

NMR Service Quick Start Guide

Before You Start

To use the NMR Service, you must have a valid SDU email account.

User Initials and Sample Naming

Your initials

- Students: Use the username from your SDU email address.
 - Example: abcde12@student.sdu.dk → initials = abcde12
- Staff: Contact Christian to choose initials.

Group initials

- Each research group has assigned group initials.
- Ask a member of your group if you do not know them.

Sample name

- Use only lowercase letters and numbers.
- Keep names short.
- Avoid symbols, spaces, and uppercase letters.

Label Your Sample Correctly

Each sample must be labelled with:

1. Your initials
2. Group initials
3. Sample name

The information on the tube must match the information entered on the requisition form.

Place the label within the marked area shown in Figure 1.



Figure 1

Complete the Requisition

A requisition form must be submitted for every sample.

Submit the form via the NMR SharePoint site:

<https://syddanskuni.sharepoint.com/sites/nmr/SitePages/Home.aspx>

Prepare Your Sample

- Dissolve the sample in a deuterated solvent.
- Fill the NMR tube with approximately 500-600 μ L solution. **Submit Your Sample**

Submission deadlines:

- Morning run: before 09:45 (Monday-Friday)
- Afternoon run: before 14:45 (Monday-Thursday) or 14:15 (Friday)

Samples can be placed:

- In the wooden block, or
- In the beaker inside the NMR closet.

Service Updates

Changes to normal operation are posted on the whiteboard on the closet door.

NMR Service availability may be reduced during holiday periods.

Accessing Data and Software

S-drive

Access via:

Staff

\\adm.c.sdu.dk\NAT\Odense - IFK

Students

\\sdu-data1.c.sdu.dk\shares\IFK

MestreNova

After connecting to the S-drive, install MestreNova version 15 from:

<https://mestrelab.com/download>

Getting Your Sample Back

Samples are normally returned to the beaker marked with your group initials after the next collection cycle. If you need a sample returned sooner, contact Christian or an authorized user.

Requesting Additional NMR Experiments

Before requesting more scans or 2D experiments:

- Review your initial ^1H and/or ^{13}C spectra.
- Request only the experiments necessary for your project.
- Consult a senior group member if you are unsure.

When requesting changes, specify exactly what you need, for example: > "Please acquire 1024 scans for the ^{13}C spectrum."

Retrieving Your Data

Processed data are uploaded to the S-drive. If data are missing or inaccessible, contact Christian

Need Help?

For questions about sample submission, NMR experiments, data access, MestreNova installation, or general use of the NMR Service, please contact:

Christian Brandt

Laborant

Email: christianbj@sdu.dk

Office: Ø11-506-1

Christian can assist with:

- User registration and initials
- Sample submission procedures
- Data access issues
- MestreNova installation
- Additional scans and experiment requests
- General NMR and service-related questions