

Milestone 2.2

**REPORT ON SURVEY OF USERS OF NMR
FACILITIES DURING THE PANDEMIC
of Remote NMR (R-NMR):
Moving NMR infrastructures to remote access capabilities**





TECHNICAL REFERENCES

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1. Executive Summary

An online survey of ‘hands-on’ users of NMR facilities was carried out in order to collect information about NMR users’ experiences with remote NMR access during the pandemic. Responses were collected from ~400 NMR users from more than 30 countries; 50% of the respondents had collected NMR data using remote access. Their detailed responses to a range of questions provide important insights into the user experience and will be a valuable resource in the development of remote access protocols within Work Packages 3 and 4. Encouragingly, 82% of the respondents using remote access have continued to do so post-pandemic and 71.5% of the respondents not using remote access during the pandemic indicated that they would be interested in using this once R-NMR has developed a standardized protocol. This confirms that there will be significant interest in the outcomes of the R-NMR project.

2. Background

This work has been carried out in the context of Task 2.2, ‘Users’ needs and stratification of users’.

With the goal of understanding remote access from the perspective of the remote users, a second survey targeting NMR facility users was designed focusing on the user experience aspects, such as facilities used during the pandemic, level of assistance provided by facilities/would additional assistance have been useful; is confidentiality of samples/experiments important; how were samples sent; likelihood of using remote access even when there are no travel restrictions; suggestions for improvement.

Contact was made with NMR users who remotely access facilities already but also those who have not yet used remote access. The survey (M2.2) aims to provide a picture of the requirements of external users and also factors that might encourage them to use remote rather than in-person access. Online discussion of their survey results with some users will provide greater insights into the user experience in a next step.

3. Survey Implementation

The survey was designed in consultation with other WP2 partners. The survey was approved by the Oxford Central University Research Ethics Committee (CUREC Reference R77838/RE002) and implemented in the Jisc online survey software. A copy of the survey, including the Participant Information Sheet, is available in Appendix 1. Potential participants in the survey were contacted in two ways. For some countries, R-NMR partners sent an email requesting participation in the survey to NMR users using national email lists (UK, Germany, France, Italy). For the remaining countries, facility manager who had been contacted about the first survey were asked, via email, to circulate information about the User Survey to users of their NMR facilities. The survey opened on January 8th and was originally designed to run until the end of January. However, the survey was only completed by 269 NMR users by the end of January. This was a lower number than expected so the survey was extended until March 29th and R-NMR partners and other NMR facility managers were contacted and asked to encourage their NMR users to take part in the survey. As a result, there was been further participation in the user survey and by the end of March the survey had been completed by 401 participants. This final report is based on these 401 survey responses.

4. Summary of NMR Users – Equipment/Software/Applications/User base

The survey was completed by 401 NMR users; the complete survey results are included in Appendix 2. They represent NMR users in 24 European countries and 8 other countries (Question 4). The highest number of participants are based in Croatia and Germany (50 responses each). More than twenty responses were obtained from the United Kingdom (49), France (40), Italy (35), Slovenia (31) and Austria (26). 32.5% of the respondents are research group leaders, 25.3% are graduate students, 15% are postdoctoral researchers, 12.5% are staff scientists, 11.5% are ‘other’ research scientist in academia and 2.8% are research scientists in industry (Question 3).

The first part of the survey included a range of questions about the NMR facilities used and the type of NMR research being carried out. Users were asked about where they collect NMR data (Question 5). 66.3% of the NMR users collect all data at a facility located in their home



university/research centre/company. Around 25% of NMR users collect data at a home facility but also at a regional/national/international facility; most of these responses (21.7%) indicated that most of their data is collected at the home facility. 8.5% of NMR users collect all NMR data at a regional/national/international NMR facility. NMR users collected data using spectrometers ranging from Benchtop NMR to 1.2 GHz NMR (Question 6). 95% of the respondents used NMR facilities equipped with Bruker spectrometers but as many as 79 respondents used facilities equipped with spectrometers from other manufacturers (Agilent, JEOL, Magritek, Tecmag, RS2D, QuOne, NanoNord Tveskaeg and Oxford Instruments) (Question 7); this result is consistent with the responses from the earlier NMR Facility Manager Survey (M2.1). The very high number of Bruker spectrometers running TopSpin in the NMR community justifies the majority of effort in Remote-NMR in the implementation of remote access using these Bruker systems. However, analysis of the survey responses of remote access users shows that remote access has been implemented on some Agilent/Varian systems. If time allows in the project, protocols for remote access to Agilent/Varian systems should be discussed with relevant stakeholders.

Solution-state NMR is the primary type of NMR being carried out by the respondents (77.2%). Only 7.4% of respondents primarily use solid-state NMR and 15.5% use both solution and solid state NMR (Question 8). The NMR users were asked about the types of NMR experiments they carry out; the responses cover all areas of biological and physical sciences (Question 9). Biomolecular NMR research was the most common response (223 users) and routine small molecule characterisation supporting organic chemistry was the next most common response (180 users). The NMR users were asked to categorize their level of expertise in operating NMR spectrometers (Question 10). 14.8% are 'non-expert' users who select from a limited list of experiments and parameters. 50.5% are 'standard' users who select from a wider list of experiments but cannot run their own pulse sequences. 32.8% are 'expert' users who can run any experiments and write their own pulse sequences. 2% of users were not sure how to categorize their level of expertise.

The NMR users were then asked if they had collected NMR data using remote access (Question 11). Remote access was defined in several ways: 1) direct remote access – users directly operate the NMR spectrometer by remote login to the NMR spectrometer computer; 2) assisted remote access – users communicate via a computer linkup (Zoom/Teams etc) or telephone with a local



operator who controls the NMR spectrometer; 3) any other type of remote access. Around 50% of the respondents had used some type of remote access to NMR spectrometers during the pandemic and around 50% had not used remote access. Of those who had used remote access, 79.1% had used remote access at their home NMR facility, 10.9% had used remote access at a regional/national/international NMR infrastructure, and 10% had used remote access at both types of facilities.

The responses to the questions that followed this are analysed according to whether remote access was or was not used for data collection.

5. Responses from NMR Users With Remote Access

There were 201 NMR users who did collect NMR data via remote access; they represent 23 European countries and 4 other countries (Question 4). The subset of responses for these 201 NMR users are included in Appendix 3. The majority of respondents collection data via remote access used direct remote access (70.1%) or both direct and assisted remote access (15.9%). Most respondents provided additional detail about their use of remote access (Questions 11a); these responses are included in Appendix 3 and may be of interest to WP3 and WP4 participants. The vast majority of remote access has been provided on Bruker spectrometers (95.2%) (Question 13). Users were asked about software used for remote access. AnyDesk, NoMachine (NX), TeamViewer and VNC were widely used for remote access. The survey also showed that around 21% of respondents also used other packages for remote access; these include DWSservice, Guacamole, Microsoft Remote Desktop, Chrome Remote Desktop and others. Details of these other packages can be found in the responses to Question 14/14a in Appendix 3. A range of software packages will need to be investigated further in WP2, and also in WP3 and WP4 in order to assess their usefulness for remote access.

The majority of users were provided with support by NMR facility staff (58.9%). This included assistance with preparation and loading of samples into the spectrometer, assistance with the setup of experiments, data processing and data transfer, and Zoom/Teams/email assistance in case of problems (Question 15). The majority of users put their own samples into the spectrometer (74.6%) and then left the NMR facility to operate the spectrometer remotely

(Question 16). Some respondents (25 of 201) shipped their samples via post/courier to the NMR facility. Samples for solution NMR were shipped in a variety of states but the most common was as a frozen solution. NMR users were asked if they consider sample shipment to an NMR facility to be a barrier to remote access (Question 18); 71.1% of respondents did not consider it to be a barrier. The 28.9% who did consider it as a barrier, identified a number of concerns which included sample degradation, NMR tube breakage, loss of sample during shipping, customs regulations and the cost of shipping. The responses relating to sample shipment have also been considered in Task 2.4 on transnational sample shipment and further analysis has been included in Deliverable 2.1 (Identification of GDPR, security needs and shipment bottlenecks (M12)).

Finally, these 201 users were asked about bottlenecks that they encountered in using remote NMR (Question 19) and for any other information that they wanted to provide (Question 21). These detailed responses will assist in development of common protocols for remote access as they highlight a range of problems that have already been encountered by users. It is encouraging to see that 82.1% of the respondents that used remote access during the pandemic have continued to do so even after ‘pandemic’ restrictions have been lifted (Question 20).

6. Responses from NMR Users With No Remote Access

There were 200 NMR users who did not collect NMR data via remote access; they represent 19 European countries and 5 other countries (Question 4). The subset of responses for these 201 NMR users are included in Appendix 4. Several reasons were given by the users in this group for not using remote access (Question 11c). The most common reasons were 1) remote access not available at the NMR facility (52.3%) and 2) there were no restrictions during the pandemic restricting in-person access (38.6%). Respondents were also invited to give more detailed information about reasons for not providing remote access. Analysis of these responses will provide valuable insights about how the R-NMR project can make remote NMR access easier for these sites to implement. NMR users who had not used remote access were also asked if they considered sample shipment to an NMR facility to be a barrier to remote access; 43.2% of respondents did consider it to be a barrier (Question 11d). The reasons given for concern were similar to those given by users of remote access; sample degradation was the biggest concern.



Encouragingly, 71.5% of the respondents not using remote access indicated that they would be interested in using this once R-NMR has developed a standardized protocol (Question 11e). This confirms that there will be significant interest in the outcomes of the R-NMR project.

7. Final Comments and Next Steps

This survey has provided valuable insights into the experiences of hands-on NMR users during the pandemic. Around 50% of respondents were provided with remote access at their facilities during the pandemic while the other 50% were not. The results presented here complement the earlier NMR facility manager survey and together they provide a snapshot, from both perspectives, of the current state of remote NMR access. The outcomes of these two surveys will feed into WP3 and WP4 and will provide important information to help in defining and implementing a common protocol for remote access to NMR instrumentation.

APPENDIX 1

Remote-NMR (R-NMR): Moving NMR infrastructures to remote access capabilities

NMR USER SURVEY (8 January -29 March 2023)

Univ. of Oxford Central University Research Ethics Committee Approval Reference: [R77838/RE002]

PARTICIPANT INFORMATION SHEET AND SURVEY



Remote-NMR (R-NMR): Moving NMR infrastructures to remote access capabilities

PARTICIPANT INFORMATION SHEET

Central University Research Ethics Committee Approval Reference: [R77838/RE002]

1. *Introductory paragraph*

Prior to the Covid19 pandemic, the overwhelming majority of NMR data collection was conducted by scientists traveling to local, national and transnational NMR facilities and sitting directly in front of the NMR console to setup data collection. The experiments were often set up together with experienced staff to ensure sample integrity, best conduct of experiments, interactive planning and peer teaching, and initial analysis of acquired data to assess the correct outcome of the experiments. Due to the lockdown restrictions in many countries during 2020-2021, this scenario had to change dramatically. The experiences of several European NMR facilities during the Covid19 pandemic have shown that remote access is feasible within the field of NMR spectroscopy. It is the aim of the Remote-NMR project to develop and exploit this type of access in full.

You are being invited to take part in the R-NMR project because you are a user of an NMR facility. Before you decide to participate in the survey, it is important for you to understand why the research is being done and what it will involve. Please take time to read the following information carefully and discuss it with others if you wish. Ask us if there is anything that is not clear or if you would like more information. Take time to decide whether you wish to take part.

2. *Why is this research being conducted?*

Remote access to NMR spectrometers has been implemented successfully at several NMR facilities around the EU/UK during the Covid19 pandemic. The R-NMR project is being conducted in order to collect information from NMR facility users about their NMR facilities and about their experiences using remote access so that a common protocol for remote access for all facilities can be developed and adopted by facilities across the EU/UK. We are also interested in feedback from users who have not used NMR spectrometers remotely.

3. Why have I been invited to take part?

You have been invited to complete this survey because you have been identified as a user of an NMR facility.

4. Do I have to take part?

No. It is up to you to decide whether or not to take part. You can withdraw yourself from the study, without giving a reason, by advising me of this decision. The deadline by which you can withdraw any information you have contributed to the research is 31 December 2023; any data that you have provided will be deleted.

5. What will happen to me if I take part in the research?

You will be invited to complete an online survey. The survey is aimed at users of NMR facilities and will ask questions about the NMR facility you use, your experiences, if any, with remote access to NMR spectrometers and for your views on how remote access can be improved in the future. The survey will be completed without providing your name or contact email address but you will be asked to indicate in which country your NMR facility is located.

6. What are the possible disadvantages and risks in taking part?

There are no disadvantages or risks in taking part in this research except that you will need to spend some time completing the surveys (no more than 15-30 minutes).

7. Are there any benefits in taking part?

The benefits to you and to the wider NMR community by taking part in this project will be the improvement of remote NMR access across the EU/UK that will be the outcome of the R-NMR project.

8. What information will be collected and why is the collection of this information relevant for achieving the research objectives?

We will not collect any information that will directly identify you. Information that all participants provide about their NMR facility and their experiences with remote access will be included in discussions with other R-NMR participants and included in reports but this information is completely anonymous. Your IP address will not be collected.

All survey data will be stored in Oxford on a secure desktop computer (password protected and behind a firewall) during the duration of the R-NMR project (until 30 June 2025). A version of the survey will be created for longer-term storage on University servers. We intend to keep this version of the survey for 3 years beyond publication of the project.

9. Will the research be published? Could I be identified from any publications or other research outputs?

The findings from the NMR user survey being carried out online by Oxford researchers as part of the R-NMR research project will be used in a report about the current protocols in place for remote access to NMR spectrometers. This report will be circulated to other R-NMR grant participants, will be

uploaded to the R-NMR website and will be used as the starting point for other work packages in R-NMR. Individuals will not be identified in the reports. It is very unlikely that the outcomes of the surveys being carried out online by Oxford researchers will be written up for publication.

10. Data Protection

The University of Oxford is the data controller with respect to your personal data, and as such will determine how your personal data is used in the study. The University will process your personal data for the purpose of the research outlined above. Research is a task that is performed in the public interest. Further information about your rights with respect to your personal data is available at <https://compliance.admin.ox.ac.uk/individual-rights>. No personal data will be collected in this survey.

11. Who is funding the research?

Remote-NMR is funded by a grant from the European Union's Horizon Europe Research and Innovation Programme under Grant Agreement No. 101058595. Participation by U.K. partners, including the University of Oxford, is funded via the Horizon Europe Guarantee scheme run by Innovate UK, part of UK Research and Innovation (UKRI).

12. Who has reviewed this study?

This study has received ethics approval from a subcommittee of the University of Oxford Central University Research Ethics Committee. (Ethics reference: R77838/RE002).

The surveys have also been approved by the Steering Board of the Remote-NMR project.

13. Who do I contact if I have a concern about the research or I wish to complain?

If you have a concern about any aspect of this study, please contact Professor Christina Redfield (see contact details in next section), and she will do her best to answer your query. I will acknowledge your concern within 10 working days and give you an indication of how it will be dealt with. If you remain unhappy or wish to make a formal complaint, please contact the Chair of the Research Ethics Committee at the University of Oxford who will seek to resolve the matter as soon as possible:

The Chair, Medical Sciences Interdivisional Research Ethics Committee;
Email: ethics@medsci.ox.ac.uk; Address: Research Services, University of Oxford, Boundary Brook House, Churchill Drive, Headington, Oxford OX3 7GB

14. Further Information and Contact Details

If you would like to discuss the research with someone beforehand (or if you have questions afterwards), please contact:

Professor Christina Redfield
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Remote-NMR: User Survey

INTRODUCTION

Remote-NMR (R-NMR): Moving NMR infrastructures to remote access capabilities

Prior to the Covid19 pandemic, the overwhelming majority of NMR data collection was carried out in-person at the NMR facility. Due to the lockdown restrictions in many countries during 2020-2021, this scenario had to change dramatically. Our experiences during Covid19 show that remote access is feasible within the field of NMR spectroscopy, and it is the aim of R-NMR to develop and exploit this type of access in full.

The purpose of this survey is to collect information from NMR users about the NMR facilities they use and about their experiences, if any, of remote access to NMR spectrometers. The survey should take no more than 15-30 minutes to complete and you can select to 'Finish later' if you wish.

Before you decide to participate in this survey, it is important for you to understand why the research is being done and what will be done with your responses to the survey. Please take time to read the information in the participant information sheet that can be accessed at [Click here](#). Ask us if there is anything that is not clear or if you would like more information.

PRIVACY NOTICE AND CONSENT TO PARTICIPATE IN THE SURVEY

You are invited to complete this online survey aimed at users of NMR facilities. We will ask questions about the NMR facility(ies) that you use, about your experiences (if any) with remote access to NMR spectrometers and for your views on how remote access can be improved in the future. The survey will be completed anonymously (you will not be asked for your name or email address) but you will be asked to indicate in which country your NMR facility is located. Information that you provide about your experiences with remote access will be included in discussions with other R-NMR project participants and in project reports. All survey data will be stored at the University of Oxford on a secure computer (password protected and behind a firewall) during the duration of the R-NMR project (until 30 June 2025). A version of the survey will also be created for longer-term storage; we intend to keep this version for 3 years beyond the end date of the project. Please confirm that you have read this information and that you are willing to continue with the survey. * *Required*

Yes

No

INFORMATION ABOUT YOU AND THE NMR FACILITY(IES) YOU USE

Please confirm that you are a user of an NMR facility. By user, we mean someone who actively collects NMR data. *(Please only complete the survey once even if you have received the link from multiple sources.)* * Required

Yes

No

INFORMATION ABOUT THE NMR FACILITY(IES) YOU USE

Please select the option that best describes you?

- Undergraduate student (studying for BA/BSc etc)
- Graduate student (studying for MSc/PhD etc)
- Postdoctoral researcher
- Research group leader (i.e. Principal Investigator)
- Staff scientist (such as NMR technician, engineer)
- Other research scientist in academia
- Research scientist in industry
- Other

If you selected Other, please specify:

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: * Required

- | | | |
|-----------------------------------|----------------------------------|--------------------------------------|
| <input type="radio"/> Austria | <input type="radio"/> Belgium | <input type="radio"/> Bulgaria |
| <input type="radio"/> Croatia | <input type="radio"/> Cyprus | <input type="radio"/> Czech Republic |
| <input type="radio"/> Denmark | <input type="radio"/> Estonia | <input type="radio"/> Finland |
| <input type="radio"/> France | <input type="radio"/> Germany | <input type="radio"/> Greece |
| <input type="radio"/> Hungary | <input type="radio"/> Iceland | <input type="radio"/> Ireland |
| <input type="radio"/> Israel | <input type="radio"/> Italy | <input type="radio"/> Latvia |
| <input type="radio"/> Lithuania | <input type="radio"/> Luxembourg | <input type="radio"/> Malta |
| <input type="radio"/> Netherlands | <input type="radio"/> Norway | <input type="radio"/> Poland |
| <input type="radio"/> Portugal | <input type="radio"/> Romania | <input type="radio"/> Serbia |
| <input type="radio"/> Slovakia | <input type="radio"/> Slovenia | <input type="radio"/> Spain |

- Sweden

 Switzerland

 United Kingdom
 Ukraine

 Other

If you selected Other, please specify:

Where do you collect your NMR data? (select one option) * *Required*

- All data collected at an NMR facility located in my home university/research centre/company.
 Most data collected at an NMR facility located in my home university/research centre/company and some data collected at a regional, national or international NMR infrastructure.
 Half of data collected at a regional, national or international NMR infrastructure and half of data collected at an NMR facility located in my home university/research centre/company.
 Most data collected at a regional, national or international NMR infrastructure and some data collected at an NMR facility located in my home university/research centre/company.
 All data collected at a regional, national or international NMR infrastructure.

If some or all of your NMR data are collected at one or more national or international NMR infrastructures, instead of your local NMR facility, please specify in which country(ies) these NMR infrastructures are located. Select all that apply:

- | | | |
|--------------------------------------|-------------------------------------|---|
| <input type="checkbox"/> Austria | <input type="checkbox"/> Belgium | <input type="checkbox"/> Bulgaria |
| <input type="checkbox"/> Croatia | <input type="checkbox"/> Cyprus | <input type="checkbox"/> Czech Republic |
| <input type="checkbox"/> Denmark | <input type="checkbox"/> Estonia | <input type="checkbox"/> Finland |
| <input type="checkbox"/> France | <input type="checkbox"/> Germany | <input type="checkbox"/> Greece |
| <input type="checkbox"/> Hungary | <input type="checkbox"/> Iceland | <input type="checkbox"/> Ireland |
| <input type="checkbox"/> Israel | <input type="checkbox"/> Italy | <input type="checkbox"/> Latvia |
| <input type="checkbox"/> Lithuania | <input type="checkbox"/> Luxembourg | <input type="checkbox"/> Malta |
| <input type="checkbox"/> Netherlands | <input type="checkbox"/> Norway | <input type="checkbox"/> Poland |
| <input type="checkbox"/> Portugal | <input type="checkbox"/> Romania | <input type="checkbox"/> Serbia |

Slovakia

Slovenia

Spain

Sweden

Switzerland

United Kingdom

Ukraine

Other

If you selected Other, please specify:

INFORMATION ABOUT THE NMR FACILITY(IES) YOU USE

At what ^1H frequencies do you collect NMR data? (select all that apply) *Optional*

- | | | |
|---|----------------------------------|----------------------------------|
| <input type="checkbox"/> 400 MHz or lower | <input type="checkbox"/> 500 MHz | <input type="checkbox"/> 600 MHz |
| <input type="checkbox"/> 700 MHz | <input type="checkbox"/> 750 MHz | <input type="checkbox"/> 800 MHz |
| <input type="checkbox"/> 850 MHz | <input type="checkbox"/> 900 MHz | <input type="checkbox"/> 950 MHz |
| <input type="checkbox"/> 1 GHz | <input type="checkbox"/> 1.1 GHz | <input type="checkbox"/> 1.2 GHz |
| <input type="checkbox"/> Benchtop NMR | | |

What type of spectrometers do you use for data collection? (select all that apply)

Optional

- | | | |
|--|---|---------------------------------|
| <input type="checkbox"/> Bruker | <input type="checkbox"/> Agilent/Varian | <input type="checkbox"/> JEOL |
| <input type="checkbox"/> GE/Omega | <input type="checkbox"/> Magritek | <input type="checkbox"/> Stelar |
| <input type="checkbox"/> Other (or don't know) | | |

If you selected Other, please specify:

INFORMATION ABOUT THE NMR FACILITY(IES) YOU USE

What type of NMR data do you typically collect? (select one) *Optional*

- Primarily solution-state NMR Primarily solid-state NMR Both solution- and solid-state NMR

What types of NMR experiments do you carry out? (select all that apply) *Optional*

- NMR associated with undergraduate/graduate teaching
- Routine small molecule characterization supporting organic chemistry
- Biomolecular NMR research
- Metabolomics research
- Micro-imaging research
- Materials Science NMR research
- Pharmaceutical NMR research
- Environmental Science NMR research
- Food research
- Relaxometry
- Hyperpolarization
- Development or maintenance of NMR hardware/software
- Other Physical Sciences NMR research
- Other Biological/Biomedical Sciences NMR research
- Other

If you selected Other, please specify:



INFORMATION ABOUT THE NMR FACILITY(IES) YOU USE

How would you categorize your level of expertise in operating NMR spectrometers? (select one) *Optional*

- Non-expert user (can select from a limited list of experiments and parameters)
- Standard user (can select from a wider list of experiments but cannot run your own pulse sequences)
- Expert user (can run any experiments and write your own pulse sequences)
- Don't know/Not sure

EXPERIENCE WITH REMOTE ACCESS TO NMR SPECTROMETERS

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. *

Required

- Yes - direct remote access.
- Yes – assisted remote access.
- Yes – both direct and assisted remote access.
- Yes - another type of remote access (please specify below)
- No

If you would like to provide more detailed information about your mode of remote spectrometer access then please fill in the text box.

Where has remote access been provided? (select one)

- At an NMR facility located in your home university/research centre/company.
- At a regional, national or international NMR infrastructure.
- At both an NMR facility located in your home university/research centre/company and at a regional, national or international NMR infrastructure.

Why have you not used remote access to NMR spectrometers? (select any that apply)

- There were no restrictions during the pandemic that prevented on-site use of spectrometers.
- Remote access was not available at the NMR facility(ies) I use.
- I was not able to install the required software for remote access on my computer.
- IT security concerns made remote access impossible.
- Remote connection was unreliable due to network or software limitations.
- Spectrometers do not have automatic tuning (ATM).
- I was not able to ship or deliver my NMR samples to the NMR facility.
- Other

If you selected Other, please specify:

Do you consider sample shipment/delivery to an NMR facility to be a barrier to remote spectrometer access?

