Training Material for remote access to NMR Facilities

General Guidelines for remote access

Provided by Remote-NMR (R-NMR):

Moving NMR infrastructures to remote access capabilities

CONTENTS

1. Preamble

General guidelines and standard operating procedures are developed in the course of the R-NMR project. This file does not provide the final solution, but is the state of the discussion as of June 2023.

Remote NMR access has always been an option, but it has gained particular significance during the COVID-19 pandemic when travel is greatly restricted. During this period, the ability to access research facilities remotely is especially valuable.

When users access a research infrastructure, their interaction with the scientific and technical staff for support and guidance is often just as important as the actual instrument time. These interactions contribute to the success of the measurements. Consequently, we are currently developing new methods to maintain productive interpersonal communication through remote access procedures.

User support can encompass various aspects, ranging from providing suggestions and advice during the initial planning stages of measurements to assisting with experimental setup. Additionally, we offer training on specific areas of interest to users.

However, the level of assistance and supervision required varies depending on the expertise of the visiting scientist using the requested technology remotely.

2. How to apply?

The application procedure may be different for each NMR facility. So, it is suggested to the user to contact the local or EU facility manager and ask for the protocols applied in the specific facility. In general, the application form for remote access does not differ from application for access in the facilities, which have an on-line application system. In any case, online systems are available for infrastructures being part of EU infrastructure projects such as i-NEXT discovery (https://inext-discovery.eu), PANACEA (https://panacea-nmr.eu/access), or Instruct-ERIC (https://instruct-eric.org/submit-proposal/)

External users may request access through one of routes the available listed on the website of each facility, choosing the one that best fits with their necessities. Otherwise, they should contact the facility manager.

3. How to prepare for the remote measurement time?

Ones you have successfully applied for remote measurement time there are a number of points to keep in mind before starting your remote NMR measurements.

Contact the NMR facility manager to schedule the allocated instrument time, providing the necessary details about the experiment and samples. Prepare the samples according to the established protocols, ensuring proper labeling and adequate quantity for the experiment. Contact the NMR facility manager/operator and organize the shipment of your sample in the appropriate packaging to secure safe delivery of the samples (in vials, falcons, eppendorfs or in NMR tubes).

Familiarize yourself with the safety guidelines specific to NMR instruments, in case that you are going to use part (software) or the entire NMR instrumentation, including handling of cryogens, flammable materials, and potential magnetic field hazards. For remote access you need to be familiar or even experienced in handling remote access software and the appropriate software (i.e. Topspin) to prepare and run the desired NMR experiments. Submit the necessary experimental details and sample information to the facility manager. Provide the information about the appropriate NMR experiment for initial quality assessment of the sample along with any specific requirements for data acquisition or processing. Coordinate with the facility manager to establish remote access to the NMR instrument, ensuring proper software installation and configuration. Access levels should be clarified and indicated by the facility manager ab initio.

Discuss the experimental parameters and requirements with the facility manager, who will assist in optimizing the NMR experiment setup remotely.

Access levels should be clarified and indicated by the facility manager ab initio.

An expert user can follow the setup of the experiments and suggest acquisition parameters to the local responsible through spectrometer screen sharing. A direct "virtual" connection can thus be established, and the spectra outcome can be commented live, with the user actively taking part to the processing of the spectra. The processed spectra and the experiment datasets are then transferred to the user.

A non-expert user can also choose to follow through screen sharing of the experiments and be trained on the set-up procedure by the infrastructure staff. Spectra analysis can be provided as well as training in the different aspects of data processing and analysis.

4. How to ship the sample?

In general, samples should be sent through one of the available couriers using safety packaging to avoid damages of the samples during transportation and safe delivery to the final destination/facility. The tracking number should be provided to the local staff to facilitate sample tracking and identification/delivery. Details on how to store the sample should be also provided to the recipient. The user should take care to cover the cost of the shipment, except if he/she uses the service of one EU Infrastructure projects, such as Instruct-ERIC, PANACEA and iNEXT-Discovery.

Within the R-NMR project we have gathered information on sample shipment which will be on the website shortly.

5. How is your sample handled at an NMR facility?

Standard workflows for solution and solid-state NMR experiments are shown in Figure 1 and Figure 2. Once the samples arrive at the facility, the state of the materials (e.g., sample, tubes, or rotors) will be visually assessed by the facility staff for signs of damage or degradation, and then documented in case something is not acceptable.

