

# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

Professor Christina Redfield  
University of Oxford  
UKMRM Meeting - Birmingham  
24 June 2024



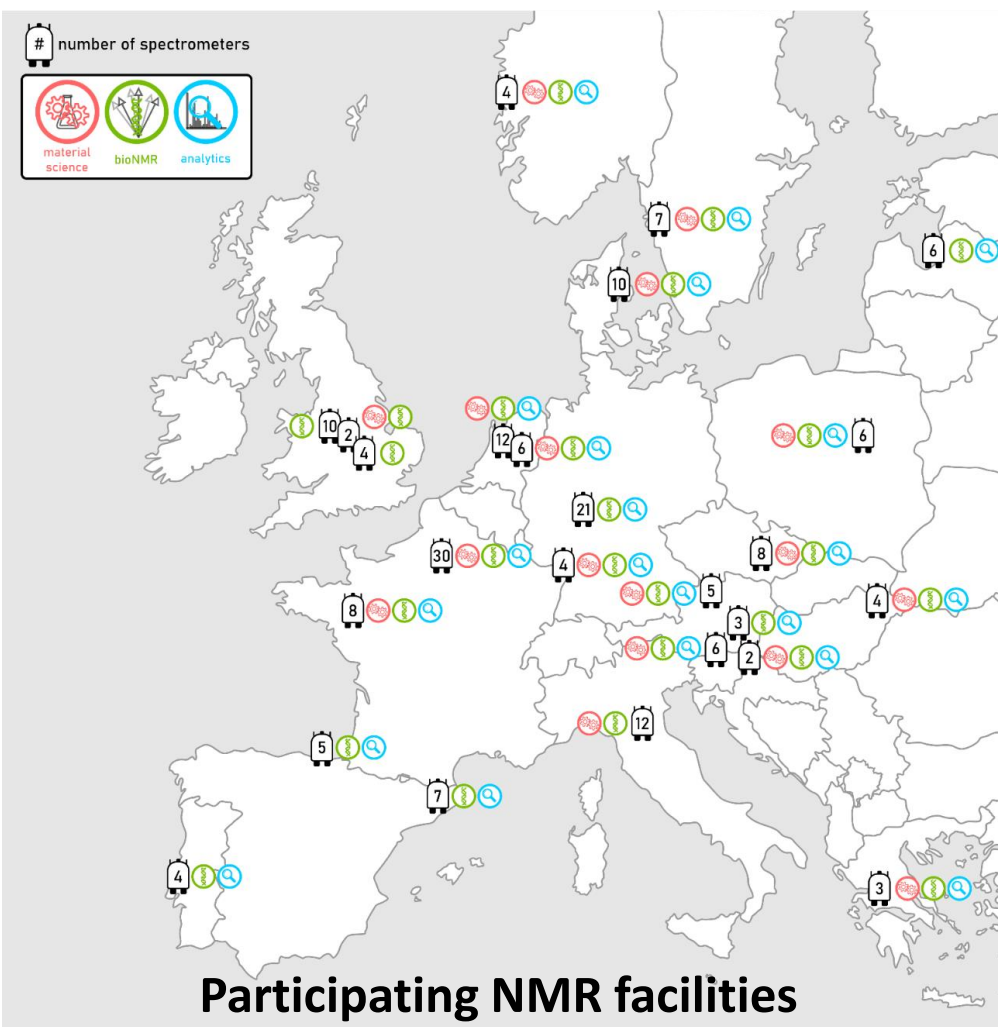


# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

Before the Covid19 pandemic, most NMR users sat in front of the NMR spectrometer for data collection.

Lockdowns and other restrictions during the pandemic made in-person NMR data collection difficult or impossible.

Very quickly many NMR facilities realised they needed to make remote access to NMR possible, particularly for Covid19 research.





# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

**Overall Goal: Introduce remote measurement at all major NMR sites throughout Europe**

**Work in R-NMR is divided into 5 Work Packages**

WP1 Project Management (BMRZ - Germany)

WP2 Remote NMR Landscape (UOXF - UK)

WP3 Defining a common procedure for remote access and measurement (CNRS - France)

WP4 Remote control of instrumentation (DEBNMR - Hungary)

WP5 Dissemination, outreach and training (UPAT - Greece)

**Project Started in July 2022 and will continue until June 2025.**



This project has received funding from the European Union's Horizon Europe research and innovation programme under Grant Agreement N. 101058595 – UK partners funded by Innovate UK



# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

## WP2 Remote NMR Landscape (UOXF - UK)

**O2.1** – Providing a detailed picture of the operation of NMR facilities in Europe during the pandemic

**Task 2.1** – Review of current protocols in place for remote access to NMR facilities, including statistics on current implementation – (M2.1)

**O2.2** – Understanding the user perception of remote access and stratification of users

**Task 2.2** – Users' needs and stratification of users – (M2.2)

**O2.3** – Mapping data protection and security need

**Task 2.3** Review of GDPR (General Data Protection Requirement) aspects – (D2.1)

**O2.4** – Identifying issues and solutions regarding sample shipments

**Task 2.4** – Transnational sample shipment – (D2.1)

**O2.5** – Monitoring the carbon footprint

**Task 2.5** – Monitoring the carbon footprint of users' travel and equipment usage.

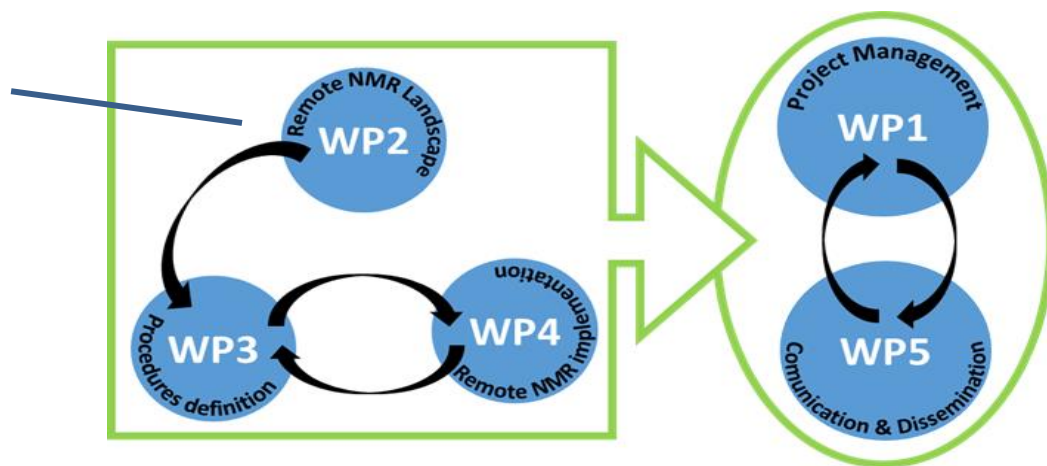
**D2.2** Remote NMR Landscape including Table of Criticalities





# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

1. Review current protocols in place for remote access
2. Identify users' needs and stratify them
3. Analyze GDPR aspects – Task 2.3 (UGOT)
4. Sample shipment – Task 2.4 (CIRMMP)
5. Carbon footprint – Task 2.5 (SloNMR)



## Milestones:

**M2.1 – Report on survey on operation of NMR facilities during pandemics (M5)**

**M2.2 – Report on survey of users' experience and expectations (M7)**

## Deliverables:

**D2.1 – Identification of GDPR, security needs and shipment bottlenecks (M12) – Tasks 2.3 & 2.4**

**D2.2 – Remote-NMR landscape including a table of criticalities (M18) – Summary of outputs from all Tasks**

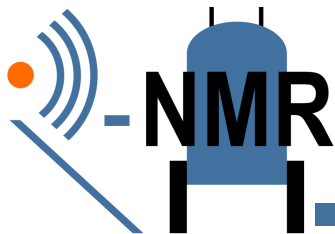




# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

- The information required to complete Tasks 2.1-2.4 was collected via online surveys of the NMR community.
- The survey of Facility Managers collected information about numbers and types of spectrometers, operating software, software used for implementation of remote access, sample handling, data security, interaction with users, and bottlenecks identified.
- The survey of NMR Users collected information about their experiences of remote access with a particular focus on how samples were shipped to the NMR facility and if users had concerns about sample shipping.
- The third survey collected information about Facility Managers' understanding and implementation of the General Data Protection Requirement (GDPR).
- The reports resulting from these surveys are available in the 'Outcome' section of the R-NMR website ( ).





# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

Jisc Online surveys

## Remote-NMR: NMR Facility Manager Survey

Showing 142 of 142 responses

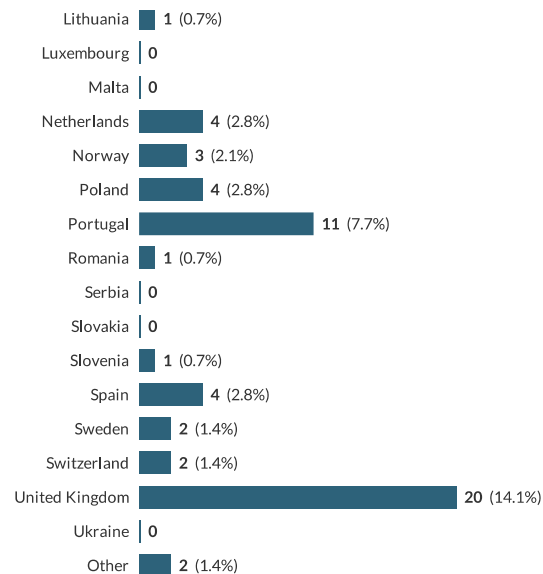
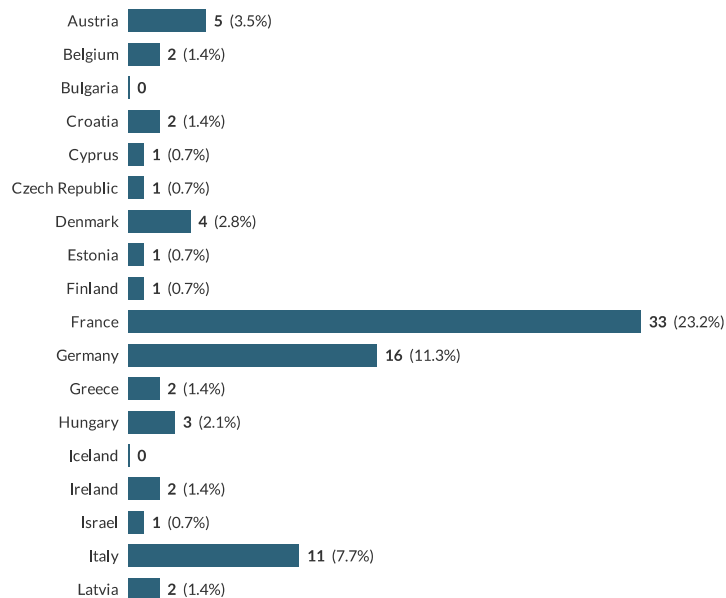
Showing **all** responses

Hiding **43** questions

Response rate: 71%

The facility manager survey was completed by 142 facility managers from ~25 countries.

3 In which country is your NMR facility located? Select one:



This project has received funding from the European Union's Horizon Europe research and innovation programme under Grant Agreement N. 101058595 – UK partners funded by Innovate UK



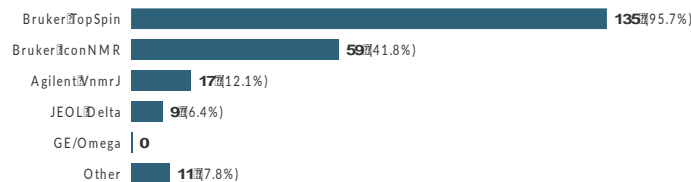
# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

7 What type of spectrometers do you have in your facility? (select all that apply)



Multi answer: Percentage of respondents who selected each answer option (e.g. 100% would represent that all this question's respondents chose that option)

8 What data acquisition software do your spectrometers run? (select all that apply)



Multi answer: Percentage of respondents who selected each answer option (e.g. 100% would represent that all this question's respondents chose that option)

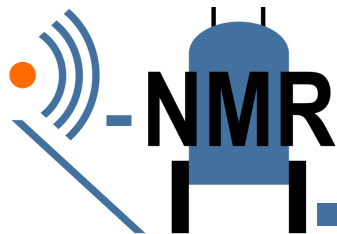
9 What operating systems do your spectrometer computers run? (select all that apply)



Multi answer: Percentage of respondents who selected each answer option (e.g. 100% would represent that all this question's respondents chose that option)