- Yes No

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

- I am concerned that the NMR tube would break during sample shipment.
- I am concerned that my sample would degrade during sample shipment.
- My samples are air sensitive and difficult to ship via a courier.
- I am concerned that my sample would be lost during sample shipment.

- The cost of shipping a sample by courier is too high.
- Customs regulations make shipping of my sample to another country difficult.
- I am concerned about the carbon footprint/environmental impact of shipping a sample by courier.
- Other

If you selected Other, please specify:

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 you be interested in remote access to the spectrometers you use?

- Yes No

EXPERIENCE WITH REMOTE ACCESS TO YOUR NMR FACILITY

If you have used any type of remote access (direct, assisted or another type) then select 'Yes' to proceed to further questions about your experiences with remote access. If you have not used any type of remote access then select 'No' to proceed to the end of the survey.

Yes

No

EXPERIENCE WITH REMOTE ACCESS TO YOUR NMR FACILITY

What type of spectrometers were available for remote access? (select all that apply)

- | | | |
|--|---|---------------------------------|
| <input type="checkbox"/> Bruker | <input type="checkbox"/> Agilent/Varian | <input type="checkbox"/> JEOL |
| <input type="checkbox"/> GE | <input type="checkbox"/> Magritek | <input type="checkbox"/> Stelar |
| <input type="checkbox"/> Other (or don't know) | | |

If you selected Other, please specify:

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

- | | | |
|---|-------------------------------------|-------------------------------------|
| <input type="checkbox"/> AnyDesk | <input type="checkbox"/> DWService | <input type="checkbox"/> Guacamole |
| <input type="checkbox"/> NoMachine (NX) | <input type="checkbox"/> Splashtop | <input type="checkbox"/> TeamViewer |
| <input type="checkbox"/> VNC | <input type="checkbox"/> Don't know | <input type="checkbox"/> Other |

If you selected Other, please specify:

EXPERIENCE WITH REMOTE ACCESS TO NMR SPECTROMETERS

As a remote user, were you provided with support by the NMR facility staff?

Yes

No

If yes, what type of support was provided? (select all that apply)

- Assistance with sample preparation (from sample material shipped to the NMR facility)
- Assistance with loading NMR samples (in NMR tubes or rotors) into the spectrometer
- Assistance with setup of NMR experiments
- Assistance with data transfer
- Assistance with data processing
- Telephone/email/online(Zoom/Teams) assistance in case of problems
- Website/YouTube videos explaining how to use remote access
- Other (please specify)

If you selected Other, please specify:

EXPERIENCE WITH REMOTE ACCESS TO NMR SPECTROMETERS

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

- You put your own samples in the NMR spectrometer and then left the facility to operate the spectrometer remotely.
- You dropped off your samples already loaded in an NMR tube/rotor at a drop-off location and then the facility staff loaded the samples into the spectrometer.
- You dropped off your samples at a drop-off location and then the facility staff loaded the samples into NMR tubes/rotors and then into the spectrometer.
- You shipped samples to the facility via post/courier and facility staff loaded NMR samples.
- Other

If you selected Other, please specify:

If you shipped samples to the NMR facility via post/courier, could you provide more information about how this was done? (select all that apply)

- Samples for solid state NMR were shipped already packed in rotors.
- Samples for solid state NMR were shipped and then packed into rotors by local facility staff.
- Samples for solution state NMR were shipped already loaded into NMR tubes.
- Samples for solution state NMR were shipped in frozen form and then thawed and placed into NMR tubes by local facility staff.
- Samples for solution state NMR were shipped as cooled solutions and then placed into NMR tubes by local facility staff.
- Samples for solution state NMR were shipped as solutions at ambient temperatures and

then placed into NMR tubes by local facility staff.

- Samples for solution state NMR were shipped as powders and then dissolved in buffer/solvent and placed into NMR tubes by local facility staff.
- Other

If you selected Other, please specify:

In the text box below, please enter any additional information about sample shipping? (such as courier company used, special packing materials used to prevent damage to samples, any other precautions taken, procedures for transnational sample shipping etc).

Are spectrometers you used for remote access equipped with automatic sample changers and were these important for your use of remote access?

- Yes automated sample changers available.
- Yes automated sample changers available and important for use of remote access.
- No sample changers were available.

If yes, was the sample changer temperature controlled (i.e. are samples stored at a specified temperature before insertion in the spectrometer)?

Yes

No

EXPERIENCE WITH REMOTE ACCESS TO NMR SPECTROMETERS

Do you consider sample shipment/delivery to an NMR facility to be a barrier to remote spectrometer access?

Yes

No

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

- I am concerned that the NMR tube would break during sample shipment.
- I am concerned that my sample would degrade during sample shipment.
- My samples are air sensitive and difficult to ship via a courier.
- I am concerned that my sample would be lost during sample shipment.
- The cost of shipping a sample by courier is too high.
- Customs regulations make shipping of my sample to another country difficult.
- I am concerned about the carbon footprint/environmental impact of shipping a sample by courier.
- Other

If you selected Other, please specify:

EXPERIENCE WITH REMOTE ACCESS TO NMR SPECTROMETERS

What bottlenecks or other problems did you identify in using NMR spectrometers by remote access? Do you have any suggestions about how remote access could be improved?



Are you continuing to use remote access to NMR spectrometers now that some/many/all 'pandemic' restrictions have been lifted?

Yes

No

FINAL QUESTIONS

If you have further information that you would like to provide, please enter this in the text box below.

A large, empty rectangular text box with a thin black border, set against a light gray background. The box is intended for the user to provide additional information.

FINAL COMMENTS AND THANKS!

Thank you very much for taking the time to complete this survey. Your responses will be important in formulating common practices for future provision of remote access to NMR spectrometers.

If you would like further information about the R-NMR project then please visit the project webpage at <https://www.r-nmr.eu> or follow the project on Twitter @RemoteNMR_eu. A summary of the results of the survey will be available on the R-NMR web site in February 2023.

APPENDIX 2

Remote-NMR (R-NMR): Moving NMR infrastructures to remote access capabilities

NMR USER SURVEY (8 January -29 March 2023)

Univ. of Oxford Central University Research Ethics Committee Approval Reference: [R77838/RE002]

SUMMARY OF RESPONSES FROM ALL NMR USERS

Introduction

Lockdown restrictions in many countries during 2020-2021 Covid19 pandemic resulted in the implementation of remote access to NMR spectrometers as a way of enabling the continuation of important research. The experiences of several European NMR facilities during the pandemic have shown that this access mode can work well within the field of NMR spectroscopy. It is the aim of the Remote-NMR project to develop and exploit remote access to NMR facilities. Work Package 2 within R-NMR focusses on the "Remote NMR Landscape". Task 2.2 within WP2 is a review of NMR users' need with respect to remote access to NMR facilities; this includes aspects such as facilities used during the pandemic, level of assistance provided by facilities/would additional assistance have been useful; is confidentiality of samples/experiments important; how were samples sent; likelihood of using remote access even when there are no travel restrictions; suggestions for improvement. This information has been collected via an online survey of NMR users.

This document is a summary of the responses from all of the 401 NMR users who completed the survey.

Remote-NMR: User Survey

Showing 401 of 401 responses

Showing **all** responses

Showing **all** questions

Response rate: 20%

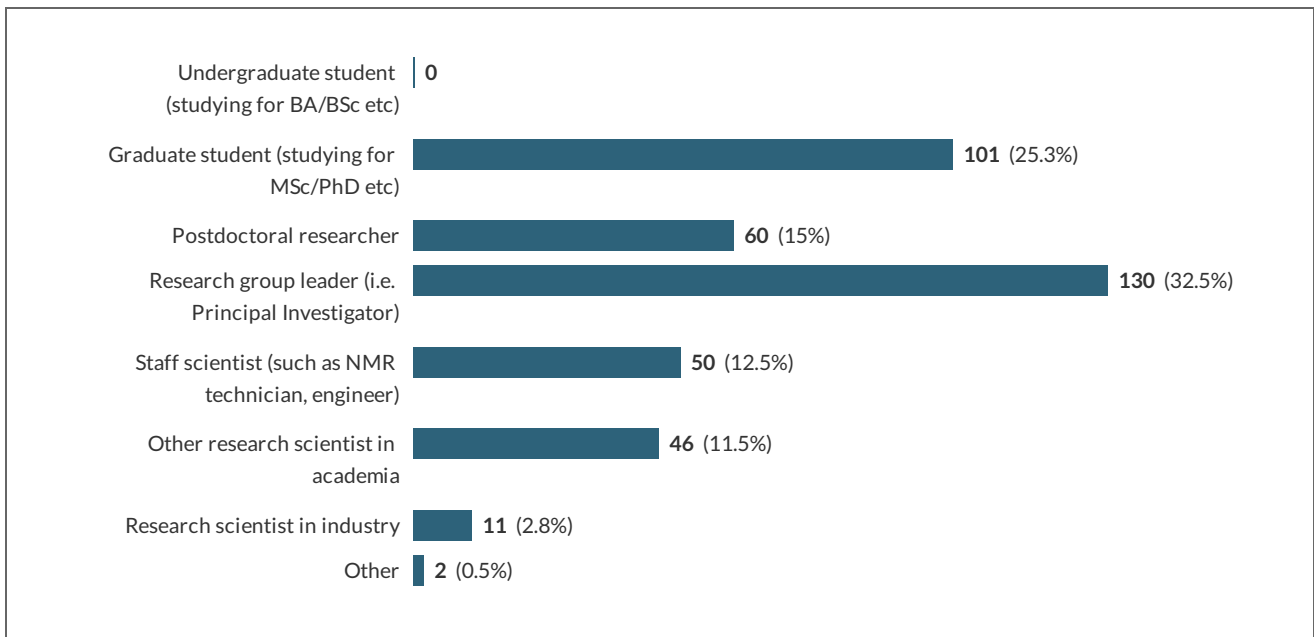
- 1** You are invited to complete this online survey aimed at users of NMR facilities. We will ask questions about the NMR facility(ies) that you use, about your experiences (if any) with remote access to NMR spectrometers and for your views on how remote access can be improved in the future. The survey will be completed anonymously (you will not be asked for your name or email address) but you will be asked to indicate in which country your NMR facility is located. Information that you provide about your experiences with remote access will be included in discussions with other R-NMR project participants and in project reports. All survey data will be stored at the University of Oxford on a secure computer (password protected and behind a firewall) during the duration of the R-NMR project (until 30 June 2025). A version of the survey will also be created for longer-term storage; we intend to keep this version for 3 years beyond the end date of the project. Please confirm that you have read this information and that you are willing to continue with the survey.

Yes  401 (100%)
No | 0

- 2** Please confirm that you are a user of an NMR facility. By user, we mean someone who actively collects NMR data. (Please only complete the survey once even if you have received the link from multiple sources.)

Yes  401 (100%)
No | 0

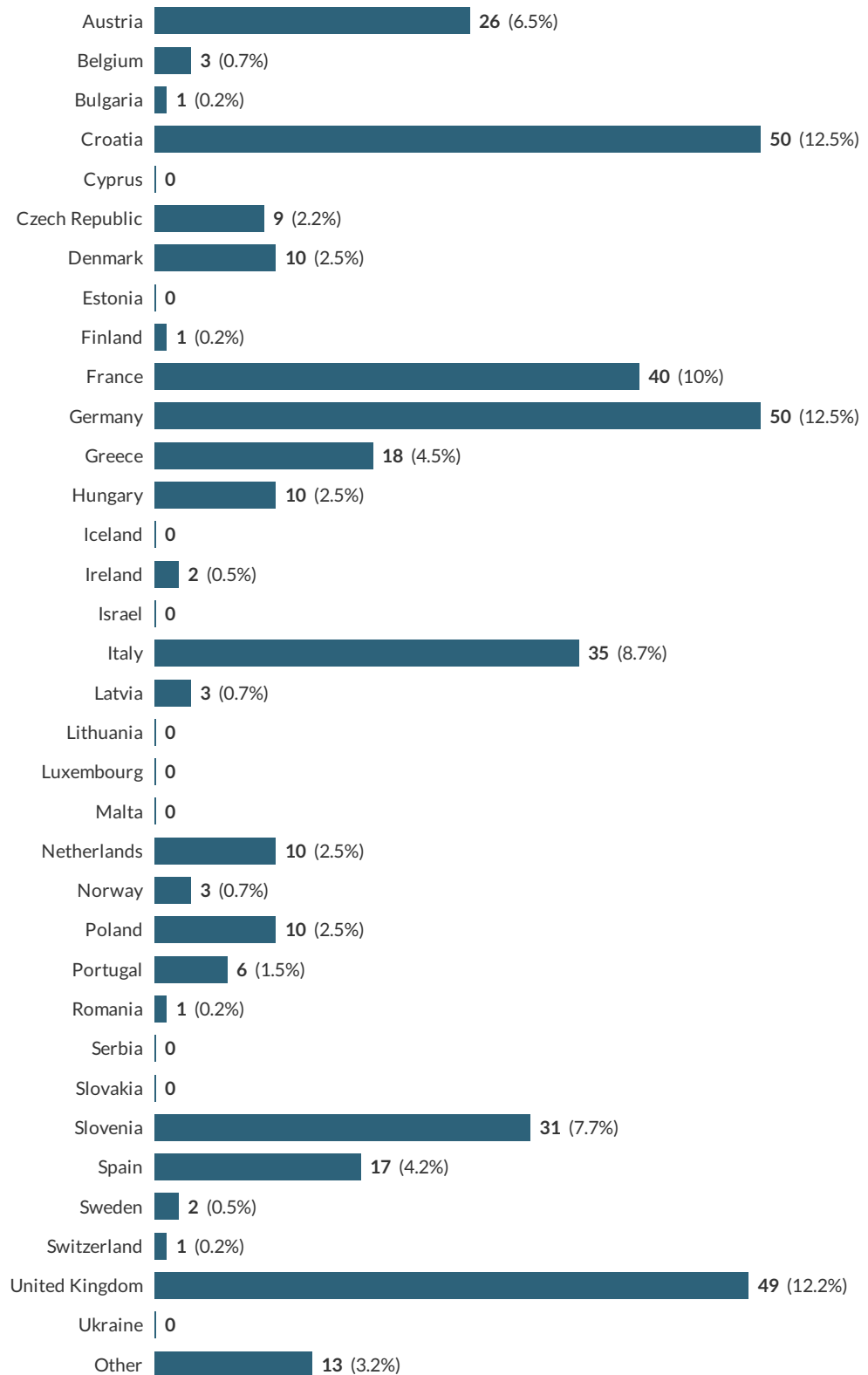
- 3** Please select the option that best describes you?



3.a If you selected Other, please specify:

Showing all 2 responses	
Research Scientist in Government	987038-987020-104036011
(Lab-)Technician	987038-987020-104772110

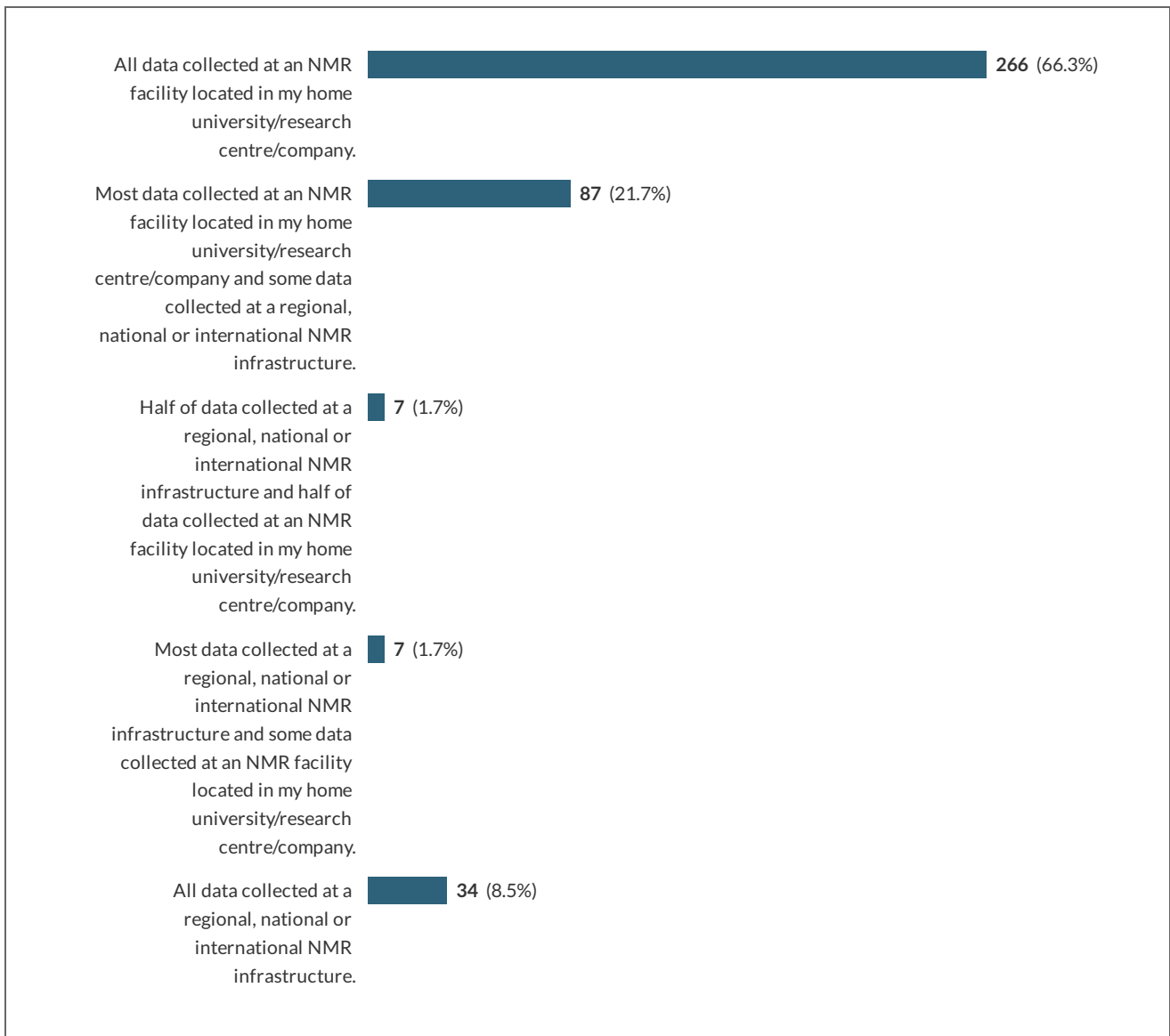
4 In which country do you carry out your NMR research? This is most likely to be the country in which you live. If you also use an NMR facility in another country you will be able to indicate that later in the survey. Select one:



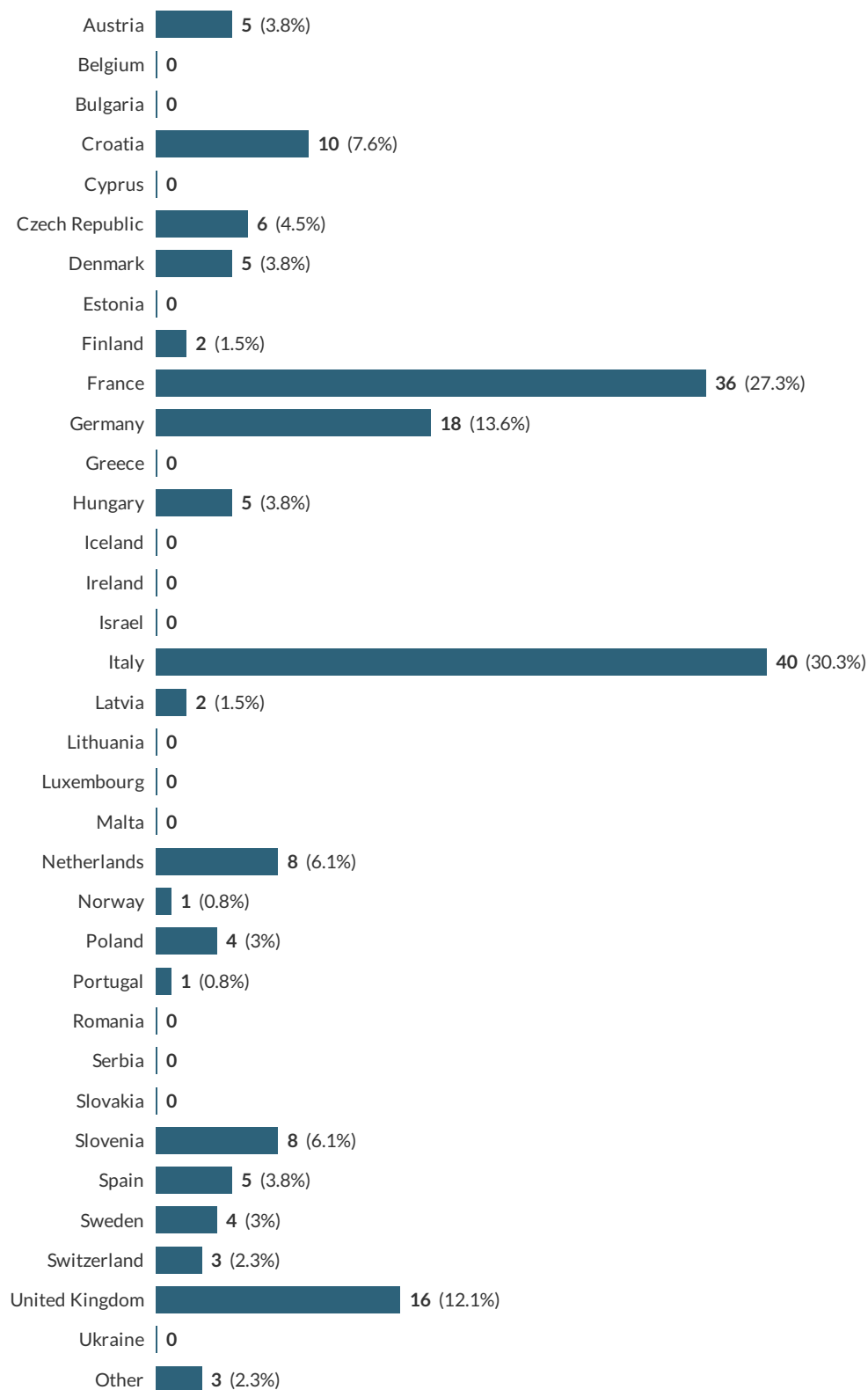
4.a If you selected Other, please specify:

Showing all 13 responses	
India	987038-987020-104033457
Brazil	987038-987020-104033656
Canada	987038-987020-104036011
Brazil	987038-987020-104066039
Canada	987038-987020-104377423
Russia	987038-987020-104378805
Turkey	987038-987020-104397267
Mexico	987038-987020-104418281
United States of America	987038-987020-104421282
Argentina	987038-987020-104423415
USA	987038-987020-104467387
Argentina	987038-987020-104756491
Argentina	987038-987020-104840209

5 Where do you collect your NMR data? (select one option)



5.a If some or all of your NMR data are collected at one or more national or international NMR infrastructures, instead of your local NMR facility, please specify in which country(ies) these NMR infrastructures are located. Select all that apply:

