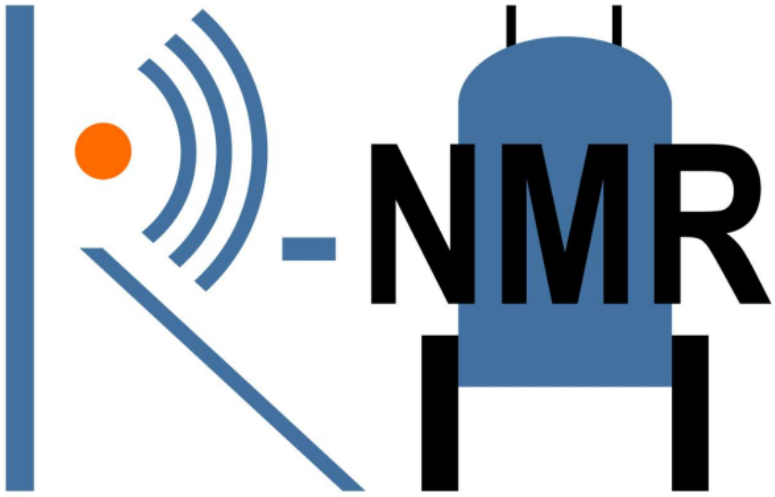

Deliverable 5.4

First report on the organization of dedicated workshops along with the annual consortium meeting of Remote NMR (R-NMR):
Moving NMR infrastructures to remote access capabilities

Authors: Georgios A. Spyroulias (UPAT), Julia Wirmer-Bartoschek (BMRZ), Francesca Morelli (CIRMMP), Antonio Rosato (CIRMMP), Harald Schwalbe (BMRZ)

This project has received funding from the European Union's Horizon Europe research and innovation program under Grant Agreement N. 101058595

TECHNICAL REFERENCES

Project acronym:	R-NMR
Project Title:	Remote NMR: Moving NMR infrastructures to remote access capabilities
Grant Agreement number:	10105859
Project coordinator:	Prof. Dr. Harald Schwalbe
Organization:	J.W. Goethe Universität, Frankfurt
E-mail:	Schwalbe@nmr.uni-frankfurt.de
Project website address:	http://www.r-nmr.eu/
Deliverable No.:	D5.4
Lead Beneficiary:	BMRZ
Type and dissemination level:	Report - Public
Due Date:	M12 (30 June 2023)
Delivery Date:	30 June 2023

CONTENTS

1. Executive summary

The purpose of this report is to describe the organization of a workshop from the R-NMR network and the presentations of different issues and achievements regarding remote access and the corresponding best practices applied in EU NMR Infrastructures.

2. Objectives

The activity reported here directly addresses project objective **O1) Establishing standardized remote access procedures**.

More specifically, the aim is to maximise the impact of the Remote-NMR project and to disseminate the remote access protocols and experience gained by NMR Infrastructures that have applied remote access practices.

3. Summary

"REMOTE-NMR Workshop"

The workshop was organized on 6th of June, 2023, from 10.00am το 12.00pm (CET) and advertised via an email to NMR facility managers that had expressed their interest in the R-NMR project previously, the Twitter account and the webpage of the R-NMR project.

A total of 102 participants attended the workshop.

The link to join the meeting and the program was the following: https://uni-frankfurt.zoom.us/j/64431618961?pwd=RVoyYit1WFpUUlBIcHBROG9FNDhWQT09

Programme (all times are CET)

10-10:15am	Christina Redfield (Oxford): Brief Introduction to the Remote-NMR project and an update on the results of the NMR Facility Manager and NMR User surveys.
10:15-10:30am	W. Trent Franks (Warwick, UK): Remote Access NMR: Experiences from a National Solid-State NMR Facility.

10:30-10:45am	Hugo van Ingen (Utrecht NL): Remote NMR experiences @ Utrecht University.
10:45-11am	Göran Karlsson (Gothenburg SE): GDPR in NMR – what does it mean?
11-11:15am	Jarl Underhaug (Bergen NO): Remote access at University of Bergen.
11:15-11:30am	Jennifer Gomez Badillo & Jop Wolffs (Radboud University NL): Tuning and Matching remotely: applications and demonstration.
11:30-11:45am	Daniel Mathieu (Bruker) - Simplifying NMR experiments for entry level users.
11:45am-12pm.	Final Questions & Discussion

4 A summary of the presentations of the workshop

1) **"R-NMR: Experience so far in assessing the remote NMR landscape in Europe"** by Christina Redfield (University of Oxford)

Christina Redfield summarized the main objectives of the R-NMR project and presented results from two surveys (for facility managers and for NMR users), that were performed to get an overview of the existing NMR landscape in Europe and the needs of the users in terms of remote NMR.

