User Rules & Regulations
Core Facility for Mass Spectrometry and Proteomics (CFMP)
at the Centre for Molecular Biology of Heidelberg University (ZMBH)

Accepted on 30. January 2017

§1 Definition and aims

1. The Core Facility for Mass Spectrometry and Proteomics (CFMP) is an infrastructure facility of the Centre for Molecular Biology of Heidelberg University (ZMBH). This central service facility supports the research facilities at the campus Heidelberg with high-performance mass spectrometry aimed at protein analytics and proteomics.
2. The user rules & regulations stated in this document regulate the organization of service and method development at the CFMP. They are mandatory for every core facility user.
3. This document is in accordance with the requirements of the Deutsche Forschungsgemeinschaft (DFG).

§2 Responsibilities of the central service facility

1. The services of the CFMP include the consultation of scientific projects, sample preparation & processing and the mass spectrometry-based protein analysis as well as the primary analysis of experimental data.
2. All services offered by the CFMP are conducted by experienced personnel of the central service facility (full service). These services are listed in the currently valid Service & Pricing List.

§3 Organization

1. The CFMP is managed by the core facility head.
2. The core facility head is accountable to the ZMBH MS-Commission (ZMBH MS-Kommission) as well as the directorate of the ZMBH.
3. The research group leaders (Forschungsgruppenleiter [FGL]) of the ZMBH appoint a scientific coordinator and pass the user rules & regulations of the CFMP.
4. The work of the CFMP is being followed by the ZMBH MS-Commission (§4), under supervision of the scientific coordinator (§5).
5. The name of the facility head and the scientific coordinator will be published online (http://www.zmbh.uni-heidelberg.de/Central_Services/Mass_Spectrometry/aboutus.html).

§4 ZMBH MS-Commission

The ZMBH MS-Commission supervises the activities of the CFMP to achieve an optimal integration of the central service facility into the research environment at the campus Heidelberg. The scientific coordinator heads the commission.
The commission consists of:

a) The director of the ZMBH or his /her representative
b) Two delegates of facility users
c) The scientific coordinator
d) The core facility head

The commission meets at regular intervals to discuss issues concerning the CFMP and to take note of the head's statement of accounts. Alternatively, this can also be handled by means of a circular resolution. The commission determines their own orders of conduct. The names of the commission members will be published on the internet (http://www.zmbh.uni-heidelberg.de/Central_Services/Mass_Spectrometry/aboutus.html).

§5 Scientific coordination

Responsibilities of the scientific coordinator are:

a) Representing and communicating the needs of the ZMBH and CFMP users to the core facility head.
b) Role of competent and approachable contact for the core facility head in all matters needed for an optimal integration of the CFMP into the research environment at the campus Heidelberg.

c) Distributing invitations to regular MS-Commission meetings as well as irregular ones that require immediate attention.
d) Prioritizing the order of sample processing in times of high demand or in urgent case.

§6 Provided services

1. The services offered by the central service facility will be regularly updated and adapted to the users' needs. The core services are being described in the current Service & Pricing List. They include the following:
    a. Consulting services during specified hours or on appointment
    b. Experimental design, sample preparation, conductance and primary data analysis of mass spectrometry-based peptide and protein analyses
2. The central service facility recommends their users to get in contact as soon as possible to avoid the occurrence of errors during experimental design or sample preparation. A detailed experiment consultation precedes any service or project requests, in which a suitable analytical strategy is being agreed upon with the user and the estimated costs of the measurements based on the Service & Pricing List are being explained to the costumer. The user agrees to cover any resulting costs before the measurements are being conducted.
3. The core facility head or his/her representative is responsible for scheduling services and projects. Generally, user requests are being processed on a first come, first served basis. In justified cases (e.g. optimization of instrument usage or to ensure the reproducibility of serial measurements) an exception can be made and a divergent scheduling order can be determined by the core facility staff. In case of doubt it is up to the scientific coordinator to decide.
4. The head of the central service facility or his/her representative reserves the right to reject requests for the provision of services in objectively justified cases. In the event of a refusal, a constructive feedback will be sent to the requester. The scientific coordinator must be notified about such a rejection too.

§7 Sample submission

1. All samples must be electronically registered under a unique and continuous identification number by the members of the CFMP.
2. Samples can be submitted to the ZMBH's CFMP, INF 282, Room 401, either by post or in person between 10 am and 5 pm. Toxic or human pathogenic as well as radioactive samples can not be processed.
3. Remaining samples continue to be property and responsibility of the users. Since the service unit has only limited possibilities for refrigerated storage of samples, a medium or long-term storage of sample sets is not possible. Therefore, no guarantee can be given for the integrity of samples beyond the immediate period of the service (1 month).

§8 Costs

A service includes the routine processing of samples, the sample preparation steps as specified in the Service & Pricing List and a primary data analysis. The fees charged, as determined by the FGL assembly, are also detailed in that list. The groups that have made a significant contribution to the equipment of the CFMP will receive a 20% discount (price in brackets). The ZMBH MS-Commission decides upon the classification of the groups. Collaborations (without the fixed fees) must be stipulated prior to the commencement of work. They are limited to projects used for method development and are generally financed through joint third-party funding. Service projects have priority over collaborations. The intellectual contribution of one or more employees of the CFMP exceeds the technical provision of a service and is therefore to be honored by a co-authorship.