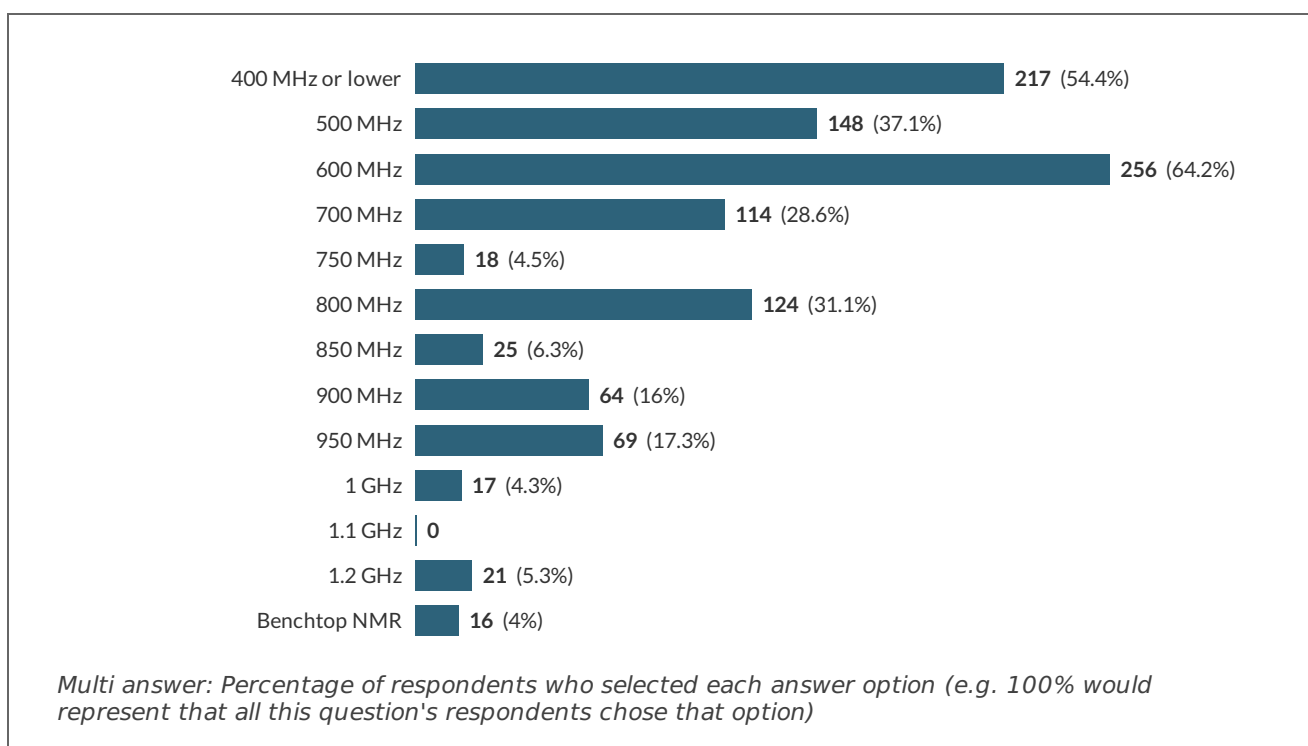


Multi answer: Percentage of respondents who selected each answer option (e.g. 100% would represent that all this question's respondents chose that option)

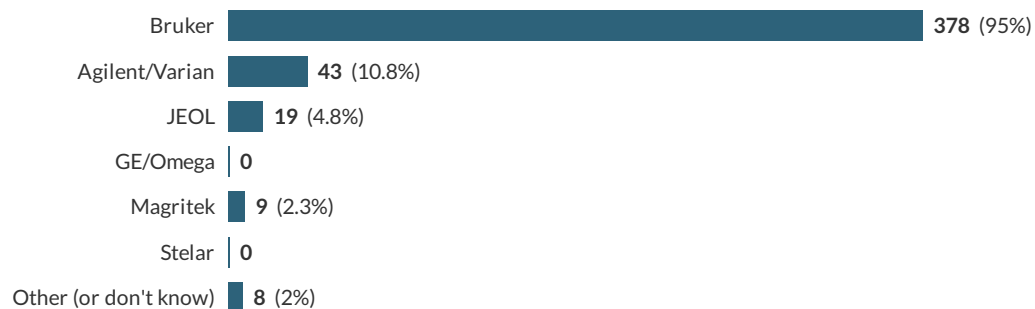
5.a.i If you selected Other, please specify:

Showing all 3 responses	
India	987038-987020-104033457
Brazil	987038-987020-104033656
United States	987038-987020-104423415

6 At what 1H frequencies do you collect NMR data? (select all that apply)



7 What type of spectrometers do you use for data collection? (select all that apply)

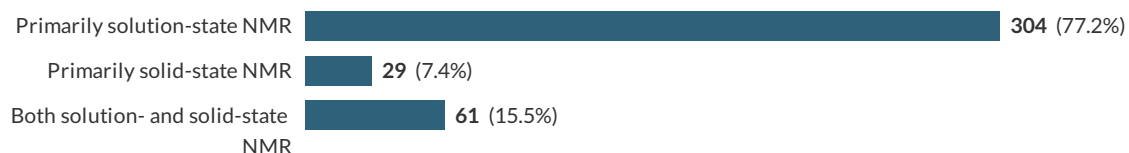


Multi answer: Percentage of respondents who selected each answer option (e.g. 100% would represent that all this question's respondents chose that option)

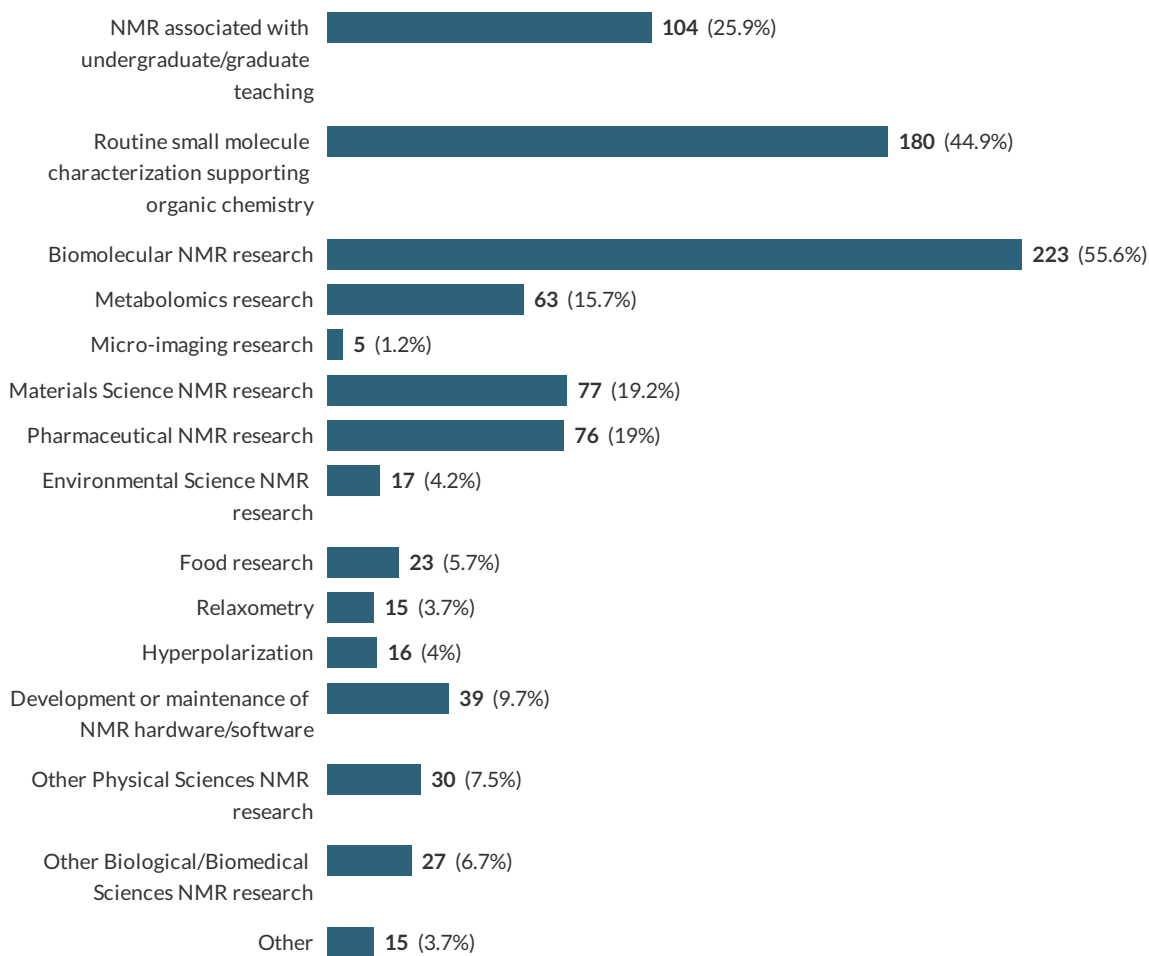
7.a If you selected Other, please specify:

Showing all 5 responses	
Tecmag	987038-987020-104037885
RS2D	987038-987020-104044047
QuOne	987038-987020-104378805
NanoNord Tveskaeg	987038-987020-106148495
Oxford	987038-987020-106173927

8 What type of NMR data do you typically collect? (select one)



9 What types of NMR experiments do you carry out? (select all that apply)

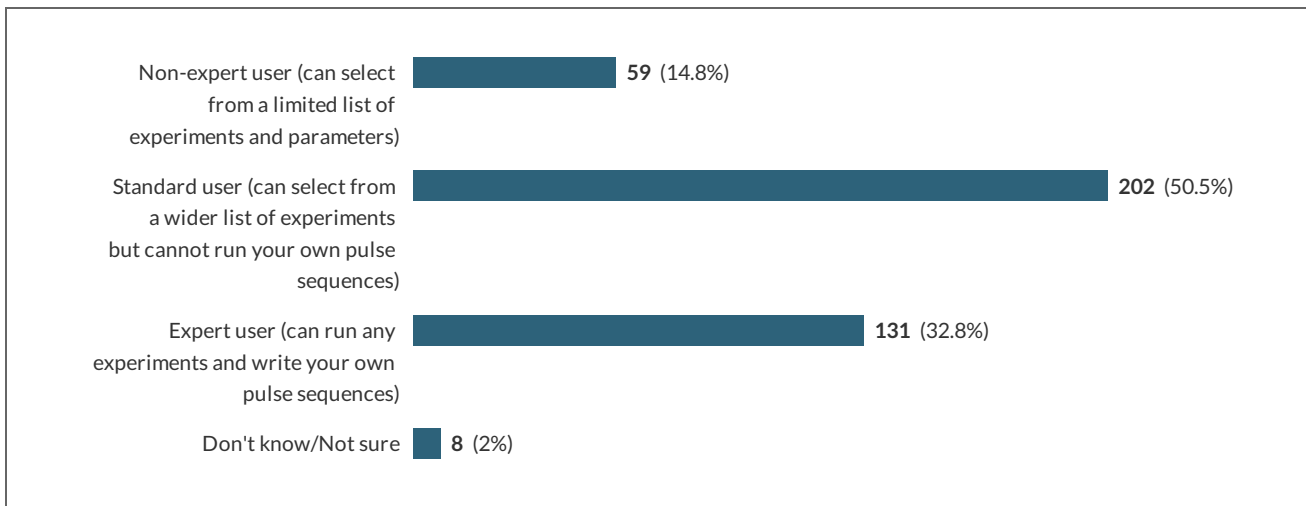


Multi answer: Percentage of respondents who selected each answer option (e.g. 100% would represent that all this question's respondents chose that option)

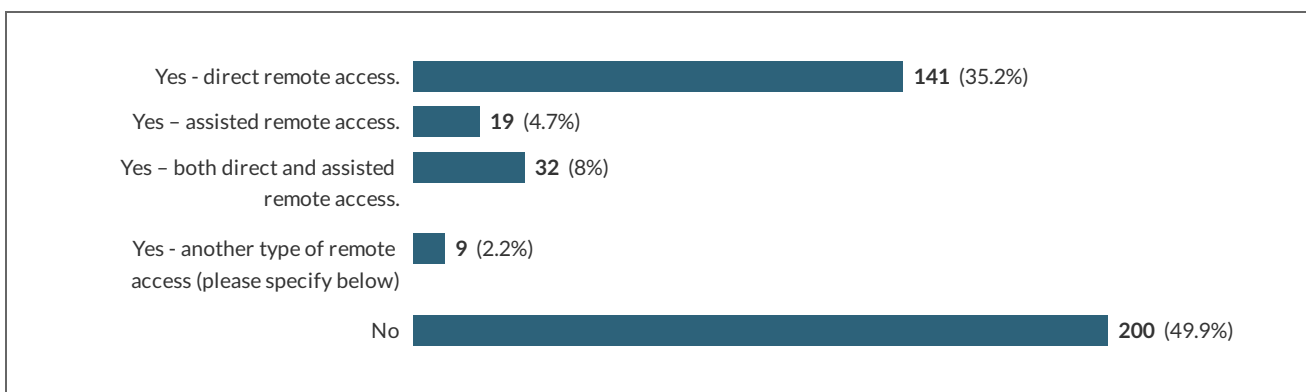
9.a If you selected Other, please specify:

Showing all 15 responses	
Structure Elucidation of Natural Products	987038-987020-104004509
Organometallics research	987038-987020-104039591
NMR on colloidal quantum dots	987038-987020-104382331
Quantitative NMR of transition metal complexes.	987038-987020-104382711
Diffusometry	987038-987020-104429762
Screening	987038-987020-104641637
Reaction monitoring	987038-987020-104677232
Routine small molecule characterization supporting inorganic/organometallic chemistry Kinetic Studies and reaction monitoring	987038-987020-104678345
Reaction monitoring and kinetics Molecular Dynamics	987038-987020-104712621
molecular synthesis	987038-987020-104851393
Polymer NMR	987038-987020-104901512
in addition to routine small molecule characterization supporting organic chemistry, my group works on organometallic (metallocenes with Fe(II), Ru(II) or Co(III)) or metal-organic samples (with diamagnetic metals like Zn, Cd, Pd(II), Pt(II), Rh(I), Re(I), Cu(I), Ag(I)...). In addition to routine 1D ¹ H, ¹³ C or ³¹ P, we also do 2D NMR for identification. For our supramolecular work DOSY is very useful. Rarely measured paramagnetic metal complexes containing Co(II).	987038-987020-104922032
NMR on polymers	987038-987020-105022810
Inorgani chemistry	987038-987020-105036238
qNMR	987038-987020-106586217

10 How would you categorize your level of expertise in operating NMR spectrometers? (select one)



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.a If you would like to provide more detailed information about your mode of remote spectrometer access then please fill in the text box.

Showing all 94 responses	
Our company shipped samples to a nearby university with listed experiments.	987038-987020-103842897
remote desktop applications (teamviewer. anydesk) or directly VNC	987038-987020-103901122
Using a home laptop to connect via a remote desktop connection directly to the spectrometer workstation. Or using my office computer to connect to the spectrometer workstation in an adjacent building.	987038-987020-103912490
remote login via vpn to the institute and through that to NMR spectrometers	987038-987020-103914070

I was accessing the spectrometer from my office above stairs, instead of operating it from its main computer in the NMR room. But it can also be done from home or anywhere that has Wi-Fi connectivity, providing you have a VPN.	987038-987020-103929106
Sending samples with detailed list of measurement information or by telephone.	987038-987020-103933604
AnyDesk in VPN mode	987038-987020-103945877
Remote access provided by TopSpin 4	987038-987020-103957208
Via locally established VPN link	987038-987020-104005042
with tight vnc	987038-987020-104009724
I sent the sample	987038-987020-104016821
The software was accessed remotely via team viewer and sample loading-unloading were carried out by the technician/students.	987038-987020-104033457
No Machine	987038-987020-104033656
TeamViewer software to access NMR computer	987038-987020-104036011
We Use a software to take control on the computer ton run experiments	987038-987020-104036680
Controlled session over TeamViewer session	987038-987020-104036746
Remote access to spectrometer via ssh and VNC viewer, enables full access of spectrometers equipped with sample changers and automatic tuning and matching.	987038-987020-104036834
Anydesk	987038-987020-104038147
Teamviewer	987038-987020-104051197
I frequently operate the 800 MHz NMR instrument using Teamviewer for remote access. Usually a technician will load the sample for me, and I will do the rest.	987038-987020-104066039
I have only used remotely to see if my experiment is running fine, after that I have transferred data remotely to access it further.	987038-987020-104130885
Tuning and matching of a probe	987038-987020-104202487
Remote access only after covid-19 pandemic Access is granted by and monitored by facility manager who decides if allowed for an individual to use independently	987038-987020-104235459
Teamviewer	987038-987020-104326713
Through the built in VNC service on the linux box.	987038-987020-104377423
assisted via teams or zoom direct - vpn and ssh + X11 and then "topspin -client" or vpn + https (iconnmr)	987038-987020-104382232
I have used AnyDesk.	987038-987020-104392826
Remote desktop application.	987038-987020-104382711

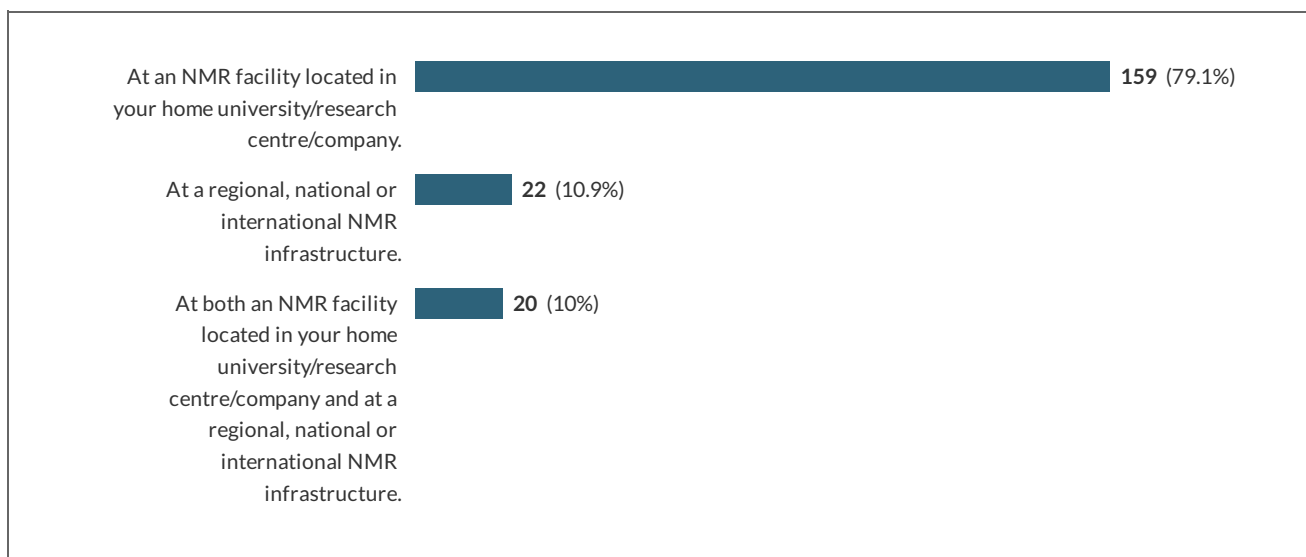
We have used Anydesk to reach the NMR spectrometer computer.	987038-987020-104392629
I submitted the sample for measurement and access to the remote inside-Lan network to collect data	987038-987020-104412732
Direct remote access at Indiana University in the USA Assisted remote access at CERM in Florence Italy	987038-987020-104423415
via the AnyDesk software that enabled remote connection to the NMR computer from my laptop	987038-987020-104425268
Via Signal Logs Portal for data and NoMachine for direct access	987038-987020-104425976
Limited access using 'anydesk' software. Most of the hardware need to be setup earlier. Temperature experiments are limited if no autotune hardware is installed.	987038-987020-104429762
We access through INSTRUCT grants. We normally discuss the experiments we need in advance and prepare a working plan. Then, we send the protein to the facility and if the local operator has questions, he/she contact us (phone/email/zoom) and we clarify the doubts. After that, we get the raw data.	987038-987020-104436599
via NoMachine	987038-987020-104438077
utilize Anydesk software to direct access to NMR spectrometers	987038-987020-104461826
teamviewer	987038-987020-104466561
In principle we have a dedicated lab technician who runs all our NMRs for us. The raw spectra are then accessed via remote access and processed individually by the researcher on his or her PC. NMR samples are being transferred to the spectrometers twice a day at given measuring time slots. In addition, night time experiments can be submitted by trained users themselves (NMR has an autosampler).	987038-987020-104487345
Access through Anydesk/Teamviewer software	987038-987020-104486977
A direct remote access has become unavailable with the evolution (sic!) of the Bruker Topspin software. The direct remote access at the user level was effectively deprecated beginning with the Topspin above ver. 3.2, and phased out with the current versions. It has complicated the remote access to the NMR spectroscope at the local facility to a great extent, now.	987038-987020-104494482
What do you mean by mode of access? If it is a question on how I access the computer from which I run NMR experiments it is either through VPN and remote desktop or through a third party software, such as AnyDesk.	987038-987020-104504200
I usually use NoMachine via a VPN	987038-987020-104541226
teamviewer	987038-987020-104568498
Prior to the pandemic we had sporadic access to NMR spectrometer computer via TeamViewer. However due to the increase of the amount of people using that access, our central NMR facility removed that access due to fear of (accidental) misuse and to keep an overview on how the spectrometer computer is being treated. The NMR facility has since been working on a more controlled alternative, but it did not materialize since then.	987038-987020-104569325

Vnc	987038-987020-104572895
I contacted the technician at the facility and we organized the set up of the experiments. To check the results, the technician uploaded the experiments on the web server and we decided how to proceed.	987038-987020-104578649
VNC over ssh tunnels, NoMachine	987038-987020-104652020
I used to have a core MRC grant but then I switched to working on systems of high MW intractable to NMR but recently wish to do NMR on nucleic acid components of the DNA-protein complexes Rusing NME	987038-987020-104651420
Remote control of NMR experiments via Anydesk session.	987038-987020-104652171
My previous remote access was via the 900 MHz NMR instrument at HWB-NMR in Birmingham. After attending for a day, setting up experiments etc I would then remote log on to monitor and set up further experiments based on the results of the initial ones. This to me was the real power of remotes access - a long block of time and interacting as if it was your own spectrometer.	987038-987020-104674153
Via Teams Login as though I was sat with the spectrometer	987038-987020-104676884
remote access to IconNMR	987038-987020-104678345
Spectrometers accessed using Chrome Remote Desktop. This has worked almost flawlessly. Issues: Samples being removed from sample changer carousel by other users If spectrometer does not have, or if sample is unstable or time critical, clearly cannot use remote access, user must be physically present at spectrometer	987038-987020-104679564
nx client	987038-987020-104680024
VPN --> RDC to virtual computer --> RDC to spectrometer computer	987038-987020-104679345
direct remote access using vpn server	987038-987020-104731960
Use VNCViewer to access the computer controlling the spectrometer remotely	987038-987020-104737700
Using softwares such as AnyDesk, TeamViwer, NoMachine	987038-987020-104742070
From a remote Bruker session in my office while the spectrometer was in another building, 300 m away.	987038-987020-104751961
NX Client for Windows Version 3.5.0.9	987038-987020-104858091
By use of the FastViewer software	987038-987020-104884554
Use of teamviewer and ssh.	987038-987020-104891596
Remote desktop (Windows 10) with VPN, Teamviever, ICON NMR (Bruker Topspin) additionally online cameras to control the hardware e.g. sample changer	987038-987020-104890370
Leaving the samples in front of the NMR facility for routine NMR data collection (small organic molecules)	987038-987020-104911443

