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

Conference Corner

The Local and International Organizing Committee is delighted to extend this invitation to you to attend Metabolomics 2019, the 15th Annual Conference of the Metabolomics Society, in The Hague, The Netherlands. The conference will be held June 23-27, 2019 at the World Forum.

Open Call to Society Members for Workshop Suggestions

We are busy planning the conference agenda and we are eager for your input on pre-conference workshops on Sunday June 23rd and Monday June 24th. The workshops will provide a terrific venue to discuss a wide range of important topics and practical aspects of metabolomics, and may include hands-on learning opportunities. You can submit your workshop application online (click here) by completing the simple form.

The deadline for submission of workshop proposals is **December 11, 2018**

Sponsorship Opportunities Now Available!

We look forward to partnering with your organization to continue the success of bringing together all the major international organizations involved in human, plant, microbial, animal and environmental metabolomics.

We expect this to be the event in 2019 for metabolomics researchers from around the world, where established experts and the rising stars of the future will present their work. The conference will attract a high proportion of senior scientists with top level purchasing authority.

We have a variety of sponsorship opportunities available to position your brand and product at the forefront of the scientific community; view them here. Opportunities are limited and available on a first-come, first-served basis; so do not delay!

NEW for 2019 – Introduction to the Field

A new element in 2019 will be "Introduction to the Field" sessions, where leading PIs will give an introduction to their field, in an interactive 90-120 minute session, for a classroom-size group of (primarily) early-career scientists. The aim is that participants are able to ask their questions, thereby creating a new platform for interactions which currently doesn't exist at Metabolomics conferences.

Conference registration and abstract submission will open in December. We look forward to welcoming you to The Hague! www.metabolomics2019.org

Jules Griffin
Metabolomics Society President

Board of Directors

Words From the President

For those that follow MetaboNews you will know that we have recently been joined by a number of new directors and said goodbye to those terms are up. If you aren't familiar with how it works, directors are elected for two years and can then stand for re-election for one other term of two years. While terms may be extended if a director becomes an officer of the board, the whole board has a limited tenure and each October/November we are faced with renewing our committee memberships. The Society's committees each carry out specific jobs for the Society and according to the bylaws can be made up of directors and members of the Society; however in practice, some committees have to be limited to directors because of reasons of confidentiality within the board. We have just completed this process and you should be able to see the current committee memberships on the Society webpages.

The next stage is to re-invigorate the task groups that the Society has. These were set up to carry out a specific set of tasks where the Society felt there was an urgent community need to make progress. For example, the Metabolite Identification task group is "working with the community to build consensus on metabolite identification reporting standards, to educate the community on best practices and current tools and resources and to provide the opportunity for inter-laboratory comparisons." You can find all the task groups under the Board & Committees tab on the website, with each task group having its own webpage listing key contacts and their mission statement. While these task groups carry out vital work for the community, one issue can be that because some of the mission statements are quite open-ended its sometimes difficult to gauge progress of these task groups. The plan is to have each task group present a progress report to the Board on a regular basis so we can let the membership know about progress and whether we need membership input into these various activities, for example in metabolite ID workshops, etc.

Members Corner

Early-Career Members Network (EMN)

EMN Bursary Program

The EMN travel award 2018 was given to two graduate students, Yannick Audet-Delage for going to the 2018 AACR Annual Meeting in Chicago with a poster titled "Metabolic biomarkers of endometrial cancer and its recurrence in postmenopausal women", and Fatema Bhinderwala for going to the 2018 Experimental NMR Conference to present her research on "Nitrogen-Based Metabolomics for functional analysis of urease in Staphylococcus aureus". Both winners appreciated the chance to present their work and the networking opportunities, as those are key elements for the next career steps after graduation.

Follow the EMN on facebook (https://www.facebook.com/EMN.MetabolomicsSociety/) for the upcoming call 2019 and apply for our travel grant to expand YOUR horizon!

Please stay tuned for our upcoming webinars. You can access the recorded videos of the past webinars on the Metabolomics Society website.

METABOLOMICS SOCIETY

METABOLOMICS SOCIETY
EARLY-CAREER MEMBERS NETWORK

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

General Enquiries
info@metabolomicssociety.org
Membership Enquiries
membership@metabolomicssociety.org

International Affiliates Corner

Réseau Français de Métabolomique et Fluxomique (RFMF)

Visit http://www.rfmf.fr/

The RFMF board, the RFMF junior and the local committees are happy to announce the organization of the **12th Scientific Conference of RFMF taking place in Clermont-Ferrand from May 21st to May 23rd 2019**. A satellite event will take place May 20th 2019 and will be dedicated to workshops and round tables. This 12th edition will again be the opportunity to stimulate exchanges within the French-speaking community by offering 4 plenary talks by internationally speakers, oral presentations, 180 seconds flash presentations, thematic and poster sessions.