The user should provide a clear description of the potential hazards of the material sent and guidelines about the handling of the sample (#1 in the Figures). Unusual requirements should be discussed in the project brief. All samples will be stored in a well labelled secure site specific for remote users (#2 in the Figures).

If the samples are not shipped in the required tubes or rotors, the recipient and the facility staff will take care to transfer the sample from the vial to the tube/rotor (#4 and #5 in the Figures); air-sensitive samples will be handled in an oxygen-free chamber if such an information is provided by the user/sender. The facility staff will operate according to the protocol for operations (air/light sensitivity, temperature of storage, etc.) provided ahead of time by the users.

Meanwhile, the user gets informed about the required software for enabling remote access. On the day of the experiment passwords for the remote session will be set and detailed to the user, also depending on the required access mode.
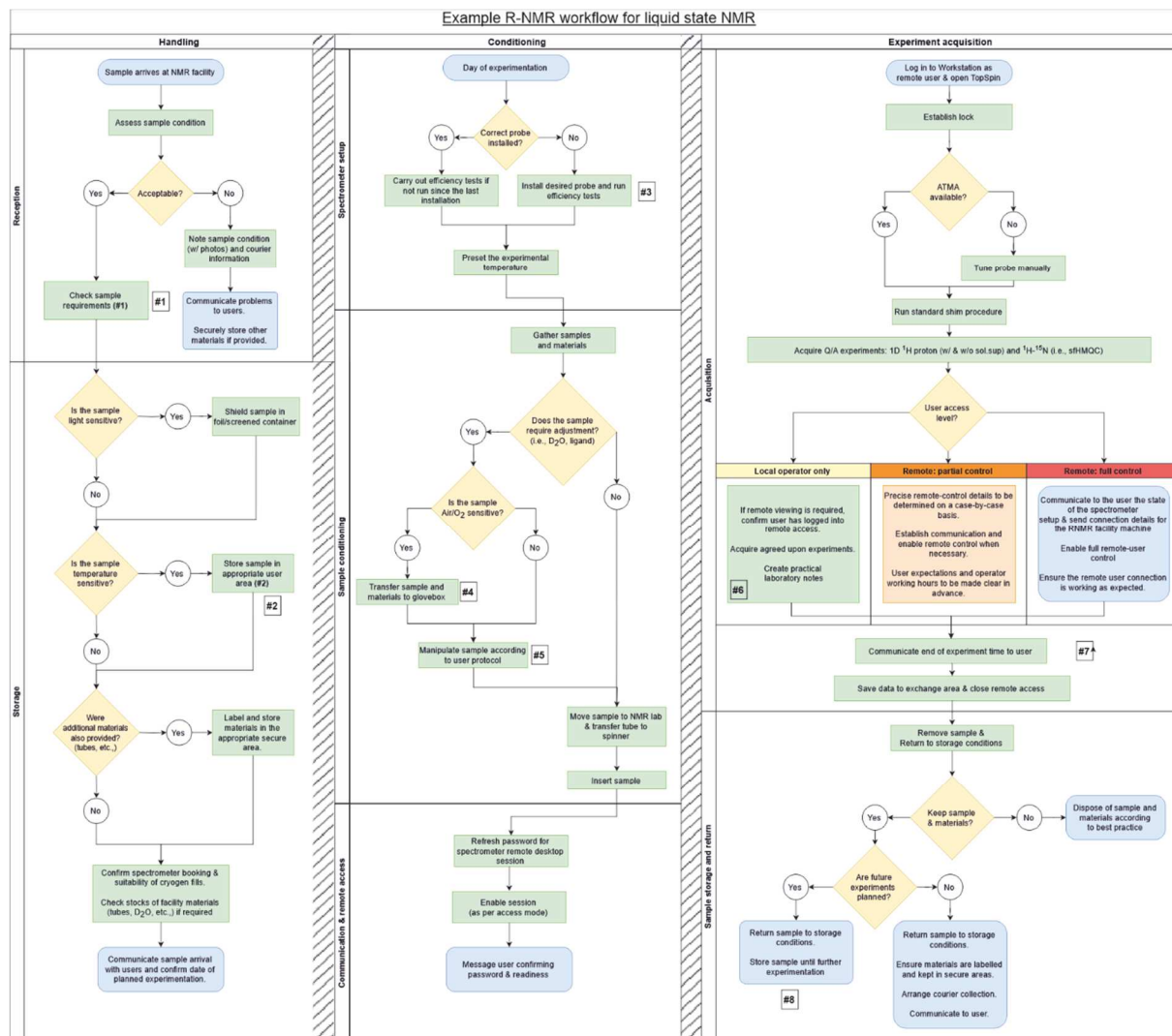
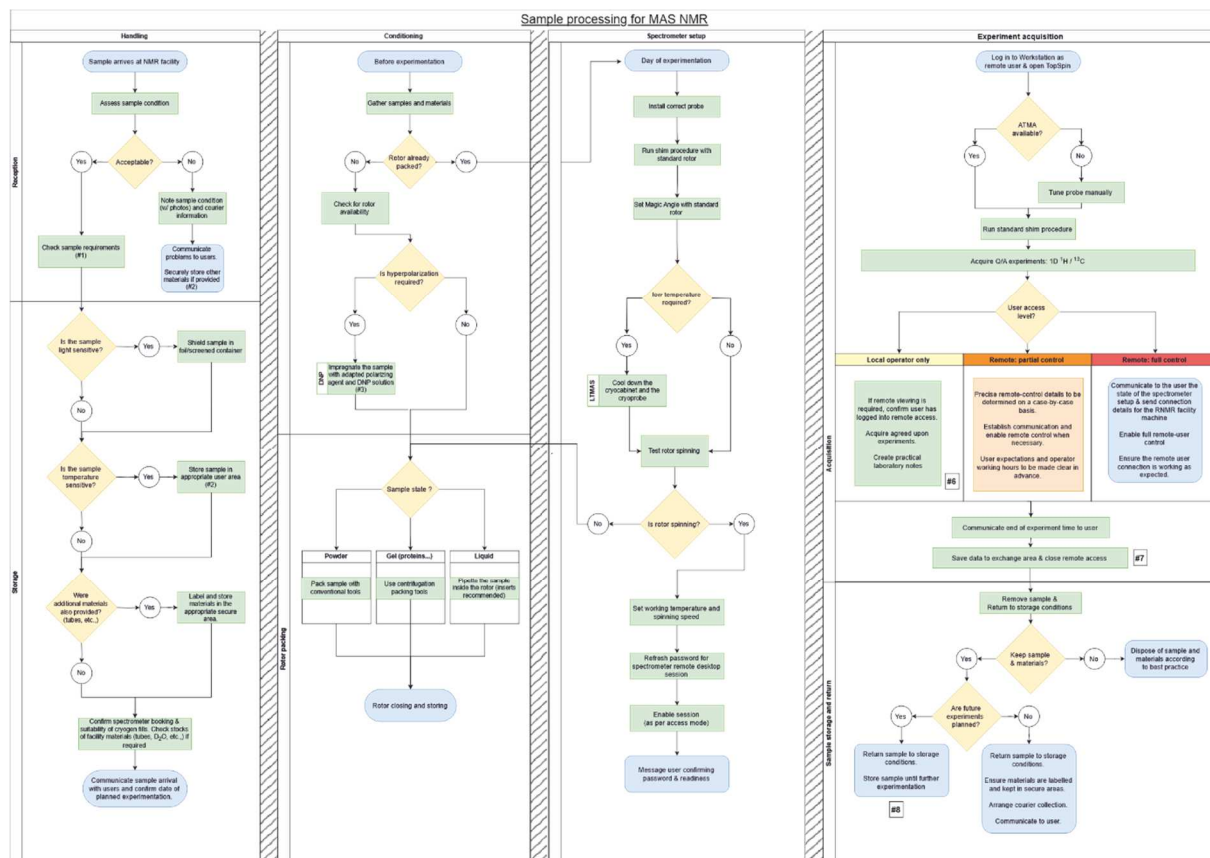Figure 1: Standard procedures for liquid state remote NMR measurements.

Figure 2: Standard procedures for solid-state remote NMR measurements.