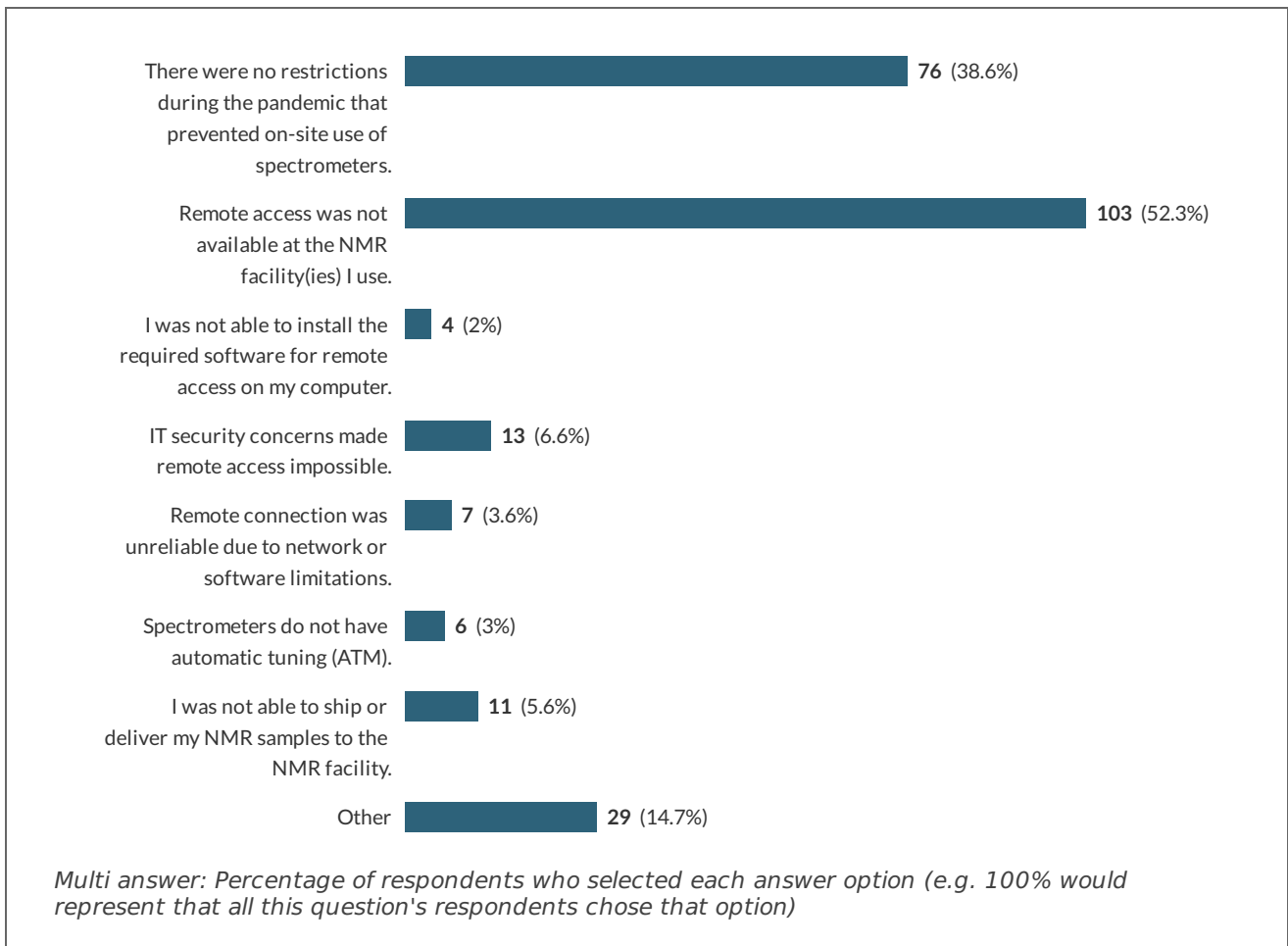
collection (small organic molecules).	
Well, I leave the samples at a specified place at the facility, the operator collects the NMR data, I analyze the data. I contact the operator if something is unclear or if I need a new, more specialized measurement. Not sure whether or not this qualifies as remote...	987038-987020-104922032
We can access our 800MHz via a VPN connection, including the SampleJet.	987038-987020-104929943
I used Team Viewer to operate the computer connected to the spectrometer.	987038-987020-104970631
Technicians put the rotor with sample (packed previously) and I set the experiments remotely	987038-987020-104987098
Remote connection via TigerVNC, RealVNC and TeamViewer	987038-987020-104995386
Pur NMR instrument can be accessed remotely through the AnyDesk software	987038-987020-105004542
Interaction with remote staff.	987038-987020-104995202
Zoom sessions with the persons operating the instruments; occasional attempts to use VNC fo direct interaction, but plagued with lag and connection reliability problems	987038-987020-105024523
access via vnc to the spectrometer	987038-987020-105024937
Access was usually via a VNC session on the computer controlling the spectrometer. Access was also performed on occasion using TeamViewer.	987038-987020-105046974
Anydesk	987038-987020-105041252
Remote login to the spectrometer from my personal laptop via Anydesk	987038-987020-105055804
By using a remote desktop	987038-987020-105056889
WE've already set up a remote access connection (via AnyDesk) to one NMR spectrometer located in another region of the institute. We only need to bring the samples and then can run any experiments remotely.	987038-987020-105087822
I operated infrastructure at my own research facility remotely using TeamViewer.	987038-987020-105197740
TeamViewer	987038-987020-105225587
Used Teamviewer.	987038-987020-105235641
For many years I have used VNC or similar to run experiments from home. This works most of the time very well.	987038-987020-105235200
All spectrometers are inducted to a local network and it is possible to acces them via nomachine even outside of the local network via IP, PW and acces file.	987038-987020-105359436
AnyDesk to control the software (pulse sequences, monitoring etc); hardware changes (including MAS speed changes, VT) on-site	987038-987020-105428768
TeamViewer	987038-987020-106146312
Grid of 30 low-field NMR spectrometers operated via robots	987038-987020-106148495

Send samples, contact via phone or email	987038-987020-106163112
We use a "remote desktop" solution that is integrated in Win10.	987038-987020-106588677
Access granted by password through firewall and further control of the instrument through Remote Desktop Connection.	987038-987020-106803889
VNC server on the NMR computer, TightVNC client on my PC	987038-987020-106835847
VPN connection to our NMR spectrometers	987038-987020-106968186
connection to X11 server installed on spectrometer computer	987038-987020-107009335
My direct remote access operates with the help of vnc. I used it already before 2020 to control the experiments from my desk in the normal laboratory and from my computer at home.	987038-987020-107339769

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



11.c Why have you not used remote access to NMR spectrometers? (select any that apply)



11.c.i If you selected Other, please specify:

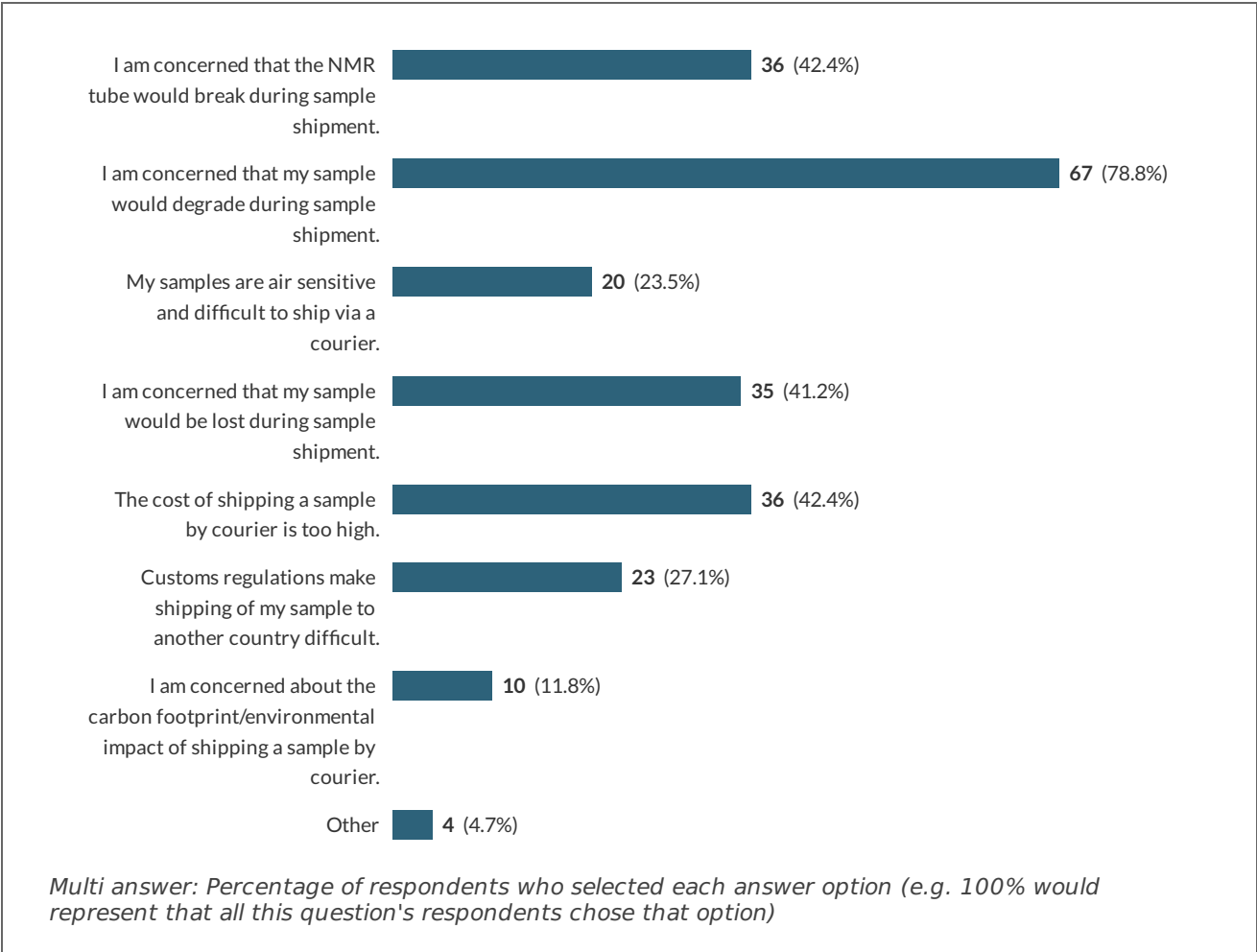
Showing all 28 responses	
I wasn't working with NMR yet.	987038-987020-103912338
I started working after the pandemic, so no restrictions that prevented on-site use of spectrometers.	987038-987020-103913260
I started after the restrictions were lifted	987038-987020-103933811
I did not need NMR data collection during the strict restriction time	987038-987020-103992982
Have not started my PhD until September 2020 and my masters project was stopped in March 2020	987038-987020-104004894
I do not need them for now	987038-987020-104013928
I have not been an NMR user for very long and so have not encountered any restrictions during my time - however my research facility was under restrictions for much of the early pandemic preventing on-site work.	987038-987020-104024542
Someone else is operating NMR spectrimeter, I send samples and get spectra by e-mail or server.	987038-987020-104036086

I did not perform any experiment during Covid-19 pandemic: restrictions to people mobility and restrictions to access to working places avoided any experiment at that time. Since Covid-19 pandemic, I had normal access to the nearest facility, so I did not need remote access.	987038-987020-104198359
I didn't start my NMR research by then and now everything can be done on campus.	987038-987020-104382331
I was not able to prepare the samples for the NMR experiments.	987038-987020-104454070
Since remote access is generally restricted, my on-site collaborating partner recorded the experiments during the pandemic.	987038-987020-104485771
I won a fellowship (Instruct ERIC) that allowed me to be physically present during data collection and analysis.	987038-987020-104545870
Staff at the facility accessed and elaborated data	987038-987020-104611593
Most of the time we are not actively operating the spectrometers at these facilities, (e.g. the actual measurements are performed by the experts there) although this via some kind of remote access could be a great option for us in the future.	987038-987020-104673945
I haven't needed to measure yet.	987038-987020-104770560
I had no need of NMR during lockdown and then the spectrometer were accessible.	987038-987020-104833479
Need to be present for titrations	987038-987020-104843071
Project had not started	987038-987020-104850009
NMR experiments that require presence (change of samples and titration experiments)	987038-987020-104864015
I did not need it, I use it only occasionally	987038-987020-104903762
During the first months of hard restrictions I had no samples to measure, later there were no restrictions anymore and i could measure on-site.	987038-987020-105233734
The consoles have been turned off for fear of power outages	987038-987020-105496764
I have waited the end of the restrictions during the pandemic period	987038-987020-106623404
I am not an expert in NMR.	987038-987020-107026866
I was not running any experiments during this period because I was an undergraduate student.	987038-987020-107385393
i was an undergraduate student	987038-987020-107385171
this was not possible / offered	987038-987020-107492647

11.d Do you consider sample shipment/delivery to an NMR facility to be a barrier to remote spectrometer access?



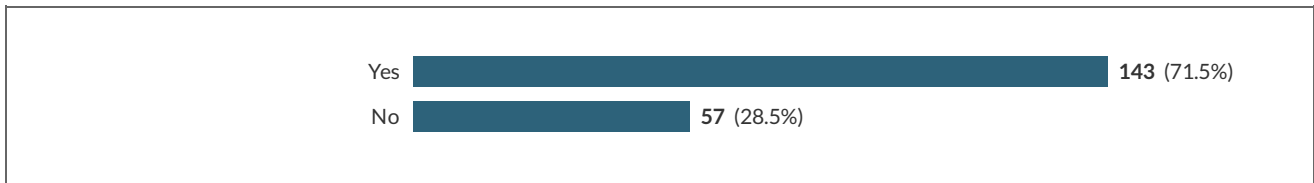
11.d.i If yes, what are your main concerns about sample shipment? (select all that apply)



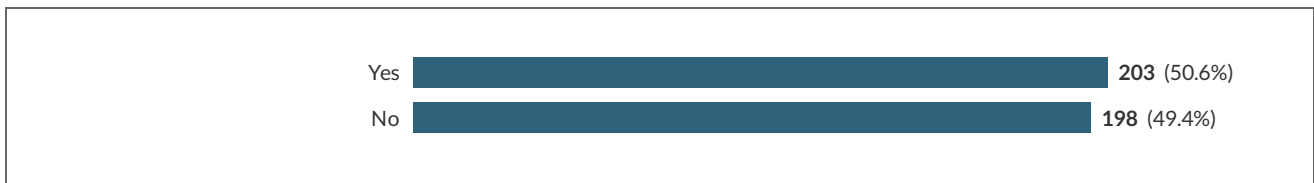
11.d.i.a If you selected Other, please specify:

Showing all 4 responses	
I like to have my results as quickly as possible	987038-987020-104042865
Clinical samples of IP sensitive samples can often not been shipped or measured outside	987038-987020-104437506
I am concerned that it is a lot of work. If I'm on site, I feel like I'm more flexible and can get my results as fast as possible. Or possibly adjust my sample.	987038-987020-104478118
Many of my samples are for kinetic studies and so need to be prepared immediately before analysis.	987038-987020-104677759

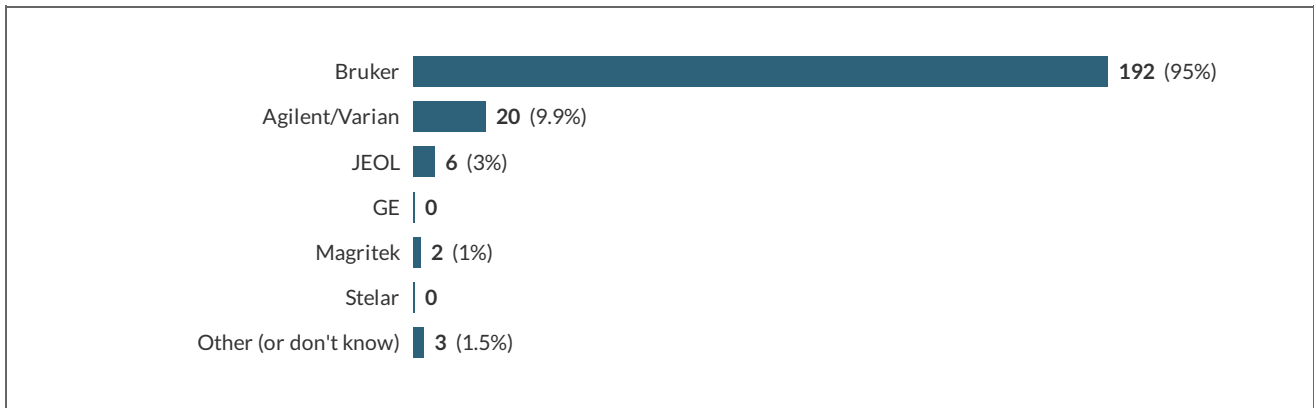
11.e The aim of the Remote-NMR project is to develop a common framework for remote spectrometer access taking into account best practice across the EU/UK. Standardized training for remote access will also be put in place. Once this has been completed, would you be interested in remote access to the spectrometers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



12 If you have used any type of remote access (direct, assisted or another type) then select 'Yes' to proceed to further questions about your experiences with remote access. If you have not used any type of remote access then select 'No' to proceed to the end of the survey.



13 What type of spectrometers were available for remote access? (select all that apply)

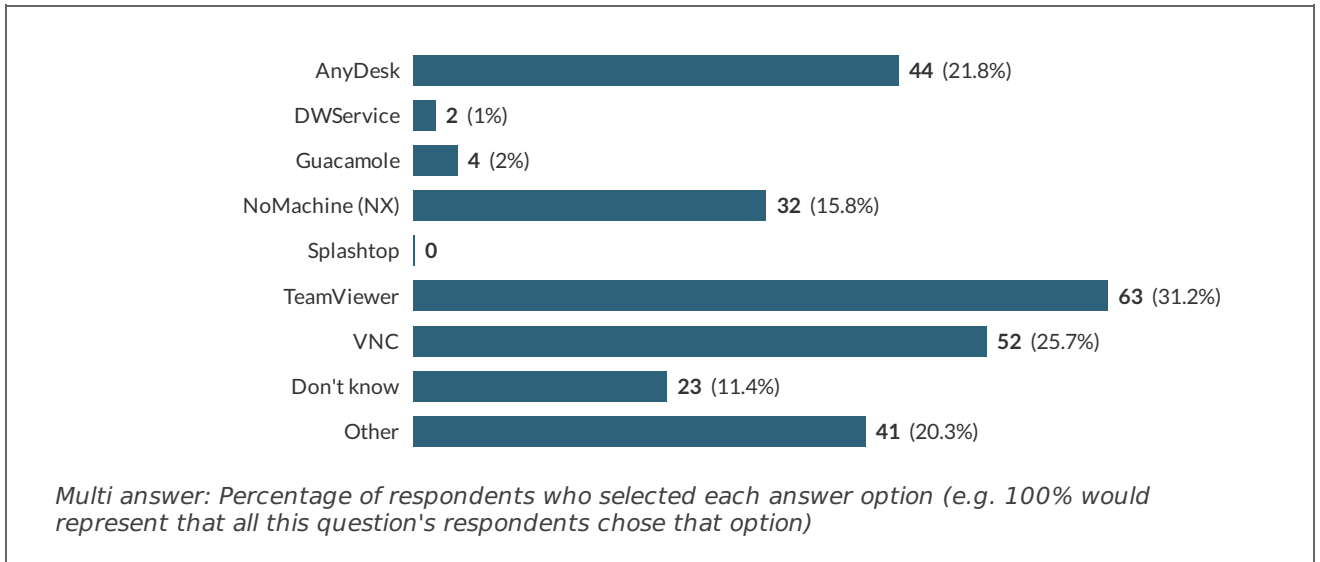


Multi answer: Percentage of respondents who selected each answer option (e.g. 100% would represent that all this question's respondents chose that option)

13.a If you selected Other, please specify:

Showing all 2 responses	
RS2D	987038-987020-104044047
NanoNord Tveskaeg	987038-987020-106148495

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



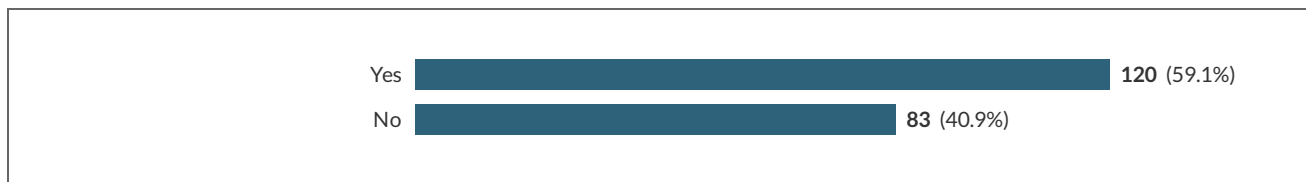
14.a If you selected Other, please specify:

Showing all 41 responses	
See previous answer for assisted remote access	987038-987020-103842897
Microsoft Remote Desktop app	987038-987020-103867866
Remote Desktop Connection	987038-987020-103875649
cisco	987038-987020-103912509
Windows remote desktop	987038-987020-103913102
Remote Desktop Connection (Windows), if working from home in tandem with Cisco Anyconnect.	987038-987020-103912490
freerdp	987038-987020-103914070

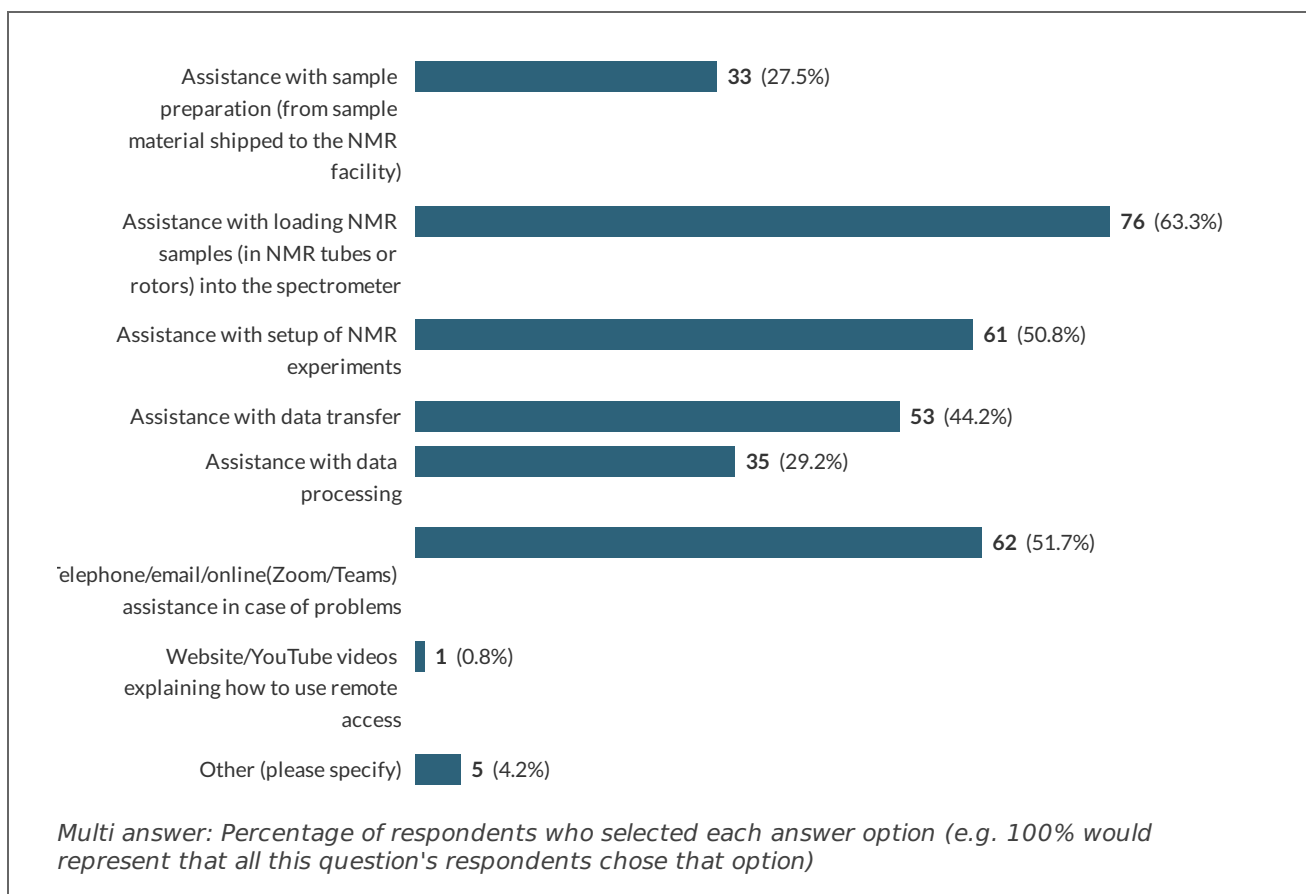
Remote control desktop and ICON NMR on Windows operating system	987038-987020-103929106
Remote Desktop Connection	987038-987020-103940038
TopSpin remote access	987038-987020-103957208
Chrome Remote Desktop	987038-987020-103971664
Microsoft Remote Desktop Protocol (RDP) via VPN	987038-987020-103988106
RDP	987038-987020-103988815
RDP	987038-987020-103988892
No software used, I sent the samples	987038-987020-104016821
Microsoft Remote Desktop	987038-987020-104038022
Windows remote desktop	987038-987020-104044047
LOGS	987038-987020-104130885
windows subsystem for Linux + GWSL (X server) and ssh for direct topspin access or vpn + chrome for iconnmr	987038-987020-104382232
Winscp	987038-987020-104412732
FileZilla FTP, MestrelNova	987038-987020-104487345
Remote access via ssh command on Linux terminal	987038-987020-104490106
A native Bruker implementation of the client-server implementation of the remote access in the Topspin software [for vers. <3.2].	987038-987020-104494482
sent samples a while back to the Utrecht facility	987038-987020-104651420
iconnmr	987038-987020-104678345
Spectrometers accessed using Chrome Remote Desktop. This has worked almost flawlessly.	987038-987020-104679564
Microsoft's Remote Desktop Connection	987038-987020-104679345
windows remote desktop	987038-987020-104700377
Microsoft Remote Desktop	987038-987020-104863090
FastViewer	987038-987020-104884554
microsoft teams	987038-987020-104890787
SSH	987038-987020-104891596
Remote desktop (Windows), ICON nmr (Bruker Topspin), Ezviz	987038-987020-104890370
Telefon + mail in sample	987038-987020-104993813
x2go	987038-987020-105263179
Zoom	987038-987020-105433478
Homebuilt software accessed via VPN/MC	987038-987020-106148495

