# MetaboNews

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

# Metabolomics Society News

### Board of Directors Election - Election Results

Thank you for your participation in the Board of Director Election in August! We are pleased to announce the results of the election and welcome some new faces to the Board.

Re-elected for another 2-year term: Caroline Johnson, Jessica Lasky-Su, Dan Raftery and Ralf Weber.

Newly joining the Board for a 2-year term:

Natasa Giallourou Roy Goodacre Matej Orešic Stacey Reinke Fidele Tugizimana Baljit Ubhi Michael Witting

We also welcome Marine Letertre to the Board as the Chair of the EMN for the next year.

The Officer Election will be open September 15 – 28, keep an eye on your e-mail for the voting announcement, as your input for Officers is greatly valuable!

### Metabolomics 2020 Online

Join your peers virtually at Metabolomics 2020 Online! Registration and Abstracts Now Open!

We still have presentation spots available and encourage you to submit an abstract for Metabolomics 2020 Online, hitting a global audience October 27 –29. Presentations will happen in several time zones, and your talk will be recorded and available for viewing online after the event. Don't miss this opportunity to publish your work!

The deadline for oral abstract submissions has been extended to September 20 and poster abstracts will be accepted through September 20 as scheduled. There are a limited number of attendee spots for this virtual conference, register soon to reserve your space. Metabolomics 2020 Online is FREE to current members of the Metabolomics Society.

The line-up of Keynote Speakers is available to view online, with additional speakers coming soon. All conference details can be found at <a href="https://www.metabolomics2020.org">www.metabolomics2020.org</a>.

### Metabolomics Society News | Notes from the Chair





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

# Metabolomics Society News

It is nearly the end of my second term as President of the Metabolomics Society and time for me to make way for a new President. We have already held our elections for new board members to start in October and we are about to hold the elections for the Officer posts. Please look out for the email detailing how to vote in the Officer elections to elect a new President, a new Treasurer and a new Secretary. I would like to take this opportunity to thank all the directors on the board that I have served with over the past four years and in particular my fellow officers, Nichole Reisdorph and Krista Zanetti who have been a huge support over my stint as President. I would also like to thank Horst Joachim Schirra, Huiru Tang and Jiang Zhu for all their work on what we hope is the delayed Shanghai meeting. I'm looking forward to the meeting already!

However, I do not want to only look back on the past this month but encourage all the membership to look forward. In the immediate future we have the online virtual meeting on 27th-29th October, 2020. You still have time to submit abstracts for talks (deadline extended to September 20th 2020) and posters (deadline 20th September, 2020). There is a cracking line up of plenary speakers which you can find at <a href="http://metabolomics2020.org/">http://metabolomics2020.org/</a> along with all the details for registering for the meeting. Looking forward we hope to be back to face to face meetings in 2021 visiting Niagara Falls, Canada and then finally get to Shanghai in 2022. This last part all depends on the current global situation but I hope we will meet again in the very near future.

Jules Griffin

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President of the Metabolomics Society



# Dr. Cristina Legido-Quigley



Photo by Lizette Skotbo

Head of Systems Medicine
Steno Diabetes Center
Copenhagen, Denmark
Associate Professor
King's College
London, United Kingdom

# Short Biography

Cristina Legido-Quigley is the Head of Systems Medicine at Steno Diabetes Center Copenhagen and an Associate Professor at King's College London. She has been a group leader in clinical biomarkers at King's College London since 2006. In 2018 she moved to Steno a hospital and research centre in Denmark to pursue her interests in Systems Medicine, especially the brain-liver axis, and finding clinical biomarkers of healthy aging, Alzheimer's, cognition, diabetes and metabolic disease. She shares her findings in publications in the biotechnology and medical fields (In the press, social media @drlegidoquigley and in peer-reviewed journals ORCID: https://orcid.org/0000-0002-4018-214X)

# Interview Q&A

# How did you get involved in metabolomics?

It was in 2006, I had worked in industry in the late 90s and did my PhD with mass spectrometry in Chemistry at Imperial College London. After a year postdoc in Italy, I came back to Elaine Holmes and Jeremy Nicholson's team at the same university, they were working with NMR so I, and my friend Cinzia Stella, started the MS side of things with a beta version UPLC-MS.

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

I now work in a hospital and collaborate in clinical trials and cohort studies, so I am able to test the biological role of metabolites in disease.

We have biomarkers that we are validating, and the idea is to implement them in our clinic. I find it exciting to be involved in the discovery and in the implementation.

# What key metabolomics initiatives are you pursuing at your research centre or institute?

I work at Steno Diabetes Center in Copenhagen and at King's College London. At Steno we work with seven clinical teams and work in systems medicine. My main interest is systems medicine, and I mostly work in metabolic disease and brain neurodegeneration.



### Metabo Interview | Dr. Cristina Legido-Quigley

### Accelerate Your Metabolomics Research

Agilent's industry-leading metabolomics portfolio just got even better





We are also part of a bigger network of Novo Nordisk Merging cohort data, sharing data with others and Foundation centers. In other centers there are systems personalising medical data many times is not possible. biology labs and metabolomics labs applied to basic science. There is a lot of expertise to collaborate in the Copenhagen area. The Danish invest in technology and science, so you are never far from a new cool technique, the omics, informaticians, etc.

At King's College London there is a lot of interest in metabolomics. The NMR facility helps many researchers, and I think that there are plans of extending to mass spectrometry. My wish would be to reproduce the Danish model at King's and bring in bioinformaticians as there are excellent researchers in-house.

