



EUROPEAN  
UNIVERSITY  
ALLIANCE



## Computational Mass spectrometry and its presentation using AI tools workshop

Computational-based Mass spectrometry (MS) is rapidly evolving, challenging us to process and interpret complex multi-dimensional data. There are many computational MS projects to aid in this process - but mastering or even starting to use them can be a challenge of its own. Therefore, we want to provide a platform in Prague to meet, discuss, and learn how to move MS-based omics forward. Additionally, we want to offer a hands-on training workshop in the use of generative AI-tools for scientific writing presentation, where we can learn their use, opportunities and ethical usage.

### *Who we are:*

We are a group of enthusiasts students from the 4EU+ universities alliance driven by sharing knowledge and international collaboration. Our presenters comprise software developers and power users of various open-source AI driven resources.

### *Who you are:*

You are a highly motivated “beginner” in the field, open to network, and dive deeper into computational tools for MS, data processing, compound annotation, and AI-Assisted tools in scientific writing.

### *Goals of the workshop:*

1. Introduce MS-based analysis and data processing
3. Provide hands-on training in the use of AI-generative tools for scientific writing
4. Connect users from different fields - to better understand trends and needs
5. Socializing & networking

We are opening this at the beginner level - no prior knowledge in computational tools or AI is required as we are starting with some basics, but the workshop will be fast-paced. However, a background in Natural Sciences (Chemistry, Physics, etc.) is the most suitable for the selection.

### *When & Where*

August 28<sup>th</sup> to 30<sup>th</sup>, 2024 in Prague, Czech Republic.

### *Registration*

The registration process will start in at the end of June. As part of the 4EU+ alliance project, the workshop is free of charge and includes the welcoming and farewell cocktails, coffee breaks and lunch. Nevertheless, the capacity is limited and therefore a selection process will take place based on your motivation to participate in this workshop. Accommodation and travel expenses in Prague are not covered by the workshop.

**Venue:**  
Kampus Hybernská  
Prague, Czech Republic



**WORKSHOP PROGRAM:**

**Wednesday (August 28<sup>th</sup>, 2024)**

Time	Event	Lecturer/ Moderator
15:00 – 16:00	Welcoming coffee	-
15:00 – 16:00	Registration	Core Team
16:00 – 16:30	Welcoming	Felipe <i>and</i> core team. (Charles University)
16:30 – 17:00 Presentation	4EU+ Alliance presentation	4EU+ team
17:00 – 17:10	Workshop general instructions and Q&A	Felipe <i>and</i> core team.
17:10 – 18:00	Welcoming cocktail (Drinks & Snacks)	-

**Thursday (August 29<sup>th</sup>, 2024)**

Time	Event	Lecturer/ Moderator
9:30 – 10:00	Registration (Cont.) and morning coffee	-
10:00 – 10:30 Lecture	Brief Introduction to Mass Spectrometry	Corinna Brungs (IOCB)
10:30 – 11:00 Lecture	Computational Mass Spectrometry Basics	Tomáš Pluskal (IOCB)
11:30 – 12:00	Coffee Break (Coffee, drinks & Snacks)	-
12:00 – 13:00 Hands-On	Exploring MS Data in MZmine	Robin Schmid (IOCB)
13:00 – 14:00 Hands-On	LC-MS/MS Data Processing using MZmine + Q&A	Robin Schmid <i>and</i> <i>col.</i> (IOCB)
14:00 – 15:00	Lunch at venue	-

15:00 – 15:30	Wake-up coffee	-
15:30 – 16:30 Hands-On	Introduction to Molecular Networking + Application Examples	Robin Schmid <i>and col.</i> (IOCB)
16:30 – 17:00 Hands-On	MZmine - LC-MS/MS Results	Robin Schmid <i>and col.</i> (IOCB)
17:00 – 17:30 Lecture	Omics using Computational MS	Matthias Mattanovich (University of Copenhagen)
17:30 – 18:30 Flash Talks	Students presentations on Computational MS and Q&A – Part I	<i>Core team</i>
18:30 – 19:30	Dinner	-

## Friday (August 30<sup>th</sup>, 2024)

8:30 – 9:00	Morning Coffee	
9:00 – 10:00 Flash Talks	Students presentations on Computational MS and Q&A – Part II	<i>Core team</i>
10:00 – 11:00 Workshop	Introduction into AI tools for academia*	Adam Urban (National Technical Library, NTK)
11:00 – 11:30	Coffee Break	
11:30 – 12:30 Workshop	AI-assisted tools in scientific writing - Part I**	Milan Jirásek (Czech Technical University)
12:30 – 14:00 Workshop	AI-assisted tools in scientific writing - Part II♦	Anna Jirásková (Czech Technical University)
14:00 – 15:00	Lunch at venue	
15:00 – 15:30	Wake-up coffee	
15:30 – 16:30 Workshop	AI-assisted tools in scientific writing - Part III▲	<i>TBD</i>
16:30 – 17:30 Workshop	Mental health and stress management for PhD students	Anna-Marie Pospíšilová (Charles University)
17:30 – 18:00	Farewell, Statistics & Prague recommendations	<i>Core team</i>
18:00 – 20:00	Farewell cocktail	

*IOCB = Institute of Chemistry and Biochemistry of the Czech Academy of Sciences.*

TBD= To be determined

\*Introduction into AI tools for academia:

Introduction into generative AI tools, prompt-based searches, mapping tools, text analysis, other resources.

\*\*Workshop on AI-assisted tools in scientific writing - Part I

Rules on AI in scientific writing, retrieving, or checking facts, processing, and interpreting data, generating computer code, processing mathematical expressions.

◆ Workshop on AI-assisted tools in scientific writing - Part II

Tools that support writing (Grammarly, Writefull, DeepL Write), dialog with a chatbot.

♠ Workshop on AI-assisted tools in scientific writing - Part III

Tools that help to organize, inspire and present: Zotero, EndNote, R Discovery, Canva, Biorender.