

3rd International Summer School on **NON-TARGETED METABOLOMICS DATA MINING** FOR BIOMEDICAL RESEARCH

21st – 25th August 2023

Statens Serum Institut, Copenhagen, Denmark

Overview

The summer school will introduce **non-targeted mass spectrometry-based metabolomics** for biomedical researchers, including **hands-on training** in **metabolomics data mining** tools.

Goals

We will briefly introduce analytical hardware, acquisition strategies, study design, sample preparation, and quality control. The main focus will be on working with state-of-the-art metabolomics data mining tools for **preprocessing**, **compound annotation**, and **statistical analysis**.

Instructors

Madeleine Ernst, Markus Fleischauer, Martin Hansen, Steffen Heuckeroth, Florian Huber, Alan Jarmusch, Scott Jarmusch, Efi Kontou, Fleming Kretschmer, Filip Ljung, Filip Ottosson, Daniel Petras, Robin Schmid, Abzer K. Pakkir Shah, Justin van der Hooft, Ming Wang, and more...

Registration

<https://en.ssi.dk/news/events/summer-school-on-non-targeted-metabolomics-data-mining-for-biomedical-research>

Course credits

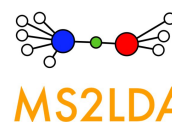
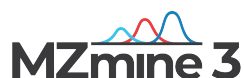
5 ECTS

Costs

Academic 400 €, Industry 700 €, waivers for low-income participants

Contact

For more information visit the registration link or contact us at metabolomics@ssi.dk



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Preliminary Program

Monday, August 21st, 2023, Introduction

8.30-9.00	Registration and Coffee	
9.00-9.30	Welcome and introduction	Madeleine Ernst, Statens Serum Institut, Denmark
9.30-11.00	Mass spectrometry basics I	Daniel Petras, University of Tübingen, Germany
11.00-11.30	Break	
11.30-12.30	Mass spectrometry basics II	Daniel Petras, University of Tübingen, Germany and Corinna Brungs, IOCB Prague, Czechia
12.30-13.30	Lunch break	
13.30-14.30	Guided tours in the Danish National Biobank and SSI's mass spectrometry facilities	Madeleine Ernst, Karina Meden Sørensen, and Bartłomiej Wilkowski, Statens Serum Institut, Denmark
14.30-15.15	Quality assurance and quality control	Martin Hansen, Aarhus University, Denmark and Morten Danielsen, MS-Omics, Denmark
15.15-16.00	Best practices in metabolomics	Filip Ljung, Filip Ottosson, Statens Serum Institut, Denmark and Justin van der Hooft, Wageningen University & Research, the Netherlands
16.00-16.30	Break	
16.30-17.00	<i>Keynote:</i> Unraveling the metabolomic architecture of autism in a large Danish population-based cohort	Filip Ottosson, Statens Serum Institut, Denmark
17.00-19.00	Ice breaker	

Tuesday, August 22nd, 2023, Data preprocessing

8.30-9.00	Coffee	
9.00-9.30	Introduction to data preprocessing	Steffen Heuckeroth, University of Münster, Germany and Robin Schmid and Corinna Brungs, IOCB Prague, Czechia
9.30-11.00	Data preprocessing in MZmine 3 I*	Steffen Heuckeroth, University of Münster, Germany and Robin Schmid and Corinna Brungs, IOCB Prague, Czechia
11.00-11.30	Break	
11.30-12.30	Data preprocessing in MZmine 3 II	Steffen Heuckeroth, University of Münster, Germany and Robin Schmid and Corinna Brungs, IOCB Prague, Czechia
12.30-13.30	Lunch break	
13.30-14.00	Keynote: Application of untargeted mass spectrometry analysis of biofluids in precision medicine	Alan Jarmusch, National Institute of Environmental Health Sciences, United States
14.00-15.00	Working on data in groups	
15.00-15.30	Break	
15.30-17.00	Working on data in groups	

* Schmid R., Heuckeroth S. et al., Integrative analysis of multimodal mass spectrometry data in MZmine 3, *Nature Biotechnology* (2023).

