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EUROPEAN UNIVERSITY FOR CUSTOMISED EDUCATION

STUDY GUIDE

LC-MS-BASED UNTARGETED AND TARGETED METABOLOMICS

Organised by

Medical University of Bialystok (MUB), Poland
within the EUNICE European University Alliance

1. IDENTIFYING DATA.	
· Course Name.	LC-MS-based untargeted and targeted metabolomics.
· Coordinating University.	Medical University of Bialystok (MUB).
· Partner Universities Involved.	No Partners involved.
· Course Field(s).	Biomedical Sciences; Biochemistry; Systems Biology; Omics Technologies.
· Related Study Programme.	Bachelor, Master and Doctoral programmes in Medicine, Pharmacy, Biotechnology, Biology, Chemistry, Biomedical Sciences and related disciplines.
· ISCED Code.	0512 – Biochemistry; 0531 – Chemistry; 0511 – Biology; 0542 – Statistics – skills and methods applicable across biomedical sciences and related analytical fields; 0912 – Medicine.
· SDG.	SDG 3 – Good Health and Well-being; SDG 9 – Industry, Innovation and Infrastructure.
· Study Level.	Open to all study levels (Bachelor, Master, Doctorate) and university staff.
· EUNICE Key Competencies	Problem solving: Strongly Teamworking: Moderately Communication: Moderately Self-management: Strongly Cognitive flexibility: Strongly Digital competence: Strongly Technical competence: Strongly Global intercultural competence: Moderately

· Number of ECTS credits allocated.	3 ECTS
· Mode of Delivery.	Online self-study (asynchronous).
· Language of Instruction.	English
· Course Dates.	Winter semester: 1 October 2026 – 14 February 2027
· Precise Schedule of the Lectures.	Self-paced online modules.
· Key Words.	Metabolomics; Untargeted; Targeted; LC–MS; Biomedical research; Data analysis.

· Catchy Phrase.	From LC–MS spectra to biological insight: untargeted and targeted metabolomics for biomedical research.

· Prerequisites and co-requisites.	B2 level English or higher. Basic knowledge of chemistry and biochemistry or life sciences is recommended.
· Number of EUNICE students that can attend the Course.	Unlimited.
· Number of EUNICE students that can attend the course per institution	Unlimited.
· Course inscription procedure(s).	Standard EUNICE procedure.

2. CONTACT DETAILS.	
· Department.	Clinical Research Centre – Metabolomics and Proteomics Laboratory.
· Name of Lecturer.	Joanna Godzien, PhD
· E-mail.	joanna.godzien@umb.edu.pl
· Other Lecturers.	Julia Zelkowska, MSc (last-year PhD student) Adrian Godlewski, MSc (last-year PhD student)

3. COURSE CONTENT.

This course provides a focused introduction to LC–MS–based metabolomics, covering both untargeted and targeted approaches in the context of biomedical and clinical research. Students will learn how LC–MS workflows are designed and implemented, from experimental design and sample preparation through data acquisition, processing and interpretation. The course emphasises untargeted metabolomics for discovery and phenotyping, as well as targeted metabolomics for quantitative validation and hypothesis-driven studies, highlighting how these strategies complement each other within a coherent workflow. Through self-paced modules and guided exercises, participants will explore practical aspects such as quality assurance and quality control, data preprocessing, basic statistics and pathway analysis for biomarker discovery and mechanism-oriented research. Real-world examples will be used to illustrate typical challenges and best practices in LC–MS–based metabolomics.

4. LEARNING OUTCOMES.

Upon successful completion of the course, students will be able to:

1) Explain the role of LC–MS–based metabolomics in biomedical and clinical research and differentiate between untargeted and targeted approaches.

