## Metabolomics Events

### 28 June to 2 Jul 2021

#### Introduction to Nutritional Metabolomics

##### Venue

Department of Nutrition Exercise and Sports, University of Copenhagen, Denmark

##### Overview

The course will provide a general overview of LC-MS based untargeted metabolomics from study design to results and will be exemplified with its specific application in nutrition. It will be delivered using a mixture of lectures, hands-on data preparation and analysis, computer-based practical sessions, and discussions. Visits to wet labs and instructions on human sample preparation procedures are included but with minimal hands-on experience.

The students will go through common steps in a typical metabolomics study using a real-life case. This case study includes collected plasma (or urine) samples from a nutritional intervention. The sample preparation and analysis on UPLC-QTOF has been conducted and the students will further process and analyze the acquired data with various freeware tools (e.g., R, XCMS, MZmine, etc). They will finally work on identification of relevant metabolites using several web-based structure elucidation tools. The course will conclude by presentations of reports generated by the students based on the case study.

The course will be structured as initial short lectures on theory followed by hands-on exercises, which will teach the students to transfer the theoretical information to practice. The students should expect a fairly technical course with a strong focus on the hands-on data analysis abilities and data interpretation skills.

##### Fee

There will be no fee for PhD students under the Open Market in Denmark and NOVA partners (Nordic Countries). Other participants are to pay a course fee of 300 EUR. Each student must pay and arrange their own travel and accommodations in Copenhagen during the course.

#### [Course Link](#)

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### 12-16 July 2021

#### 2021 EMSL Summer School

##### Venue

Online, Pacific Northwest National Laboratory, Richland, Washington, USA

#### Virtual Multi-omics Modeling of Biochemical Pathways Summer School

Researchers interested in modeling of multi-omics data are invited to attend the virtual Multi-omics Modeling of Biochemical Pathways Summer School July 12-16, 2021. Presentations given during this week-long event are free and open to the public.

Learn from world-class national laboratory and academic researchers how to use visualization tools, analysis, and modeling of multi-omics data for understanding biochemical pathways. Hosted by the Environmental Molecular Sciences Laboratory (EMSL) and Agile Biofoundry groups, this event will feature lectures on software and data analysis.

## Metabolomics Events

Overview of daily topics covered during this Summer School event:

- Experimental Design
- Transcriptome & Proteome Data
- Metabolomics and Lipidomics Data
- Metabolic Modeling
- Fluxomics

Visit [pnnl.cventevents.com/2021summerschool](http://pnnl.cventevents.com/2021summerschool) for information about speakers, topics covered, applications for the competitively-selected tutorials, and much more.

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### 5 Aug 2021

Identification of Unknown Compounds in Untargeted Metabolomics using Freely Available Software for Compound ID

#### Venue

Online, University of California, Davis, California, USA

#### Instructor

Dr. Arpana Vaniya, UC Davis

#### Registration

**Required software:** [MS-FINDER](#) & [SIRIUS+CSI:FingerID](#). CFM-ID will be the web-based tool. Versions of tools to be used will be announced closer to the course date.

**Participant prerequisites:** Basic knowledge of computer skills. No coding experience needed.

**Short description of the course:** Compound identification is known as the bottleneck in metabolomics. However, there are many approaches one may consider while tackling this challenge (i.e., mass spectral library search, in silico fragmentation tools, or database searching). This short course will provide an overview on the current status of compound ID in metabolomics, participants will learn how to use some current tools for compound ID (i.e., CFM-ID, MS-FINDER, and SIRIUS+CSI:FingerID), and apply those skills to some unknown challenges.

For more information, please visit the [Bits & Bites: Short Course Series 2021 website](#).

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### 30 Aug-10 Sep 2021

International Summer Sessions in Metabolomics

#### Venue

Online, University of California, Davis, California, USA

#### Registration

## Metabolomics Events

The course will include:

1. Study design, including pitfall analysis and hidden biases in studies from microbial, plant, mouse and human cohort research
2. Sample preparation and quality control
3. In-laboratory detailed discussions standard operating procedures for GC-MS and LC-MS data acquisitions
4. Targeted metabolomics, including monitoring charts and use of isotope labeled internal standards
5. Exercises on flux analysis in cancer cells by isotope tracer analysis
6. Untargeted data processing and exercises on MS-DIAL software
7. Exercises on identification of unknowns by cheminformatics software workflows (incl MS-FINDER, CFM-ID, and various databases and small software routines)
8. Data normalization and transformation with and without internal standards and quality controls
9. Multivariate and univariate statistics
10. Pathway mapping

For information and registration click [here](#).