The facility manager survey was launched in November 2022 and got 142 responses from 25 countries. The questions of the survey concerned, amongst others the:

- provider of spectrometers in use
- acquisition software and the operating system
- levels of users' expertise and the levels of access
- implementation of remote access at each facility, the intention to continue to be used after the pandemic, or the intention to be used in the case that it was not implemented at all
- software that is used for the remote access

The user survey took place in January–March 2023 and got 401 responses. The main aspects presented were about:

- the level of the user (bachelor student, PhD student…)
- the type of NMR data that is collected
- the level of NMR expertise of the user
- the experience of remote access, the reasons if there was no experience, and the intention to use or continue to use it after the pandemic

Further, ongoing tasks of WP2 of the project were mentioned involving:

- GDPR-related survey and analysis for the identification of GDPR and security needs
- sample shipment
- and the carbon footprint of NMR

2) "Experiences from a National Solid State NMR Facility" by W. Trent Franks (University of Warwick)

W. Trent Franks presented the *Remote Access Options of the NMR facility at Warwick* University. Three different software packages have been tested: x2go, Tiger VNC Server and TeamViewer

He also presented the Network Configuration, consisting of a firewall with a file server that people from university can access, and a local server. The NMR lab computers are behind this firewall.

He explained that the network configuration when using x2go & TigerVNC goes through the University of Warwick through a local server to the NMR lab computers. Whereas the TeamViewer is connected directly to the NMR lab computers (bypassing the firewall).

He also presented a brief comparison of remote access tools, advantages and disadvantages. Furthermore, he outlined the TeamViewer details regarding remote access and how it is implemented in their daily routine.

The following concept was about the *Mode of operation during lockdown with TeamViewer*. This part of the presentation included statistics from 2021 regarding only Warwick employees that were fully remote.

Finally, the ways in which someone can access their data were demonstrated:

a. Through TeamViewer's file transfer
b. Account request (only data access account)

3) "Remote NMR experiences @ Utrecht University?" by Hugo van Ingen (Utrecht University)

Hugo van Ingen presented, on behalf of the Utrecht NMR Group, the remote access setup implemented by Andrei Gurinov and Johan Ban der Zwan. He introduced the Utrecht University NMR "environment," which includes ten NMR machines ranging from 400 to 1200 MHz (used in the uNMR-NL, INSTRUCT-ERIC, and iNEXT projects) for solid and solution analysis, accompanied nowadays by a remote access setup.

He explained that they started using Teamviewer and then turned to other alternatives due to Teamviewer's free version limitations,despite the many advantages that Teamviewer has (high quality, fluent connection, cross-platform, and connection from anywhere).

They have created two setups and a remote magnet monitoring system.

The first remote access configuration, "Alternative 1: vcn via ssh tunnel" (developed by Johan van der Zwan), was presented as a graphical representation in which the spectrometers are behind the university's firewall and connected to a local server that must be accessible for the users. He mentioned the advantages (amongst others: free and connection from anywhere) and the disadvantages of this alternative, explained the spectrometer, server, and remote user set-ups, and referred to the requirements (i.e., x0vncserver for spectrometer set-up and ssh-VNC client for user set-up). The server set-up of Alternative 1 allows:

- the open connection from server to user
- only ssh connections from the user to the server
- user-specific IP address to control and define every user

The presentation was followed by a live demonstration covering the steps from login to the server and the navigation at Topspin for processing as an example. Moreover, during this demonstration, he referred to useful "macros" that he set up to help the remote users specify meta-data (creating directories with name consistency including all the needed information for each sample) and others that contain analytic explanations and instructions of *what to do* and *how to use* a spectrometer about standard procedures and experiments.

The second configuration, "Alternative 2: vcn via ZeroTierVPN" (developed by Andrei Gurinov), was also presented in a graphical representation in which the spectrometers are behind the university's firewall and connected to a VPN server (zerotier.com), being thus completely independent from the university's control and allowing the direct connection of the users to the spectrometer (via VPN). This is also a free option with good quality that can be used by anyone anywhere without the barrier of a specified port (presented for Alternative 1).

