

Fakultät für Chemie und Mineralogie MS Core Facility "MS-UL" 01.06.2020

MS Core Facility an der Fakultät für Chemie und Mineralogie der Universität Leipzig

Universität Leipzig, Institut für Analytische Chemie Technikum/Analytikum in der Linnestr. 3, 04103 Leipzig

Terms of use

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1. Foreword and scope of the terms of use

The MS Core Facility MS-UL is a facility of the Faculty of Chemistry and Mineralogy at the University of Leipzig. These regulations govern the use of the equipment available in this equipment center. They are binding for all users of the Core Facility "MS-UL" at the Faculty of Chemistry and Mineralogy at the University of Leipzig. The terms of use apply to the mass spectrometry laboratories belonging to the Core Facility in the Technikum/Analytikum in Linnestr. 3, 04103 Leipzig, including the equipment available there as well as the professional environment required for sample preparation and analysis.

2. Responsible persons

- Dr. rer. nat. Claudia Birkemeyer for scientific advice on planning and evaluation of experiments, strategic requests and financial organisation
- Ramona Oehme and Dr.-eng. Susan Billig for technical requests

3. Models of use

Following usage models apply:

- "Service operation": The samples are submitted after suitable preparation and employees of the instrument center carry out the analysis. This usage model is available to all users of the Core Facility.
- "Self operation": Users work independently on the devices (with less supervision by employees of the Core Facility). This usage model is only available to members of the "MS User Community" (see point 6. of the terms of use) by prior agreement and only to trained users in accordance with our safety regulations after initial instruction in the laboratory. Different, individual usage concepts for individual devices can also be agreed upon request.

Thereby

- the DFG recommendations on good scientific practice (https://www.dfg.de/foerderung/grundlagen_rahmenbedingungen/gwp/) are complied with,
- any technical problem and possible damage to the equipment must be reported immediately to the responsible manager of the Core Facility,
- the work (including the appropriate sample preparation) is carried out in such a way as to avoid any instrument malfunctions.

4. Detailed services

The following services are offered in the "service operation" model:

- Scientific consulting on experimental questions and data evaluation
- Determination of the (accurate) mass of a target substance in sufficiently clean samples suitable for *automated measurement*
- Determination of the (accurate) mass of samples that are generally suitable for measurement but difficult to detect for *manual measurement*
- Measurements using hyphenated techniques (mass spectrometry coupled with liquid or gas chromatography) of suitable samples on request and subject to availability of the technology
- Automated generation of a pdf report of the results after target peak control
- Booking of computers in the rooms of the Core Facility for self-guided evaluation of measurement data by users using the vendors softwares
- Training on equipment and data evaluation according to the needs of the respective user and the time capacities of the Core Facility employees

The following services are offered in the "self-operation" model:

Services desired on a larger scale (>500 samples/year), which are also offered in service operations

- Installation of equipment within the rooms of the facility including operation, maintenance and minor
 repairs by the Core Facility. Requires the allocation of the consumables costs to the users including the
 owner of the equipment and individual agreements on major repairs (sharing or full settlement of the
 costs). If only a part of the usage time of the device is shared by the facility, only this part is regulated by
 these terms of usage.
- Larger experiments involving instruments of the Core Facility require the share of consumable and repair costs and an agreement to the reimbursement of damages to the used device caused by user errors.
- In the "self-operation" mode we offer selected representatives of the using working groups training on the devices and for data evaluation. A prerequisite is the appropriate professional qualification (completed vocational training in the field of chemistry or a master's degree in the natural sciences) and the anticipated use of the Core Facility for at least half a year.

In addition, we offer scientific consulting and the preparation of quotes to advise applicants on the feasibility of the planned project if the expected costs of use exceed EUR 10,000.

The equipment currently available to the Core Facility and its specifications are described on our home page. In the Core Facility, a distinction is made between devices for service operation ("service devices") and self operation ("project devices"); the distinction can also be found in the list of devices on the Core Facility homepage.

5. Access to our services and booking system

In the automated *service operation*, each —clearly labeled— sample comes with a completely and correctly filled out MS order form, available on demand as a download on the homepage. Alternatively, an online mask is available on the homepage to replace the form sheet printout. For special consumables and time-consuming sample preparation, users need to care on their own. The samples have to be deposited in the designated rack in front of room 173a in the Technikum/Analytikum, Linnéstr. 3, 04103 Leipzig, Germany, or sent by mail to the AK Mass Spectrometry at this address to the attention of the head of the facility.