### What is happening in your country in terms of metabolomics?

In Denmark we started a network and have had an annual meeting in which we invite international speakers <a href="https://">https://</a> clime.dk/. We organise two local meeting and we recently had a Zoom to organise virtual seminars while we are taking measures for the pandemic worldwide. We did the same in London. We started the London metabolomics network few years back <a href="http://londonmetabolomicsnetwork.com/">http://londonmetabolomicsnetwork.com/</a>, both networks are going strong thanks to metabolomics group leaders and ECR volunteers.

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

It will be applied in our clinic to stratify patients into treatments and to monitor them before they get complications. In cases we will need genetics or other omics to make better decision panels.

I see lipidomics enhancing clinical lipid data already, but we must discover the function of lipids before we start modulating them.

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

It's a fast track to discovery of disease mechanisms, its impact to society will be big.

Sometimes we can't even peruse our own data which is sitting in a federated database in another EU country. I'm hoping someone in the EU will work to make GDPR easier to use for research.

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

I think metabolomics has taken off already, but you can always ask for more accurate data, new metabolites in all tissues, defined concentrations and functions, easier ways of sharing and more collaboration to validate results.

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

I'm hoping it's good!

Obviously, it is up to us to show funding bodies its utility. Then, many countries are cutting funding or hardly fund science, in those cases it will be impossible to produce hightech data. Luckily, it will be possible to do data analyses and discovery. Industry will play a role too, as they work in an international environment, they can make sure that funding is invested wisely.

### What role can metabolomics standards play?

An important role to be able to share data and validate results. Similar to the GDPR we can't be too strict, as this can stall progress, it is a tricky one. To me the question is, who is to set these standards? Will this mean that those with less resources won't be able to do metabolomics?

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

Yes, one pet peeve of mine is when people doing metabolomics and talk about data like it is an absolute accurate measurement. By now, people outside our field are very confused and are doing work that they think is deterministic when at best it is an approximation.

I am worried that the difficult research times that we are experiencing with Covid-19 will impact mostly women and BAME, we must keep an eye for this. Some positive action by established scientists can go a long way.



# Recent Publications

### Recently published papers in metabolomics

- <u>Metabolic Signatures of 10 Processed and Non-processed Meat Products after In Vitro Digestion</u>
- <u>Volatile Organic Compounds Analysis optimization and biomarker discovery in urine of Non-Hodgkin Lymphoma patients before and during chemotherapy</u>
- NMR-based metabolomics analysis of Calabrian citrus fruit juices and its application to industrial process quality control
- Metabolic perturbations prior to hepatocellular carcinoma diagnosis: Findings from a prospective observational cohort study
- The Metabolomic Underpinnings of Symptom Burden in Patients With Multiple Chronic Conditions
- MetaboShiny: interactive analysis and metabolite annotation of mass spectrometrybased metabolomics data
- <u>Longitudinal change of metabolite profile and its relation to multiple risk factors for</u> the risk of developing hepatitis B-related hepatocellular carcinoma
- Warmth Prevents Bone Loss Through the Gut Microbiota
- <u>Distinct serum metabolomic signatures of multiparous and primiparous dairy cows</u> switched from a moderate to high-grain diet during early lactation
- Metabolomics for Biomedical Research



### 12 Oct-6 Nov 2020

### Metabolomics Data Processing and Data Analysis

### Venue

Online, Birmingham Metabolomics Training Centre, University of Birmingham, United Kingdom

### **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
- 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



### **Metabolomics Events**

### 20 Nov-18 Dec 2020

### Quality Assurance and Quality Control in Metabolomics

### Venue

Online, Birmingham Metabolomics Training Centre, University of Birmingham, United Kingdom

### **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

https://www.birmingham.ac.uk/facilities/metabolomics-training-centre/courses/2020/Quality-Control-and-Quality-Assurance-in-Metabolomics.aspx



### **Metabolomics Events**

# Postponed/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/

## 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).

Abstract submission deadline is Monday, June 15, 2020, 11:59pm CST.

### Course link

https://www.soc-neuro-onc.org/SNO/2020METAB/Home.aspx



### **Metabolomics Events**

# 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.

### Course link

 $\underline{https://www.wur.nl/en/Education-Programmes/Wageningen-Academy/Plant/Course-Data-analysis-for-Metabolomics.htm}$ 



### **Metabolomics Jobs**

# Metabolomics Jobs & Collaborations

If you have a job you would like posted, please email Shelby Soke (soke@ualberta.ca).

# Jobs Offered

Job Title	Employer	Location	Posted	Closes	Source
Various Positions			9-Sep-20		Metabolomics Association of North America Jobs
Researcher in Metabolomics/ Computational Metabolomics	Institute for Biomedicine, Eurac Research	Bolzano, Italy		Until filled	<u>MetaboNews</u>
Postdoctoral scholar	University of California San Francisco (UCSF)	San Francisco, CA, USA	24-June-20	31-Dec-20 or until filled	Metabolomics Society Jobs
Are you a skilled metabolomics expert/ analytical chemist?	MS-Omics	Vedbaek/ Copenhagen, Denmark	26-May-20	1-Sep-20	Metabolomics Society Jobs



### **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 Shelby Soke (<u>soke@ualberta.ca</u>). Upon review, a limited number of job submissions will be selected for publication in the Jobs Wanted section.

