Pharma-Zentrum Bonn

UNIVERSITÄT BONN

Rheinische Friedrich-Wilhelms-Universität Bonn

User regulations

of the "Chemical Analysis" service area at the Department of Pharmaceutical & Medicinal Chemistry

of the Pharmaceutical Institute of the Faculty of Mathematics and Natural Sciences, University of Bonn

Preamble

The **analysis of chemical compounds** plays an important part in **pharmaceutical research** and teaching. One of the original tasks of pharmacists is to supply the population with high-quality drugs. Apart from qualitative analysis, also quantitative analysis plays an important role in this respect. Pharmacists are trained to become experts in analytics.

Pharmacy at the **Excellence University of Bonn** plays a central role in life sciences and is anchored in the *Transdisciplinary Research Area* (TRA**) Life & Health**. In research and teaching, the interdisciplinary Pharmacy has a broad-based network, both within the Faculty of Mathematics and Natural Sciences and across faculty boundaries, especially within the Faculty of Medicine. The **PharmaCentre Bonn**, a research centre for innovative drugs and pharmacotherapy (Pharma-Zentrum Bonn, PZB, www.pharmazentrum.uni-bonn.de), which was founded jointly by professors of Pharmacy and Medicine, networks the working groups interested in drug research.

The Department of Pharmaceutical & Medicinal Chemistry (Head: C.E. Müller) and the Department of Pharmaceutical & Cell Biological Chemistry (F. Hansen, successor to M. Wiese) have already centralized large-scale chemical analysis **more than 20 years ago** and offered **analytical services** for the whole Division of Pharmacy, the PharmaCentre Bonn and other interested parties and cooperation partners. This **Chemical Analysis Centre**, which includes high-field NMR spectrometers, mass spectrometers and the capillary electrophoresis equipment of the Division of Pharmacy, works closely together with the analytical departments of the neighbouring Chemical Institutes. In the field of mass spectrometry, the priorities are complementary: While the Chemistry Division focuses on **qualitative MS analysis** and **MS imaging**, the Pharmacy Division has many years of expertise in the field of **quantitative analysis**.

§ 1 Scope of application

These user regulations describe the use of the resources and services offered by the service area "Chemical Analysis" at the Department of Pharmaceutical & Medicinal Chemistry of the Pharmaceutical Institute of the University of Bonn. The regulations cover the use of the equipment provided, of the connected control and evaluation computers, the software installed on them, of the laboratory rooms and the advice and instruction provided by the service staff. The regulations are binding for all users of the service area. The service area is available to the working groups of the University of Bonn and external users. Additional cooperation agreements are concluded with external institutions, such as the partners of the PharmaCentre Bonn (PZB), which regulate the use of the services in detail.

§ 2 Equipment and contact persons

The "chemical analysis" platform of the Department of Pharmaceutical & Medicinal Chemistry consists of several high-quality analytical instruments: NMR spectrometers (500 and 600 MHz), mass spectrometers (triple-quadrupole LC-ESI-MS; single-quadrupole LC-ESI-MS; DC-MS) and several capillary electrophoresis (CE) devices with UV and fluorescence detectors.

Professional staff and established operating protocols are available to operate the devices. The existing equipment and facilities of the chemical analysis platform enable the precise quantitative and qualitative analysis of a large number of chemical samples and are performed according to current scientific guidelines and standards. The service department is headed by Prof. Dr. Christa E. Müller and Prof. Dr. Finn Hansen.

§ 3 Services

The services offered by the chemical analysis platform are:

1. Qualitative NMR spectroscopy with modern 500 and 600 spectrometers. ^{1}H, ^{13}C, ^{15}N, ^{19}F and ^{31}P measurements can be performed including 2D techniques such as NOESY, TOCSY, COSY, HSQC and HMBC. This allows the structural elucidation of natural and synthetic compounds, small molecules and compounds of higher molecular masses (oligo- and polypeptides, oligonucleotides).
2. Qualitative and quantitative LCMS analyses with the existing systems. In addition to classical analyses, analytes from biological matrices such as blood and tissue are also determined. This includes the professional establishment of an extraction procedure and suitable analytical MS methods, both in negative and positive MS modes as well as MS-MS analyses. LCMS analyses can also be used for purity control and stability determination of samples.
3. Separation and detection methods using capillary electrophoresis (CE) and UV or fluorescence detection. Charged analytes can be enriched by electrokinetic injection and then quickly separated. Various stacking methods as well as fluorescence detection lead to high sensitivity.

The users of the chemical analysis platform are advised and supported both technically and scientifically by employees of the service area as to the conception, implementation and result analysis. In individual cases, a kind of "driving licence" can be obtained after a briefing, in order to use the respective equipment independently.

§ 4 Conditions for use

Before using the service area for the first time, a personal or telephone discussion of the measurements must take place between the user and the service area manager or the relevant contact person. During this meeting, the experimental question and the resulting requirements for the sample material for the measurement are discussed. All members of the service area commit themselves to treat the user's data confidentially.

For this purpose, the user independently contacts the corresponding contact person, who is listed on the website. Before using the services of the service area, the user must give a written statement that they are willing to accept the terms of use and agree to pay the costs incurred.