The local operator takes care that the proper probe head is in the spectrometer and necessary tests have been applied before the sample of the user is brought into the spectrometer. Once the sample is in the spectrometer, experiments can be run remotely depending on the level of expertise of the user. For very inexperienced users, a local operator will run the experiment and remote viewing of the experiment setup will be enabled by the local operator (#6 in the Figures). Partial control is possible for more experienced users allowing the local operator to assist when needed from case to case. Full remote-user control can be enabled for very experienced users following discussion with the facility staff. In this case, local operators will confirm the established software and protocols for remote access and ensure adherence to the scheduled time slot.

After the end of the experiments, data will be transferred securely and stored in accordance with GDPR (#7). If future experiments are not explicitly planned, samples should be sent back to the user after the end of the measurements (#8).

6. Short checklist for remote NMR

SOP Remote NMR user

1.   Organize the NMR Schedule: Contact the NMR facility manager to schedule the allocated instrument time, providing the necessary details about the experiment and samples.

2.   NMR Sample Preparation: Prepare the samples according to the established protocols, ensuring proper labeling and adequate quantity for the experiment.

3.   NMR Sample shipment: Contact the NMR facility manager/operator and organize the shipment of your sample in the appropriate packaging to secure safe delivery of the samples (in vials, falcons, eppendorfs or in NMR tubes).

4.   Safety Measures: Familiarize yourself with the safety guidelines specific to NMR instruments, in case that you are going to use part (software) or the entire NMR instrumentation, including handling of cryogens, flammable materials, and potential magnetic field hazards. For remote access you need to be familiar or even experienced in handling remote access software and the appropriate software (i.e. Topspin) to prepare and run the desired NMR experiments.

5.   Data Submission: Submit the necessary experimental details and sample information to the facility manager. Provide the information about the appropriate NMR experiment for initial quality assessment of the sample along with any specific requirements for data acquisition or processing.

6.   Remote Access Setup: Coordinate with the facility manager to establish remote access to the NMR instrument, ensuring proper software installation and configuration. Access levels should be clarified and indicated by the facility manager ab initio.

7.   Experimental Setup: Discuss the experimental parameters and hardware requirements with the facility manager, who will assist in optimizing the NMR experiment setup remotely.

8.   Data Acquisition: Ensure that the NMR experiments will be running/performed remotely using the established software and protocols, ensuring adherence to the scheduled time slot.

9.   Data Analysis: Retrieve the acquired data and perform the required analysis using suitable software tools. Seek assistance from the facility manager for any data processing or interpretation queries.

10.   End of measurements/Logoff: After completing the experiment, follow the instructions provided by the facility manager to ensure proper instrument use and wrap up any specifications.

11.   Feedback: Provide feedback to the facility manager regarding the instrument performance, any issues faced, or suggestions for improvement.

SOP Remote facility manager

1.   NMR user Communication: Coordinate with remote NMR users to schedule their instrument usage time and gather necessary details about their experiments and samples.

2.   Sample Submission Guidelines: Provide clear instructions to users regarding sample preparation, labeling, and quantity requirements to ensure compatibility with the NMR instrument and the NMR probe.

3.   Safety Guidelines: Ensure users' level about the safety protocols and precautions specific to NMR instruments, including cryogen handling, flammable material storage, and magnet safety.

4.   Remote Access Setup: Assist users in setting up remote access to the NMR instrument, guiding them through software installation, user authentication, and necessary configurations.

5.   Experiment Optimization: Collaborate with users to optimize their NMR experiments remotely, advising on suitable experimental parameters, pulse sequences, and acquisition protocols.

6.   Monitoring and Troubleshooting: Schedule regular monitoring intervals to supervise remote experiments, ensuring prompt detection of any technical issues or instrument errors. Provide timely assistance and troubleshooting support to users.

7.   Data Retrieval: Provide all the needed information regarding each access level and help users retrieve the acquired data remotely, ensuring its integrity and availability for further analysis.

8.   Data Processing Support: Offer guidance and support to users in processing and analyzing the acquired NMR data using appropriate software tools and techniques.

9.   Instrument Maintenance: Regularly control cryogenic liquids' levels and organize/perform maintenance tasks on the NMR instrument, including cryogen refills, calibration checks, technical services and routine system inspections.

10.   User Feedback and Documentation: Encourage users to provide feedback on their experience and the instrument's performance. Set up and maintain proper documentation of user interactions, instrument maintenance, and troubleshooting logs.