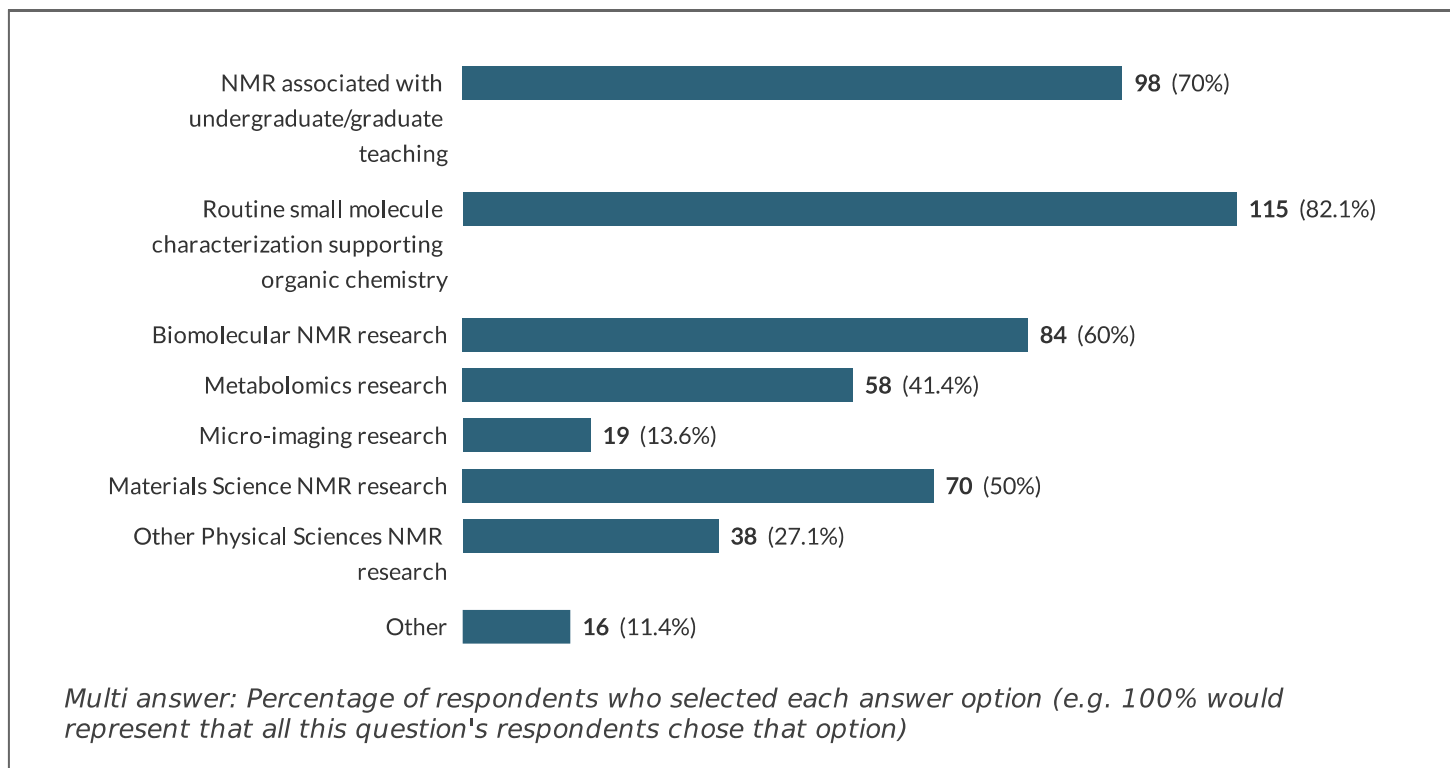






# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

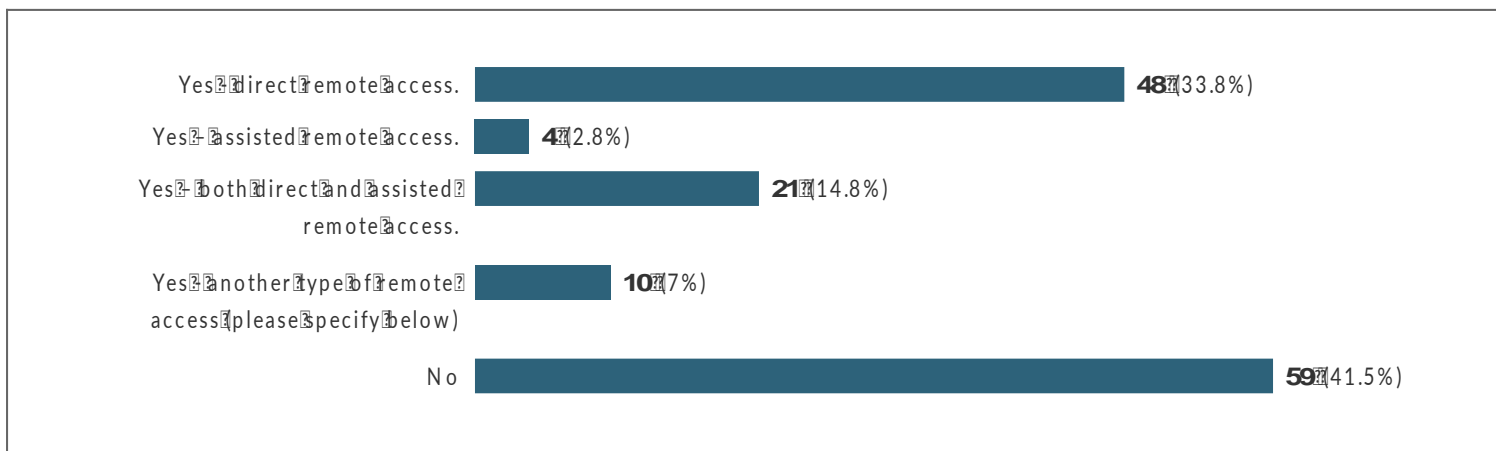
12 What types of NMR experiments do your users carry out? (select all that apply)