International renowned speaker venue is already confirmed

- **Coral Barbas** (University of San Pablo Madrid)
- **Pieter Dorrestein** (University of California)
- **Claudio Luchinat** (Unversity of Florence)
- **Konstantinos A. Aliferis** (University of Athens)

Main thematic research areas covered during the 12th RFMF conference will be applications of metabolomics and fluxomics in the areas of:

- Nutrition
- Environment
- Pharmacology/toxicology
- Plants
- Health
- Food product quality
- Biotechnologies

RFMF will promote methodological and technological developments for metabolomics, fluxomics, lipidomics and volatilomics with new:

- Analytical developments
- Data pre- and post-processing
- Statistics and data integration

Both English and French will be spoken during the conference.

There will be the opportunity for RFMF to award several prizes during the conference proceedings: PhD award 2019, poster prizes and best flash presentation.

We hope that the conference will continue to provide a friendly atmosphere for networking within the French-speaking Community.

SpOtlight

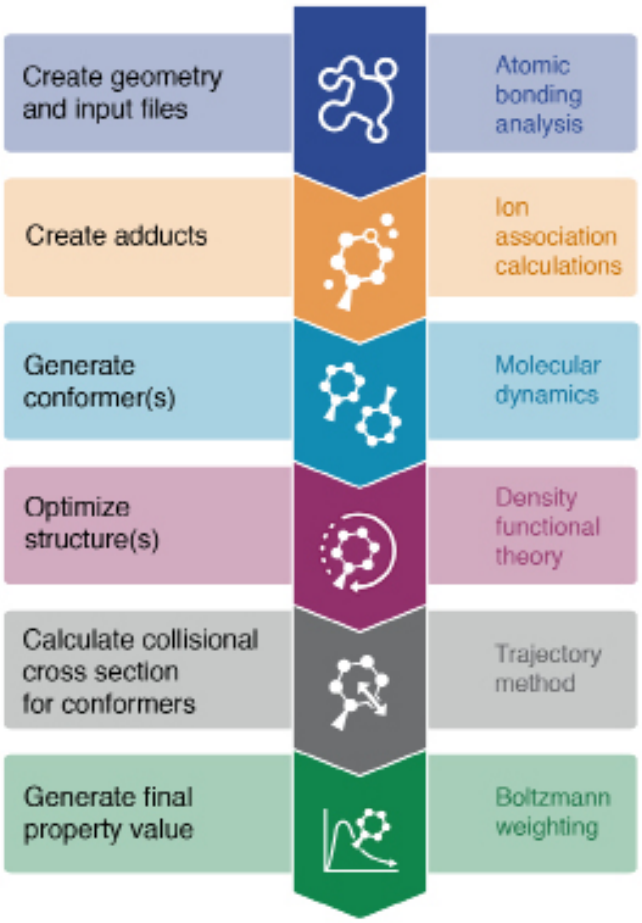
Pushing toward standards-free metabolomics with ISiCLE, the in silico chemical library engine

Sean Colby, Thomas Metz, and Ryan Renslow

Overview

Current gold-standard methods for identification of small molecules in complex samples rely on comparison of experimental features to libraries of reference data derived from analysis of authentic chemical materials. However, most molecules have yet to be characterized, and of those that are known, most are not available for purchase as standards. This represents a currently insurmountable problem: the majority of small molecules cannot be identified.

A step towards overcoming this barrier is to use computational methods, instead of laboratory-based methods, to build libraries. Chemical properties that can be **(i)** consistently measured experimentally and **(ii)** accurately calculated computationally can be used to build evidence towards identification, without reliance on traditional libraries. We call this approach "standards-free" metabolomics. Successful development and validation of standards-free methods will dramatically expand the number of identifiable compounds and bring the metabolomics field up to a level commensurate of that which is currently enjoyed in proteomic and genomic fields.



To advance standards-free metabolomics, we have developed the in silico chemical library engine (ISiCLE, now freely available on GitHub) as a way to automate the calculation of chemical properties using high-performance computing resources. These properties can subsequently be used to aid identification of molecules after experimental analysis of samples. Currently, ISiCLE can be used to calculate collision cross sections (CCS) for use in ion mobility spectrometry measurements and chemical shifts for use in nuclear magnetic resonance (NMR) spectroscopy. Future versions of ISiCLE will focus on adding additional properties and increasing throughput and accuracy. Confidence in molecular identification can be increased by adding additional dimensions of chemical properties as evidence. We envision a future where molecular identification can be performed without any use of standards, with confidence on par with, or exceeding, current gold-standard (i.e., standards-based) approaches.

