Workshop 1: EMN Workshop – Career Development

Organizers

Nicola Gray (Shimadzu UK) and Justin van der Hooft (University of Glasgow)

Abstract

This session will focus on job prospects for early-career scientists considering career pathways in both academia and industry, and discuss the challenges and opportunities in transitioning between these sectors. We will be joined by experts from academia (Jules Griffin, University of Cambridge) and non-academic scientific recruitment (Sinead Cullen, Life Science Recruitment) who will discuss how to develop a skill set for career progression within various sectors and activities to aid successful career progression. The session will cover skills and qualities sought after by recruiters in these sectors, including tailored CV writing, finishing with a discussion and Q&A session.

Workshop Objectives

This workshop is targeted at the early-career scientists of the Metabolomics Society and will provide information on career options in both academia and industry. The session will allow attendees to gain an insight into career progression within academia, with advice on honing a skill set for career progression. This will be balanced by information on alternative career choices with a focus on industry, with advise on how to transition between different sectors.

Learning Outcomes

By the end of this session, attendees will have been received information about:

1. The current status of the scientific workforce in academia and industry
2. Opportunities and challenges in switching between academic and industry career pathways
3. Advise on developing a skill set for a career in academia or industry and how to transition between one sector and another
4. CV writing for academia and industry – some concrete tips on what recruiters look for

Schedule

Time	Speaker	Topic
0:00 – 0:05	Nicola Gray and Justin van der Hooft	Introduction
0:06 – 0:31	Dr Jules Griffin (MRC HNR, University of Cambridge, UK)	Career Progression in Academia
0:35 – 1:00	Sinead Cullen (Life Science Recruitment, Ireland)	Career Pathways in Industry
1:00 - 1:30	Nicola Gray and Justin van der Hooft	Open discussion and questions

Workshop 2: Data Sharing and Standardisation

Organisers and Speakers

Reza Salek (Chair), Steffen Neumann, Philippe Rocca-Serra, Tim Ebbels, Mark Viant, Saravanan Dayalan, Oliver Jones, Juan Antonio Vizcaíno, Andrew Jones, Masanori Arita.

Abstract

There is still a great need in standardisation and data sharing in the metabolomics field. The metabolomics community saw its first round of standardisation efforts, culminating in a set of publications, in 2007. We now have several data sharing platforms such as MetaboLights and Metabolomics Workbench that aim to make use of such standards to promote data-sharing but they are not as wll used as they could be. We will discuss data sharing as well as metabolomics data formats, much of which are adopted from the efforts in the proteomics HUPO-PSI initiative. We will also discuss the importance of capturing metadata in an electronic, sharable format. We hope to get the metabolomics community to to be aware of, and get more involved in, and ongoing efforts in this area.

Workshop Objectives

In this workshop, participants will be able to learn about the current status of the development of a worldwide network of databases and data standards initiatives - such as COSMOS), HUPO-PSI the NIH Common Fund's Metabolomics Program, MassBank and MetabolomeXchange. All of these aim to provide metabolomics researchers with high quality metabolite data standards. These initiatives build on the earlier developments, and improve standardisation of reporting requirements for data and metadata, and to establish best practices and workflows for metabolomics data capture, deposition, and dissemination.

Learning Outcomes

To give an overview of the current state of the art in metabolomics standards and to get anyone interested in metabolomics data sharing and standards, ranging from PIs to PhD and graduate students to participate.

Schedule

5 min - **Data standards in metabolomics, current and future!** Reza Salek, EMBL-EBI, Cambridge, UK
10 min - **Why you should care about recording (and reporting) your experimental metadata**.
Oliver Jones, RMIT University, Australia
10 Min - **Be FAIR: Publish experiment descriptors and data in ISA format, get indexed, get cited, get noticed**.
Philippe Rocca-Serra, Oxford e-Research Centre (University of Oxford, UK) and Biocrates AG
10 min - **Complying with international data standards through data management software - an automated approach** Saravanan Dayalan, Metabolomics Australia, The University of Melbourne
15 min Short Discussion (meta-data): **Mutual Benefit for metabolomics community, instrument vendors, publishes and public repositories -gathering interest and suggestion**- Short survey using https://kahoot.it/#/
10 min "**Experiences to learn from the mass spectrometry proteomics field**"
Juan Antonio Vizcaino, EMBL-EBI, Hinxton, Cambridge, UK
10 min - "**Data exchange formats - Why, how and a plea to the MS instrument vendors**"
Steffen Neumann, Leibniz Institute of Plant Biochemistry (IPB Halle, Germany)
10 min - "**Complying with standards in a multi-user environment: the case of MassBank**" Masanori Arita (National Institute of Genetics, Japan)
15 min Discussion and questions