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### 27-30 Sep 2021

CliMetabolomics

#### Venue

Leipzig and Halle / Saale, Germany

#### Overview

CliMetabolomics aims to better understand the plasticity of plants and to develop sustainable plants adapted to climate change. The event consists of seminars, discussions and many practical courses. The workshop is aimed at doctoral students, post-docs and young researchers working in France or Germany. It is funded by INRAE, Science Campus and the Franco-German University.

#### [Event Link](#)

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### 17-19 Oct 2021

3rd Annual MANA Conference: Foods for Health Discovery Theme

#### Venue

The Ohio State University, Columbus, Ohio, USA

[MANA 2021 conference website](#)

If you seek to get *your* planned metabolomics event endorsed by MANA and receive MANA funds, please [contact us!](#)

## Metabolomics Events

# 1-5 Nov 2021

## Hands-On Mass Spectrometry Course

### Venue

Department of Animal Science, Aarhus University, Blichers Allé 20, Tjele, Denmark

At Aarhus University, Department of Animal Science, we are organizing a “Hands-on mass spectrometry course”, which will give insight in the use of mass spectrometry for a range of analyses with relevance in animal science. The course will take place November 1-5, 2021.

### [Course Flyer](#)

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**Metabolomics Jobs**

# Metabolomics Jobs

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

## Jobs Offered

Job Title	Employer	Location	Posted	Closes	Source
Various Positions			19-May-21		<a href="#">Metabolomics Association of North America Jobs</a>
Postdoctoral Researcher	IARC	Lyon, France	27-Apr-21	Until Filled	<a href="#">IARC</a>
Senior/Principal Research Associate, Metabolomics	Calico Life Sciences	South San Francisco, CA, USA	26-Apr-21	Until Filled	<a href="#">Calicolabs.com</a>
Marketing Specialist – Metabolomics (150945BR)	Thermo Fisher Scientific	San Jose, California, USA	20-Apr-21	Until Filled	<a href="#">ThermoFisher.com</a>
PhD Student and Post-doctoral Fellow Positions in Mass Spectrometry Metabolomics and Proteomics	Technion – Israel Institute of Technology	Haifa, Israel	29-Mar-21		<a href="#">MetaboNews Jobs</a>
Research Associate, Entomology Department	Cornell University	Ithaca, NY, USA	22-Mar-21	Until Filled	<a href="#">AcademicJobs Online.org</a>
Business Development Manager	TMIC, Faculty of Science, University of Alberta	Remote	17-Mar-21	Until Filled	<a href="#">University of Alberta Careers Page</a>
Postdoctoral R&D Scientist - NMR-based metabolomics	Lesaffre	Loos, France	16-Mar-21	Until Filled	<a href="#">SmartRecruiters.com</a>
PhD Research Project Opportunities, Centre for Integrative Metabolomics and Computational Biology	Edith Cowan University	Joondalup, Australia	16-Mar-21	Until Filled	<a href="#">Edith Cowan University</a>

**Metabolomics Jobs**

<b>Job Title</b>	<b>Employer</b>	<b>Location</b>	<b>Posted</b>	<b>Closes</b>	<b>Source</b>
Postdoctoral Research Fellow, Metabolomics and Nutritional Epidemiology	McMaster University	Hamilton, ON, Canada	23-Feb-21	5-Jul-21	<a href="#">TMIC Careers Page</a>
Research Technologist	Cold Spring Harbor Laboratory	Cold Spring Harbor, NY, USA	17-Jan-21	Until Filled	<a href="#">Cold Spring Harbor Laboratory</a>
Post-doctoral Fellow / Staff Scientist – Metabolomics	Oklahoma Medical Research Foundation	Oklahoma City, Oklahoma, USA	17-Dec-20	Until Filled	<a href="#">Metabolomics Society Jobs</a>
Postdoctoral Researcher in Analytical Environmental Cheminformatics	University of Luxembourg	Belval Campus, Luxembourg	Dec-20	Until Filled	<a href="#">University of Luxembourg</a>
Postdoctoral Position	NIH	Rockville, Maryland, USA	20-Nov-20	Until Filled	<a href="#">Metabolomics Society Jobs</a>
Post-Doctoral Position with influence of multiple 'omics' datatypes on the development of respiratory and/or neurological disease	Brigham and Women's Hospital and Harvard Medical School	Boston, MA, USA	20-Nov-20	31-May-21	<a href="#">Metabolomics Society Jobs</a>

## Metabolomics 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](mailto:metabolomics.innovation@gmail.com)). Upon review, a limited number of job submissions will be selected for publication in the Jobs Wanted section.

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