



EUROPEAN
UNIVERSITY
ALLIANCE



Computational Mass spectrometry and its Scientific communication using AI tools

Dear Colleagues,

We are pleased to invite you to a hands-on training workshop on Computational Mass Spectrometry and its Presentation using AI Tools, organized in collaboration with Charles University under the 4EU+ Alliance. This workshop will be held at Kampus Hybernská, Prague, Czech Republic, and is mainly intended for students and educators in the fields of analytical chemistry, biochemistry, or biotechnology, though other fields are equally welcome.

The workshop aims to provide beginner-level training, with no prior knowledge of MS computational tools required, though a basic understanding of mass spectrometry is highly recommended. The second half of the workshop will focus on using Generative AI for scientific communication and publication, providing practical information and training in this field as well. The event will span three days and feature lectures and practical sessions conducted by esteemed trainers from the Institute of Organic Chemistry and Biochemistry (IOCB), Czech Technical University in Prague (CTU), University of Copenhagen (KU), Charles University (CU), and the National Library of Technology (NTK). Towards the end of the event, we will have a workshop in Mental health and stress management.

We look forward to welcoming you to an enriching and collaborative learning experience in the beautiful city of Prague.

Who we are:

We are a group of enthusiasts doctoral students from the 4EU+ universities alliance driven by sharing knowledge and international collaboration. Our presenters comprise software developers, professors 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. You possess a minimum basic knowledge in MS and are highly motivated to participate. Although it is obvious, we would like to remind you that you must bring your own laptop (preferably charged). The targeted computational tools are adapted to iOS, Windows and Linux.

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. Learn and understand stress management
6. Socializing & networking

We are opening this hands-on training at the beginner level where 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, Biology, etc.) is the most suitable for the participation.

When & Where

August 28th to 30th, 2024 in Prague, Czech Republic.

Venue:

Kampus Hybernská
Prague, Czech Republic

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| H | Y | KAMPUS HYBERNSKÁ |
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Registration

As part of the 4EU+ alliance project, the workshop is free of charge and includes the welcoming and farewell cocktails, coffee breaks, dinner and lunch (as marked in the program). Nevertheless, the capacity is limited to 30 seats and therefore, a selection process will take place based on your motivation to attend the workshop and your active participation. Important to notice, the accommodation and travel expenses in Prague are not covered by the workshop.



WORKSHOP PROGRAM:

Wednesday (August 28th, 2024)

| Time | Event | Lecturer/Moderator |
|-------------------------------|---|--|
| 15:00 – 16:00 | Registration & Welcoming coffee | - |
| 16:00 – 16:30 | Welcoming meeting | Core Team |
| 16:30 – 17:00 Presentation | 4EU+ Alliance presentation | Kristýna Kolínová (4EU+ Alliance Project Officer) |
| 17:00 – 17:10 | Workshop general instructions and Q&A | Core Team |
| 17:10 – 18:00 | Welcoming cocktail (Drinks & Snacks) | - |

Thursday (August 29th, 2024)

| Time | Event | Lecturer/Moderator |
|---------------|---|--|
| 9:30 – 10:00 | Registration (Cont.) | - |
| 10:00 – 10:30 | Brief Introduction to Mass Spectrometry | Corinna Brungs (IOCB) |
| 10:30 – 11:00 | Computational Mass Spectrometry Basics | Tomáš Pluskal (IOCB) |
| 11:30 – 12:00 | Coffee Break (Coffee, drinks & Snacks) | - |
| 12:00 – 13:00 | Exploring MS Data in MZmine | Robin Schmid (IOCB) |
| 13:00 – 14:00 | LC-MS/MS Data Processing using MZmine + Q&A | Robin Schmid <i>and col.</i> (IOCB) |
| 14:00 – 15:30 | Lunch at the venue | - |
| 15:30 – 16:30 | Introduction to Molecular Networking + Application Examples | Robin Schmid <i>and col.</i> (IOCB) |
| 16:30 – 17:00 | MZmine - LC-MS/MS Results | Robin Schmid <i>and col.</i> (IOCB) |
| 17:00 – 17:30 | Omics using Computational MS | Matthias Mattanovich (University of Copenhagen) |
| 17:30 – 18:30 | Students presentations on Computational MS <i>TBD – Part I</i> | Core Team |

Friday (August 30th, 2024)

| Time | Event | Lecturer/Moderator |
|---------------|--|---|
| 9:00 – 10:00 | Students presentations on Computational MS <i>TBD – Part II</i> | Core Team |
| 10:00 – 11:00 | Introduction into AI tools for academia* | Adam Urban (National Technical Library, NTK) |
| 11:00 – 11:30 | Coffee Break (Coffee, drinks & Snacks) | - |

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|---------------|---|--|
| 11:30 – 12:30 | AI-assisted tools in scientific writing - Part I** | Milan Jirásek (Czech Technical University) |
| 12:30 – 14:00 | AI-assisted tools in scientific writing - Part II♦ | Anna Jirásková (Czech Technical University) |
| 14:00 – 15:30 | Lunch at the venue | |
| 15:30 – 16:00 | AI-assisted tools in scientific writing - Part III♠ | Felipe Martínez-Ramírez (Charles University) |
| 16:00 – 17:30 | Stress management workshop | Anna-Marie Pospíšilová (Mental health counsellor at FSV UK) |
| 17:30 – 18:00 | Farewell, Statistics & Prague recommendations | Core team |
| 18:00 – 20:00 | Farewell cocktail and dinner | |

TBD = To be determined

The lunch at the venue will include vegetarian options

*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.