

Research Software Engineer (Open to all genders)

Expansion of Python Library for Mass Spectral Data Analysis ("matchms")

We are currently building a new data science and research software engineering group at the Centre for Digitalisation and Digitality (ZDD) in Düsseldorf. Our core research focus is on the development of algorithms and research software to facilitate better - often entirely novel - analysis of biochemical and biomedical data. Join our team as Research Software Engineer (RSE) to develop open source software and data science techniques in a truly interdisciplinary setting and in close collaboration with a very active and welcoming international research community.

Responsibilities

As a key member of our development team, you will be integral in advancing the open-source library **matchms**¹. This library, created in collaboration with researchers from fields like metabolomics, cheminformatics, and environmental sciences, is tailored towards importing, processing and comparing tandem mass spectrometry data ("MS/MS" data). With increasing adoption among developers and researchers, our goal for the next three years is to expand and enhance the library's capabilities, as well as stimulate its application within relevant research projects.

As one of the main developers your role will involve:

1) Research Software Development

- Enhancing software scalability and performance, potentially through parallelization.
- Adding new features aligned with current research projects.
- Exploring ways to refine the user interface.

2) Involvement in current research projects

- Contribute to the development and implementation of novel data science methods for analyzing large-scale MS/MS datasets.
- Depending on your background and interests, this can, for instance, be related to data visualization, machine learning and deep learning, or statistical and graph-based approaches.

3) Community engagement

- Offer support and training to new software users.
- Help broaden the library's user and co-developer communities.

There is also an option to pursue a PhD, provided the necessary criteria are met.

¹ See <https://github.com/matchms/matchms> to get a first impression, but also several libraries build on top, e.g., Spec2vec (<https://github.com/iomega/spec2vec>) or MS2Query (<https://github.com/iomega/ms2query/>).

Requirements

- Master's degree in a field related to quantitative science, engineering, or software development.
- Study or project-based background in a pertinent scientific field (e.g., biochemistry, bioinformatics, medicine) **OR** proven experience in software development projects.
- Hands-on experience with Python
- Very good communication skills in English, German is a bonus.
- Ability and willingness to work cooperatively as part of a team.
- Strong motivation and ability to acquire new skills, be it data science algorithms, software development techniques, or domain knowledge relevant to the project.

Employment conditions

You will be joining a small, emerging team at the newly founded Centre for Digitalisation and Digitality (ZDD) in Düsseldorf. The ZDD considers itself a radically interdisciplinary research center with expertise spanning from design to ethics, and informatics to engineering.

In addition, you will -as one of the main developers- become part of a very lively and welcoming international open science community. You will interact with (and get help from) our collaboration partners in the Netherlands, Denmark, Belgium, France, Switzerland, Czech Republic, Italy, and USA.

While the intended cooperative and creative character requires a regular presence at the ZDD in Düsseldorf, the position offers flexible hours and remote work options. We will provide extensive onboarding to familiarize you with our projects and our workplace. We encourage continuous learning and provide opportunities for skill enhancement and career advancement. Whether you're deepening your technical expertise or exploring new areas within our interdisciplinary setting, we're here to support your professional journey.

The position can be full-time or part-time. Remuneration will be based on the candidate's qualifications according to TV-L up to EG13. You are welcome to start immediately, but the exact starting date can be agreed individually. The position, funded by a third-party project (DFG), is initially for a three-year term.

If you are interested, please send your application, quoting *****Matchms-RSE-2023*****, with a letter of motivation and a detailed curriculum vita to florian.huber@hs-duesseldorf.de. Please also provide links to repositories from prior software projects, if available.

Applications can be in English or German.

Also feel free to reach out to the same mail address for further information or questions.