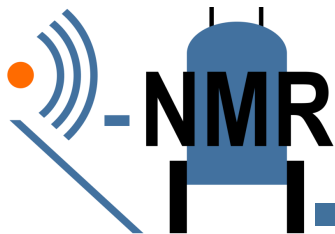




# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

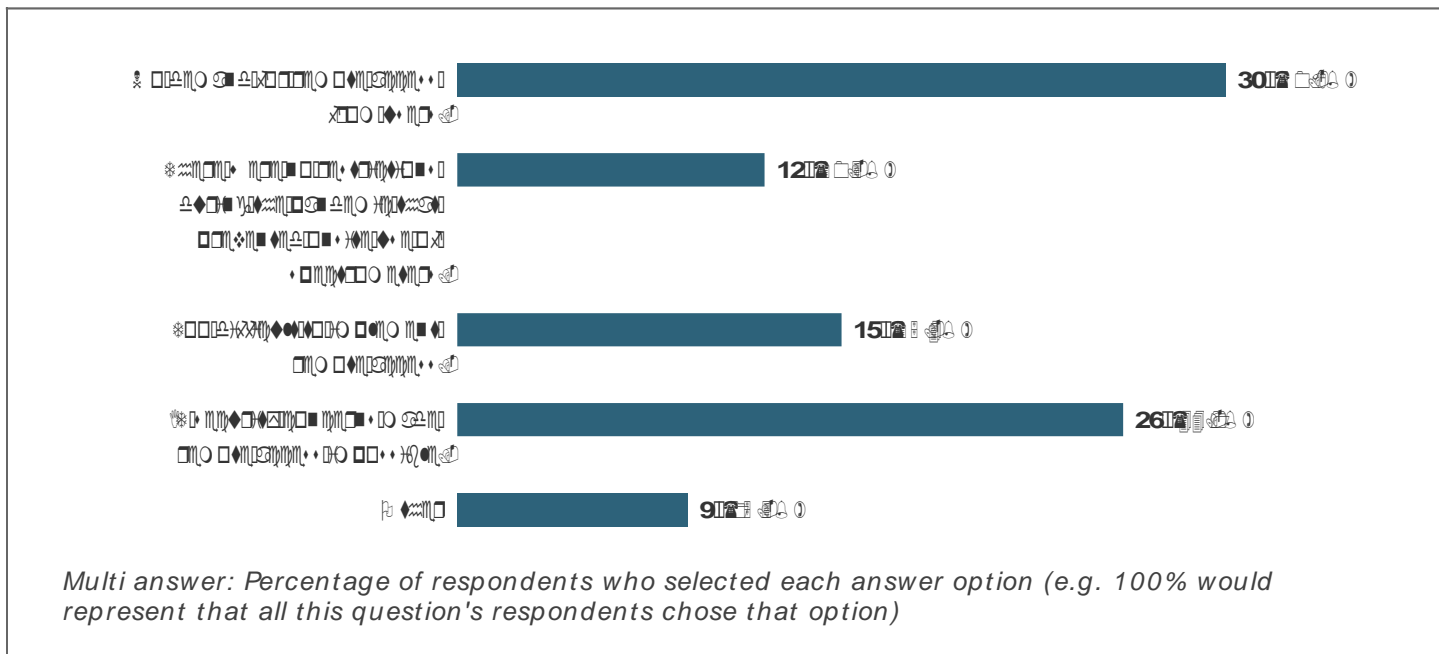
23 Prior to, during and since the Covid19 pandemic, did you provide remote access to one or more of the NMR spectrometers in your facility? By remote access, we mean that either: 1) users could directly operate the NMR spectrometer by remote login to the NMR spectrometer computer (direct remote access), or 2) users could communicate via a computer linkup (Zoom/Teams etc) or telephone with a local operator who controlled the NMR spectrometer based on the information provided by the remote user (assisted remote access), or 3) some other type of remote access.





# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

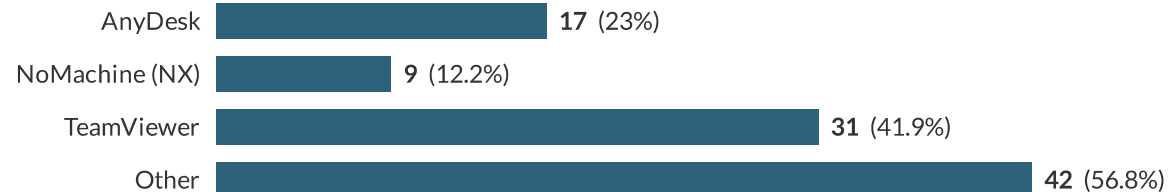
23.b Why has remote access to spectrometers not been implemented in your facility? (select any that apply)





# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

32 What software was used for remote access? (select all that apply)



*Multi answer: Percentage of respondents who selected each answer option (e.g. 100% would represent that all this question's respondents chose that option)*

Other software packages used for remote access include: DWService, VNC, FastViewer, Splashtop, and Guacamole. These other software packages are being investigated in order to assess their usefulness for remote access. (More information on a range of software options in Appendix 1 of D2.2 - "Remote NMR Landscape Including Table of Criticalities")



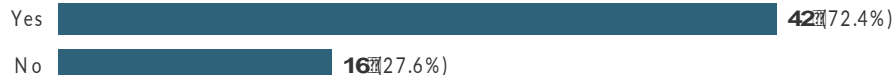


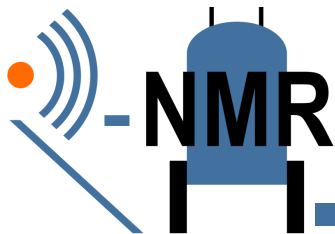
# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

42 Is your facility continuing to provide remote access to NMR spectrometers now that some/many/all 'pandemic' restrictions have been lifted?



23.c The aim of the Remote-NMR project is to develop a common framework for remote spectrometer access taking into account best practice across the EU/UK. Standardized training for remote access will also be put in place. Once this has been completed, would your NMR facility be interested in implementing remote spectrometer access?





# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

Jisc Online surveys

## Remote-NMR: User Survey

Showing 401 of 401 responses

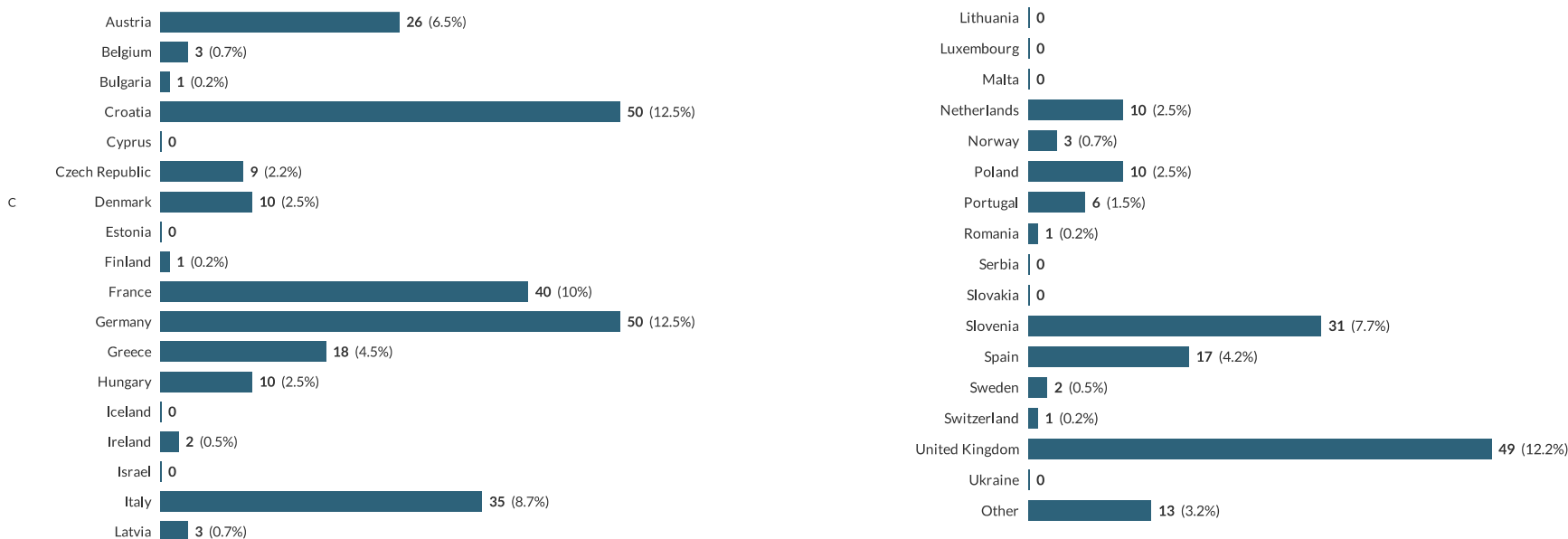
Showing **all** responses

Hiding **20** questions

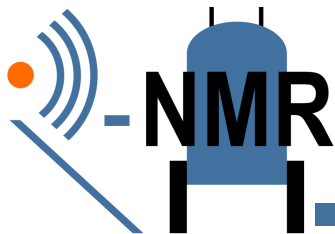
Response rate: 20%

The user survey was completed by 401 NMR users.

4 In which country do you carry out your NMR research? This is most likely to be the country in which you live. If you also use an NMR facility in another country you will be able to indicate that later in the survey. Select one:

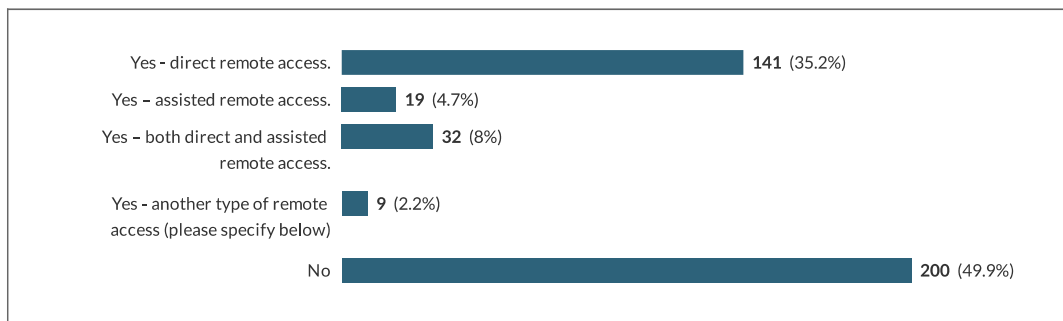


This project has received funding from the European Union's Horizon Europe research and innovation programme under Grant Agreement N. 101058595 – UK partners funded by Innovate UK

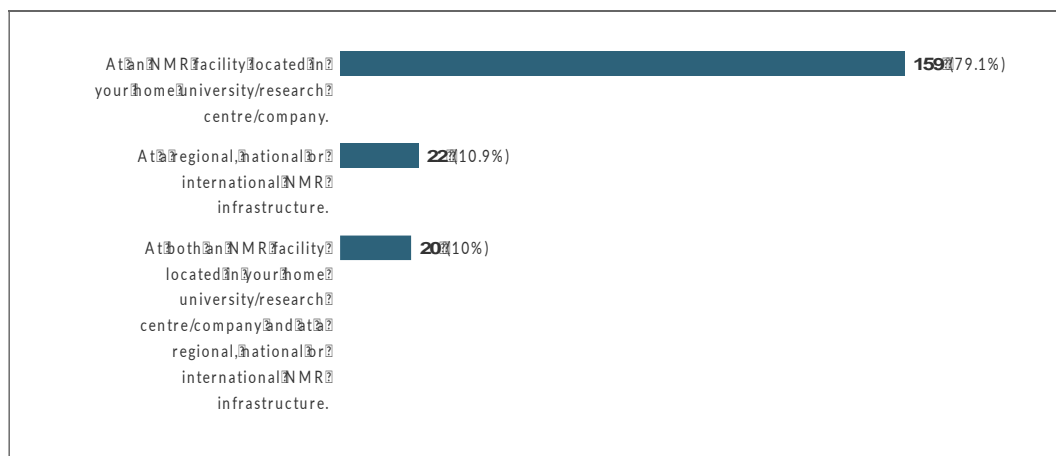


# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

11 Prior to, during and since the Covid19 pandemic, have you collected NMR data via remote access? By remote access, we mean that either 1) you directly operated the NMR spectrometer by remote login to the NMR spectrometer computer (direct remote access), or 2) you communicated via a computer linkup (Zoom/Teams etc) or telephone with a local operator who controlled the NMR spectrometer based on the information you provided (assisted remote access), or 3) some other type of remote access.



