Nontarget Chemical Analysis using High Resolution Mass Spectrometry, 6.0 credits

Förutsättningslös kemisk analys med högupplösande masspektrometri, 6.0 hp

Third-cycle education course

6FIFMB5

Department of Physics, Chemistry and Biology

Valid from: First half-year 2026

Approved by **Approved**

Registration number

Entry requirements

Entry requirement for studies on third-cycle education courses

- second-cycle degree,
- 240 credits in required courses, including at least 60 second-cycle credits, or
- acquisition of equivalent knowledge in some other manner

For this course, basic knowledge of analytical chemistry as well as advanced-level mass spectrometry is also required.

Learning outcomes

By the end of the course the students will be able to:

- describe the physical and chemical principles underlying high-resolution mass spectrometry,
- explain the difference between targeted and non-targeted analysis and when each strategy is appropriate,
- describe the key steps in HRMS-based workflows: sample preparation, chromatographic separation, ionization, mass analysis, data preprocessing, and statistical strategies,
- explain the principles of molecular formula prediction, fragmentation mechanisms, library searching, and *in silico* annotation,
- describe established standards for annotation levels (e.g. the Schymanski classification).
- plan and carry out an HRMS-based experimental design for non-targeted analysis of complex chemical samples,
- independently perform basic and advanced data preprocessing: noise reduction, peak finding, alignment, normalization, and batch correction,
- use relevant software and bioinformatics tools (e.g. MZmine, SIRIUS/CSI:FingerID, MetFrag) for annotation and hypothesis generation,
- interpret MS and MS/MS spectra to justify possible structures and chemical identities,
- critically analyze results, uncertainties, and limitations in non-targeted workflows,
- interpret MS and MS/MS spectra to justify possible structures and chemical identities,
- critically analyze results, uncertainties, and limitations in non-targeted workflows.
- formulate scientifically robust arguments regarding the level of identification and the validation of proposed structures.
- critically and independently evaluate the quality, reproducibility, and reliability of data from non-targeted HRMS analysis,
- assess the method’s capabilities and limitations in relation to specific research questions, particularly in environmental analysis, exposomics, metabolomics, and chemical contaminants,
- reflect on how algorithms, databases, and machine learning models influence objectivity and bias in the annotation of unknown compounds,
- address research-ethical aspects such as data management, traceability, open data, and reproducibility in mass spectrometry–based research,
- demonstrate the ability to communicate and defend results in written and oral scientific form.

Contents

The course provides a concentrated introduction to non-targeted chemical analysis using high-resolution mass spectrometry (HRMS). Students gain an overview of key instrumental principles of HRMS, ion mobility mass spectrometry, and the importance of ionization methods for the analysis of complex samples. The workflow for non-targeted analysis is covered from experimental design to the acquisition of MS and MS/MS data, with a focus on data preprocessing steps such as peak detection, alignment, normalization, and the handling of batch effects.
The course also addresses strategies for annotation and structural elucidation, including molecular formula prediction, fragmentation analysis, spectral libraries, and in silico methods. Students are introduced to relevant databases and tools such as GNPS, MassBank, and SIRIUS/CSI:FingerID. The importance of established identification levels, in particular the Schymanski framework, is discussed together with aspects of quality, reproducibility, and transparency. Through practical computer-based exercises and a project component, students apply a complete HRMS-based workflow to realistic datasets.

Educational methods

The teaching and learning methods in this course include lectures, workshops, computer-based laboratory exercises, seminars, literature studies, and a project assignment.

Examination

An individual project assignment including data analysis, presented in an oral presentation. Active participation in seminars and exercises.

Grading

Two-grade scale

Course literature

A list of recommended literature will be provided by the course coordinator.

General information

The course is planned and carried out according to what is stated in this syllabus. Course evaluation, analysis and suggestions for improvement should be fed back to the Research and PhD studies Committee (FUN) by the course coordinator.