2) Describe key components of untargeted LC–MS metabolomics workflows, including experimental design, sample preparation, chromatographic separation, high-resolution MS/MS acquisition, and quality control procedures.
3) Describe the key components of targeted LC–MS metabolomics workflows, including analyte panel selection, sample preparation, chromatographic separation, the use of internal standards, targeted acquisition modes (e.g. MRM and SRM), and quantitative validation.
4) Summarise the main steps in LC–MS metabolomics data processing (peak detection, alignment, normalisation, filtering) and recognise common issues that affect data quality.
5) Interpret basic LC–MS metabolomics outputs (e.g. ion chromatograms, feature tables, quality control metrics) and understand their relevance for downstream statistical analysis.
6) Apply core concepts of univariate and multivariate analysis (e.g. t-tests, PCA, supervised classification) to assess metabolic differences between study groups.
7) Discuss how untargeted discovery and targeted confirmation can be combined in metabolomics workflows for biomarker discovery and validation.
8) Extract and apply relevant information from LC–MS metabolomics publications, particularly in relation to study design, analytical methods, data processing and interpretation, to support their own research.
9) Reflect on reproducibility, reporting standards and ethical aspects of generating and sharing metabolomics data.

5. OBJECTIVES.

The main objectives of the course are to:

1) Provide a solid conceptual foundation in LC–MS–based untargeted and targeted metabolomics for biomedical applications.
2) Familiarise students with the design and execution of LC–MS metabolomics studies, from research question to experimental design and data acquisition.
3) Introduce common strategies for processing, analysing and interpreting LC–MS metabolomics data, including pathway analysis and potential biomarker evaluation.
4) Highlight how untargeted and targeted metabolomics workflows can be combined for discovery, confirmation and quantitative validation of metabolic biomarkers.
5) Develop students' ability to critically read and evaluate scientific literature in LC–MS–based metabolomics.
6) Enable students, especially at Master's and Doctoral levels, to critically evaluate whether and how LC–MS–based metabolomics can be meaningfully applied in their own or planned research projects, including recognising when such approaches are not appropriate or informative.

6. COURSE ORGANISATION.

UNITS

1.	**Introduction to LC–MS based Metabolomics and Study Design** Overview of metabolomics and its applications in biomedicine; position of LC–MS among metabolomics platforms; basic principles of LC and MS; study design (case–control, cohort, longitudinal); sample collection, storage and pre-analytical factors; introduction to quality assurance and quality control in metabolomics.
2.	**Untargeted LC–MS Metabolomics Workflows** Untargeted metabolomics strategy; sample preparation for broad metabolite coverage; high-resolution LC–MS acquisition (positive/negative ion modes, MS/MS); quality control samples and batch structure; conceptual overview of molecular feature, alignment, feature filtering and normalisation; introduction to metabolite annotation and identification levels.
3.	**Targeted LC–MS Metabolomics Workflows** Rationale for targeted metabolomics; selection of analyte panels; optimisation of sample preparation method; optimisation of LC–MS/MS method parameters; internal standards and calibration strategies; LC–MS/MS methods using triple quadrupole instruments; quantitative validation and performance metrics; examples of targeted panels (e.g. amino acids, acylcarnitines, lipids, commercial) in clinical research.
4.	**Data Analysis, Interpretation and Integrated Workflows** From feature/metabolite tables to results: univariate and multivariate analysis; batch effects; identification based on MS/MS spectra, biological interpretation using pathway analysis, ROC curve analysis.

LEARNING RESOURCES AND TOOLS.

The course's learning resources and assessment tools are available on the EUNICE Moodle Platform.

PLANNED LEARNING ACTIVITIES AND TEACHING METHODS.

Students will have access to written course contents, video explanations, and an automatic online exam in the EUNICE Moodle online environment. The course is fully asynchronous and self-paced; students can review materials and complete assessments at their own convenience during the course delivery period.

Student activities in EUNICE Moodle will include:

- Reading and familiarization with text materials available on the course site.
- Watching short video presentations from MUB Metabolomics and Proteomics Laboratory available on the course site.
- Taking the exam, which assesses students' knowledge and understanding of metabolomics concepts.

The course is completed by working independently and taking the exam, which consists of multiple-choice questions covering the course topics. The course is graded “passed” or “failed”.

