

User Rules

1) User Projects and Organization of the Platform

The Biocenter-MS platform offers all researchers, particularly those of the Biocenter Cologne and the CEPLAS cluster, the possibility to identify and quantify metabolites and inorganic molecules (e.g., metabolites, peptides). The CEPLAS MS Facility [Secondary metabolites Laboratory], is part of the Biocenter-MS platform and therefore based on the same concept. The platform is a merger of the existing mass spectrometric facility of the Biocenter. This combination provides operators and users the use of existing devices to efficiently and optimally solve analytical problems.

The user enters the facility by approaching the coordinator with their analytical question/s. As part of the consultation, options from the objective of the project to sample volumes and extraction procedures are discussed. For specific questions the corresponding equipment operator can be contacted directly.

The cooperation between the user and platform includes, in principle, the analysis of the desired substances by chromatographic and / or mass spectrometric methods. Depending on needs, the researcher is supported in the discussion of sample preparation, experimental design, data analysis and processing of the raw data by the operator.

You are given the opportunity to high throughput sampling with an automated evaluation of baselines and the identification and structural elucidation of unknown substances using high-resolution MS and MSⁿ.

The user provides already extracted samples into the provided containers from the platform and will get the results of the analyses in the pre-agreed format (see Cost agreement).

2) Equipment

For mass spectrometric measurements, the following equipment / connection options are available:

A QTRAP 5500 system (ABSciex), a hybrid triple quadrupole / linear ion trap mass spectrometer, which can be coupled to a 1260 HPLC (Agilent) or a Advion TriVersa nano mate. The ion source allows both electrospray ionization (ESI) and Atmospheric Pressure Chemical Ionization (APCI), further, a nano - ESI ion source can be connected.

The A maXis 4G (Bruker Daltonics), a Quadrupole / time-of-flight mass spectrometer device, which can be coupled to a 3000 Ultra UHPLC (Dionex) or a 450 GC (Bruker Daltonics). The ion source also allows ESI and APCI ionization.

Another coupling option is the QExactive, a Orbitrap system (Thermo Scientific) and/or an Accela UPLC (Thermo Scientific). Fractions can be collected parallel to the MS analysis. Furthermore a nano - ESI source can be used.

ICP (inductively coupled plasma) MS-7700 (Agilent), an inductively coupled plasma mass spectrometer for total element analysis is also available for use.

Two MALDI (matrix-assisted laser desorption / ionization) time-of-flight mass spectrometers (Voyager STR, ABSciex; ultrafleXtreme, Bruker Daltonics), which are preferred for the analysis of peptides, are available.

The above mentioned devices are normally operated by the equipment staff responsible the requested analyses. In individual cases, exceptions may be granted after consultation and briefing by the operator. The operation of the devices by students / PhD students / postdocs in the context of courses and internships are given under supervision by the operator.

3) User authorization and priorities

Normal sample processing is based on the delivery date. However, at full capacity, the order in which the samples are to be analyzed is determined by the following key priorities:

- i) Working groups of the Biocenter Cologne as well as the CEPLAS cluster.
- ii) Analysis for currently open projects that are already in manuscript revision processes.
- iii) External academic partners.

If there is an overload, so not all requests can be fulfilled, only those of high priority (i) can reserve the right for analysis.

The final decision on the order of processing is with the operator to ensure efficient use of the equipment.

4) User costs

The platform collects fees for routine ongoing analysis. These fees are used for the purchase of software and updates as well as standard substances, chemicals, consumables and method development.

For analyses, which are not yet routinely running or for only one method that needs to be developed there cannot be guaranteed from the outset that the user receives useful results. Details of the costs incurred for the development of methods will be explained in the context of a user agreement during the consultation session with the equipment operator and jointly determined.

Costs for measurements within the scope of teaching have to be discussed with the appropriate contact person in advance.

Costs for the use of LC / MS GC devices are estimated for 8 h (test run) or 24 (measurement). It should be noted that not only the actual measurement period is involved, but also equilibration and calibration times. For the use of ICP / MALDI MS, the cost per sample will be charged.

5) Contact information and sample delivery

Before Initiating a new project, the coordinator and operator of the respective MS field has to be contacted to discuss project details.

Contacts

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In this confidential conversation, the planned experiments are discussed and the most suitable method for measurement will be investigated. In addition, the time and financial frame will be determined. Technical personnel as well as operators may be consulted by the coordinator to the meeting. The submission of samples for mass spectrometry analysis and the use of devices are only possible after prior consultation or notification of the respective operator.

Before submitting the samples, users need to sign the cost agreement and hand in a detailed documentation about sample preparation.

In addition, the signature confirms that the samples are chemically and biologically safe and do not endanger the health or safety of employees. Without a completed and signed form the samples will not be processed (see cost agreement).

6) Data analysis and storage

The acquired data is immediately stored on the local machine. This raw data with the corresponding analytical data is stored on long term storage servers ("scale out file services")

(SOFS)) at the University of Cologne. The synchronization of the drives is effected by the device operator. Data backup is achieved by the data center, in multiple copies, so that a complete data loss is virtually eliminated. The users do not have access to the data stored on the data center. The use of SOFS is not currently charged. The agreed quality controls to check the integrity of the measurement method / device are provided to the user in an already analyzed form. The data analysis is subject of the agreement between the operators and users. After completion of the project, the user receives a copy of all raw data and the pre-agreed form of data analysis.

7) Publication of experimental results

If the participation of the platform personal has profoundly contributed to the scientific success of the project (e.g., development of new methods, elaborate evaluations (graphics), interpretations of results), co-authorship is justified. Any other form of participation has to be mentioned in the acknowledgments. The publications should be published on the website of the platform. The signature of the acknowledgment agreements is a prerequisite for the analysis (see acknowledgement agreement).

8) Consequences of abuse

If these guidelines are repeatedly ignored, the group can be excluded from further use of the platform.