UNIVERSITY OF COLOGNE

Department of Chemistry and Biochemistry

Terms of Use

NMR Facility at the Department of Chemistry and Biochemistry

University of Cologne

06/2026

1. Mission and Objectives

The NMR Facility is a central research infrastructure of the Department of Chemistry and Biochemistry within the Faculty of Mathematics and Natural Sciences at the University of Cologne. It operates as an independent scientific institution within the Department of Chemistry and Biochemistry, conducts independent research in the field of NMR spectroscopy, and enables all academic members of the Department as well as external researchers to access and use NMR spectroscopy instrumentation.

This includes the application of NMR spectroscopy in both analytical and research contexts, as well as the teaching of the necessary methodological knowledge within the degree programmes of the Department of Chemistry and Biochemistry.

In addition, the NMR Facility collaborates in research projects with national and international research institutions and thereby contributes to the scientific networking of the Department of Chemistry and Biochemistry.

The Head of the NMR Facility strives to ensure that all spectrometers remain at the cutting edge of technology, to implement and develop new NMR methods, and to make these accessible to the Department of Chemistry and Biochemistry.

2. Structure and Organization

The NMR Facility is headed by a scientist who is responsible for its activities in research and teaching, administration, personnel management, and the appropriate instrumentation and technical equipment of the facility.

In particular, the Head is supported by an engineer responsible for ensuring the operation of routine analytical services as well as the maintenance of hardware and

software, and by two technical assistants responsible for conducting NMR measurements.

3. Instrumentation

The NMR Facility currently operates six spectrometers with different magnetic field strengths (one 300 MHz spectrometer, two 400 MHz spectrometers, two 500 MHz spectrometers, and one 600 MHz spectrometer; see https://nmr.chemie.uni-koeln.de/en/).

The instrumentation of the NMR spectrometers is designed to be as complementary as possible and to enable high sample throughput in order to provide access to a broad range of NMR methodologies.

Two spectrometers (300 MHz and one 400 MHz instrument) are available as open-access instruments for routine analytical measurements following instruction by the Head and staff members of the NMR Facility.

Four additional instruments (one 400 MHz, two 500 MHz, and one 600 MHz spectrometer) are operated as research instruments by the staff of the NMR Facility for commissioned measurements on behalf of users.

4. Operating Concept

The open-access instruments may be used by registered users at any time, except during periods in which maintenance work (e.g. repairs or refilling of cryogens) must be carried out.

In addition, all users may request measurements with special requirements on the research instruments (e.g. heteronuclear experiments, dynamics measurements, or measurements of samples with low substance quantities). These measurements are performed by the staff of the NMR Facility using an appropriate instrument. By prior arrangement, appointments for commissioned measurements may also be scheduled, for example for titration experiments, time-series measurements, measurements of unstable substances, or similar applications.

After agreeing to comply with the rules for spectrometer usage established by the Head of the NMR Facility, each user receives an individual account in the laboratory information and management system (LIMS) (https://laplace.nmr.uni-koeln.de/) of the

NMR Facility. These rules are specified by the Head of the NMR Facility and are communicated during an individual introduction to the use of the NMR instruments. They concern the handling of NMR samples and spectrometers and are a prerequisite for the smooth operation of the analytical service. Routine measurements and measurement requests can be carried out via the LIMS.

For scientific questions, the Head of the NMR Facility provides advice both on the selection or development of suitable NMR methods and on the interpretation and analysis of NMR spectra. Within the degree programmes offered by the Department of Chemistry and Biochemistry, the Head of the NMR Facility teaches the necessary knowledge for the application of NMR spectroscopy. In addition, the Head provides interested users with an introduction to NMR spectroscopy whenever required. The contact persons of the NMR Facility are listed at https://nmr.chemie.uni-koeln.de/en/.

5. User Fees

The operating costs of the NMR Facility are charged annually to the research groups of the Department of Chemistry and Biochemistry in proportion to their usage of the facility. The guidelines of the German Research Foundation regarding equipment-related usage costs and core facilities serve as a reference for the fee structure (see DFG guidelines on equipment-related usage costs and core facilities (https://www.dfg.de/resource/blob/168406/55-04-en.pdf). The costs for cryogens (liquid nitrogen and liquid helium) are covered by the Department of Chemistry and Biochemistry. All spectrometers of the NMR Facility are connected to the helium reliquefaction system of the Department of Physics at the University of Cologne, allowing the procurement of liquid helium to be realized cost-efficiently through cooperative collaboration with the Department of Physics.

6. Data Management

Users are responsible for backing up the NMR data made available through the LIMS. For data processing and analysis, the Department of Chemistry and Biochemistry provides access to the MestReNova software package Mnova NMR, the licensing and administration of which are organized and managed by the NMR Facility. Alternatively,

the use of the freely accessible NMR data analysis software TopSpin by Bruker, available through an academic license, is recommended.

7. Safety

Operation of the NMR spectrometers is permitted only after prior instruction in the use of the instruments, including a safety briefing provided by the Head of the NMR Facility. NMR laboratories may pose specific hazards associated with the use of high-field magnets, particularly for persons with magnetic field-sensitive implants (e.g. pacemakers), as well as hazards related to the cryogens used (liquid nitrogen and liquid helium).

8. Authorship and Publications

Unless a scientific collaboration extending beyond routine analytical measurements has been agreed upon, sole ownership and authorship of the NMR data remain with the users. The general handling of NMR data, their authorship, the publication of such data in journal articles, book chapters, and monographs, as well as the presentation of research results at scientific conferences (e.g. posters, oral presentations, etc.), is governed by the overarching Regulations of the Analytical Platforms of the Department of Chemistry and Biochemistry at the University of Cologne.

<u>The following principles apply:</u>

1. Personnel in the NMR Facility provide essential services to their users. It is important to recognize their contributions to the scientific advancement of the research projects. References to analytical facilities are a crucial metric of their value and enables them to demonstrate the importance for the Department of Chemistry and Biochemistry and the Faculty of Mathematics and Natural Sciences. This ultimately helps to justify the need for existing and new equipment. For our records, we kindly ask the authors to send us the reference of the papers or thesis.

2. The use of the services provided by the NMR Facility of the Department of Chemistry and Biochemistry entails the obligation to acknowledge this support appropriately in any subsequent publications. The type of appropriate appreciation may differ depending on the

projects and input. At a minimum, the contribution of the NMR Facility must be acknowledged in the *Acknowledgements* section. This requirement applies irrespective of any co-authorship of the Head of the NMR Facility, Daniel Friedrich, or other members of the NMR Facility resulting from scientific contributions. If the NMR Facility members have made a substantial intellectual and/or experimental contribution to a publication, they should be treated as any other co-author.

3. Each principal investigator is always requested to recognize the contributions of the NMR Facility in producing data for publication or theses in the acknowledgement section of the manuscript. A template sentence for use in acknowledgements is given below.
   "*NMR spectroscopy was performed in the NMR Facility of the Department of Chemistry and Biochemistry at University of Cologne which benefits from generous funding by the German Research Foundation (Deutsche Forschungsgemeinschaft, DFG). The contribution of the NMR Facility is kindly acknowledged*."