As an optional additional activity, each module will include a discussion forum for students to share questions, reflections, or experiences. These forums will be moderated by the course lecturer, who may contribute responses when appropriate.

7. ASSESSMENT METHODS, CRITERIA AND PERIOD.

This course will be assessed on a pass/fail basis only. No grades or marks will be awarded.
To complete the course and receive a certificate, students must:
1) Review at least 90% of the course materials across all four Modules, going through all Sub-Topics.
2) Successfully pass the Automatic Online Assessment by correctly answering at least 8 out of 12 questions. Please note: students have only two attempts to complete the assessment.
3) Complete both the pre-course and post-course surveys. These surveys take approximately 3–5 minutes each and are essential for issuing the free certificate and for reporting and evaluation purposes.
Upon meeting all course completion criteria, students can download their Course Certificate directly from the EUNICE Moodle Platform.

OBSERVATIONS.

8. BIBLIOGRAPHY AND TEACHING MATERIALS.

Recommended literature:
Books

1. Ivanisevic, J., Giera, M. A Practical Guide to Metabolomics Applications in Health and Disease: From Samples to Insights into Metabolism. Springer, 2023.
2. Jaumot, J., et al. Data Analysis for Omic Sciences: Methods and Applications. Comprehensive Analytical Chemistry, Vol. 82. Elsevier, 2018.
3. Siuzdak, G. Activity Metabolomics and Mass Spectrometry. MCC Press, 2025.
4. Sussulini, A. Metabolomics: From Fundamentals to Clinical Applications. 1st ed. Advances in Experimental Medicine and Biology, Vol. 965. Springer, 2017.
5. Lutz, N. W., et al. Methodologies for Metabolomics: Experimental Strategies and Techniques. 2013.
6. Wehrens, R., Salek, R. Metabolomics: Practical Guide to Design and Analysis. Chapman & Hall, 2021.
7. Hyotylainen, T., Wiedmer, S. Chromatographic Methods in Metabolomics. RSC, 2013.
8. Winkler, R. Processing Metabolomics and Proteomics Data with Open Software: A Practical Guide. RSC, 2020.
9. Lämmerhofer, M., Weckwerth, W. Metabolomics in Practice: Successful Strategies to Generate and Analyze Metabolic Data. Wiley-VCH, 2013.
10. Lindon, J. C., et al. The Handbook of Metabolic Phenotyping. Elsevier, 2019.

Articles

1. Alseekh, S., et al. “Mass spectrometry-based metabolomics: a guide for annotation, quantification and best reporting practices.” Nature Methods 18, 747–756 (2021).
2. Mosley, J. D., et al. “Establishing a framework for best practices for quality assurance and quality control in untargeted metabolomics.” Metabolomics 20, 20 (2024).
3. Goodacre, R., et al. “Proposed minimum reporting standards for data analysis in metabolomics.” Metabolomics 3, 231–241 (2007).
4. Goodacre, R., et al. “Metabolomics by numbers: acquiring and understanding global metabolite data.” Trends in Biotechnology 22(5) (2004).
5. Dunn, W. B., et al. “The importance of experimental design and QC samples in large-scale and MS-driven untargeted metabolomic studies of humans.” Bioanalysis 4(18), 2249–2264 (2012).
6. Xia, J. “Translational biomarker discovery in clinical metabolomics: an introductory tutorial.” Metabolomics 9, 280–299 (2013).
7. Dunn, W. B., et al. “Procedures for large-scale metabolic profiling of serum and plasma using gas chromatography and liquid chromatography coupled to mass spectrometry.” Nature Protocols 6, 1060–1083 (2011).
8. Broadhurst, D., et al. “Guidelines and considerations for the use of system suitability and quality control samples in mass spectrometry assays applied in untargeted clinical metabolomic studies.” Metabolomics 14, 72 (2018).
9. Beger, R. D. “Metabolomics enables precision medicine: ‘A White Paper, Community Perspective.’” Metabolomics 12(9), 149 (2016).