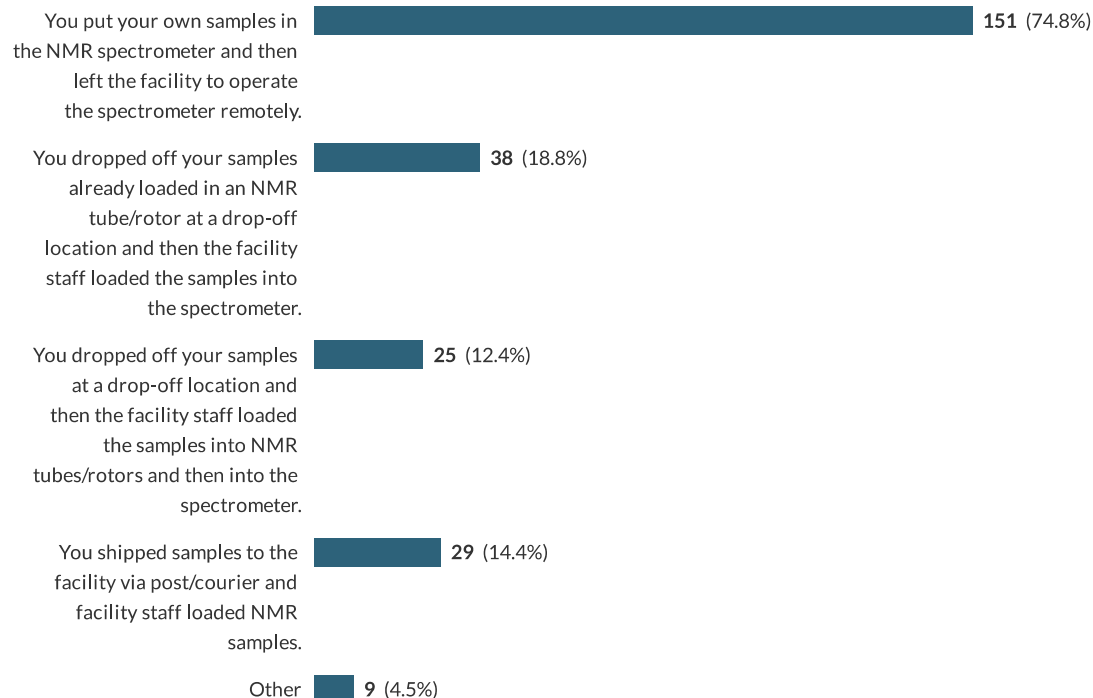
11.b Where has remote access been provided? (select one)





# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

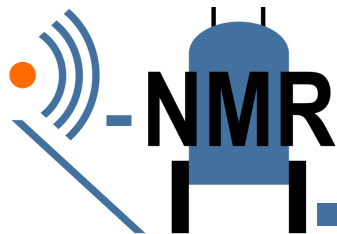
16 How were your NMR samples delivered to the NMR facility and loaded into the NMR spectrometers? (select all that apply)



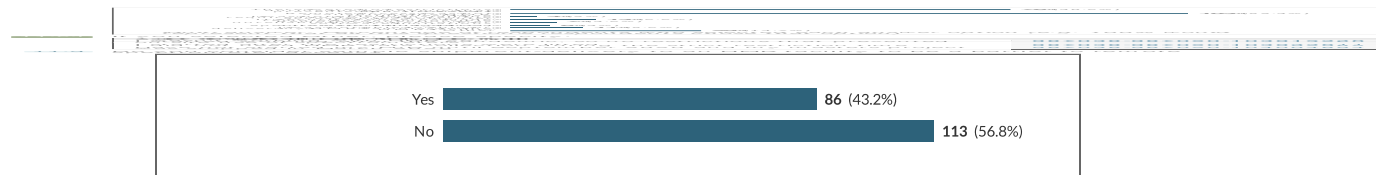
*Multi answer: Percentage of respondents who selected each answer option (e.g. 100% would represent that all this question's respondents chose that option)*



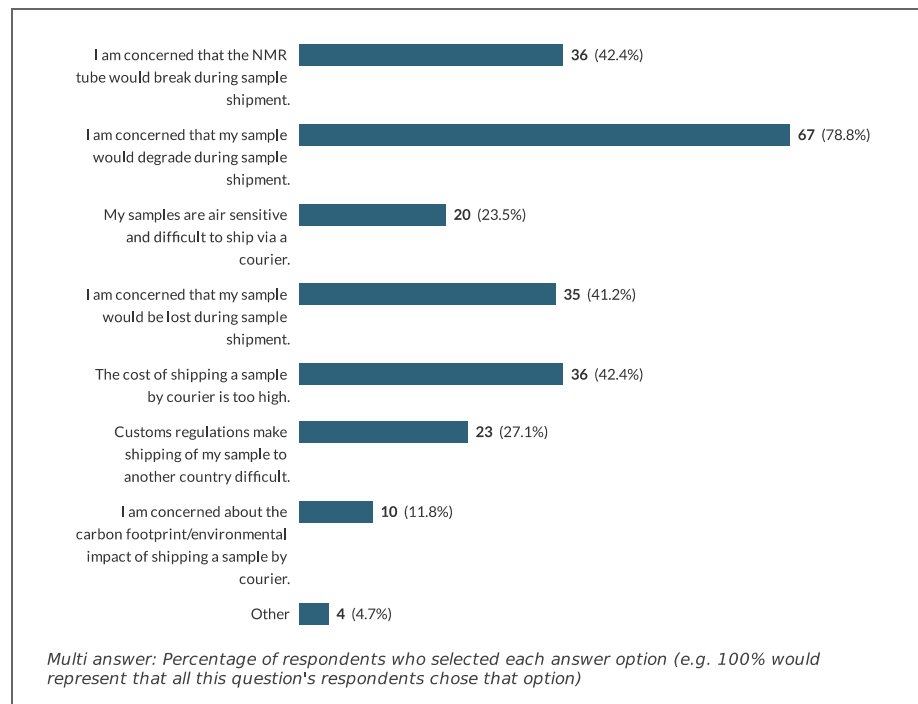




# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities



11.d.i If yes, what are your main concerns about sample shipment? (select all that apply)





# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

- **Task 2.3 – A ‘Fact Sheet and Guidelines on GDPR as it relates to NMR Facilities’** is available on the R-NMR website Outcome page.
- **Task 2.4 – Transnational sample shipment** – A standard operating procedure (SOP) for sample shipment, with guidelines for shipment of samples for both solution-state and solid-state NMR and a flowchart for determining the best procedures is included in WP3 Deliverable 3.1.
- **Task 2.5 – Monitoring the carbon footprint** – A report investigating the ‘carbon footprint’ of various aspects of NMR spectroscopy is included as Appendix 4 in D2.2 and also as a standalone document (both available on the R-NMR website). The report includes links to websites for estimating the carbon footprint associated with travel and parcel shipment. A carbon footprint calculator has been developed and will be rolled out to the NMR community before the end of the R-NMR project.