Homebuilt software accessed via VPN/VNC	987038-987020-100148499
Remote desktop	987038-987020-106165519
"Remote Desktop" in Windows	987038-987020-106588677
Desktop Remote Connect	987038-987020-106803889
moba xterm ssh session	987038-987020-107025498

15 As a remote user, were you provided with support by the NMR facility staff?



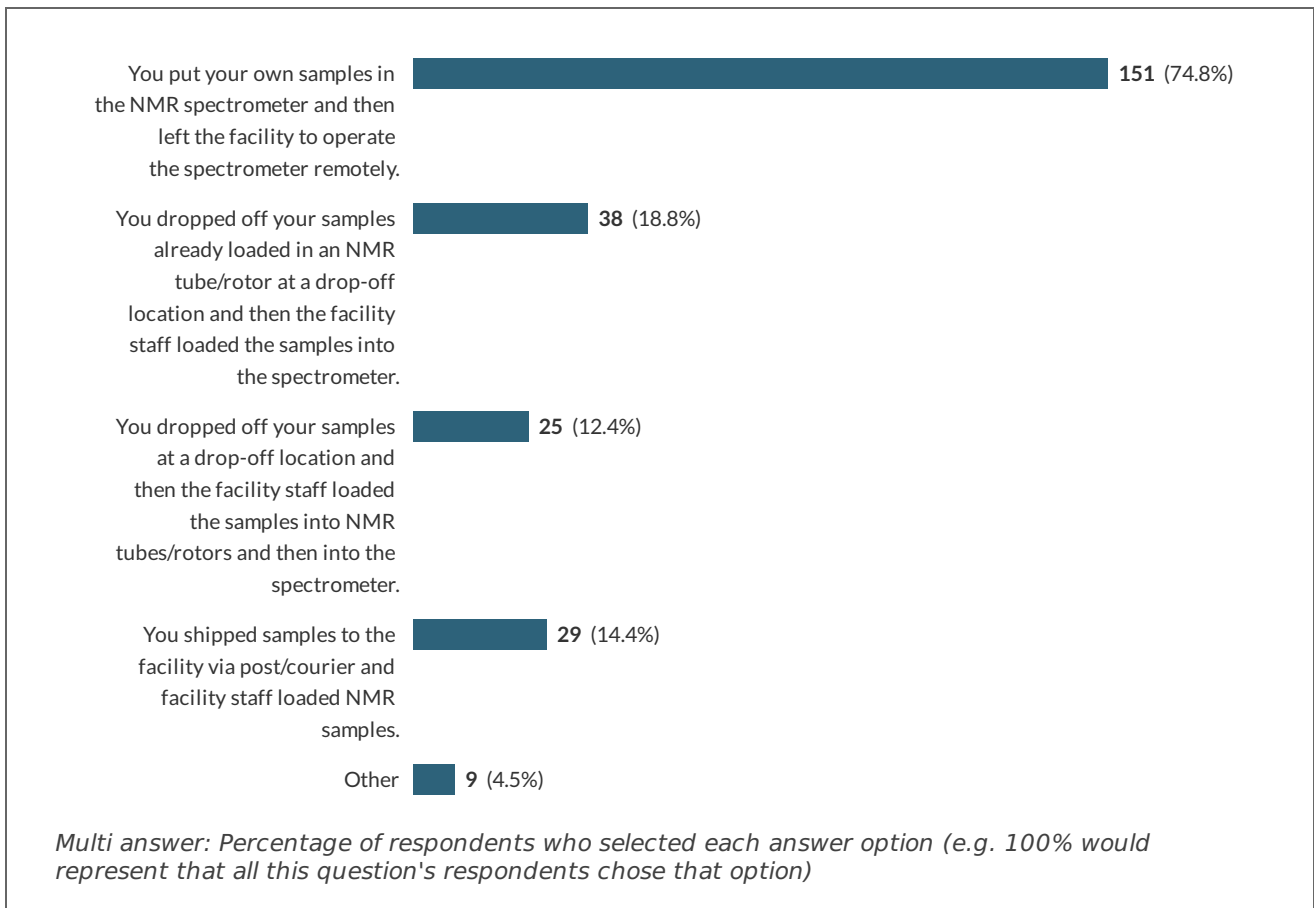
15.a If yes, what type of support was provided? (select all that apply)



15.a.i If you selected Other, please specify:

Showing all 5 responses	
Assistance with connecting to the spectrometer and assistance with data transfer via the remote connection.	987038-987020-103912490
Training in how to connect to the spectrometers from a remote location	987038-987020-104004509
Made up the samples and sent them through to the EU facility in Utrecht and in the past made up the samples and went to B'ham where they were shimmed and recorded by Sara Whittaker	987038-987020-104651420
Description of how to setup remote access on my computer	987038-987020-104737700
I am the person who bought and installed the software for remote use of the NMR spectrometers. Therefore, I was not assisted by other persons but assisted other persons.	987038-987020-104884554

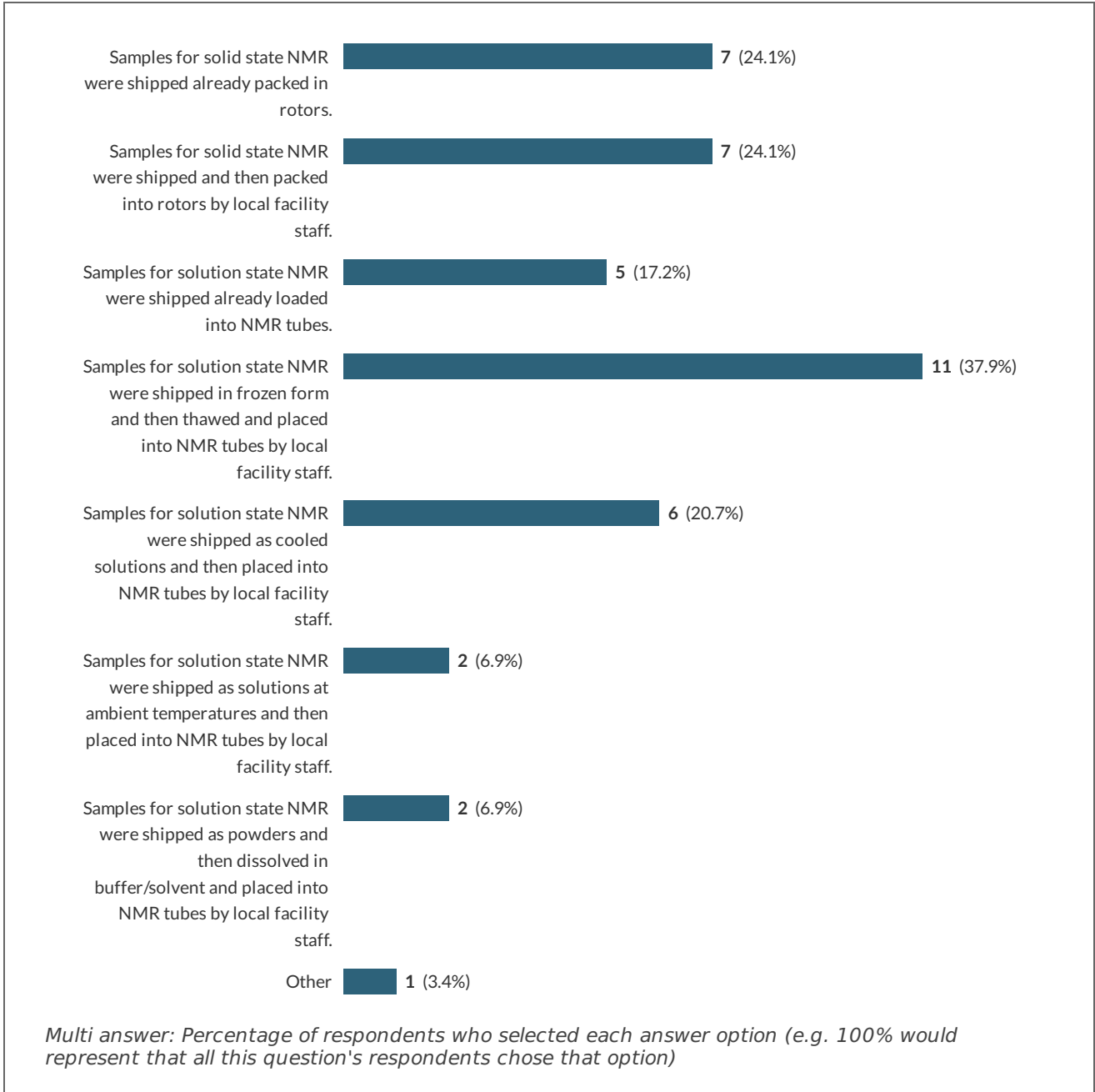
16 How were your NMR samples delivered to the NMR facility and loaded into the NMR spectrometers? (select all that apply)



16.a If you selected Other, please specify:

Showing all 9 responses	
I work on other peoples samples. Either they or other facility staff load the sample into a sample changer and provide me with information on its location	987038-987020-104004509
I put my own sample in the NMR spectrometer, started experiment and once its started, used remote facility to check if the experiment is running fine and to access results further.	987038-987020-104130885
Nice colleagues put my samples in the spectrometer	987038-987020-104409197
That was done by my colleagues who were working in person	987038-987020-104486977
I put the samples in an autosampler next to the NMR and an automated system (roboter) is loading and processing the sample	987038-987020-104772110
I put my own samples in the NMR spectrometer and then I operate the spectrometer remotely.	987038-987020-104858091
The samples were made in the wetlab of the facility and placed in the NMR spectrometer. I operated the spectrometer remotely.	987038-987020-105055804
I work in the same location as NMR facility, so was happy to run all experiments myself.	987038-987020-105235641
Students prepared and delivered sample to rack in SampleJet.	987038-987020-106588677

16.b If you shipped samples to the NMR facility via post/courier, could you provide more information about how this was done? (select all that apply)



16.b.i If you selected Other, please specify:

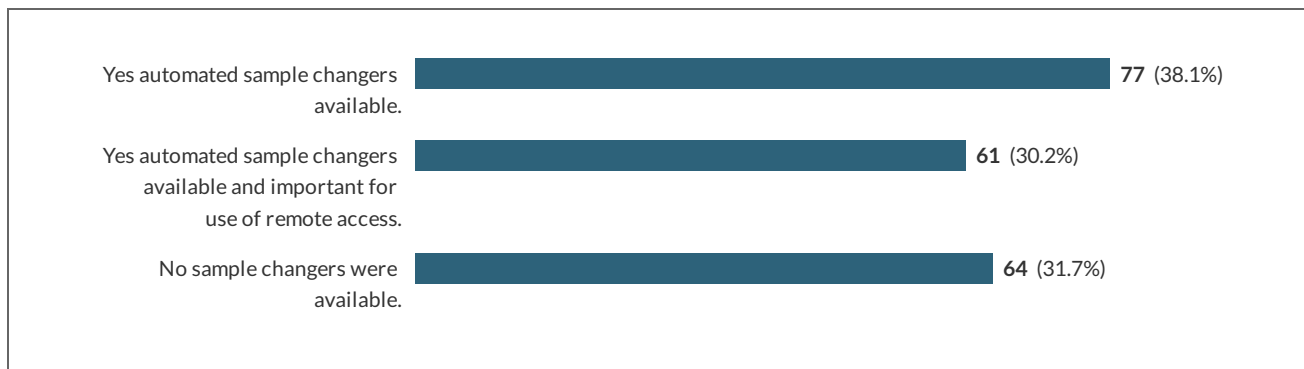
Showing 1 response	
Metabolism of cells	987038-987020-104995202

16.c In the text box below, please enter any additional information about sample shipping? (such as courier company used, special packing materials used to prevent damage to samples, any other

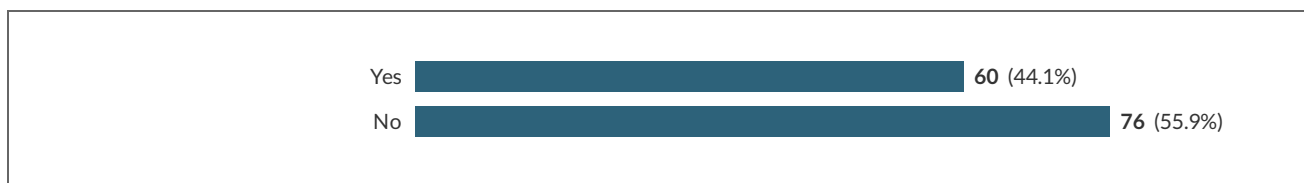
precautions taken, procedures for transnational sample shipping etc).

Showing all 8 responses	
ample prepared self and stored in 4 C	987038-987020-104130885
standard shipping via PostNord (Postal service)	987038-987020-104382232
FEDEX The procedures for transnational sample shipping from Argentina to Italy did not work properly and the sampled thaw in the process.	987038-987020-104423415
We use FEDEX and ship samples frozen on dry ice or as lyophilized powder. We very rarely ship refrigerated solutions. We always ship samples in an eppendorf, stored inside a falcon tube to make sure it does not break during shipment. We usually ship two tubes, one of them as a backup.	987038-987020-104436599
DHL	987038-987020-104439880
TnT (reliable, but expensive), FEDEX, DHL (not recommended...)	987038-987020-104680024
Companies used were FedEx, Roadrunners (Nottingham), BioCair	987038-987020-105046974
A good hard case protecting for the already packed rotors were sent. But, there is always some problems associated with couriers in general, they never deliver thing properly and on time. So, a good protecting packing, especially air tight if needed, is always done in my case.	987038-987020-106870635

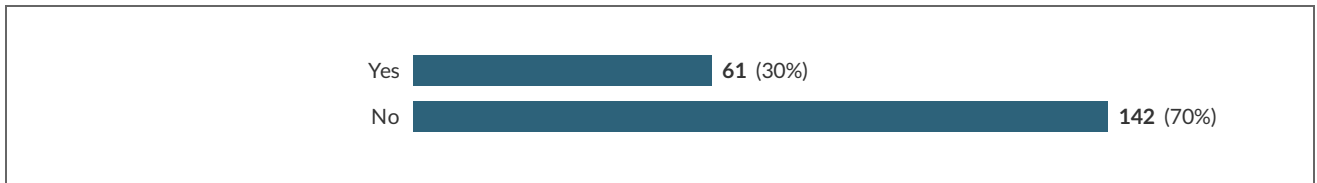
17 Are spectrometers you used for remote access equipped with automatic sample changers and were these important for your use of remote access?



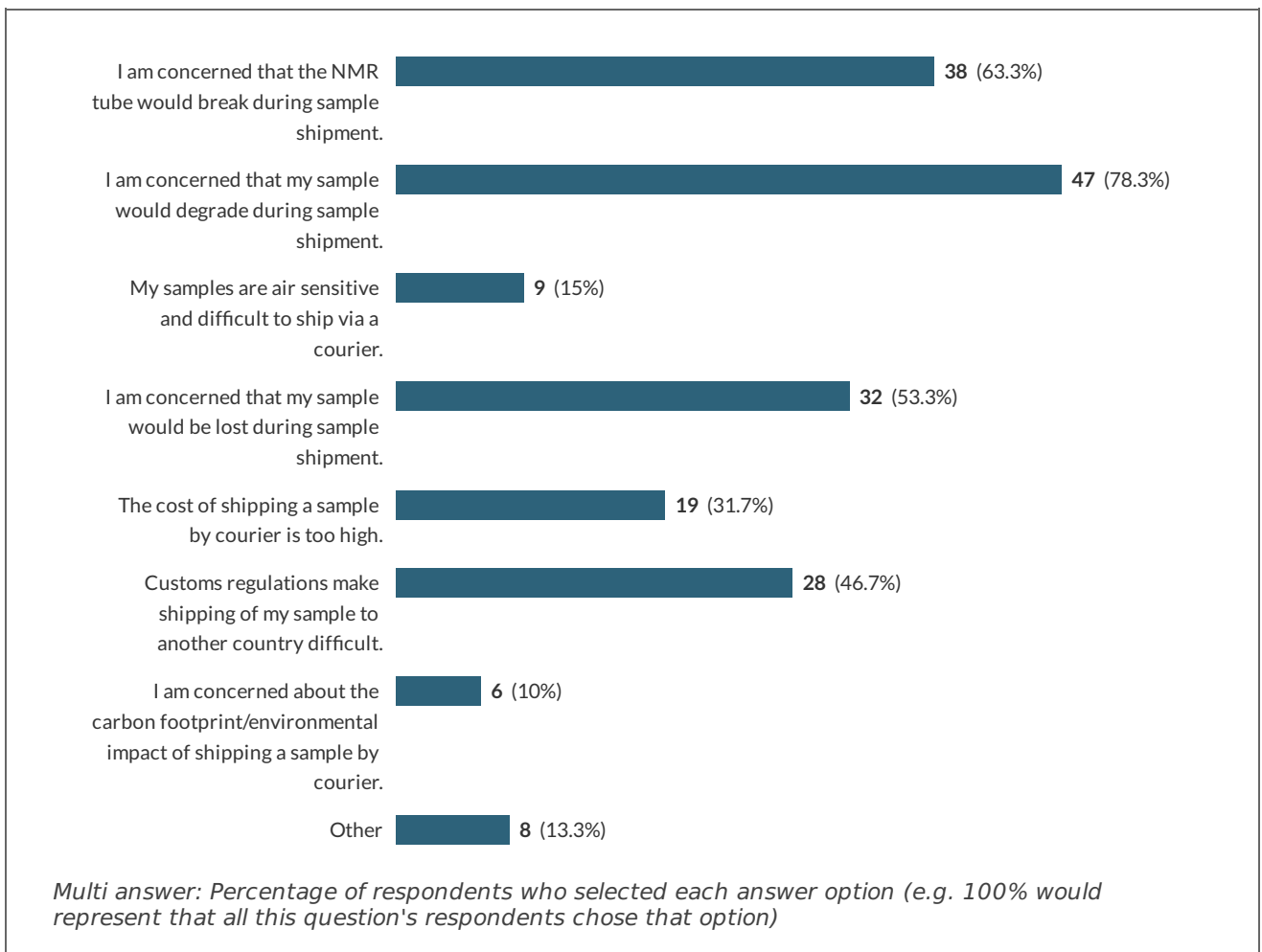
17.a If yes, was the sample changer temperature controlled (i.e. are samples stored at a specified temperature before insertion in the spectrometer)?



18 Do you consider sample shipment/delivery to an NMR facility to be a barrier to remote spectrometer access?



18.a If yes, what are your main concerns about sample shipment? (select all that apply)



18.a.i If you selected Other, please specify:

Showing all 8 responses	
An effective 24 h turnaround on NMR samples was very disruptive to working.	987038-987020-103842897
Some clinical samples are not allowed to be shipped.	987038-987020-104106458
Clinical and IP sensitive samples can often not be measured outside our own facility.	987038-987020-104437506
I want to use my samples multiple times. Personally readjusting a sample in the magnet or shigemi if needed is not possible.	987038-987020-104673241
Safety. Many samples will be in chloroform or other controlled solvent	987038-987020-104679564
In a way, all of the above may be true, depending on sample and urgency. I would still always take the option and in most cases shipment has worked before.	987038-987020-104680024
The hassle with preparing a package and organize shipment.	987038-987020-104679345
My samples (live cells) have to be freshly made at the NMR facility.	987038-987020-105055804

- 19 What bottlenecks or other problems did you identify in using NMR spectrometers by remote access? Do you have any suggestions about how remote access could be improved?

Showing all 104 responses	
I think sample shipping is the biggest problem. I run experiments for external users and many/most of these would rather travel to our facility with their sample than shipping the sample.	987038-987020-103832699
None, generally it was excellent and I would be happy to do all my research remotely	987038-987020-103832964
A view of the automatic sample changer (through a webcam) is advisable.	987038-987020-103841365
NO	987038-987020-103866692
absence of automated tuning&matching If something goes wrong, it is much more difficult to trouble shoot. Knowledgeable staff is required to be present by the spectrometers anyway, otherwise we may wait too long for local assistance...	987038-987020-103901122
A bottleneck is a slight delay in the connection which makes interactive phasing a bit tedious. However, taking your time/phasing slowly alleviates the problem. Other than this, no problems were identified during my use.	987038-987020-103912490
Unwanted change of samples in the sample changer by other users.	987038-987020-103914070
Clearly the position(s) of the sample(s) in the 'sample changer' is crucial and it may represent an issue during an intense and combined 'direct'	987038-987020-103933631

and 'remote' usage of NMR spectrometers. The related problems can be avoided by people awareness, by respecting a pre-established protocol for handling the NMR samples.	
Very time consuming.	987038-987020-103933604
no	987038-987020-103945877
The main problem, by far, was convincing our IT department to open the ports necessary to access the spectrometers. It took us years to convince them that this was safe.	987038-987020-103947685
Auto sampler and auto tuning would be beneficial.	987038-987020-103971664
Develop secure, reliable and inexpensive software for usage	987038-987020-103971785
For my home institution there were no bottlenecks.	987038-987020-103989826
I have no experience with an NMR facility outside my home institution.	
Remote access was mostly for monitoring experiments set up in person (i.e. not remote).	987038-987020-104005042
Interactive operations such as Phasing can be tricky due to the slower response. A fast internet connection is a pre-requisite.	987038-987020-104004509
No problems	987038-987020-104016821
Speed of Internet connections and restriction of access for multiple users. This is because I have archaic systems.	987038-987020-104030135
It's time consuming.	987038-987020-104033457
I am the head of the facility. We use No Machine for remote access, protected by a VPN. It is stable and it works well. So far, we imposed no restriction of access. The main problem is the lack of control of many no expert users using the remote access to copy datasets. We are considering restricting the access.	987038-987020-104033656
Software issues that arise when no one is around to resolve	987038-987020-104036011
Lag on the internet connections was the main issue. Nice computers with good graphic cards and top quality internet connection will help.	987038-987020-104036746
Unable to perform hyperpolarization experiments remotely. Operation of hyperpolarization infrastructure is manual.	987038-987020-104036834
The critical point is regarding the internet connection, it depends from the building where the facility is located	987038-987020-104039216
data protection issue	987038-987020-104051197
The bottle neck is the sample shipment. I shipped samples under dry ice within Brazil, prices were too expensive and samples arrived at room temperature.	987038-987020-104066039
if the sample does not spin for MAS, then cannot be done anything remotely unless , we check rotors if we need to acquire reference spectra then we need to change samples manually and operate further	987038-987020-104130885

manually and operate further sometimes the software freezes when you access remotely , o better and fast computer required	
Bottleneck: Being extra carefull since sometimes the active window through AnyDesk in reality stuck and the command hasn't been applied.	987038-987020-104215034
In Canada, we have national facilities in Edmonton and Montreal that have worked well for years. They have technical people who will run your requested experiments although I prefer remote access so I can ensure all my parameters are set and make adjustments in real time.	987038-987020-104377423
less bureaucracy to get a measurement time in other facilities.	987038-987020-104381797
Primary bottleneck is not software/IT but Legal - standard contracts with clear identification over who owns what available from the outset (combination of corporate legal and university legal is a big barrier)	987038-987020-104382232
The lack of fund for international remote access is a bottleneck.	987038-987020-104392826
The remote acces by AnyDesk is just fine. The bigger problem is that we have an old instrument with manual tuning and multiple probes. Remote acces is used regardless of Covid. It is a great help to check on the measurements after work or running long experiments on weekends.	987038-987020-104382711
Only the lack of an automatic sample changer	987038-987020-104402900
Alternate remote and in-person would enhance training and facilitate transport.	987038-987020-104423415
At NoMachine there is the problem of newest log-in gets access. So people are able to shut out users. This can cause problems if people want to process at spectrometer, but next one is doing experiments.	987038-987020-104425976
Some initial setup need to be performed by host facility staff.	987038-987020-104429762
If the protein behaves well and can be frozen/thawed or resuspended after lyophilization (without precipitation), there is no bottleneck for using remote NMR spectrometers in our experience. We have started using remote access before covid. It saves time and economical resources (travel, hotel...).	987038-987020-104436599
it is better if the teams at both sites have had the chance to meet and interact often.	987038-987020-104439880
--	987038-987020-104466561
accidental interference with non-self measurements	987038-987020-104477989
Actually I like our system as it saves a lot of time, even if sometimes one has to wait a bit for the available time slot, or if the queue is longer. During my PhD I ran all NMR samples myself, which in the end was very time consuming (walking to the NMR and typing in the samples into the software).	987038-987020-104487345
I am concerned that the magnet is correctly calibrated, configured and working properly when the samples are to be analyzed. I am also concerned about the conservation and/or preparation of the samples.	987038-987020-104486977
The main bottleneck is the diversity of software platforms that could possibly be used for remote access. The phasing out of the native support	987038-987020-104494482