Wednesday, August 23rd, 2023, Metabolite annotation

8.30-9.00	Coffee	
9.00-9.30	Introduction to metabolite identification	Alan Jarmusch, National Institute of Environmental Health Sciences, United States; Scott Jarmusch, Technical University of Denmark and Daniel Petras, University of Tübingen, Germany
9.30-10.30	Introduction to GNPS**	Alan Jarmusch, National Institute of Environmental Health Sciences, United States; Scott Jarmusch, Technical University of Denmark and Daniel Petras, University of Tübingen, Germany
10.30-11.00	Break	
11.00-12.30	Sirius+CSI:FingerID***	Markus Fleischauer and Fleming Kretschmer, Friedrich-Schiller University Jena, Germany
12.30-13.30	Lunch break	
13.30-14.00	Introduction to Cytoscape	Madeleine Ernst, Statens Serum Institut, Denmark
14.00-16.00	Working on data in groups	
16.00-16.30	Break	
16.30-17.30	Keynote: Advanced metabolite annotation tools and newest developments within GNPS2	Mingxun Wang, University of California - Riverside, United States (online)
17.30-19.30	Happy hour	

** Wang M., et al. Sharing and community curation of mass spectrometry data with Global Natural Products Social Molecular Networking, *Nature Biotechnology* **34**, 828-837 (2016); Nothias, L.F. et al., Feature-based molecular networking in the GNPS analysis environment, *Nature Methods* **17**, 905-908 (2020).

*** Dührkop K., Fleischauer M., et al., SIRIUS 4: a rapid tool for turning tandem mass spectra into metabolite structure information, *Nature Methods* **16**, 299-302 (2020).

Thursday, August 24th, 2023, Substructure discovery and advanced metabolite annotation

8.30-9.00	Coffee	
9.00-9.30	Intro to Jupyter notebooks	Eftychia Eva Kontou, Technical University of Denmark and Abzer K. Pakkir Shah, University of Tübingen, Germany
9.30-11.00	Matchms ⁺	Florian Huber, Düsseldorf University of Applied Sciences, Germany
11.00-11.30	Break	
11.30-12.30	MS2Query ^{**}	Florian Huber, Düsseldorf University of Applied Sciences, Germany and Justin van der Hooft, Wageningen University & Research, the Netherlands
12.30-13.30	Lunch break	
13.30-14.00	Keynote: Spatial and single-cell metabolomics: technology, applications, and computational challenges	Theodore Alexandrov, European Molecular Biology Laboratory, Heidelberg, Germany & BioInnovation Institute, Copenhagen, Denmark
14.00-15.00	MS2LDA ^{***}	Justin van der Hooft, Wageningen University & Research, the Netherlands
15.00-15.30	Break	
15.30-17.00	Working on data in groups	

⁺ Huber F., et al. matchms - processing and similarity evaluation of mass spectrometry data, *Journal of Open Source Software* **52**, 2411 (2020).

^{**} De Jonge N., et al. MS2Query: reliable and scalable MS2 mass spectra-based analogue search, *Nature Communications* **14**, 1752 (2023).

^{***} Van der Hooft, J.J.J., et al., Topic modeling for untargeted substructure exploration in metabolomics, *PNAS* **113**, 13738-13743 (2016).

Friday, August 25th, 2023, Statistical analysis and data visualization

8.30-9.00	Coffee	
9.00-10.00	Data normalization	Filip Ottosson and Madeleine Ernst, Statens Serum Institut, Denmark and Alan Jarmusch, National Institute of Environmental Health Sciences, United States Abzer K. Pakkir Shah, University of Tübingen, Germany
10.00-11.00	Multivariate statistical analyses	Filip Ottosson and Madeleine Ernst, Statens Serum Institut, Denmark; Alan Jarmusch, National Institute of Environmental Health Sciences, United States; Abzer K. Pakkir Shah, University of Tübingen, Germany
11.00-11.30	Break	
11.30-12.30	Univariate statistical analyses	Filip Ottosson and Madeleine Ernst, Statens Serum Institut, Denmark; Alan Jarmusch, National Institute of Environmental Health Sciences, United States; Abzer K. Pakkir Shah, University of Tübingen, Germany
12.30-13.30	Lunch break	
13.30-14.30	Biological interpretation and conclusions	Madeleine Ernst, Statens Serum Institut, Denmark
14.30-15.30	Working on data in groups	
15.30-16.00	Break	
16.00-17.00	Project presentations in groups	