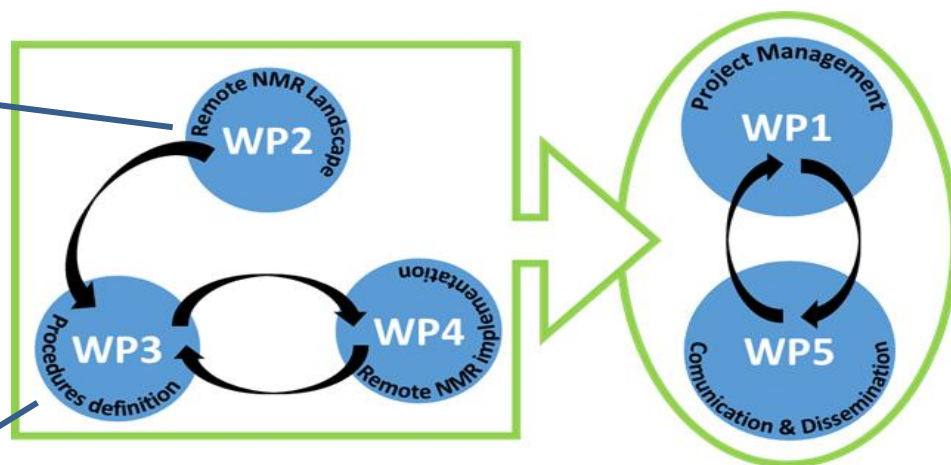


# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

1. Review current protocols in place for remote access
2. Identify users' needs and stratify them
3. Analyze GDPR aspects
4. Sample shipment
5. Carbon footprint



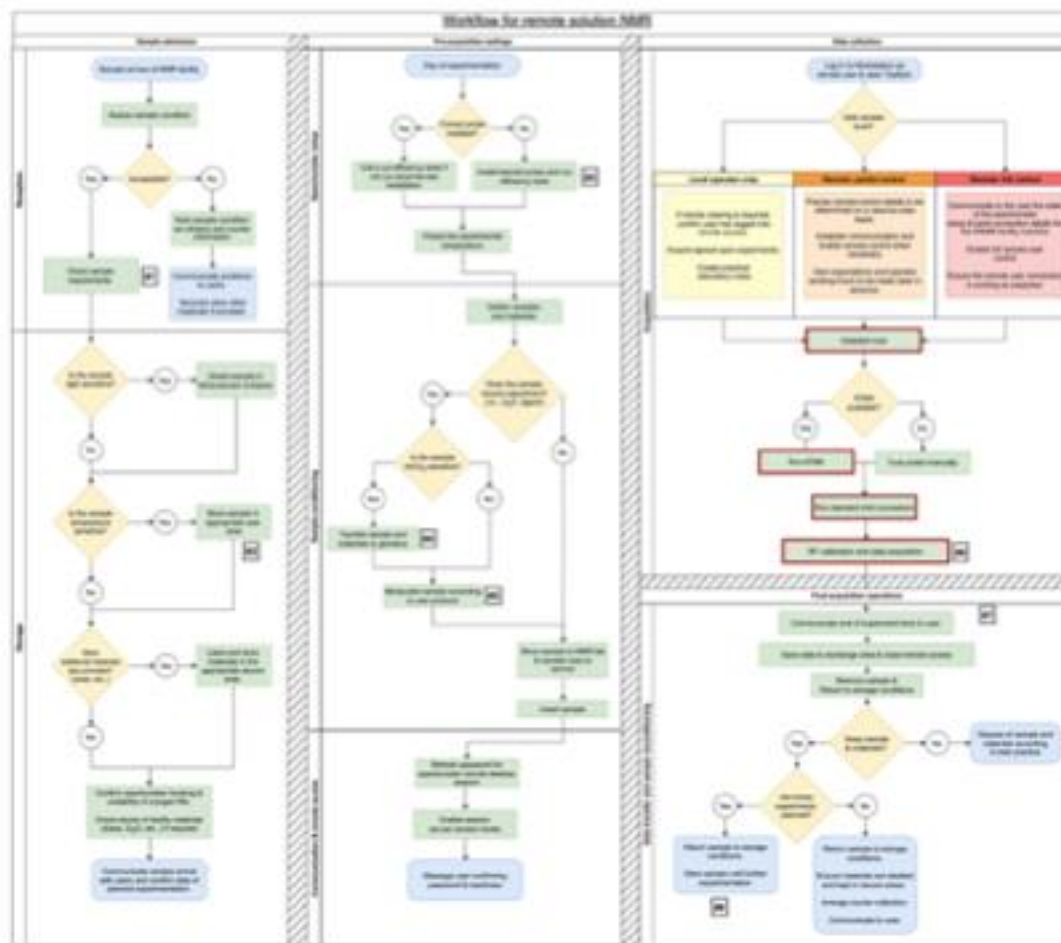
1. Define a general workflow
2. Define a strategy for evaluating the users' expertise and the corresponding support needs
3. Identify technical solutions for remote operation of spectrometers