<p>In the Bruker Topspin is a serious drawback, as one cannot maintain the old versions of Topspin [supporting the reemote access directly], as there is a requirement for the new versions of the acquisition software, that follows the new trends in pulse programming, bugs correction and firmware updates.</p> <p>In my view, the client-server architecture of the Topspin remote access was an advantage and should be re-implemented.</p>	
<p>Sample preparation:</p> <ul style="list-style-type: none"> -Special conditions: buffers, salt. etc -high number of samples -Weighting samples 	987038-987020-104501448
<p>Changing solid-state samples is an issue, in particular if experiments are to be run using very fast MAS. This is because of limited number of 1.3 mm rotors (price!) and also because samples have to be loaded manually into the probe.</p>	987038-987020-104504200
<p>As a user I did not perceive difficulties during times in which the spectrometer functioned normally. Using Topspin software via TeamViewer proved no problem. Some people managing the NMR computers were however concerned about misuse/ accidental deletion of data.</p> <p>However, during times when the cryoprobe we are using was defective/ in repair, automatic tuning/matching was not implemented for the replacement probe, therefore measurements of samples of different composition via the automation and remote access was no longer possible.</p>	987038-987020-104569325
<p>Lack of auto tuning and matching in solid state</p> <p>Some manual Processing e.g. Phase correction (screen lag makes it difficult to fine adjust)</p>	987038-987020-104572895
<p>I did not have problems in using remote access to NMR spectrometers, I received an excellent assistance. How feel not comfortable in performing NMR titration experiments because there is too much sample handling. I believe remote access is perfect to run long lasting experiments.</p>	987038-987020-104578649
<p>If the sample changer doesn't work anymore, remote access doesn't help, so I need to go to the spectrometer anyway.</p>	987038-987020-104606871
<p>Sample stability is a big concern. Most of my samples have to be freshly prepared and cannot stay for long periods at RT (>72h)</p>	987038-987020-104619504
<p>air bubble inside the nmr tube, somebody needs to be at the spectrometer in case having this problem</p>	987038-987020-104650540
<p>Navigating vnc port setups, ssh connections, tunnels, firewalls etc is not for the beginner!</p> <p>Equally, I'd be concerned to let inexperienced users loose remotely without supervision. The potential to get something wrong due to network lag, or a small screen size, is higher than physical presence next to the spectrometer.</p>	987038-987020-104652020
<p>I have been doing NMR for the past 42 years, at the start on</p>	987038-987020-104651420

<p>100 MHz and then during a 3 year postdoc in the Netherlands on the Groningen 360 MHz in Rob Kaptein's lab and then on the 500 MHz on the Netherlands facility in Kees Hilbers lab in Nijmegen Shimming and collecting myself. Then I used a 500MHz at Yale which was a home built spectrometer and moved to doing more crystallography due to the size and correlation time of the complex. Worked with students on the MRC NMR spectrometers to solve several protein complexes in the HIV area where we made the samples and let the expert spectroscopists shim and record spectra as well as use the Utrecht NMR EU facility with local experts recording and the same in B'ham at 900 MHz them.</p>	
<p>Kinetic studies almost impossible via R-NMR.</p>	<p>987038-987020-104652171</p>
<p>Sample readjusting (in the shigemi or the magnet) is not possible.</p>	<p>987038-987020-104673241</p>
<p>Perhaps engage with a specialist shipping company that would serve universities, be well versed in what these samples entailed - are simple to use as there is some form of agreement governing their use so arranging the shipment is seamless. I would like it to be as simple as ordering a takeaway but you know the sample will be delivered same day to an NMR centre.</p>	<p>987038-987020-104674153</p>
<p>for routine air/moisture/temperature stable samples i do not see any bottlenecks. However my samples are air/moisture sensitive and frequently only stable at lower temperatures and therefore i like to run samples myself, and in as shorter time as possible to get the best data. I dont think it is possible to get any quicker than the computer directly at the machine. For those that are more on the stable side, it is handy to be able to add additional experiments remotely</p>	<p>987038-987020-104678345</p>
<p>Samples being removed from sample changer carousel by other users and/or technical staff</p> <p>If spectrometer does not have, or if sample is unstable or time critical, clearly user must be physically present at spectrometer</p>	<p>987038-987020-104679564</p>
<p>-Stability of connection (most likely at the own end)</p> <p>-sometimes incompatibility of typing languages/keyboard settings</p>	<p>987038-987020-104680024</p>
<p>Over time, Topspin slows down and becomes impossible to use with Remote Desktop for the spectrometer running Topspin 3.6 and Windows 7. No problem with Topspin 4.2 and Windows 10.</p>	<p>987038-987020-104679345</p>
<p>I believe remote access removes bottlenecks rather than creates them and would not want to go back to pre-covid days when we did not have remote access to our spectrometers.</p>	<p>987038-987020-104700377</p>
<p>software issues--handling is less "smooth" than direct operation at the console computer</p>	<p>987038-987020-104712621</p>
<p>Overall, it's OK and possible to do for an experience user.</p> <p>it's very useful to have a facility manager on the site in case any network/hardware problems.</p> <p>tuning could be quite painful and slow sometime</p>	<p>987038-987020-104731960</p>

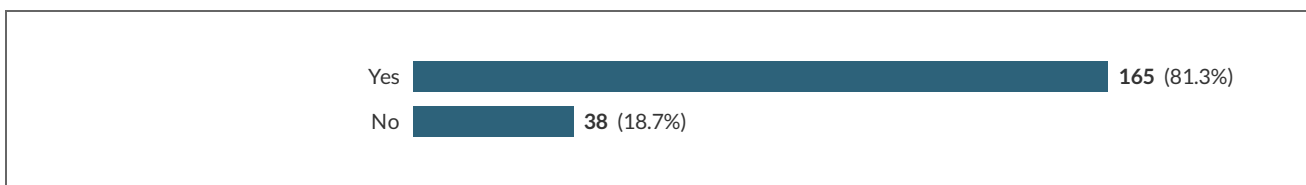
tuning could be quite painful and slow sometime.	
it's relatively easy to do a standard setup but it's difficult to do anything more complicated (e.g., a new pulse-sequence setup, etc).	
big screen on home computer is definitely a benefit.	
Occasional drop outs which require being in the facility to reset the remote access software.	987038-987020-104737700
the reactivity of the graphical interface and mouse sensitivity can be slow or badly controlled in remote accesses.	987038-987020-104742070
Bandwidth to download the data	987038-987020-104844176
At my non-home facility, remote access was indeed not available then. Fortunately, covid restrictions were already lifted and I could go to the spectrometer to further set up experiments.	987038-987020-104858892
operating lagtime during the remote connexion	987038-987020-104858091
Assistance needed for changing rotors and starting the spinning for newly packed rotors (all rotors should be spun before running experiments to ensure good spinning)	987038-987020-104874197
Remote access could be improved by the availability of automatic sample changers for all kinds of NMR tubes and MAS rotors. Furthermore, as many NMR probes as possible should contain motors to have to possibility for remote or automatic tuning and matching.	987038-987020-104884554
Some equipment problems cannot be solved remotely. Sometimes the network can be unstable.	987038-987020-104890370
For a routine usage I do not see any barriers but for the measurements regarding scientific research one should work on site with the technician	987038-987020-104903762
In our lab, the fragile VPN connection makes things a bit more complex. At the remote IR-RMN Lille site, the engineer was there to help.	987038-987020-104929943
Sometimes you dont have access to the probe especifications when you operate the spectrometer remotely. It would help to have access to the safe limits values to operate the probe.	987038-987020-104987098
The already discussed ones	987038-987020-104995386
Internet connection might be unstable or might cause some lag causing issues (also quite dangerous) in the set-up	987038-987020-105004542
Complicated in terms of secure access. Vnc gives best performance but must be run via a vpn.	987038-987020-104995202
Verification of sample state (optical check for precipitate, color) Network reliability, in particular from home and if high network load on campus due to live streaming of lectures during the pandemic remedy: reserved bandwidth, network separation from streaming network	987038-987020-105024523
The main thing is that you do not see the things going on in the lab. So when people walk close to the magnet, activities going on, temperature drop etc etc. Of course a camera can help but this is not workable on all systems. Systems need to be up to date. For example, we work with an attached	987038-987020-105024937

<p>apparatus to our Bruker 600 which does not (yet) allow upgrade of the CentOS 5.9 operating system. This means that old web browser won't work, anydesk is not operational at this version and teamviewer can handle older systems connect to newer ones. Same is true for an inova500 system. The NMR part works perfectly providing high ranked papers but the operating system is old ... very old</p>	
<p>Automatic sample changers should be present in all the spectrometers with the possibility to store the sample refrigerated.</p>	987038-987020-105005282
<p>At the moment the system used required a physical login to the spectrometer computer. This require a site visit or passing on login details to a staff member which compromises security.</p> <p>A method of securely logging in from a remote location would greatly aid the utility of the remote access whilst retaining security.</p>	987038-987020-105046974
<p>Anydesk on the spectrometer (linux OS) sometimes stops working and has to be manually restarted by someone with superuser privileges.</p>	987038-987020-105055804
<p>Based on my experience with a remote desktop, I do not need any improvement</p>	987038-987020-105056889
<p>Poor performance of the remote connection apps.</p> <p>Sometimes, the console or PC should be restarted and, consequently, the remote connection is lost.</p>	987038-987020-105087822
<p>Issues with "only" seeing the computers interface with the instrument. For example He and N2-Levels are not part of the software, air-flow rates for cooling are sometimes inaccurate, samples have been stuck in the sample changer. Maybe the addition of webcams might help (at least for some issues).</p>	987038-987020-105197740
<p>I am happy to run all my own experiments, however I would prefer if all our NMR spectrometers had Teamviewer.</p>	987038-987020-105235641
<p>The quality of remote access to research infrastructures heavily depends on the quality of the person who supports the access locally (staff/facility manager).</p> <p>I have mixed experience with access in Lyon (little support) and good experience in Grenoble.</p> <p>Making sure that a person locally feels in charge of the experiment is really crucial.</p> <p>Moreover, I find it really important that a good library of experiments is available. For example, NMRLib (solution and solids) is a good basis, in my opinion.</p>	987038-987020-105235200
<p>The biggest bottleneck is of course a spectrometer that is not able to auto tune and match.</p> <p>And if you're not measuring via automation with a sample changer, you have to put the sample into the spectrometer at least.</p> <p>There are no further suggestions in these cases.</p>	987038-987020-105359436
<p>Hardware changes (VT, tuning/matching, MAS control) were either not possible remotely or considered too risky (no-one around if something goes wrong)</p>	987038-987020-105428768

goes wrong).	
Remote sample loading/removing is due to special sample handling requirements not an option.	
No bottlenecks, what it would be nice to have an autosampler in other instruments	987038-987020-105433478
The limitation comes from the fact that the network must be opened to external users.	987038-987020-105704489
A stable connection was not always guaranteed in my own experience. I used VNC. Then I had to pop into the lab and re-establish the connection.	987038-987020-106138336
When spinning the sample, it is nice to be able to hear the spinning.	987038-987020-106146312
None for the present low-field applications, for high-field solid-state NMR experiments it is important to have video monitoring to avoid physical problems with sample spinning etc.	987038-987020-106148495
The bottlenecks are connected with the use of old instruments and the lack of autosample changers. Moreover, beside the optimization of the remote access, one technician should be around for every "strange" possible situation	987038-987020-106373721
Sometimes, lags made it impossible or at least very difficult to work. Small laptop screen size was a nuisance and kids on top of my head provided a new layer of difficulty.	987038-987020-106588677
Company IT security policy is the major obstacle	987038-987020-106801443
Software issues, Remote Desktop Connection does not work well with IconNMR, it freezes and crashes.	987038-987020-106803889
loss of flexibility. You usually have to write a proposal, wait to get it approved (even if that is rather unbureaucratic), send a sample, get the data. It is OK for routine stuff, but you cannot quickly try something.	987038-987020-106835847
A good, simple and efficient shipping procedure should be developed for scientific samples delivery. And a good guidance at the facility by staff is always appreciated/needed for remote users. A dedicated (experimental) experienced staff should be hired at each university/ facility, the work should not be given to existing PhD students or postdocs with non-direct experience, wherever the remote access is allowed for external users. This, otherwise, will result in time experimental wasting or non-conclusive NMR research, especially for non-NMR experts, which is currently mostly the case when measuring at different facilities, as per my personal experience. Otherwise, I am in very favor of remote NMR. It is exceptionally useful for the researchers especially from the developing countries, who does not have a in-person access to high tech NMR instrumentation.	987038-987020-106870635
Insertion of samples if no autosampler. Tuning and matching probehead if no automatic device present	987038-987020-106968186

normally you see only the desktop of the spectrometer computer but if samples are not correctly lifted into the magnet or you have other issues with the sample case you are lost if possible some kind of video control to see the sample case or magnet could improve trouble shooting	987038-987020-107009335
If problems come up with the sample changer (that happens quite often with our nmr) you are not able to eliminate the defects on a remote way. You would need a camera to supervise the operation of the sample changer but that is a problem in Germany because of forbidden work control/surveillance and you can't help a sample which is sticking in the tube anyway if you are at home.	987038-987020-107339769

20 Are you continuing to use remote access to NMR spectrometers now that some/many/all 'pandemic' restrictions have been lifted?



21 If you have further information that you would like to provide, please enter this in the text box below.

Showing all 42 responses	
Remote access is an excellent option. Works great with liquids where ATM and sample changers are available. For solids, usefull for long studies (multiple experiments) with a single sample.	987038-987020-103901122
Although I don't have much experience working remote I think that it's beneficial in many ways and should be encouraged.	987038-987020-103912338
Remote NMR access is a great thing, even if it is more or less a by-product of the COVID-19 pandemic. It simplifies both office/lab work and work-from-home. However, I think that sooner or later, users will run into problems with either the hardware or experiment setup. Good troubleshooting support is therefore necessary.	987038-987020-103912490
no	987038-987020-103945877
It would be better to have possibility to take NMR spectra ourselves then to use the service, which is currently the only option	987038-987020-103949594
R-NMR is a great idea, specially since less time is wasted for travel so you can be more efficient. But for newbies in the field it might be less educative.	987038-987020-103971664
For me Remote working is now the norm.	987038-987020-104004509
pointless survey	987038-987020-104008044

None	987038-987020-104016821
High time remote access for NMR users is sorted. So well done for doing this survey and thinking about remote access NMR. Good luck with your initiative.	987038-987020-104030135
There should be a visible indicator of the queue line that you should expect if you submit a project to a given NMR facility. Like that you could chose the facility in function not only of the field and experiments that you want to perform, but also control better the time-window to have the experiments done.	987038-987020-104036746
/	987038-987020-104042865
I think remote access is a good idea and I would be keen to see this installed in my working institute.	987038-987020-104069999
Looking forward to have remote acces to the NMR spectrometers of my facility. This project is really needed.	987038-987020-104237975
The 700 MHz that I use is on the 4th floor and my lab is on the 3rd floor. If my sample is already in the magnet, I will use remote access every time from the comfort of my own office!	987038-987020-104377423
Thanks a lot for presenting such a facility.	987038-987020-104397267
Would this be internationally available?	987038-987020-104421282
some of my 'remote access' occurs through the shipment of sample+student	987038-987020-104424796
I am aware of remote control software but never used in NMR. The idea of remote-NMR is wise.	987038-987020-104437114
--	987038-987020-104466561
My group also does X-ray crystallography or SAXS at synchrotron facilities.. remote access is a very good option once it is properly set-up. It is, however, still crucial, to have a contact person on-site - often to get started or in case there are some truly mechanical issues that require human intervention.	987038-987020-104467387
Another advantage of the remote access only-one-person-is-in-charge procedure in my opinion is the limited access of less-frequent NMR users, which limits poential problems by wrong usage of the machines. Only experienced users, who regulary go to the NMR, should really use it.	987038-987020-104487345
I would prefer to use remote access most of the time.	987038-987020-104485771
It would be good if quality control and process traceability protocols were integrated and standardized. Including for example things such as the naming of the experiments, names assigned to the samples, file formats, etc.	987038-987020-104486977
no	987038-987020-104578649
There are two problems that I would like to use the highest fields at 1 GHz to solve as I need the dispersion for these DNA systems. They are part of a DNA-protein complex for which we wish to study the DNA component in solution as so far we have not been able	987038-987020-104651420

<p>to crystallise them - and anyway we would like to see them independent of the crystal lattice</p>	
<p>In fact, we are currently not routinely run our own experiments but we are very much interested to do so in the future. Currently, we send the samples to our partners and get back the spectra for further analysis. Some of our lab members, however, have some experience in the setup of biomolecular NMR measurements and we would welcome any future possibility of remote use.</p>	987038-987020-104673945
<p>I mostly use NMR for synthesis reaction/purity control, so most of the time I measure samples immediately parallel to working in the lab, therefore remote measuring is not really necessary for the workflow (as we can't work anyway if we don't get results fast). What we have is remote access to all NMR-results which is really great.</p>	987038-987020-104673898
<p>The remote option of NMR device would be better for my studies, even if I did not used in-person. I am encouraging to build an infrastructure about R-NMR. Cheers.</p>	987038-987020-104682518
<p>The choice of "remote access" has nothing to do with Covid-19 but is bare convenience because it is possible to fill waiting times (inevitably with NMR) with other work</p>	987038-987020-104712621
<p>Remote access in our facility in Leeds, UK was initiated during the pandemic, but has since proven extremely useful. In particular, the ability to set up and run experiments/change samples at anti-social hours from home has been very helpful.</p>	987038-987020-104737700
<p>I believe that remote access will solve some or probably a lot of problems. This approach is fine for NMR users. But, R-NMR should not stop the ability of NMR experts to visit European Infrastructures. This process gives the opportunity to the NMR experts to meet and exchange their thoughts on problem solving.</p>	987038-987020-104737415
<p>The spectrometers that I have used have been piloted by the local team, my input in the experiments performed has been limited to discussing the type of results desired and debating the advantages or disadvantages of different techniques and the required samples.</p>	987038-987020-104850009
<p>Independent of pandemic restrictions, I regard remote-NMR as a very helpful possibility for an effective use of working time. It is possible to work with (more than one) spectrometer with the own workstation in the office or at home and simultaneously deal with other work. We used remote-NMR already before Covid-19.</p>	987038-987020-104884554
<p>for basic science one should allow the access with the expert technician</p>	987038-987020-104903762
<p>Reference spectra help for less experienced users - just copy the directory, and adjust p1 and spectral widths.</p> <p>Changing samples is always a bit of a worry - if problems with the SampleJet, you are stuck.</p> <p>Don't leave the guacamole on in your office - you can only log in once!</p>	987038-987020-104929943
<p>Remote access is great for monitoring and setting up simple sequences, but the physical presence has a huge benefit when it involves hardware-related things and troubleshooting</p>	987038-987020-105428768

related things and troubleshooting.	
The closest I got to remote access was receiving data via e-mail. But I guess that does not count.	987038-987020-105575669
None	987038-987020-105582613
Remote access is important for national, transnational instrumentation, but also a potential asset locally to ensure optimal use of time	987038-987020-106148495
Remote access is great, difficulties can be overcome.	987038-987020-106588677
<p>Direct remote access is like being there yourself. However, it is often prohibited due to IT-security concerns (and those concerns are of course justified). Access through others is not like being there yourself, the possibility of experimenting with the spectrometer is lost. Then, remote NMR (outside my own university) is good for larger routine measurements (e.g. running all experiments necessary for protein assignment), but not for trying something new.</p> <p>Remote NMR does not replace a local NMR, but the local NMR can be of lower field strength, and the remote NMR of higher field strength.</p> <p>Remote NMR must be free of charge, otherwise no one will use it.</p>	987038-987020-106835847

APPENDIX 3

Remote-NMR (R-NMR): Moving NMR infrastructures to remote access capabilities

NMR USER SURVEY (8 January -29 March 2023)

Univ. of Oxford Central University Research Ethics Committee Approval Reference: [R77838/RE002]

SUMMARY OF RESPONSES FROM NMR USERS COLLECTING DATA WITH REMOTE ACCESS

Introduction

Lockdown restrictions in many countries during 2020-2021 Covid19 pandemic resulted in the implementation of remote access to NMR spectrometers as a way of enabling the continuation of important research. The experiences of several European NMR facilities during the pandemic have shown that this access mode can work well within the field of NMR spectroscopy. It is the aim of the Remote-NMR project to develop and exploit remote access to NMR facilities. Work Package 2 within R-NMR focusses on the "Remote NMR Landscape". Task 2.2 within WP2 is a review of NMR users' need with respect to remote access to NMR facilities; this includes aspects such as facilities used during the pandemic, level of assistance provided by facilities/would additional assistance have been useful; is confidentiality of samples/experiments important; how were samples sent; likelihood of using remote access even when there are no travel restrictions; suggestions for improvement. This information has been collected via an online survey of NMR users.

This document is a summary of the responses from the subset of 201 NMR users who completed the survey and indicated that they had used remote access for NMR data collection.

Remote-NMR: User Survey

Showing 201 of 401 responses

Showing **all** responses

Hiding question **12**

With filter **q11-is-yes-direct-remote-access-or-yes-assisted-remote-access-or-yes-both-direct-and-assisted-remote-access-or-yes-another-type-of-remote-access-please-specify-below** applied

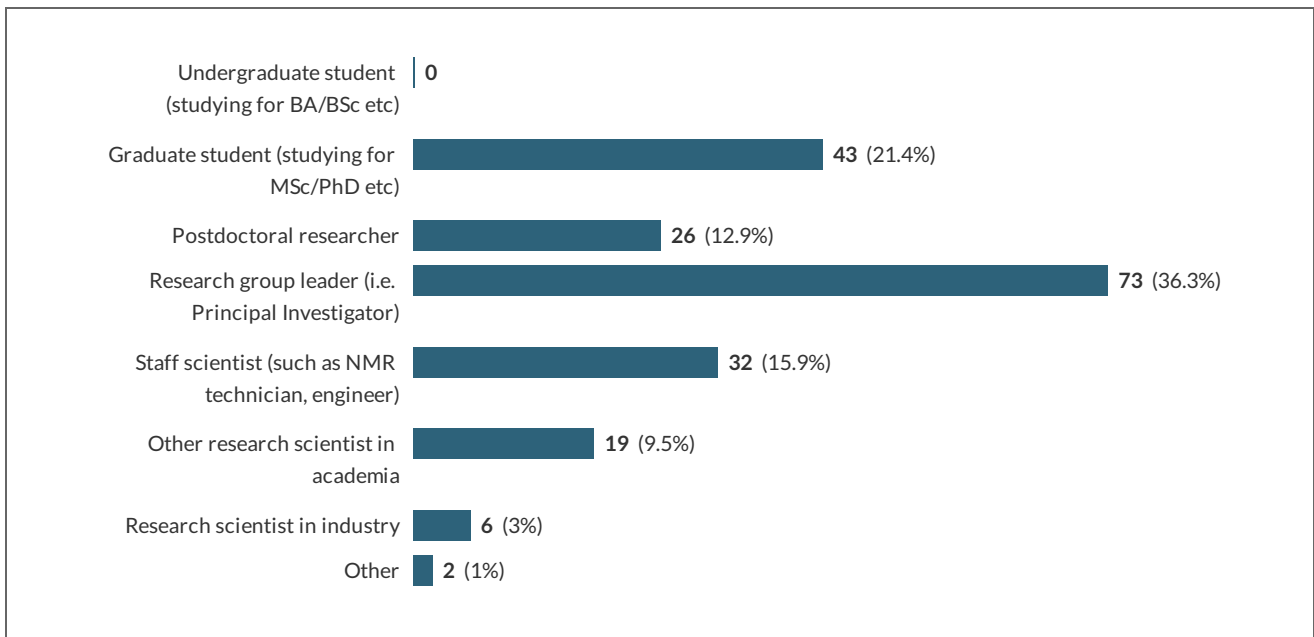
- 1** You are invited to complete this online survey aimed at users of NMR facilities. We will ask questions about the NMR facility(ies) that you use, about your experiences (if any) with remote access to NMR spectrometers and for your views on how remote access can be improved in the future. The survey will be completed anonymously (you will not be asked for your name or email address) but you will be asked to indicate in which country your NMR facility is located. Information that you provide about your experiences with remote access will be included in discussions with other R-NMR project participants and in project reports. All survey data will be stored at the University of Oxford on a secure computer (password protected and behind a firewall) during the duration of the R-NMR project (until 30 June 2025). A version of the survey will also be created for longer-term storage; we intend to keep this version for 3 years beyond the end date of the project. Please confirm that you have read this information and that you are willing to continue with the survey.