ISiCLE was evaluated on the largest set of experimental collision cross section (CCS) values to-date, spanning molecular classes and sizes, and achieved a mean absolute percent error of 3.2%, besting similar methods in the literature and competing machine-learning approaches.

Implementation

ISiCLE employs state-of-the-art first-principles calculations in an easy-to-use package that scales, without modification, from desktops to supercomputers to the cloud. The pipeline takes an InChI (International Chemical Identifier) or SMILES (simplified molecular-input line-entry system) string as input, generates an initial 3D conformation, and subsequently optimizes this initial structure through molecular dynamics simulations and quantum chemistry calculations. Finally, ISiCLE simulates desired properties for each conformer yielded during molecular dynamics simulations to produce a single value, Boltzmann-weighted by Gibb's free energy, giving emphasis to properties from highly probable conformations. Currently, properties include CCS and NMR chemical shifts, but we are rapidly expanding the base framework to include MS/MS spectra, IR spectra, and more.

ISiCLE was developed using the Snakemake workflow management system, enabling scalability, portability, provenance, fault tolerance, and automatic job restarting. Snakemake provides a readable Python-based workflow definition language and execution environment that scales seamlessly to HPC architectures. Users simply provide input structures defined by InChIs, optionally tweak a single configuration file, and their simulations are then scheduled automatically, ultimately yielding desired properties.

In silico library

ISiCLE was used to calculate CCS values for the Human Metabolome Database (HMDB) 4.0, Universal Natural Product Database (UNPD), and the Distributed Structure-Searchable Toxicity (DSSTox) Database. Combined, nearly 1 million values are now available at metabolomics.pnnl.gov, which is being regularly updated to expand the number of compounds and, as ISiCLE is further developed, the number of calculated properties.

The first is a preprint paper describing ISiCLE for CCS, the second describes ISiCLE for NMR chemical shifts, and the third is to cite the software package (update version and access date appropriately).

Referencing ISiCLE

If you would like to reference ISiCLE in an academic paper, we ask you to include the following references:

• Colby, S.M., Thomas, D.G., Nunez, J.R., Baxter, D.J., Glaesemann, K.R., Brown, J.M., Pirrung, M.A., Govind, N., Teeguarden, J.G., Metz, T.O. and Renslow, R.S., 2018. ISiCLE: A molecular collision cross section calculation pipeline for establishing large in silico reference libraries for compound identification. arXiv preprint arXiv:1809.08378.

• Yasemin Y., Jamie R.N., Sean M.C., Dennis G.T., Mark I.B., Patrick N.R., Nancy M.W., Thomas O.M., Justin G.T., Niranjan G., Ryan S.R. An automated framework for NMR chemical shift calculations of small organic molecules. Journal of Cheminformatics. In press.

• ISiCLE, version 0.1.0 http://github.com/pnnl/isicle (accessed Oct 2018)

Recent Publications

Recently published papers in metabolomics

- A Sensitive, High-Throughput LC-MS/MS Method for Measuring Catecholamines in Low-Volume Serum.
- Advances in Mass Spectrometry-Based Single-Cell Metabolomics.
- A Plasma Metabolite Panel as Biomarkers for Early Primary Breast Cancer Detection.
- A Foodomics Approach: CE-MS for Comparative Metabolomics of Colon Cancer Cells Treated with Dietary Polyphenols.
- Metabolomics in the Study of Retinal Health and Disease.
- Machine Learning in Untargeted Metabolomics Experiments.
- Cluster Analysis of Untargeted Metabolomic Experiments.
- Determining the Mode of Action of Antimalarial Drugs Using Time-Resolved LC-MS-Based Metabolite Profiling.
- Quantitative Profiling of Endogenous Metabolites Using Hydrophilic Interaction Liquid Chromatography-Tandem Mass Spectrometry (HILIC-MS/MS).
- Worldwide Variation in Human Milk Metabolome: Indicators of Breast Physiology and Maternal Lifestyle?

Metabolomics Events

Imperial College London

3-7 Dec 2018

Hands-on LC-MS for Metabolic Profiling

Venue:
Imperial College London, Exhibition Road, London, United Kingdom

This week-long course aims to cover how to perform a metabolic profiling experiment, from start to finish. It will cover study design, sample preparation, the use of mass spectrometry for global profiling and targeted methodologies and data analysis.

