

Standard Operating Procedure (SOP)

Booking the nano-ultrahigh-performance liquid chromatography - high-resolution mass spectrometry (nUHPLC-HRMS) system for (phospho-) proteomics and metabolomics

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1. Introduction and Purpose

This SOP describes how to book measurements on the nano-ultrahigh-performance liquid chromatography - high-resolution mass spectrometry (nUHPLC-HRMS) system for (phospho-) proteomics and metabolomics.

2. Scope and Application

The SOP was designed to ensure an open, non-discriminatory access to the nUHPLC-HRMS system acquired within the CELLCOMM grant, which is embedded and

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operated by the Bioanalytical Research Labs within the Department of Biosciences and Medical Biology of the University of Salzburg.

3. The nUHPLC-HRMS instrument

The nUHPLC-HRMS system allows (phospho-) proteomics and metabolomics analysis. The instrument acquired within CELLCOMM (Thermo Fisher Scientific Orbitrap Ascend Tribrid Mass Spectrometer) in short is called “M11”. The nUHPLC system Thermo Fisher Scientific Vanquish Neo acquired within CELLCOMM in short is called “H16”. In combination the instrument is termed “M11H16”.

4. Booking the instrument

Infos on the booking of the instrument can be found on the homepage of the Bioanalytics Core Facility: <https://www.plus.ac.at/biosciences/facilities/core-facilities/cf-bioanalytik/contact/?lang=en>. The contact for booking the instrument via eMail is: cf_bioanalytik@plus.ac.at. eMails sent to this address will reach the director of the core facility (Univ. Prof. Mag. Dr. Christian Huber), the technical expert (Dipl.-Ing. Aleksandar Paunovic) and the scientific expert (Dr. Christof Regl). Upon contact a meeting will be scheduled to discuss the type of samples, required preparation steps and a time plan for the experiments.

5. Open, non-discriminatory access to the nUHPLC-HRMS system

The access to the nUHPLC-HRMS system is open and non-discriminatory. This means that any interested client will be given access to the device and, if necessary, training in its use. However, operating the nHPLC-MS technology is technically highly demanding. It requires a solid foundational knowledge of analytical techniques as well as extensive training in the computer-based operation of the instruments. Due to the enormous amount of data generated, data evaluation is usually only possible using specialized software, the handling of which must also be practiced. Therefore, the device itself is only operated under the supervision of the technical or scientific expert and may only be accessed upon prior agreement with them.

Independent use of the infrastructure requires proof of proficiency in analytical techniques and instrument operation (e.g., through courses at the University of Salzburg or training provided by the staff of the Core Facility).

6. Correct naming of files and sequences

Data acquisition on the M11 is done within the Xcalibur software. The instruments supervisor (e.g. Christof Regl) will generate a dedicated folder assigned to the client on the D hard drive, e.g. “D:\Data\Christof\Client1”. Within the folder, the data are ordered in sequences, which have to be named as described in 4.1.

5.1 Correct naming of sequences and files

The sequences have to be named easily understandable, containing the **date**, whereby the order is **YYYYMMDD**, **the users abbreviation**, the used **instruments**, the

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column and the samples and the client them. All separated by “_”. E.g.:
“20250801_CR_M11H16_Aurora258_PMU_MigraineEVs”.

Injectons within the sequence are named accordingly to the samples by another extension of “_” and ideally the sequential number. E.g.:
“20250801_CR_M11H16_Aurora258_PMU_MigraineEVs_Control_001”.

6. Archiving of files

Data storage is done as described in the SOP Acquisition, backup and archiving of HPLC-MS datasets Version 2.0; 2026.31.08