§ 5 Authorisation of use and prioritisation

The services and resources of the service area are available to all research groups within and outside the University of Bonn. The services can be used within a reasonable period of time after receipt of the first request. If the capacities of the service area are fully utilized, the requests are prioritised as follows:

1. requests from the departments of Pharmacy and members of the PharmaCentre Bonn
2. requests from the University of Bonn
3. external requests

If it is not possible to meet all requests due to overbooking, the management of the service area decides on the allocation of service times for the devices (and follows the above-mentioned prioritization). In justified cases, priority can be given to certain projects by the management of the service area.

§ 6 Time of use and device bookings

The measurement is ordered by submitting a sample together with a completely filled-out order form. The assignment to a specific device, the allocation of the measuring time as well as the execution of the measurement is carried out by the service staff. In the event of a one-sided overload of measuring devices, the managers in the service departments can arrange a reallocation in order to use the pool of devices as efficiently as possible. The order for a justified measurement on a specific device must be explicitly noted on the order form. An NMR service measurement in automation is started with an automatic sample changer. The measurement time starts when the sample is inserted into the device and ends when the sample is ejected. For complicated measurements, it is possible that measurements are performed manually by the service personnel. For this purpose, the users must arrange an appointment with the service personnel. The measurement time is the time during which the instrument is not available for other measurements.

Provided that all requirements mentioned in § 4 are met, the user is granted a usage time, e.g. for measurements of the desired samples. The measurement time can be cancelled by the user. This cancellation must be communicated to the service department at the earliest possible time. Cancellations at short notice (less than 24 hours prior to the booked period) may be subject to cancellation fees. In case of unannounced non-compliance with the measurement times, the full user fee will be charged.

§ 7 Data storage and data provision

The service area assures the confidential treatment and storage of the collected data. The data will be stored for at least 1 year on an access-restricted server of the Pharmaceutical Institute. The collected raw data is converted into a form usable for all common standard evaluation programs with the help of the software of the service area. The evaluation of the data is usually carried out outside the service area, but can be accompanied by the service area on request.

The service area undertakes to grant users access to the stored measurement data at short notice.

§ 8 Fees

Fees are charged as a contribution to the costs of using the equipment, including consumables. For all academic and non-commercial users, a binding fee table applies, the latest version of which can be viewed on the website. For external commercial companies, different fee rates apply. After clarifying the experimental requirements and their scope, an estimate of the expected fees can be made and communicated to the user.

§ 9 Duties of the users

The users are obliged to use the laboratory equipment of the service department and its control and evaluation computers exclusively after prior instruction and on the basis of the operating instructions.

The workplace must be left in perfect condition. Foreseeable impairments of the laboratory operation are to be avoided. In addition, any actions that could lead to damage to the infrastructure or impair the work of other users must be avoided. If a device or workplace is left behind heavily soiled, the time required for cleaning will be charged. Should this occur repeatedly despite a corresponding reminder, the user's measurement permit will be withdrawn.

The general safety precautions for working in laboratories have to be observed. In the event of a publication of results obtained with significant involvement of the service department, its contribution must be indicated. Upon request, the user undertakes to identify publications containing data generated with the support of the service area.

When making use of the resources of the service area, the "Guidelines for Safeguarding Good Scientific Practice" of the DFG (https://www.dfg.de/en/research_funding/principles_dfg_funding/good_scientific_practice/index.html) must be observed.

§ 10 Liability

The service area does not guarantee that the special requirements of the users can be fully met. It also does not guarantee that the resources can be used at all times without error and without interruption, or that the data obtained will be saved error-free and permanently.

If required, the service department supports its user with the interpretation of the measurement data within the limits of its capacities. However, the responsibility for the interpretation lies with the user.

The service area is not liable for any damage caused to the user by the use of the services. Excluded are damages to life and limb caused intentionally or through gross negligence on the part of the service area.

Attachment

Price list for research groups of the University of Bonn and for research groups of external institutions

The fees listed below are charged for the use of the equipment and services. The basic prices shown include proportional personnel costs and typical consumables.

Please note that the user fees are evaluated regularly and can be adjusted accordingly. All operating, maintenance and repair costs of the service areas are borne by the users of the institutes or departments of the Pharmacy Division. The costs incurred for the operation of the service areas are split between the institutes and Pharmacy departments according to regulations defined within the Division of Pharmacy. The classification of the user groups takes into account the contributions of current and former research groups of the Division of Pharmacy when a device is first purchased. Each registered research group regularly receives a detailed list of the measurements/usage times and the resulting costs (at least annually). This list will be sent to the heads of the research groups.

The following fees per are charged for the use of the instruments of the platform chemical analytics:

1. Section NMR

NMR fees per measurement:

for members of the Pharmacy departments:
first hour: **25 €**
each additional hour started: **5 €**

for external research groups:
upon request

Complex NMR experiments require considerably more effort and, if necessary, scientific support as to the preparation, execution and data processing. Accordingly, hourly rates up to max. 40 Euro (average field strength, 500 MHz) can be applied. Therefore, price requests for special measurements should be made in advance.

2. Section Mass Spectrometry

for members of the Pharmacy departments:

LC-ESI-MS: SQ-measurements with LC/MSD **24 €/h**
This means a fee of 6 to 12 € per measurement in standard mode.

QTRAP: **35 €/h**, or upon request

Advion Expression cms: **3 €** per measurement in self-measuring mode

for external research groups:
upon request

3. Section capillary electrophoresis

Calculation of costs upon request