

Postdoctoral position

Development of novel ML-based algorithms for automated method selection and optimization in LC/SFC-MS/DAD/ELSD and ESI-IM-Q-TOF analysis

The EPFL Swiss Cat+ West Hub laboratory ^{1,2} offers a 1-year postdoctoral position in analytical chemistry, renewable. The position focuses on developing novel machine-learning (ML) algorithms for automated method selection and optimization in LC/SFC-MS/DAD/ELSD and ESI-IM-Q-TOF analysis.

The overall goal is to help speed up qualitative and quantitative analysis, as well as structural data acquisition, in the automated high-throughput synthesis of small organic molecules. You will work with the laboratory's synthetic chemists, computer scientists and robotics engineers, in line with the distributed-intelligence self-driving laboratory concept. ³ Together, you will develop autonomous algorithms for tasks such as:

- frugal LC-MS method selection based on molecular descriptors
- method optimization using Bayesian optimization ⁴
- full molecule purification that combines analytical LC with preparative LC through deconvolution algorithms ⁵
- digital data processing and structuration⁶

A second line of research is part of a collaboration with Agilent Technologies. You will help fully automate our SFC-IM-Q-TOF instrument, including calibration and quantification.

Alongside the research, you will supervise the day-to-day operation of the analytical platform for our service, together with our laboratory technician.

The position also includes some teaching, mainly supervising student projects. Beginning: 1st of Jan 2027.

For more information, or to send your CV, please contact Dr. Pascal Miéville, MER (pascal.mieville@epfl.ch).

1. [doi: 10.2533/chimia.2023.154](https://doi.org/10.2533/chimia.2023.154)
2. epfl.ch/research/facilities/swisscat/
3. [doi: 10.26434/chemrxiv.15003459/v1](https://doi.org/10.26434/chemrxiv.15003459/v1)
4. [doi: 10.1016/j.chroma.2024.464941](https://doi.org/10.1016/j.chroma.2024.464941)
5. [doi: 10.1021/acscentsci.2c01042](https://doi.org/10.1021/acscentsci.2c01042)