Standard: £1950
Registration: Register using this link

For further information and registration details, please visit http://www.imperial.ac.uk/imperial-international-phenome-training-centre/courses/hands-on-lc-ms-for-metabolic-profiling/

Metabolomics Events

MetaboMeeting 2018 17-19 December University of Nottingham, UK

17-19 Dec 2018

Metabomeeting 2018

Venue:
University of Nottingham, United Kingdom

Welcome to MetaboMeeting 2018. The Metabolic Profiling Forum is delighted to announce the 11th Metabomeeting which is to be held at the University of Nottingham in the UK on the 17th-19th December 2018.

The meeting will bring together research scientists and practitioners from all areas of application and development of metabolic profiling, covering a wide range of experience from early career scientists to experts from throughout the international metabolomics field.

MetaboMeeting 2018 continues to highlight the work of its attendees through both oral platform presentation and poster sessions.

Oral presentation and poster abstract submission 30 September 2018

For further information and registration details, please visit:
http://thempf.org/mpf_cms3/index.php

Metabolomics Events

31 Jan - 30 June 2019

Research Hotel Application

Venue:
The Metabolomics Innovation Centre. Edmonton, Canada
Application deadline is Sept. 30 2018

The Metabolomics Innovation Centre (TMIC) at the University of Alberta, in Edmonton, Alberta, Canada offers hands-on training opportunities in metabolomics and bioinformatics to qualified scientists. To apply, please complete the application here.
For more information, contact dchamot@ualberta.ca.

3-8 Feb 2019

Understanding Human Diseases Through Metabolomics: Interactions Among the Genome, Proteome, Gut Microbiome and Nutrition (Gordon Conference Series on Metabolomics and Human Health)

Venue:
Four Points Sheraton / Holiday Inn Express
1050 Schooner Drive
Ventura, CA, USA

Application Information

Applications for this meeting must be submitted by January 6, 2019. Please apply early, as some meetings become oversubscribed (full) before this deadline. If the meeting is oversubscribed, it will be stated here. Note: Applications for oversubscribed meetings will only be considered by the conference chair if more seats become available due to cancellations.

Conference Description

Metabolomics is the comprehensive study of the metabolome, the repertoire of biochemicals present in cells, tissues, and body fluids. The study of metabolism at the global or "-omics" level is a rapidly growing field that has the potential to have a profound impact upon medical practice. At the center of metabolomics, is the concept that a person's metabolic state provides a close representation of that individual's overall health status. This metabolic state reflects what has been encoded by the genome, and modified by diet, environmental factors, the gut microbiome among other influences. The metabolic profile provides a quantifiable readout of biochemical state from normal physiology to diverse pathophysiologies in a manner that is often not obvious from gene expression analyses. In this Gordon Conference series, we highlight state of the art metabolomics technologies and their applications to the study of human health and disease.

We will cover most recent developments in the field covering applications of metabolomics for deeper understanding of disease mechanisms, disease heterogeneity and disease progression; variation in treatment outcomes and enablement of precision medicine approaches; connections between metabolome, proteome and genome and atlases being created; effects of exposome, diet and gut microbiome on human metabolome and health. We will highlight large consortia initiatives which enable epidemiology and clinical studies, functional genomics, nutrigenomics, pharmaceutical applications including toxicology studies, systems pharmacology, environmental exposures effects on health (exposome) and beyond. We invite established as well as early career members to attend this meeting from academia industry and regulatory agencies.

For further information, please visit:
https://www.grc.org/metabolomics-and-human-health-conference/2019/

Metabolomics Events

Imperial College London

25 Feb to 1 Mar 2019

Hands-on NMR Spectroscopy for Metabolic Profiling

Venue:
Imperial College London, Exhibition Road, London, United Kingdom

This week long course aims to cover how to perform a metabolic profiling experiment, from start to finish. It will cover study design, sample preparation, NMR spectrometer set up for global profiling, 2-dimensional NMR experiments and spectral data analysis.

Earlybird: **£1750**
Standard: **£1950**
Registration: Register using this link

For further information and registration details, please visit http://www.imperial.ac.uk/imperial-international-phenome-training-centre/courses/hands-on-nmr-spectroscopy-for-metabolic-profiling/

UF Clinical and Translational Science Institute
UNIVERSITY of FLORIDA

11-13 March 2019

5th Annual Metabolomics Symposium on Clinical and Pharmaceutical Solutions through Analysis (CPSA Metabolomics 2019)

Venue:
The University of Florida Clinical & Translational Science Institute, Gainesville, Florida USA

Make plans to attend the 5th Annual Metabolomics Symposium on Clinical & Pharmaceutical Solutions through Analysis (CPSA Metabolomics 2019). This unique event is highly interactive and dedicated to the needs of the clinic. The program features updated perspectives and experiences on clinical and pharmaceutical analysis. Imagination and stimulating discussion are central to each CPSA Metabolomics session and event.