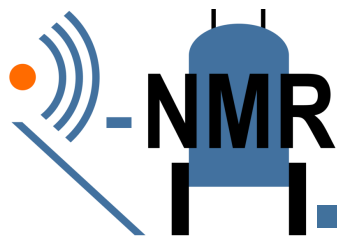


# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

## WP3 – Workflow for remote solution-state NMR

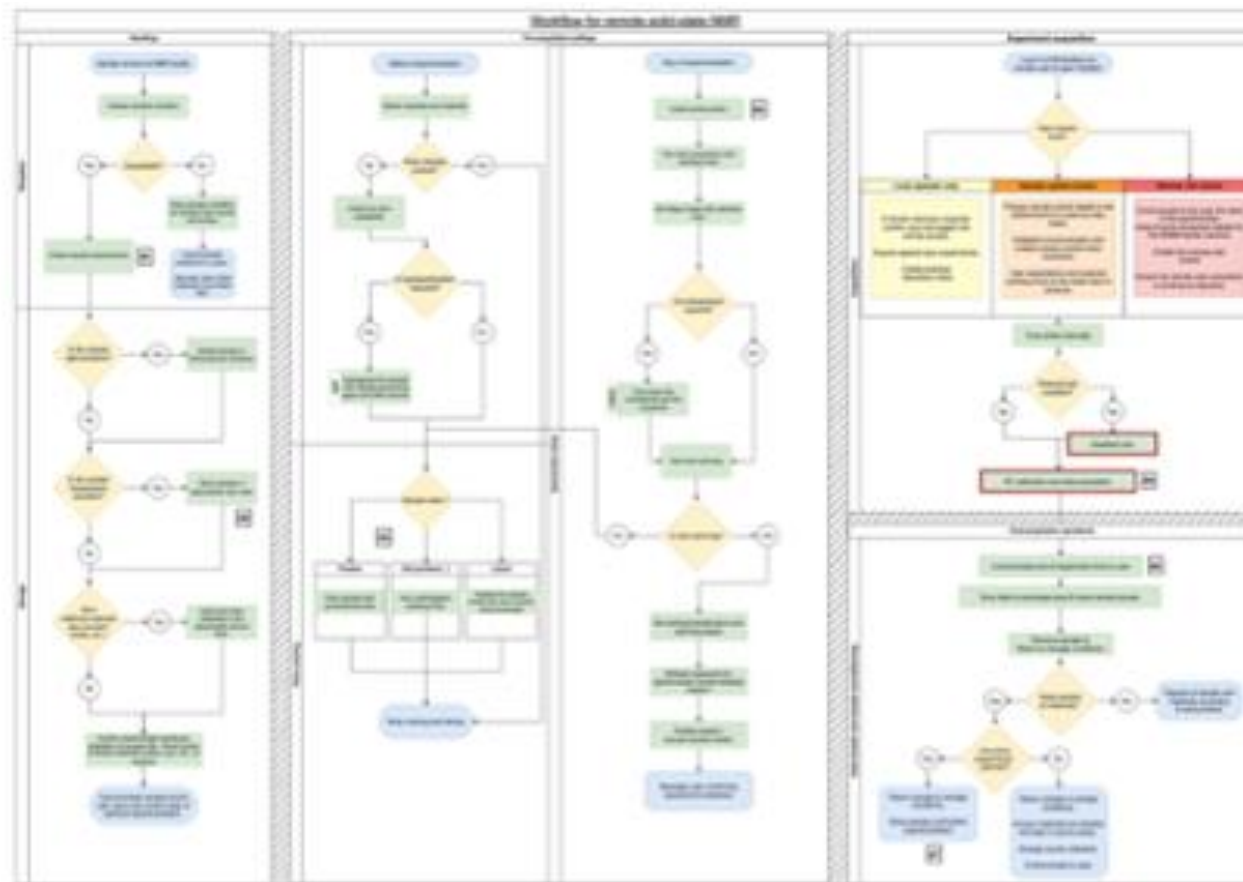


This project has received funding from the European Union's Horizon Europe research and innovation programme under Grant Agreement N. 101058595 – UK partners funded by Innovate UK



# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

## WP3 – Workflow for remote solid-state NMR



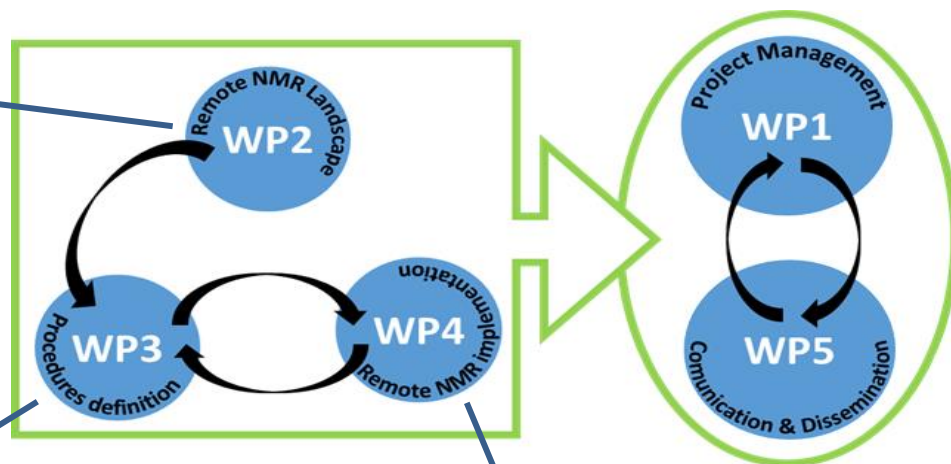


# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

1. Review current protocols in place for remote access
2. Identify users' needs and stratify them
3. Analyze GDPR aspects
4. Sample shipment
5. Carbon footprint



1. Define a general workflow
2. Define a strategy for evaluating the users' expertise and the corresponding support needs
3. Identify technical solutions for remote operation of spectrometers



1. Implement standardized experiments
2. Implement data & metadata standards
3. Implement data access interface
4. Implement mechanisms to modulate users' freedom depending on expertise
5. Utilize existing facilities

**WP 4 is currently in progress**



The logo for R-NMR features a blue stylized Android robot head with a white antenna emitting three blue curved lines representing a signal. To the right of the robot, the text 'R-NMR' is displayed in a bold, black, sans-serif font. A thick blue horizontal bar extends from the right side of the logo across the top of the slide.

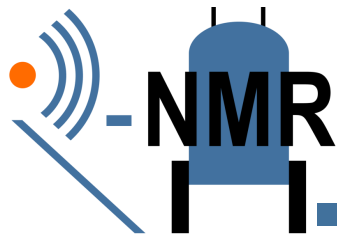
# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

R-NMR website : <https://r-nmr.eu>



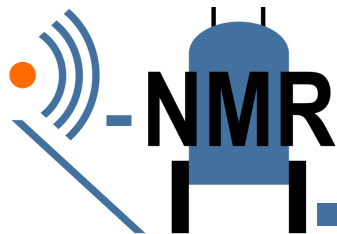
This project has received funding from the European Union's Horizon Europe research and innovation programme under Grant Agreement N. 101058595 – UK partners funded by Innovate UK

# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities



This project has received funding from the European Union's Horizon Europe research and innovation programme under Grant Agreement N. 101058595 – UK partners funded by Innovate UK





# Remote NMR (R-NMR): Moving NMR Infrastructures to Remote Access Capabilities

If you'd like to learn more about the R-NMR project or to follow our progress then visit [and/or follow the project on Twitter @RemoteNMR\\_eu](#)

If you'd like UK-specific responses to the Facility Manager and NMR user survey then send me an email ([christina.redfield@bioch.ox.ac.uk](mailto:christina.redfield@bioch.ox.ac.uk))

Thank you for your attention!