Yes  201 (100%)
No | 0

- 2** Please confirm that you are a user of an NMR facility. By user, we mean someone who actively collects NMR data. (Please only complete the survey once even if you have received the link from multiple sources.)

Yes  201 (100%)
No | 0

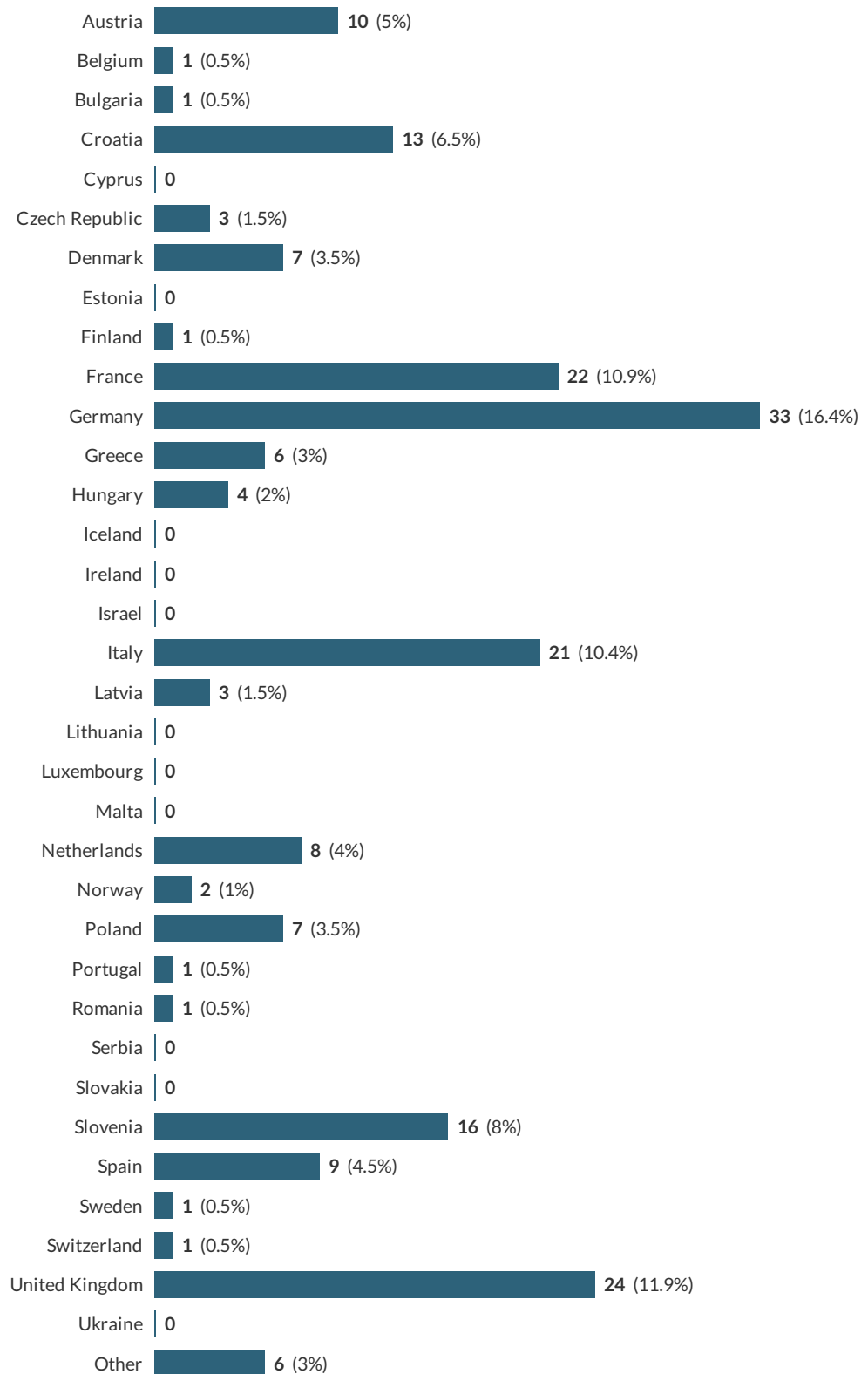
- 3** Please select the option that best describes you?



3.a If you selected Other, please specify:

Showing all 2 responses	
Research Scientist in Government	987038-987020-104036011
(Lab-)Technician	987038-987020-104772110

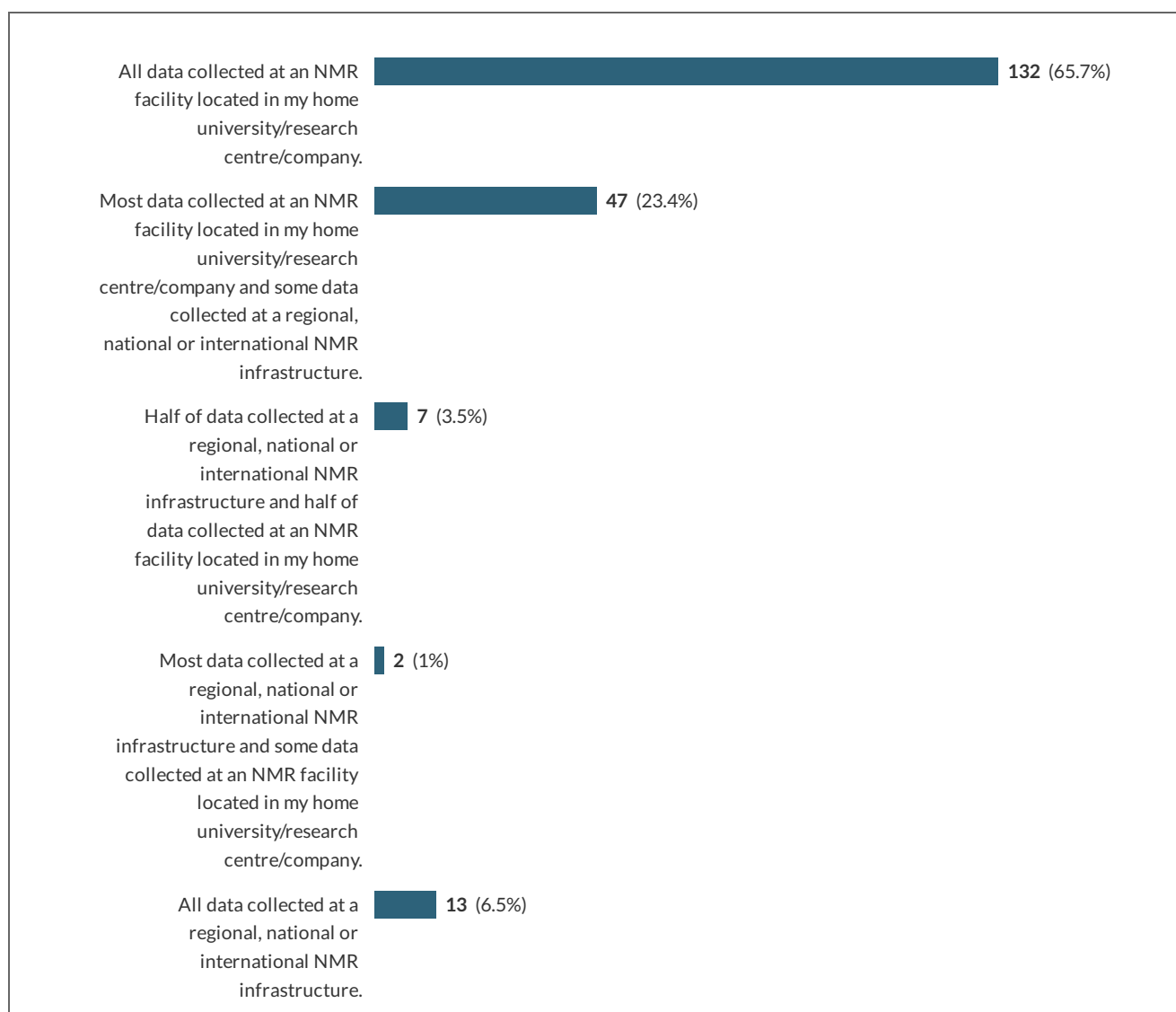
4 In which country do you carry out your NMR research? This is most likely to be the country in which you live. If you also use an NMR facility in another country you will be able to indicate that later in the survey. Select one:



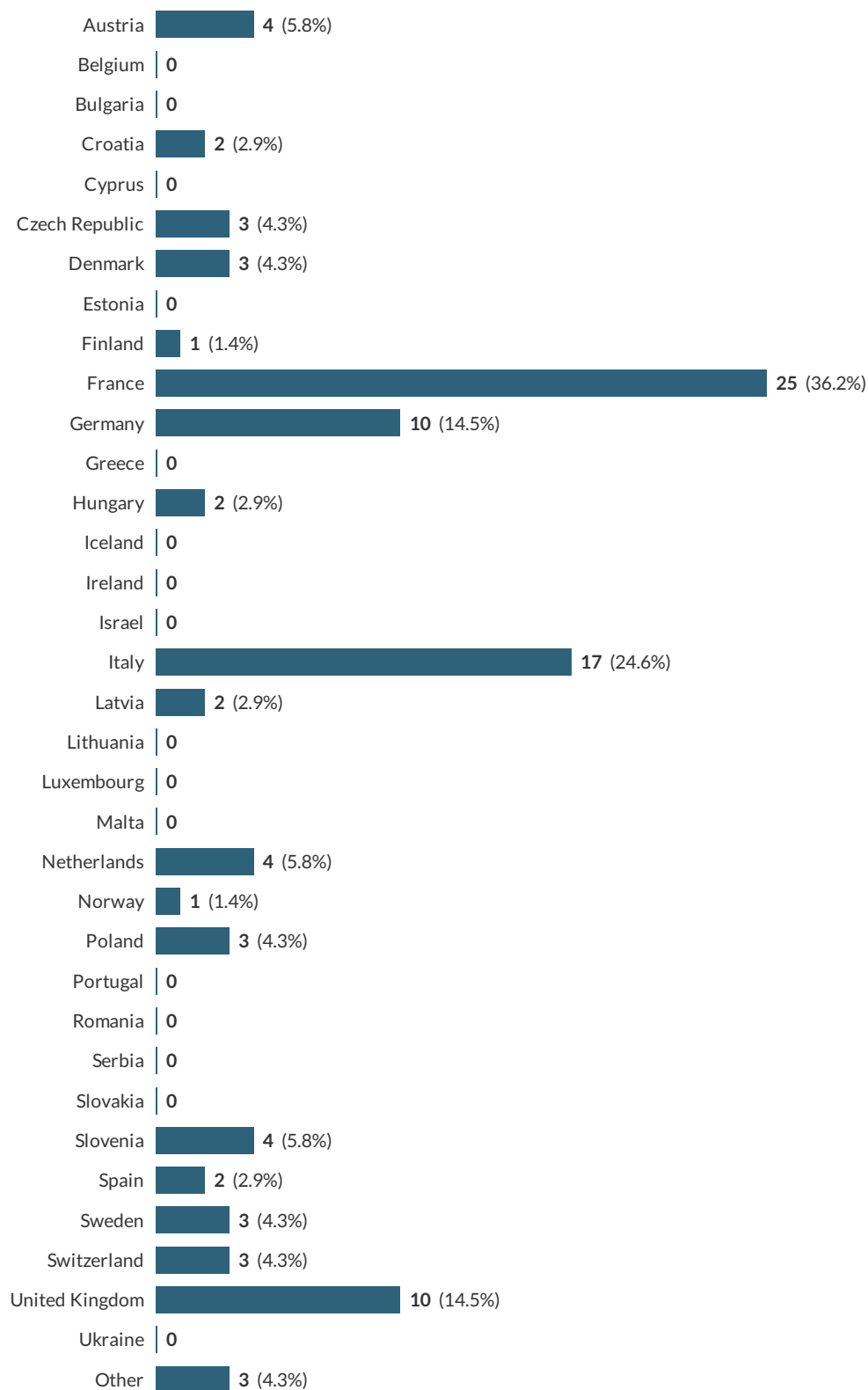
4.a If you selected Other, please specify:

Showing all 6 responses	
India	987038-987020-104033457
Brazil	987038-987020-104033656
Canada	987038-987020-104036011
Brazil	987038-987020-104066039
Canada	987038-987020-104377423
Argentina	987038-987020-104423415

5 Where do you collect your NMR data? (select one option)



5.a If some or all of your NMR data are collected at one or more national or international NMR infrastructures, instead of your local NMR facility, please specify in which country(ies) these NMR infrastructures are located. Select all that apply:

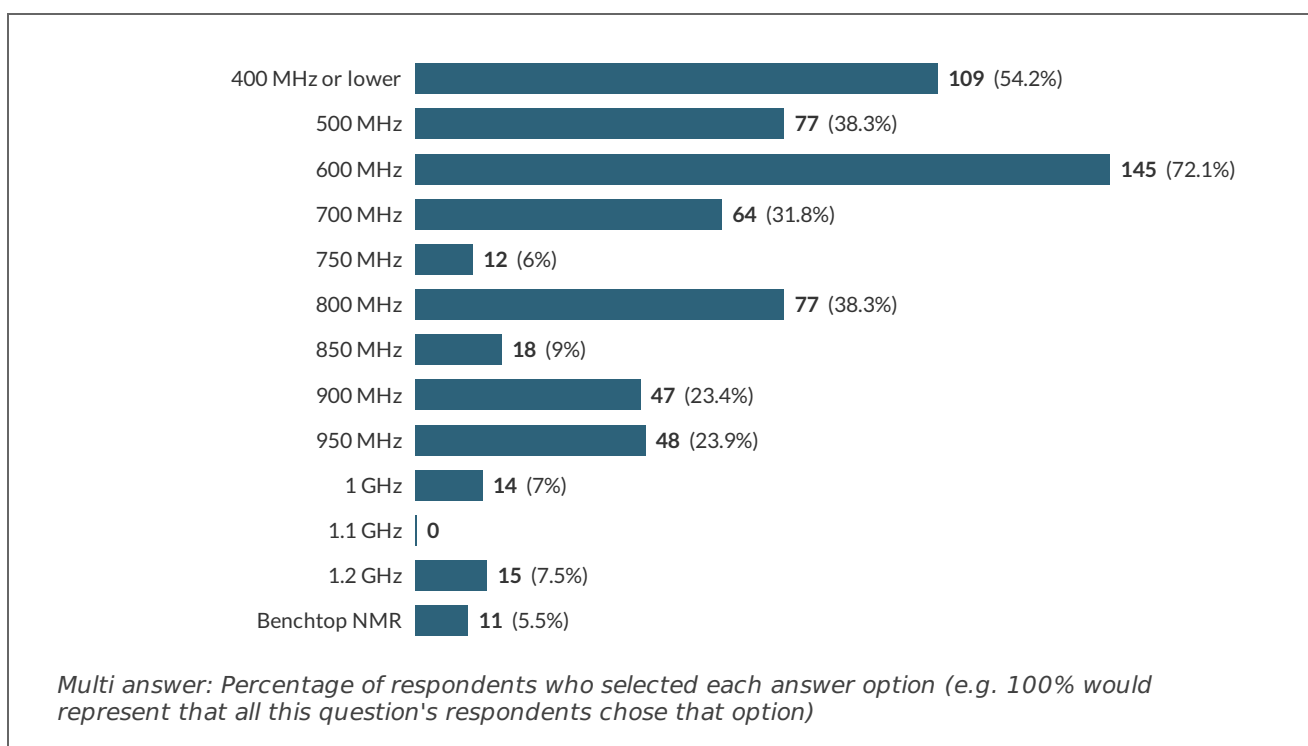


Multi answer: Percentage of respondents who selected each answer option (e.g. 100% would represent that all this question's respondents chose that option)

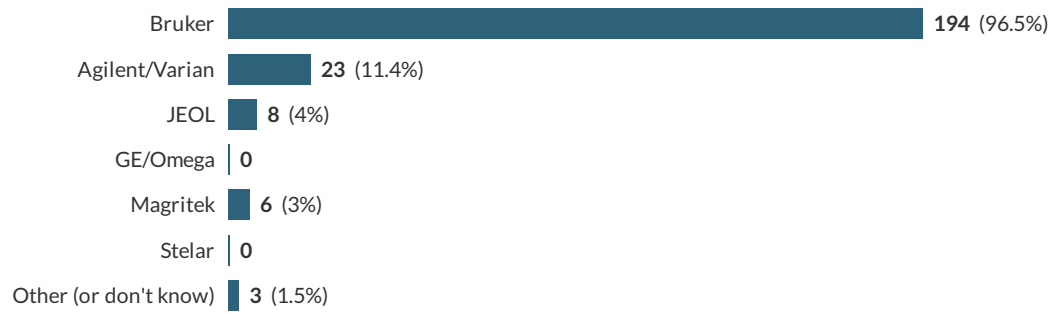
5.a.i If you selected Other, please specify:

Showing all 3 responses	
India	987038-987020-104033457
Brazil	987038-987020-104033656
United States	987038-987020-104423415

6 At what 1H frequencies do you collect NMR data? (select all that apply)



7 What type of spectrometers do you use for data collection? (select all that apply)

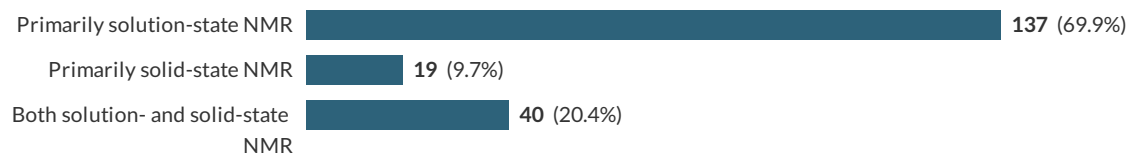


Multi answer: Percentage of respondents who selected each answer option (e.g. 100% would represent that all this question's respondents chose that option)

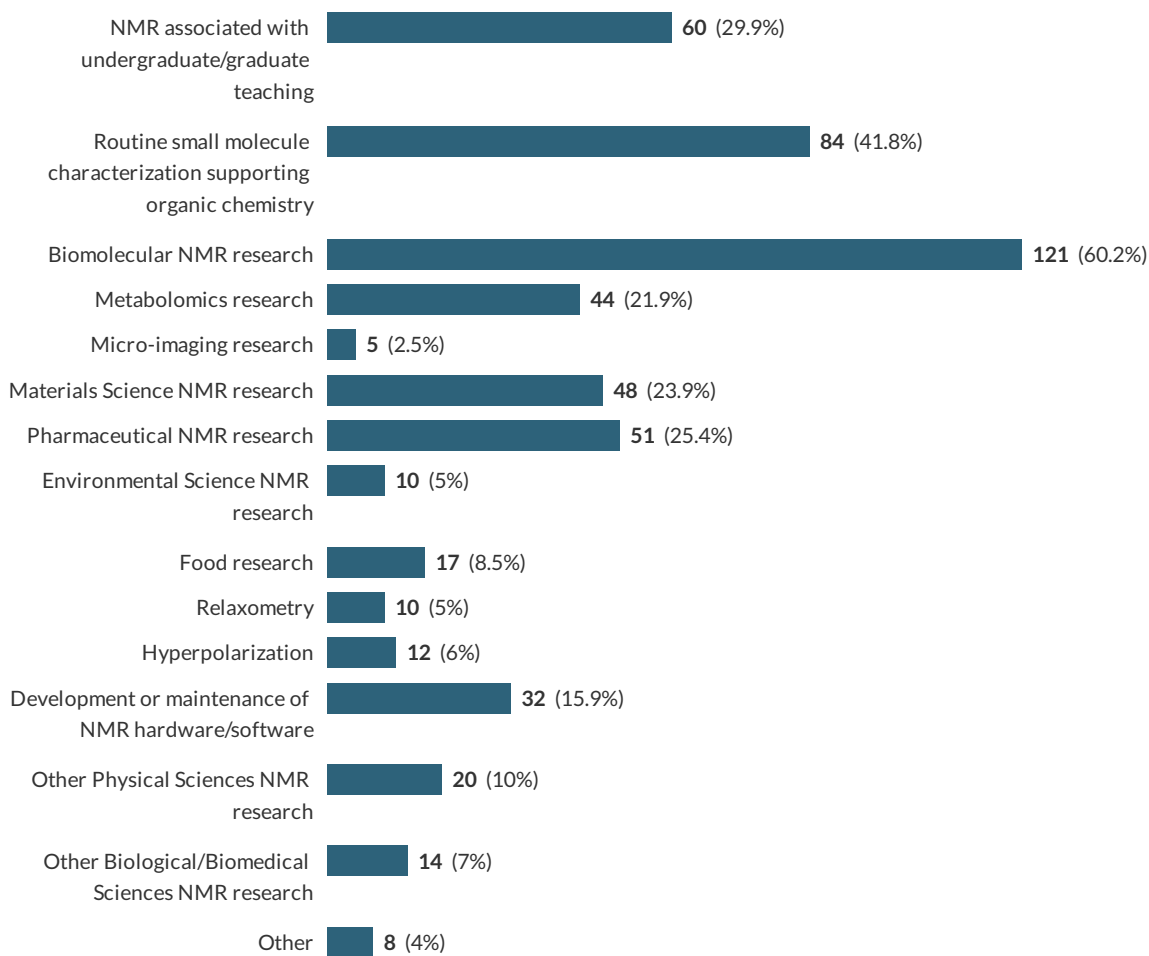
7.a If you selected Other, please specify:

Showing all 2 responses	
RS2D	987038-987020-104044047
NanoNord Tveskaeg	987038-987020-106148495

8 What type of NMR data do you typically collect? (select one)



9 What types of NMR experiments do you carry out? (select all that apply)

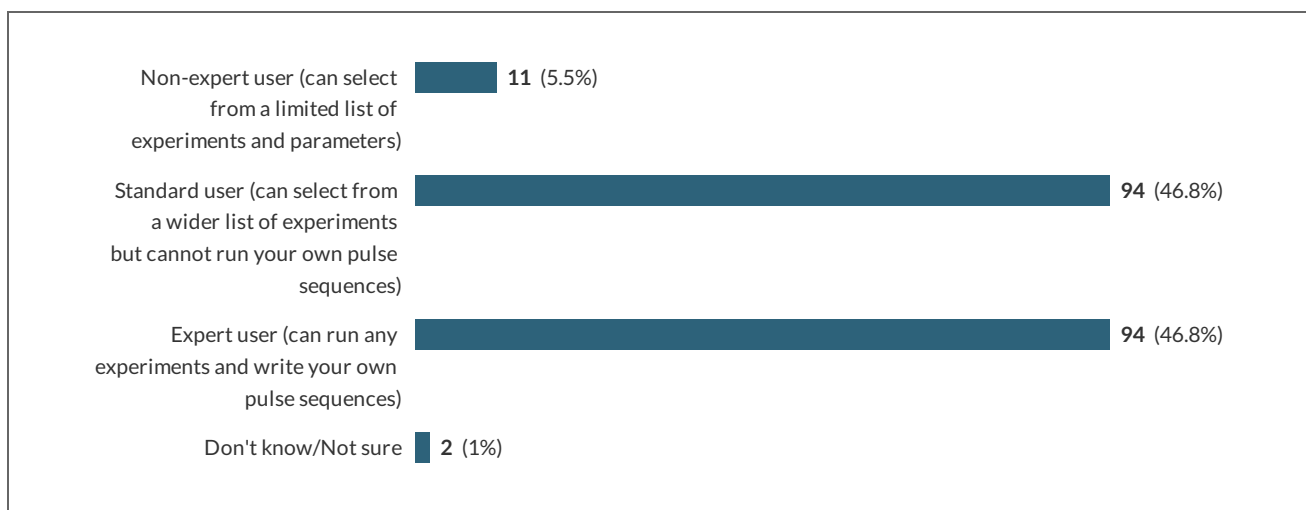


Multi answer: Percentage of respondents who selected each answer option (e.g. 100% would represent that all this question's respondents chose that option)

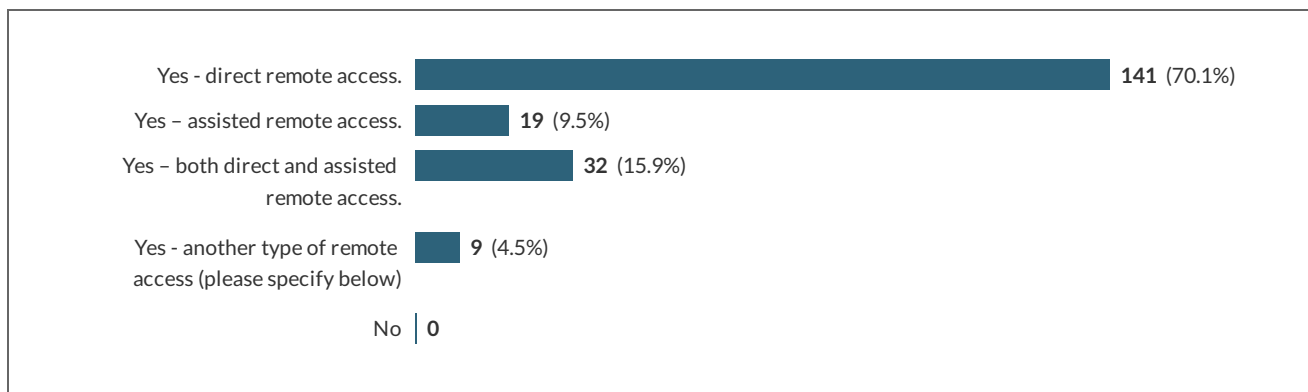
9.a If you selected Other, please specify:

Showing all 8 responses	
Structure Elucidation of Natural Products	987038-987020-104004509
Quantitative NMR of transition metal complexes.	987038-987020-104382711
Diffusometry	987038-987020-104429762
Screening	987038-987020-104641637
Routine small molecule characterization supporting inorganic/organometallic chemistry Kinetic Studies and reaction monitoring	987038-987020-104678345
Polymer NMR	987038-987020-104901512
in addition to routine small molecule characterization supporting organic chemistry, my group works on organometallic (metallocenes with Fe(II), Ru(II) or Co(III)) or metal-organic samples (with diamagnetic metals like Zn, Cd, Pd(II), Pt(II), Rh(I), Re(I), Cu(I), Ag(I)...). In addition to routine 1D 1H, 13C or 31P, we also do 2D NMR for identification. For our supramolecular work DOSY is very useful. Rarely measured paramagnetic metal complexes containing Co(II).	987038-987020-104922032
Inorgani chemistry	987038-987020-105036238

10 How would you categorize your level of expertise in operating NMR spectrometers? (select one)



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.a If you would like to provide more detailed information about your mode of remote spectrometer access then please fill in the text box.