Goal
The goal of CPSA Metabolomics is to provide in-depth review of innovative technology and industry practices through open discussion of industry-related issues and needs. This annual event is specifically geared to the needs of professionals attempting to keep pace with faster development times and technology marketing managers attempting to benchmark emerging trends.

For further information, please visit http://www.cpsa-metabolomics.com/2019/index.shtml.

Metabolomics Events

13-15 May 2019

Challenges in Analysis of Complex Natural Mixtures Faraday Discussion

Venue:
John McIntyre Conference Centre, University of Edinburgh, 18 Holyrood Park Road, Edinburgh, EH16 5AY, United Kingdom

Structure determination of molecules contained within unresolved complex mixtures represents an unsolved question that continues to challenge physical and analytical chemistry. Most naturally occurring systems can be characterised as complex mixtures. These can be broadly divided according to the molecular sizes of their constituents, into mixtures of small or large molecules. The focus of this Faraday Discussion will be on the former, while the latter such as biomacromolecules, industrial polymers, or solid matrices are outside of its scope as such. Nevertheless, the processes that are used in analysing the data originating from these studies may be of interest.

Examples of small molecule mixtures include:

- Environmental matrices such as soil, dissolved organic matter, organic molecules contained in atmospheric aerosol particles, or crude oil
- Biofluids
- Man-made mixtures of small molecules such as food, beverages or plant extracts

These systems are generally classed as “complex mixtures” or “unresolved complex mixtures (UCM)”, emphasising our current inability to separate their individual components.

The techniques best positioned to tackle such mixtures experimentally include mass spectrometry, chromatography, NMR spectroscopy, or new alternative techniques, including combinations of the above methods. For the most part, people who work on the analysis of complex mixtures are driving the progress in exploiting new methodologies and their creative combinations.

For further information and registration details, please visit http://www.rsc.org/events/detail/29574/challenges-in-analysis-of-complex-natural-mixtures-faraday-discussion

Metabolomics Jobs & Collaborations

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
Postdoctoral Researcher Position	UCSF	San Francisco, USA	01-Mar-18	Until filled	Metabolomics Society Jobs
Senior Scientific Officer (Lipidomics/ Metabolomics)	Nanyang Technological University	Singapore	12-Feb-18	Until filled	Metabolomics Society Jobs
Postdoc Position in Cheminformatics and Computational Metabolomics	Friedrich-Schiller-University	Jena, Germany	09-Feb-18		Friedrich-Schiller-University
Ph.D. Position on Mass Spectrometry-Based Analysis of Metabolites	University of Basel	Basel, Switzerland	31-Jan-18	Until filled	Metabolomics Society Jobs
Various Positions			16-Nov-18		Metabolomics Association of North America
Postdoctoral Fellow in Metabolomics and Exposomics	Icahn School of Medicine at Mount Sinai	New York, USA	21-Sep-18	Until filled	Metabolomics Society Jobs
Multiple bioinformatics positions	Emory University	Atlanta, GA, USA	17-Sep-18	Until filled	Metabolomics Society Jobs
PhD in Clinical Metabolomics, Metabolomics Unit, Faculty of Biology and Medicine	University of Lausanne, Switzerland	Lausanne, Switzerland	30-Aug-18	Until filled	Metabolomics Society Jobs
Postdoctoral Fellow	National Institutes of Health	Bethesda, Maryland, USA	9-Nov-18	Until filled	Metabolomics Society Jobs
Postdoctoral researcher in Metabolomics, Synthetic Biology and Metabolic Engineering	University of Luxembourg	Belvaux, Luxembourg	29-Oct-18	31-Dec-18 or until filled	University of Luxembourg
Postdoctoral Appointee in Metabolomics Data Integration/Analysis	Indiana University	Indianapolis, Indiana, USA	26-Oct-18	15-Dec-18	Metabolomics Society Jobs
Research Postdoctoral Scientist	Beaumont Health, Research Institute	Royal Oak, MI, USA	15-Oct-18	Until filled	Metabolomics Society Jobs
Assistant Professor in Chemistry	University of Nebraska-Lincoln	Lincoln, Nebraska, USA	10-Oct-18	Until filled	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 Ian Forsythe (metabolomics.innovation@gmail.com). Upon review, a limited number of job submissions will be selected for publication in the Jobs Wanted section.