All samples will be processed in the *order of their submission* date on the respective instruments with the required ionization mode. Unsuccessful measurements will be reanalyzed using alternative ionization techniques without further notice. *Larger sample batches* (>10) can be put on hold depending on the instruments availibility. In the event of an overbooking, the *service operation* takes precedence over the *self-operation*. Likewise, analyses involving upstream separation techniques are subordinated to flow injection analyses and as well as orders from *external users* not belonging to UL.

In the *self-operation* mode, users are granted access to internal booking systems for project instruments on a *first come first serve* basis; frequent blocking without using the instrument will result in controlled booking by the facility employees for the respective user.

6. Data exchange, security and archiving policy

Ownership and data security

All measurement results from the service requests are the property of the client, treated confidentially and only transferred to authorized users. Contact details of customers such as name, business address, telephone number and e-mail address, are only collected for service-relevant communication and billing. These data is only accessible to the responsible persons of the facility and will never be passed on to third parties.

Type of data, transfer and evaluation

Results from requested measurements come in form of an automatic report (.pdf) submitted together with the raw data file. In addition to the submission date and the name and contact details of the customer, the file name contains only a short sample identifier selected by the user. In the *service operation* mode, data can be delivered as .txt upon request of the respective user. Results are provided copied to a password-secured server that is only accessible to users. For access to the server, please contact the Core Facility staff. In exceptional cases with reasonable effort for the Core Facility staff, data can also be encrypted and exchanged by e-mail, if explicitely requested by the user. For limited use of the Core Facility (for up to 5 individual experiments per year), other data transfer options can be provided upon request, e.g., cloud-based transfer. Agreements beyond these standards, such as non-disclosure agreements, can also be agreed on considering higher operational costs.

All users are welcome to contact the staff of the Core Facility for information on further processing of the measurement data (scientific advice on free ressources) or to request access to the computers of the Facility for their evaluations.

Data storage and archiving

The data obtained during *service operation* measurements are first stored on the computers of the respective instrument, sorted by date. In the *self-operation* (project) mode, the data is sorted by user and project. The data must be backuped by the users within 3 months at the latest. After that, the data is deleted from our data exchange server and instruments computers and, unless otherwise agreed, archived by the Core Facility for 10 years.

7. Costs of use

Accounts are settled according to the following user categories:

- Working groups at the Faculty of Chemistry and Mineralogy and other faculties of the University of Leipzig
- Working groups at other public institutions
- External users

For all user groups fees are charged according to an annually updated <u>price list</u> deposited on the facility's homepage.

As a general concept, all working groups from the UL have the *right*, and working groups from other public institutions can be proveded the *possibility* to become members of the "Nutzergemeinschaft MS". In this user community, an annual membership fee is charged as a repair cost advance, while an averaged, fixed amount of consumables cost is charged for each individual sample as announced on the current <u>price list</u>. For non-members, repair costs are charged as an averaged, fixed amount per sample.

Measurements for external users must be charged according to the full cost calculation.

8. Acknowledgement of the facility staff in publications

The recognition of achievements of the facility is mainly done through acknowledgements in publications of scientific articles as well as co-authorships for staff members of the Core Facility. Recommendations with regard to acknowledgements and co-authorships are outlined in a separate <u>document</u>, which can be viewed on the homepage. Essentially, in accordance with generally accepted guidelines, a distinction is made here between routine contributions, for which an acknowledgement is appropriate and scientific-creative collaboration by Core Facility staff, for which a co-authorship is anticipated.

Publication of data generated with the participation of the Core Facility is to be indicated accordingly in the acknowledgements section and the reference is to be made available to the staff of the Core Facility. If the work of the Core Facility represents a decisive part of the publication, the persons involved are to be considered as coauthors in the sense of good scientific practice and to participate in the preparation of the manuscript. The compensation of analysis costs does not replace the obligations mentioned above.

Projects from which patents or similar may arise are not provided as a service but carried out based on individual cooperation agreements.

Leipzig, 31.01.2021

Dr. Claudia Birkemeyer, Head of the Core Facility