Workshop 3: Metabolite Profiling in Population-Based Studies: Key Concepts, Pitfalls and Best Practices

Abstract
In recent years, the application of metabolite profiling in population-based studies has become possible due to technological advancements in the field. This is of particular interest due to the potential of metabolomics in evaluating the biological effects of exposures and identifying biomarkers for disease prediction and diagnosis using large-scale, well-designed epidemiological studies. Therefore, it is important for investigators to be familiar with epidemiological and biostatistical approaches for applying metabolite profiling within population-based settings, which will be the focus of this workshop.

Workshop Objectives
The objectives of this workshop are to: 1) address fundamental epidemiological and biostatistical study design issues that must be considered for metabolomics research; 2) highlight key concepts, pitfalls and best practices for performing metabolite profiling in large, population-based studies; and 3) discuss current efforts to build capacity and infrastructure to support these types of studies, including the recently established International COnsortium of METabolomics Studies (COMETS). COMETS leverages resources and metabolomics data from 25 prospective cohorts and two consortia spanning the United States, Europe, Asia, and South America with cardiovascular, cancer, diabetes, and aging outcomes.

Learning Outcomes
By the end of this session, attendees will be able to:
1. Identify key epidemiological study design issues that need consideration when performing metabolite profiling large-scale studies;
2. Understand fundamental biostatical concepts for performing metabolite profiling in large-scale epidemiology studies;
3. Recognize common pitfalls to performing metabolite profiling in these studies; and
4. Become familiar with the COnsortium of METabolomics Studies (COMETS).

Schedule:

Time	Speaker	Topic
0:00 – 0:05	Krista Zanetti	Introduction
0:05 – 0:35	Marc Gunter, Ph.D. Section and Group Head International Agency for Research on Cancer Nutritional Epidemiology Group Lyon, FR	Epidemiological Study Design
0:35 – 1:05	Pietro Ferrari, Ph.D. Statistician International Agency for Research on Cancer Nutritional Epidemiology Group Lyon, FR	Biostatistical Approaches
1:05 - 1:15	Krista Zanetti Program Director National Cancer Institute Division of Cancer Control and Population Sciences Rockville, Maryland, USA	COnsortium of METabolomics Studies (COMETS
1:15-1:30	Panel Discussion with Speakers	

Workshop 4 – EMN- The Importance of Experimental Design, Data Acquisition, Quality Assurance and Quality Control in Metabolomics

Organizers

Stacey Reinke (Karolinska Institutet) and Fidele Tugizimana (University of Johannesburg)

Overview

Metabolomics is a powerful and exponentially growing field of science, continuously attracting new researchers from different scientific fields. This emerging 'omics' approach, being at the interface between biology, chemistry, statistics, and computer science requires multidisciplinary skill-sets. As such, metabolomics poses many challenges, which if not considered lead to erroneous data and poor experimental outcomes. As shown in this workshop, a strong understanding of study design, sample preparation, analytical platforms, data processing and data analysis is essential for obtaining meaningful results in metabolomics.

Workshop Objective

This workshop will provide education on experimental design, data acquisition, and quality assurance/quality control in metabolomics experiments. Possible solutions for commonly encountered challenges in the abovementioned study aspects will be addressed.

Learning Outcomes

1. Sources of experimental error and consequences of poor study design
2. Experimental design strategies and how they can affect the outcome
3. Data acquisition considerations and quality assurance measures
4. Quality control assessment and data cleaning

Schedule

Time	Speaker	Topic
0:00 – 0:05	Stacey Reinke and Fidele Tugizimana	Introduction
0:06 – 0:30	Prof. David Broadhurst (Edith Cowen University, Australia)	#1,2
0:31 – 0:55	Dr. Warwick Dunn (University of Birmingham, UK)	#3
0:56 – 1:15	Dr. Julia Kuligowski (Health Research Institute La Fe, Spain)	#4
1:16 - 1:30	Stacey Reinke and Fidele Tugizimana	Open discussion and questions

Workshop 5: metaRbolomics: The R toolbox for Metabolomics

Organisers

Jan Stanstrup (Steno Diabetes Center, Denmark) and Steffen Neumann (Leibniz Institute of Plant Biochemistry, Germany)

Abstract

R is a statistical and graphical environment, for which almost 10,000 add-on packages have been developed to extend the functionality of the core language. These include more than a thousand packages for the life sciences and bioinformatics area, and dozens (if not more) of packages applicable to metabolomics data processing and analysis. While the R language is not known for an easy learning curve, once the user have learned the basic syntax it is incredibly empowering and the possibilities become almost limitless.