Among the requirements are the x0vncserver, a defined network interface for VPN, and the installation of the ZeroTier application. The disadvantages include, amongst others, the limitation of the number of devices per VPN (free version) and the fact that all the computers within the same VPN can be connected to each other.

He continued his talk with general information about Utrecht University's remote experience about users' positions and levels (PhDs, Post-Docs, etc.), while mentioning the main reasons for the main usage of the remote access by internal and not external users.

The last part of his presentation was dedicated to the development (by Johan van der Zwan and Andrei Gurinov) of the remote magnet monitoring set-up through which they are capable of monitoring all the magnets, including the helium recovery system (Quantum technology), and collecting and storing the data on a webserver.

4) "GDPR in NMR – What does it mean?" by Göran Karlsson (Swedish NMR Center, University of Gothenburg)

Göran Karlsson's presentation aimed at explaining the General Data Protection Regulation (GDPR) and how it is linked to NMR in order to introduce the community to specific terms.

The first part of his talk was dedicated to the clarification of commonly used definitions such as *personal data, anonymization, pseudoanonymization, data processing, data subject, data controller, and data processor*. The basic principles for personal data (Lawfulness, accuracy, safety, storage limitation, etc.) and the special category of *sensitive personal data* (i.e., racial or ethnic origin, health, sex life, orientation, etc.) were explained. The latter is particularly important in metabolomics studies, because these studies involve biomaterials that could provide information about health or drug use. *Sensitive personal data* is governed by the same principles as the general category of *personal data,* but the rules are stricter. For example, he explained how the lawfulness is fulfilled only by two requirements concerning either the case in which the data are processed for *public interest in the field of public health* reasons or for archiving scientific, historical, or statistical research purposes, both based on EU or national law.

Then, he pointed out what GDPR compliance means for NMR-based research using specific examples. He concluded by mentioning the aspects that must be taken into account in the context of the remote NMR project regarding the GDPR that concern raw and meta-data collection, processing, analysis, storage, reporting, and erasure. He referred to the related survey that has to be completed anonymously by the community to assess the goal of WP2-Task 2.3: Review of GDPR aspects.

5) "Remote access in a walk-up environment" by Jarl Underhaug (University of Bergen)

The presentation started with an overview of the spectrometers that include: a 500MHz wide-bore AVANCE III HD, a 600MHz AVANCE NEO and a 850MHz AVANCE III HD. He focused on the 600MHz, where no booking is required, all is walk-up.

Then he proceeded to discuss the classification of data, as:

1. Open

2. Limited
3. Confidential
4. Strictly confidential

For the ‘’**limited**’’ type of data, the data is available for all NMR users, but only upon authentication. Another type of data limitation is that there is restricted access to the NMR room. Furthermore, there is one common user account on the spectrometer computer, which is always logged on, but users have their individual IconNMR accounts. All users have only read access to all NMR data (e.g., they can’t delete).

A modest amount of data is ‘’**confidential**’’, for which and the system requires strict authentication. There are individual user accounts on the spectrometer computer and there is no automatic backup. Finally, the user needs to encrypt data before transfer to storage server.

For the **“strictly confidential**” data (such as the metabolomics data) the storage server is not used nor is remote access to the spectrometer allowed.

Remote access – Restrictions

The IT department restricts access to the network for computers not maintained by the university. The IT department ‘Lab-IT’ provided some solutions:

- Separate network for instrumentation
- This network has limited access to the internet.
- Remote access to the instruments is provided by Lab-IT
- Storage and backup

Currently there are 50 labs in the University of Bergen that use this service and the NMR lab is one of them. He also presented an overview of what the service looks like and the interface of the Lab-IT manager.

If someone is accessing the NMR lab from outside from the university network, then there is a need to set a VPN tunnel to the university network using a two-factor identification. Whereas from the NMR server they provide access through TeamViewer (e.g., giving access to Bruker for the spectrometer)

Remote NMR measurements are performed using a build-in web server in Icon NMR. Jarl Underhaug did a demonstration of how the IconNMR web interface works and summarized the advantages and disadvantages:

- Works well in a walk-up environment.
- Familiar user interface.
- Multiple simultaneous users.
- Local users minimally affected.
- Slightly slow response time.
- Slows down over time.
- Advanced IconNMR is not possible.