§9 Data storage & security

1. The analysis results are being made available to the respective members of the research groups in adequate form (e.g.: e-mail, cloud).
2. All measured data (spectra and database search results) obtained during routine operations are to be stored on a server. On request, they will be made available to the respective members of the research groups in a suitable way.
3. Archiving obtained data is carried out in cooperation with the university data center (Universitätsrechenzentrum). Data are to be stored for a minimum of 10 years.

§10 Publication of data

1. Acknowledgment: In principle, contracted services, as provided by a central service facility are to be indicated in scientific publications at the appropriate position. A compensation of costs for services provided does not replace a corresponding quotation in scientific publications. More specifically, any work that originated in a service facility must be clearly identified and cited in the acknowledgments of scientific publications.
2. Co-authorship: If the development of new analytical methods or significant, intellectual contributions by service facility employees become necessary for the design of the experiments or the generation and/or evaluation of the data, the users commit themselves to include these employees in the publication or patent of the results as co-authors according to good scientific practice whether or not the technical service had been charged. As far as possible, the question of intellectual ownership or rather a contribution by a co-author must be clarified and agreed upon by mutual consent prior to the conduction of services.

Service & Pricing List
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All prices listed below are in Euro (€). The discount rates shown in brackets apply only to "groups which have made a significant contribution to the equipment of the CFMP" - see User Rules & Regulations -§8.

a) Pre-Cast Gel & Run (SDS-PAGE)	25.00	(20.00)
b) MALDI-TOF analysis without tryptic digest and database search e.g.: purity control of synthetic peptides	25.00	(20.00)
c) Usage of MALDI-TOF mass spectrometer (per hour)	25.00	(20.00)
d) Accurate mass determination of intact and purified protein via LC-MS (2 h instrument time)	62.50	(50.00)
e) Purity control of synthetic peptides via LC-MS (2 h instrument time)	62.50	(50.00)
f) In-Solution protein digest + peptide purification	62.50	(50.00)
g) In-Gel protein digest: costs are included in instrument time	---	
h) Stable isotope labeling via reductive dimethylation	62.50	(50.00)

i) LC-MS/MS analysis: Based on total instrument time needed (number in brackets; includes: sample loading on column, chromatographic peptide separation and MS/MS analysis, equilibration of HPLC for next sample) and the DFG-reimbursable flat fee (25,- Euro / hour instrument time) the following prices apply:

ProteinID:	Identification of a purified protein from a Coomassie-stained gel band; effective separation time: 25 minutes (125 min)	65.00	(52.-)
LCMS_60:	Low complexity sample; effective separation time: 60 minutes (165 min)	86.25	(69.-)
LCMS_120:	Medium complexity sample; effective separation time: 120 minutes (225 min)	117.50	(94.-)
LCMS_180:	High complexity sample; effective separation time: 180 minutes (285 min)	148.75	(119.-)
LCMS_240:	Very high complexity sample; effective separation time: 240 minutes (345 min)	180.00	(144.-)
LCMS_360:	Ultra high complexity sample; effective separation time: 360 minutes (465 min)	242.50	(194.-)

Specification of services:

a) Pre-Cast Gel & Run (SDS-PAGE):
The sample is being delivered in the form of a protein solution in SDS-sample buffer: This service includes protein electrophoresis using a commercial mini gel. The length of separation is based on the prior agreement. Gel staining is achieved using a commercial colloidal Coomassie solution (3 h), destaining using water (overnight).

b) and c) MALDI-TOF analyses:
The sample is taken up in a suitable solvent and pipetted onto the target together with the MALDI matrix, usually HCCA. The spectrum is recorded and sent to the user in electronic form. Protein identification by peptide mass fingerprint is no longer supported. In the case of a peptide mass fingerprint for protein identification, the user can perform a data search with Mascot himself/herself in the core facility.
There is the possibility that a user performs analyses independently after proper training.

d) and e) Accurate mass determination/Purity control
For analysis, proteins (purity at least 80%) and peptides are delivered in lyophilized form. The user specifies a suitable solvent. The sample is analyzed by LC-MS. The user receives the chromatogram and the relevant mass spectra in a suitable form.

Document version: January 2017

f) In-Solution protein digest + peptide purification:

The sample is lyophilized. A first digestion is performed with Lys-C in the presence of 8 M urea, followed by a trypsin digestion after dilution to 2 M urea. Peptides are enriched by solid-phase extraction and are taken up in appropriate solutions for nanoHPLC-MS analysis. The additional fee is charged due to of the high amount of trypsin used compared to In-Gel digestion.

g) In-Gel protein digest:

A polyacrylamide gel is delivered after Coomassie staining (silver staining possible only after consultation). The service includes excision of the bands / spots from the gel, reduction and alkylation of cysteines and subsequent tryptic digestion.

h) Stable isotope labeling via reductive dimethylation:

After trypsin digestion the peptide solution is treated with the appropriate reagents. Following removal of the excess reagents, the standard LC-MS analysis is carried out as described under i)

i) LC-MS/MS analysis:

The peptide sample is loaded directly onto the separation column for best possible performance and is, depending on the complexity of the sample, eluted with a correspondingly long acetonitrile gradient. The analysis is carried out using a mass spectrometer of the highest performance class. The following systems are available:

- nanoAcquity ESI LTQ Orbitrap XL
- Ultimate RCLC 3000 ESI LTQ Orbitrap Elite with ETD
- Ultimate RCLC 3000 ESI QExactive HF
- nanoAcquity ESI QTrap5500

A first automated data analysis is carried out using suitable software (Mascot, MaxQuant, Proteome Discoverer). Depending on the software, the results of the database search are provided in user-friendly form, .

The data files are stored in two independent folders for at least 10 years at the data center of Heidelberg University.