

Novel tools for high throughput metabolomics in the Multiomics Laboratory.

Dariusz Kruszka

Institute of Plant Genetics Polish Academy of Science

Contemporary mass spectrometry techniques—such as high-resolution mass spectrometry (HRMS), tandem and hybrid mass spectrometry, and ion mobility spectrometry—enable the detection of hundreds of metabolites within a single chromatographic run, making them powerful tools for metabolomics research. However, a major challenge in HRMS-based studies remains the accurate identification and annotation of metabolites, particularly in complex matrices such as plant extracts, clinical samples, and environmental samples. This issue is especially critical in the context of biomedical research conducted in accordance with FAIR principles [1] and the guidelines of the Metabolomics Standards Initiative (MSI) [2].

These challenges are addressed by the project entitled **“An Integrative Multi-Omics Platform Based on High-Resolution Mass Spectrometry for Metabolome and Microbiome Research with the Application of Machine Learning”**, co-financed by the European Union under the European Funds for a Modern Economy programme. The aim of the project is to develop an innovative, high-throughput bioanalytical platform and to advance omics methodologies in biomedical, biological, and agricultural research, with particular emphasis on studies of human, plant, and environmental microbiota. The platform integrates high-throughput microbial cultivation under aerobic, anaerobic, and hypoxic conditions with metabolomic, lipidomic, and proteomic analyses, enabling comprehensive biochemical characterization of microbiomes and the identification of potential biomarkers.

As part of the project, the Multiomics Laboratory has been equipped with state-of-the-art instrumentation, including a mass spectrometer with ion mobility (Select Series Cyclic IMS, Waters), DESI-MS imaging, UPLC, low-flow UHPLC, and APGC. This advanced infrastructure significantly enhances the laboratory’s analytical capabilities, particularly in the identification and annotation of metabolites. In addition, metabolomic analyses are supported by chemoinformatics and bioinformatics tools, facilitating efficient data processing and interpretation. The processing pipeline may incorporate commercial or open-source software solutions.

The resulting research platform is intended for scientists working in biological, medical, and agricultural fields. The project will collaborate with other research institutions in Poland and internationally, as well as partnerships with industry stakeholders in the biomedical, pharmaceutical, agricultural, and food sectors.

[1] Alseekh, S., et al. Mass spectrometry-based metabolomics: a guide for annotation, quantification and best reporting practices. *Nat Methods* 18, 747–756 (2021). <https://doi.org/10.1038/s41592-021-01197-1>

[2] Fiehn, O., et al. The metabolomics standards initiative (MSI). *Metabolomics* 3, 175–178 (2007). <https://doi.org/10.1007/s11306-007-0070-6>