

## EuBIC-MS Annual report 2021-2022

The European Bioinformatics Community for mass spectrometry (EuBIC-MS) is the EuPA initiative for mass spectrometry (MS)-related bioinformatics. Its aim is to improve bioinformatics for MS-based research through the setup of community-driven dynamics, thereby improving collaboration, funding, publication, and training activities. Through its different activities, EuBIC-MS aims to raise awareness for the benefits of open science and continuously supports open software. It was started in November 2015 (Vaudel, 2016) to bring together the MS and bioinformatics communities in an open, collaborative and constructive environment. The initiative is carried enthusiastically by the bioinformatics community and welcomes everyone willing to help.

EuBIC-MS organizes a dedicated yearly conference, bringing together researchers in the fields of mass spectrometry and bioinformatics, junior scientists and industry partners from across Europe. Every year, this conference alternates between a Winter School with keynote talks and workshops, and a Developers Meeting consisting of collaborative project sessions with the participants (hackathons). EuBIC-MS also actively contributes to bioinformatics hubs, and provides various workshops and presentations during international MS (e.g. annual conference of American Society of Mass Spectrometry) and proteomics (e.g. Human Proteome Organization congress, EuPA congress) conferences. Additionally, EuBIC-MS coordinates research projects conducted by the community.

Here is the report of our activities and achievements between October 2021 and September 2022.

### **Winter Schools**

The EuBIC-MS Winter Schools on computational MS are sponsored by the European Proteomics Association (EuPA) and several other parties, including but not limited to companies with interest in proteomics. They bring together scientists from both academia and industry to present and discuss their research in workshops, keynote lectures, flash talks and poster presentations. We hosted three Winter Schools, the first one in Semmering, Austria in 2017

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(Willems et al., 2017) and the second in Zakopane, Poland in 2019 (Kopczynski et al., 2019). Due to the Corona pandemic, the 2021 Winter School was postponed to 2022, and took place in person on 21-24 March 2022 at the Instituto Gulbenkian de Ciência in Oeiras (Portugal) ([eubic-ms.org/events/2022-winter-school](https://eubic-ms.org/events/2022-winter-school)). Unfortunately, some speakers could not attend the event, hence their presentations were done online. The Winter School was sponsored by Bruker (gold sponsor), and co-organised by EuPA and Gulbenkian Science. As usual, the first day was dedicated to educational workshops invited or organized by EuBIC-MS. The participants could choose between the two following full-day workshops entitled “A tour of machine learning” (Sven Degroeve, Ghent University/VIB-UGent Center for Medical Biotechnology, Belgium) and “Differential abundance analysis for proteomics” (Lieven Clement, Ghent University, Belgium); or two successive half-day workshops entitled “STRING and Cytoscape for proteomics data analysis” (Nadezhda Doncheva and Rebecca Kirsch, University of Copenhagen, Denmark) and “Biological interpretation by clustering and protein complex analysis” (Veit Schwämmle, University of Southern Denmark).

This first educational day was followed by two and a half days of keynotes (morning) and parallel workshops (afternoon). In total, there were eight keynote talks given by Lennart Martens (Ghent University/VIB-UGent Center for Medical Biotechnology, Belgium –online–), Isabell Bludau (Max Planck Institute of Biochemistry, Germany), Magnus Palmblad (Leiden University Medical Center, Netherlands), Matthew The (Technical University Munich, Germany), Sebastian Böcker (FSU Jena, Germany), Pedro Beltrao (ETH Zürich, Switzerland –online–), Aurelien Dugourd (Heidelberg University, Germany –online–), and Marc Vaudel (University of Bergen, Norway).

EuBIC-MS invited all keynote speakers (or members of their team) to organize a workshop on any topic or tool that they deem relevant to the field. In 2022, the participants could choose among the following parallel workshops:

Tuesday:

- Tackling identification ambiguity in immunopectidomics and in open modification searches with machine learning (Lennart Martens)

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- Introduction to the AlphaPept ecosystem for proteomics data analysis and visualization (Isabell Bludau)
- Cytoscape Automation in R (Magnus Palmblad)

Wednesday:

- The revamped ProteomicsDB API (Matthew The)
- The SIRIUS software suite (Sebastian Böcker), which was the first metabolomics workshop held in a EuBIC-MS conference
- PaSER™ 2022: real-time search solution for PASEF-enabled DDA and DIA data, which was held by our sponsor Bruker.

This program was completed by 47 posters that were presented Tuesday evening in a long and active poster session. Among these, 8 were selected for flash talks presented to the entire audience. Overall –and despite the difficulties associated with organizing an in-person conference during the pandemic– the EuBIC-MS Winter School was a success and we just started planning the next one, which will take place in 2024. The main organizers are Viktoria Dorfer, Dominik Lux and Veit Schwämmle.