Workshop Objectives

This workshop aims to highlight the tools available for metabolomics in the first part, and then proceed beyond the existing tools to emphasize the versatility of working in this environment, how existing packages can be combined and to envision future developments and synergies.

Target Audience

Biologists, Bioinformaticians, and Chemists interested in applying freely available high-throughput analyses to their metabolomics data to maximize efficiency, transparency, and reproducibility in data processing.

Schedule

Etienne A. Thévenot <etienne.thevenot@cea.fr> and Philippe Rinaudo: **(O)PLS(-DA) analysis and signature discovery with ropls and biosigner R/Bioconductor packages.**

Michael Witting <michael.witting@helmholtz-muenchen.de>, Michael Stravs, Emma Schymanski, Andrea Thum, Christoph Böttcher & Steffen Neumann: **Semi-automated MS/MS database generation using the R packages MetShot and RMassBank**

Augustin Luna <aluna@jimmy.harvard.edu>, Ozgun Babur, Bulent Arman Aksoy, Emek Demir and Chris Sander: **paxtoolsr: Access Pathways from Multiple Databases through BioPAX and Pathway Commons**

Tyler Backman <tbackman@ucr.edu>, Thomas Girke: **Analysis of Small Molecules and High-Throughput Screens with R/Bioconductor**

Code examples from presenters will be available for own experiments. The workshop will also include room for discussions on challenges and opportunities for more metabolomics developments in R and Bioconductor.

Workshop 6: Computational Workflows and Workflow Engines

Organisers

Mark Viant, Ralf Weber, Warwick Dunn, Pablo Moreno, Reza Salek, Christoph Steinbeck and the PhenoMeNal consortium

Abstract

Computational analysis of high-dimension and high-volume metabolomics data is a complex, time-consuming process including many steps, some of which still being the focus of intense research. Workflow management environments applied in metabolomics and cross-omics analyses are therefore an essential requirement to allow standardisation of bioinformatics analysis, provide access to the metabolomics community, and produce high-quality, reproducible results in a time-effective manner: on the one hand, experimenters should be able to easily select the tools via a graphical interface, choose the parameters, run the workflow and save/share the results; on the other hand, developers should be able to integrate new tools seamlessly into the environment. A few open-source workflows have recently been applied in different environments including Galaxy-M, Workflow4Metabolomics, MetaDB and MetaboAnalyst. There is a growing need for the international metabolomics community to understand the availability and capability of these workflow environments, and provide input into on-going development and interoperability.

Target Audience

The target audience will be metabolomics data producers interested in the post-wet lab phase of LC-MS, GC-MS, direct infusion MS and NMR data analysis as well as researchers involved in the computational aspects of metabolomics (data handling/analysis, tool developers).

List of speakers

1. Ralf Weber, University of Birmingham
2. Etienne Thevenot, CEA/ Yann Guitton, Laberca
3. Christoph Steinbeck, European Bioinformatics Institute (EMBL-EBI)
4. David Wishart, Edmonton, Canada
5. Reza Salek, European Bioinformatics Institute (EMBL-EBI)
6. Pietro Franceschi (Fondazione Edmund Mach)
7. Theodore Alexandrov (EMBL)

Schedule

Short talks/demos (10 minutes) on the following platforms:

- Workflow4Metabolomics (MetaboHub - IFB Galaxy Metabolomics Workflow)
- MassCascade-KNIME (Steinbeck group, EMBL-EBI)
- Galaxy-M (Birmingham Galaxy Metabolomics Workflow)
- PhenoMeNal (PhenoMeNal-H2020 consortium)
- MetaboAnalyst (Wishart Group, Edmonton, Canada)
- MetaSpace(EMBL, Germany)

Round table discussion/QAs on:

- Current shortcomings and improvements that could help widen the adoption of these type of tools within the metabolomics community.
- Interoperability between these technologies.
- General concerns from users.