Finally, he mentioned that University has also started *Splashtop* as an alternative to remote control which is similar to TeamViewer and more affordable and it seems to work very well.

6) "Tuning and matching remotely: applications and demonstration" by Jop Wolffs & Jennifer Gomez Badillo (Radboud University)

Jennifer Gomez Badillo gave an introduction to how Solid-state NMR measurements with remote tuning and matching are performed at the NMR Center of Radboud University, Nijmegen. She briefly introduced the NMR instruments and facilities and the employees (academic & technical staff, PhD's, post docs and masters students) of the NMR Center at Radboud University, in Nijmegen (The Netherlands):

- Solid & liquid state NMR
- 300-950MHz spectrometers
- DNP system - 600MHz

She mentioned that remote access is mainly achieved through AnyDesk, with good results. In addition, remote tuning and matching of solid-state NMR measurements can be achieved by using an external Automatic Tuning and Matching robot (ATM robot), which also extends the measurement time to non-business hours or weekends. This is particularly useful for performing wide line experiments in solid-state NMR (e.g. quadrupolar nuclei) and NQR (Nuclear Quadrupolar Resonance). The combination of Anydesk and the ATM robot allowed the recording of wideline ^{127}I NQR experiments on perovskites, with potential application to other nuclei and systems.

Jop Wolffs presented the ATM robot in more detail. He explained how the ATM robot (in this case a product of NMR Service) connects to a probe, and showed how it was compatible with both Varian and Bruker NMR probes. A diagram of the complete setup, showed that:

- The robot connects to the console.
- The console is controlled by regular PC.
- The PC is internet accessible.

After this, Jop discussed the two modes of operation:

a. The ''manual'' mode (simple and robust).
b. The ''automatic'' mode (more complex and less reliable).

For both modes there is a need for an edited pulse sequence, it also requires experiment-specific settings of the ATM software. The remote user must have some level of expertise of the ATM to spot potential problems before they damage anything, particularly in the automatic mode, which is currently "a bit glitchy".

He then gave a real-time *demonstration* on automatic matching and tuning with the ATM robot through AnyDesk and performed ^{127}I NQR measurements of a perovskite. To make use of the robot, it is convenient to setup the experiment *via* a python code that interfaces between the ATM and the acquisition, signalling to start tuning and matching every time it is necessary. He also presented some *Additional Applications* where ATM is useful:

- Wideline NMR
- Nuclear Quadrupolar Resonance (NQR)
- Large Quadrupole NMR (e.g. quadrupolar nuclei)

- Paramagnetic NMR
- Alternating between isotopes (e.g., ^{6}Li and ^{7}Li, if probe allows)
- Long experiments with unstable T/M in solid state NMR
- In-situ experiments

In summary, ATM robots increase the number of possible remote experiments by enabling remote or even fully automatic tuning and matching in solid-state NMR. The two (current) modes of operation are:

- Manual mode: reliable, minimal local support, but labour intensive.
- Automatic mode: not perfect, more local support, but real time-saver.

Since these robots are a flexible extension to existing equipment (Bruker and Varian probes), it is also relatively easy to start using them.

7) "Simplifying NMR experiments for entry level users" by Daniel Mathieu (Bruker BioSpin)

Daniel Matthieu, presented the use and the advantages for the remote access/users of the BIOTOP module of TopSpin software. This module is implemented in Topspin3.6 and later versions and provides possibilities for optimization and customization of NMR experiments for users (onsite or remote users).

Among the optimization options the following are included:

- Proton parameters and effective water suppression (pulsecal, paropt,…etc.)
- Carbon and Nitrogen pulses optimization (1D SOFAST HMQC sequences etc.)
- Carbon and Nitrogen offsets and spectral widths for 2D HN correlation, 2D HNCO / HNCA projections, for various HSQC versions, such as TROSY, BEST or BEST-TROSY based on molecules with different size and labelling patterns, etc.

Daniel Matthieu, also did a demonstration of the graphical interface of BIOTOP and the way to use its features for parameter handling and editing to set up, organize, optimize and customize the experiments according to the needs of different users. He also presented the capabilities of the TopSpin BIOTOP in processing and referencing to import and use external sources to (a) import assignments from the BMRB, either by ID or using a fasta search, (b) structures from the PDB, and to facilitate, for example, a protein dynamics center analysis.