### Developers Meetings

The Developers Meetings is an event dedicated to computer scientists and developers, in the field of bioinformatics applied to MS, where they can discuss and work together in an open and constructive spirit. The program is split between keynote lectures and multiple hackathon sessions where the participants develop bioinformatics tools and resources that address outstanding needs in the bioinformatics community and among biologists using MS data. Our first Developers Meeting took place in Ghent, Belgium in 2018 (Willems et al., 2018), and the second took place in Nyborg (Denmark) in 2020 (Ashwood et al., 2020). The most recent publication of a tool developed during one of these meetings was this year in the Journal of Proteome Research: “A Comprehensive Evaluation of Consensus Spectrum Generation Methods in Proteomics” (Luo et al., 2022).

The Developers Meeting 2023 will be held on 15-20 January 2023 at the ETH meeting platform Congressi Stefano Franscini (CSF), Monte Verità, Ticino (Switzerland). The registrations are

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open, it is powered by the Functional Center of Genomics in Zurich, ETH Zurich, Congressi Stefano Franscini and EuPA, and sponsored by Matrix Science, Biognosys, and MSAID. More information can be found on the official website: [eubic-ms.org/events/2023-developers-meeting](https://eubic-ms.org/events/2023-developers-meeting).

### Community achievements and outreach

#### *EuBIC-MS strategy*

We held a strategic meeting to amend the visions and missions of EuBIC-MS. These will be available soon on the EuBIC-MS website. We are also working on a code of conduct that will be available to all soon.

#### *The SDRF-Proteomics format*

The EuBIC-MS community worked together with the Human Proteome Organization Proteomics Standards Initiative (HUPO-PSI) (Deutsch et al., 2017) to define a standard for metadata annotation of proteomics data: The Sample and Data Relationship Format for Proteomics file format (SDRF-Proteomics) (Dai et al., 2021). This should increase data interpretability, as well as facilitating data reuse in an automated fashion. We remain very active in the development of this format ([github.com/bigbio/proteomics-metadata-standard](https://github.com/bigbio/proteomics-metadata-standard)) and promoted it in collaboration with ELIXIR Germany at the Proteomic Forum 2022 in a well-attended workshop.

#### *EuBIC-MS seminars 2022*

EuBIC-MS organized a series of seminars that took place at the VIB center in Ghent the 14<sup>th</sup> of September 2022. Five speakers were selected to present their work and promote EuBIC-MS to researchers and students of the institute. The information regarding this meeting can be found here: [eubic-ms.org/events/ghent-2022-seminar](https://eubic-ms.org/events/ghent-2022-seminar).

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### *EuPA early career researcher (ECR) day 2022*

The EuPA ECR day took place online on the 28<sup>th</sup> of June 2022. EuBIC-MS was present in a dedicated space in Proteopolis (set up with gathertown.org). This meeting was a perfect occasion to advertise our activities and virtually interact with potential new members.

### *Our current projects*

Two new EuBIC-MS projects emerged this year:

- Seven EuBIC-MS members started to work on the “Rusteomics” project, which aims at developing, in a collaborative manner, new Rust-based and open-source components for computational MS. This will encompass the creation of packages specialized for reading and/or writing popular MS file formats, as well as providing low-level and well established algorithms for MS spectra processing (deisotoping, deconvolution, MS/MS spectra annotation, etc...). While similar solutions exist in various programming languages, this project will be the opportunity to tailor these open-source packages to be highly compatible with scripting languages like Python / R, or being designed for specific use cases, such as the analysis of MS data during acquisition.
- Sixteen EuBIC-MS members gathered to work on a community-curated benchmark platform for comparing MS data analysis workflow. This project is named “ProteoBench”.

These two projects are driven by the community for the community. The number of people involved should increase in the next months as the projects develop, and their outputs will be presented to the EuBIC-MS members and the community.

### *Our website and resources*

In partnership with the EuPA Educational Committee (EC), the Proteomics Academy web resource (<https://www.proteomics-academy.org>) has become the central communication portal for EuBIC-MS since its creation in 2015. To increase the visibility of EuBIC-MS itself, we also

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maintain a website dedicated to the initiative at <https://eubic-ms.org>. There, people find all information regarding past and upcoming EuBIC-MS activities, including this annual report.

### How to get involved?

The EuBIC community is open to everybody working in computational proteomics and mass spectrometry. You can join us by sending an email at [info@eubic-ms.org](mailto:info@eubic-ms.org) or by using the contact form available from the eubic-ms.org website. We will then send you an invitation to join our Slack workspace (<http://eubic.slack.com>), which is our extensively used platform to interact with other EuBIC members. Additionally, you can follow and retweet our latest activities from our Twitter account ([@EuBIC\\_ms](https://twitter.com/EuBIC_ms)). By joining us, you will be part of a community effort, and thus contribute to the sustainability of these scientific activities, which we expect to foster the development of the computational MS field.

### Acknowledgments

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