Showing all 94 responses	
Our company shipped samples to a nearby university with listed experiments.	987038-987020-103842897
remote desktop applications (teamviewer. anydesk) or directly VNC	987038-987020-103901122
Using a home laptop to connect via a remote desktop connection directly to the spectrometer workstation. Or using my office computer to connect to the spectrometer workstation in an adjacent building.	987038-987020-103912490
remote login via vpn to the institute and through that to NMR spectrometers	987038-987020-103914070
I was accessing the spectrometer from my office above stairs, instead of operating it from its main computer in the NMR room. But it can also be done from home or anywhere that has Wi-Fi connectivity, providing you have a VPN.	987038-987020-103929106
Sending samples with detailed list of measurement information or by telephone.	987038-987020-103933604
AnyDesk in VPN mode	987038-987020-103945877
Remote access provided by TopSpin 4	987038-987020-103957208
Via locally established VPN link	987038-987020-104005042
with tight vnc	987038-987020-104009724
I sent the sample	987038-987020-104016821
The software was accessed remotely via team viewer and sample loading-unloading were carried out by the technician/students.	987038-987020-104033457
No Machine	987038-987020-104033656
TeamViewer software to access NMR computer	987038-987020-104036011
We Use a software to take control on the computer ton run experiments	987038-987020-104036680
Controlled session over TeamViewer session	987038-987020-104036746

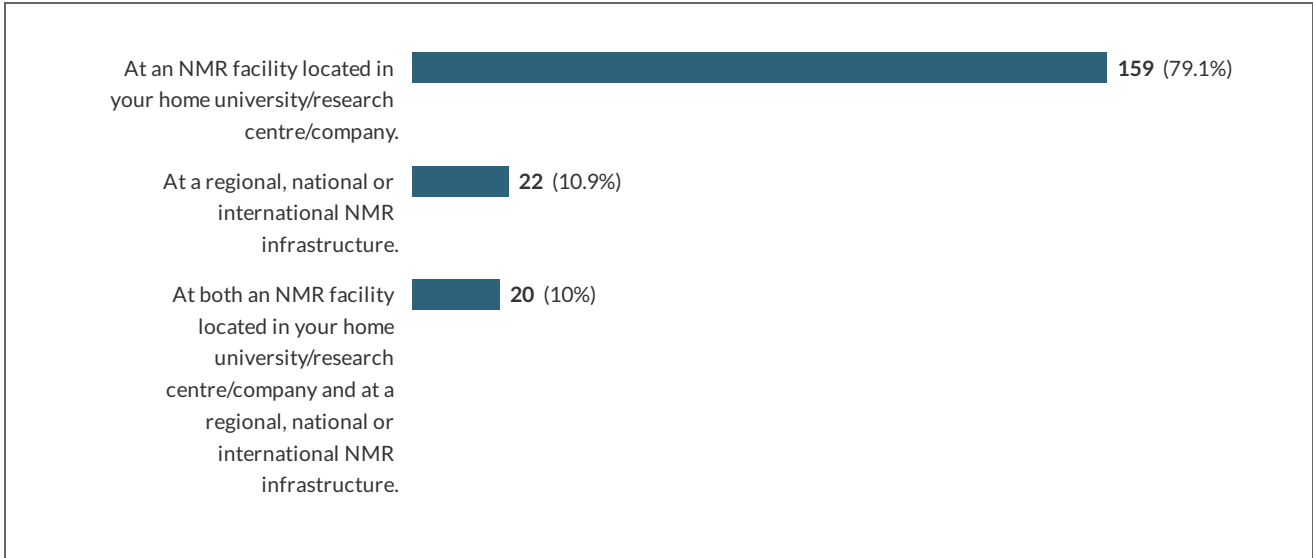
Remote access to spectrometer via ssh and VNC viewer, enables full access of spectrometers equipped with sample changers and automatic tuning and matching.	987038-987020-104036834
Anydesk	987038-987020-104038147
Teamviewer	987038-987020-104051197
I frequently operate the 800 MHz NMR instrument using Teamviewer for remote access. Usually a technician will load the sample for me, and I will do the rest.	987038-987020-104066039
I have only used remotely to see if my experiment is running fine, after that I have transferred data remotely to access it further.	987038-987020-104130885
Tuning and matching of a probe	987038-987020-104202487
Remote access only after covid-19 pandemic Access is granted by and monitored by facility manager who decides if allowed for an individual to use independently	987038-987020-104235459
Teamviewer	987038-987020-104326713
Through the built in VNC service on the linux box.	987038-987020-104377423
assisted via teams or zoom direct - vpn and ssh + X11 and then "topspin -client" or vpn + https (iconnmr)	987038-987020-104382232
I have used AnyDesk.	987038-987020-104392826
Remote desktop application.	987038-987020-104382711
We have used Anydesk to reach the NMR spectrometer computer.	987038-987020-104392629
I submitted the sample for measurement and access to the remote inside-Lan network to collect data	987038-987020-104412732
Direct remote access at Indiana University in the USA Assisted remote access at CERM in Florence Italy	987038-987020-104423415
via the AnyDesk software that enabled remote connection to the NMR computer from my laptop	987038-987020-104425268
Via Signal Logs Portal for data and NoMachine for direct access	987038-987020-104425976
Limited access using 'anydesk' software. Most of the hardware need to be setup earlier. Temperature experiments are limited if no autotune hardware is installed.	987038-987020-104429762
We access through INSTRUMENT grants. We normally discuss the experiments we need in advance and prepare a working plan. Then, we send the protein to the facility and if the local operator has questions, he/she contact us (phone/email/zoom) and we clarify the doubts. After that, we get the raw data.	987038-987020-104436599
via NoMachine	987038-987020-104438077
utilize Anydesk software to direct access to NMR spectrometers	987038-987020-104461826
teamviewer	987038-987020-104466561

In principle we have a dedicated lab technician who runs all our NMRs for us. The raw spectra are then accessed via remote access and processed individually by the researcher on his or her PC. NMR samples are being transferred to the spectrometers twice a day at given measuring time slots. In addition, night time experiments can be submitted by trained users themselves (NMR has an autosampler).	987038-987020-104487345
Access through Anydesk/Teamviewer software	987038-987020-104486977
A direct remote access has become unavailable with the evolution (sic!) of the Bruker Topspin software. The direct remote access at the user level was effectively deprecated beginning with the Topspin above ver. 3.2, and phased out with the current versions. It has complicated the remote access to the NMR spectroscope at the local facility to a great extent, now.	987038-987020-104494482
What do you mean by mode of access? If it is a question on how I access the computer from which I run NMR experiments it is either through VPN and remote desktop or through a third party software, such as AnyDesk.	987038-987020-104504200
I usually use NoMachine via a VPN	987038-987020-104541226
teamviewer	987038-987020-104568498
Prior to the pandemic we had sporadic access to NMR spectrometer computer via TeamViewer. However due to the increase of the amount of people using that access, our central NMR facility removed that access due to fear of (accidental) misuse and to keep an overview on how the spectrometer computer is being treated. The NMR facility has since been working on a more controlled alternative, but it did not materialize since then.	987038-987020-104569325
Vnc	987038-987020-104572895
I contacted the technician at the facility and we organized the set up of the experiments. To check the results, the technician uploaded the experiments on the web server and we decided how to proceed.	987038-987020-104578649
VNC over ssh tunnels, NoMachine	987038-987020-104652020
I used to have a core MRC grant but then I switched to working on systems of high MW intractable to NMR but recently wish to do NMR on nucleic acid components of the DNA-protein complexes Rusing NME	987038-987020-104651420
Remote control of NMR experiments via Anydesk session.	987038-987020-104652171
My previous remote access was via the 900 MHz NMR instrument at HWB-NMR in Birmingham. After attending for a day, setting up experiments etc I would then remote log on to monitor and set up further experiments based on the results of the initial ones. This to me was the real power of remotes access - a long block of time and interacting as if it was your own spectrometer.	987038-987020-104674153
Via Teams Login as though I was sat with the spectrometer	987038-987020-104676884
remote access to IconNMR	987038-987020-104678345
Spectrometers accessed using Chrome Remote Desktop. This has worked almost flawlessly.	987038-987020-104679564

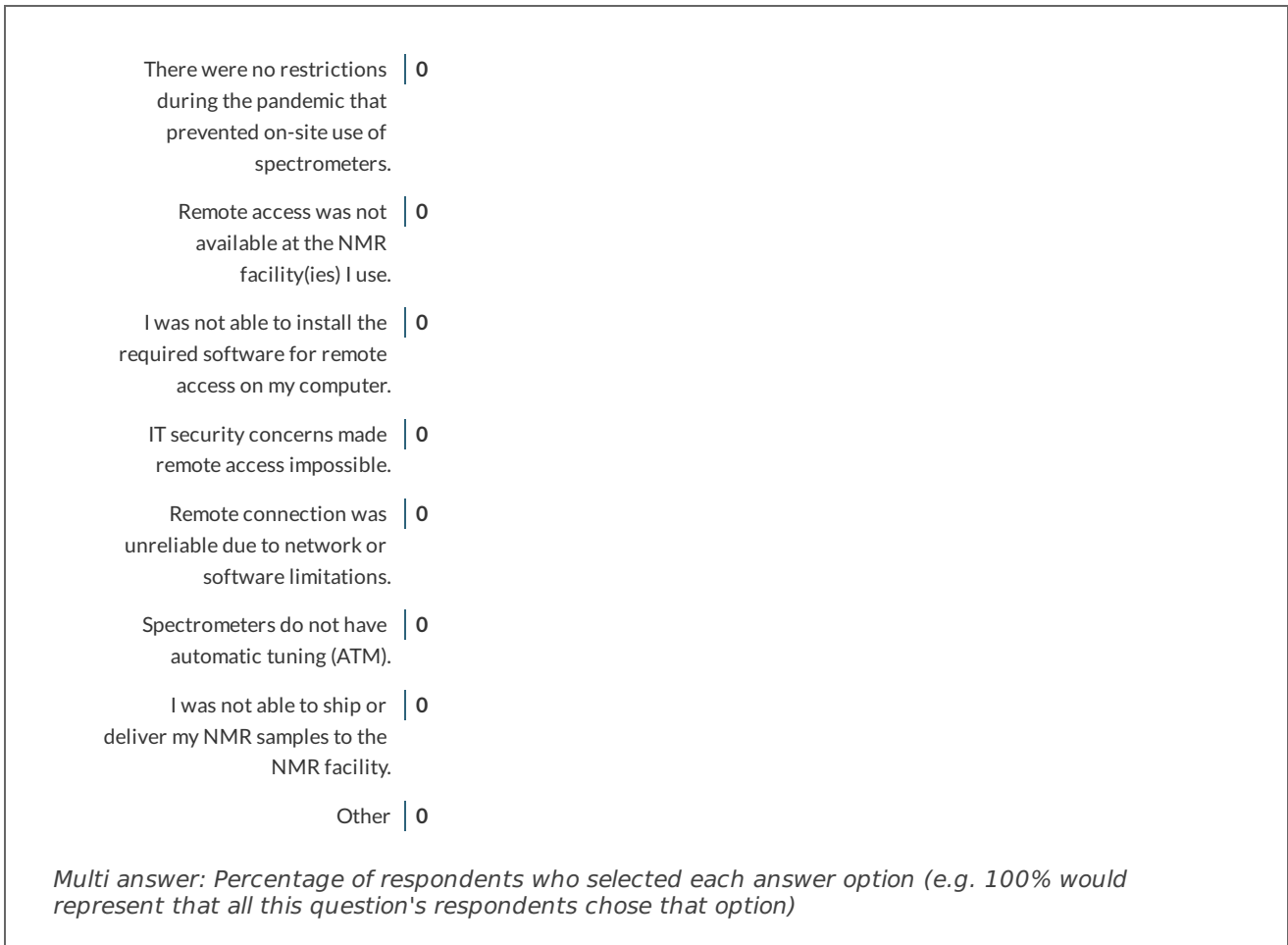
Issues: Samples being removed from sample changer carousel by other users If spectrometer does not have, or if sample is unstable or time critical, clearly cannot use remote access, user must be physically present at spectrometer	
nx client	987038-987020-104680024
VPN --> RDC to virtual computer --> RDC to spectrometer computer	987038-987020-104679345
direct remote access using vpn server	987038-987020-104731960
Use VNCViewer to access the computer controlling the spectrometer remotely	987038-987020-104737700
Using softwares such as AnyDesk, TeamViwer, NoMachine	987038-987020-104742070
From a remote Bruker session in my office while the spectrometer was in another building, 300 m away.	987038-987020-104751961
NX Client for Windows Version 3.5.0.9	987038-987020-104858091
By use of the FastViewer software	987038-987020-104884554
Use of teamviewer and ssh.	987038-987020-104891596
Remote desktop (Windows 10) with VPN, Teamviever, ICON NMR (Bruker Topspin) additionally online cameras to control the hardware e.g. sample changer	987038-987020-104890370
Leaving the samples in front of the NMR facility for routine NMR data collection (small organic molecules).	987038-987020-104911443
Well, I leave the samples at a specified place at the facility, the operator collects the NMR data, I analyze the data. I contact the operator if something is unclear or if I need a new, more specialized measurement. Not sure whether or not this qualifies as remote...	987038-987020-104922032
We can access our 800MHz via a VPN connection, including the SampleJet.	987038-987020-104929943
I used Team Viewer to operate the computer connected to the spectrometer.	987038-987020-104970631
Technicians put the rotor with sample (packed previously) and I set the experiments remotely	987038-987020-104987098
Remote connection via TigerVNC, RealVNC and TeamViewer	987038-987020-104995386
Pur NMR instrument can be accessed remotely through the AnyDesk software	987038-987020-105004542
Interaction with remote staff.	987038-987020-104995202
Zoom sessions with the persons operating the instruments; occasional attempts to use VNC fo direct interaction, but plagued with lag and connection reliability problems	987038-987020-105024523
access via vnc to the spectrometer	987038-987020-105024937

Access was usually via a VNC session on the computer controlling the spectrometer. Access was also performed on occasion using TeamViewer.	987038-987020-105046974
Anydesk	987038-987020-105041252
Remote login to the spectrometer from my personal laptop via Anydesk	987038-987020-105055804
By using a remote desktop	987038-987020-105056889
WE've already set up a remote access connection (via AnyDesk) to one NMR spectrometer located in another region of the institute. We only need to bring the samples and then can run any experiments remotely.	987038-987020-105087822
I operated infrastructure at my own research facility remotely using TeamViewer.	987038-987020-105197740
TeamViewer	987038-987020-105225587
Used Teamviewer.	987038-987020-105235641
For many years I have used VNC or similar to run experiments from home. This works most of the time very well.	987038-987020-105235200
All spectrometers are inducted to a local network and it is possible to access them via nomachine even outside of the local network via IP, PW and access file.	987038-987020-105359436
AnyDesk to control the software (pulse sequences, monitoring etc); hardware changes (including MAS speed changes, VT) on-site	987038-987020-105428768
TeamViewer	987038-987020-106146312
Grid of 30 low-field NMR spectrometers operated via robots	987038-987020-106148495
Send samples, contact via phone or email	987038-987020-106163112
We use a "remote desktop" solution that is integrated in Win10.	987038-987020-106588677
Access granted by password through firewall and further control of the instrument through Remote Desktop Connection.	987038-987020-106803889
VNC server on the NMR computer, TightVNC client on my PC	987038-987020-106835847
VPN connection to our NMR spectrometers	987038-987020-106968186
connection to X11 server installed on spectrometer computer	987038-987020-107009335
My direct remote access operates with the help of vnc. I used it already before 2020 to control the experiments from my desk in the normal laboratory and from my computer at home.	987038-987020-107339769

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



11.c Why have you not used remote access to NMR spectrometers? (select any that apply)



11.c.i If you selected Other, please specify:

No responses

11.d Do you consider sample shipment/delivery to an NMR facility to be a barrier to remote spectrometer access?

Yes		0
No		0

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

I am concerned that the NMR tube would break during sample shipment.		0
I am concerned that my sample would degrade during sample shipment.		0
My samples are air sensitive and difficult to ship via a courier.		0
I am concerned that my sample would be lost during sample shipment.		0
The cost of shipping a sample by courier is too high.		0
Customs regulations make shipping of my sample to another country difficult.		0
I am concerned about the carbon footprint/environmental impact of shipping a sample by courier.		0
Other		0

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

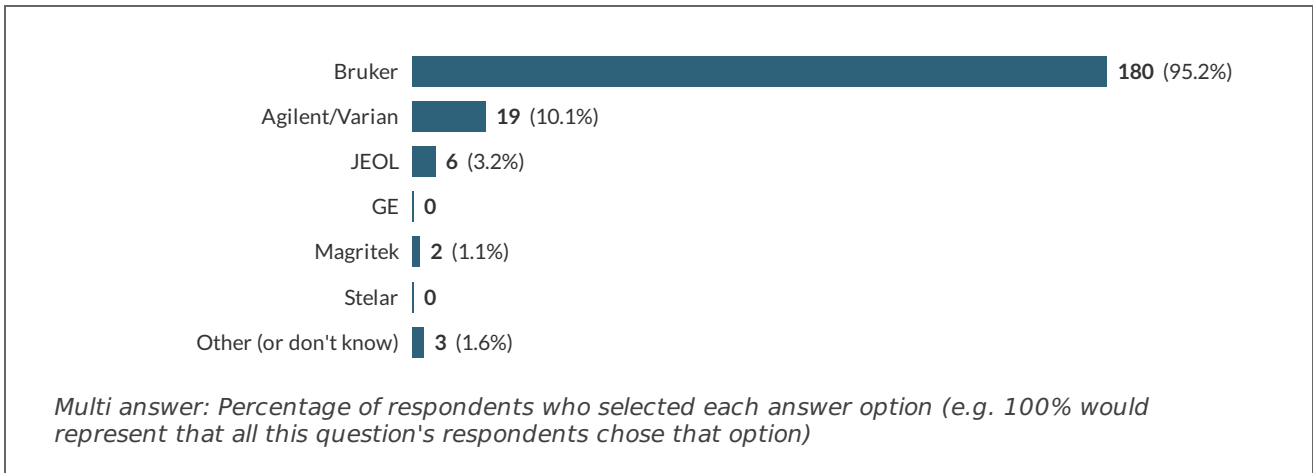
11.d.i.a If you selected Other, please specify:

No responses

11.e 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 you be interested in remote access to the spectrometers you use?

Yes		0
No		0

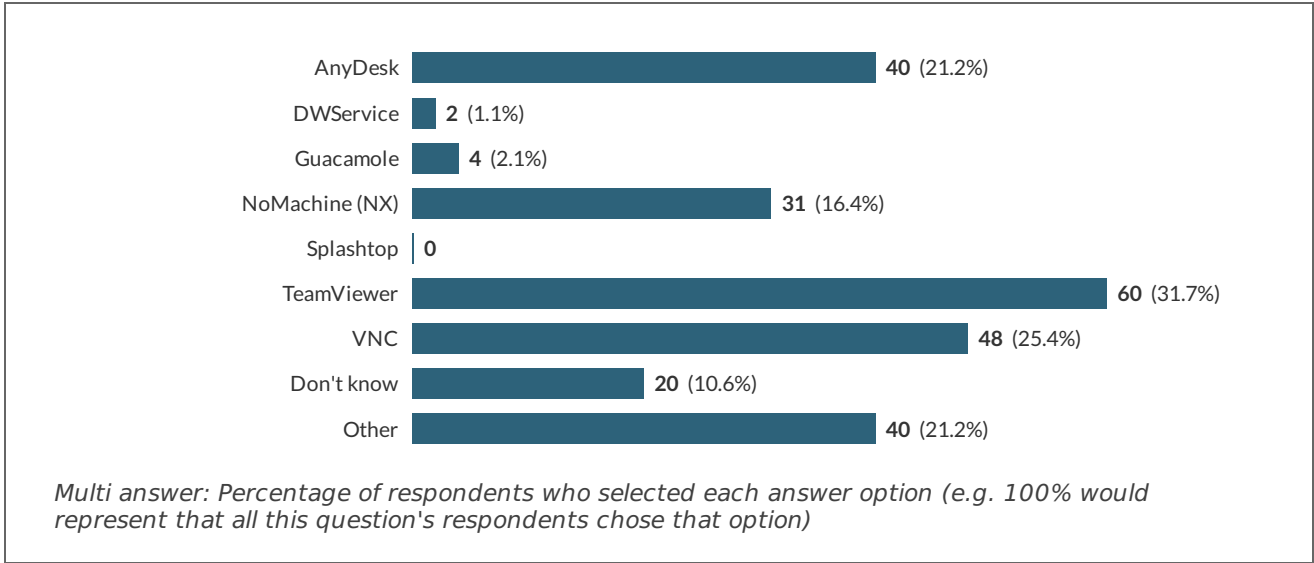
13 What type of spectrometers were available for remote access? (select all that apply)



13.a If you selected Other, please specify:

Showing all 2 responses	
RS2D	987038-987020-104044047
NanoNord Tveskaeg	987038-987020-106148495

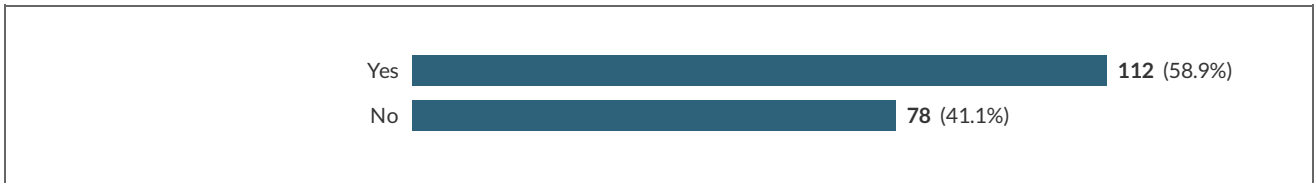
14 What software was used for remote access? (select all that apply)



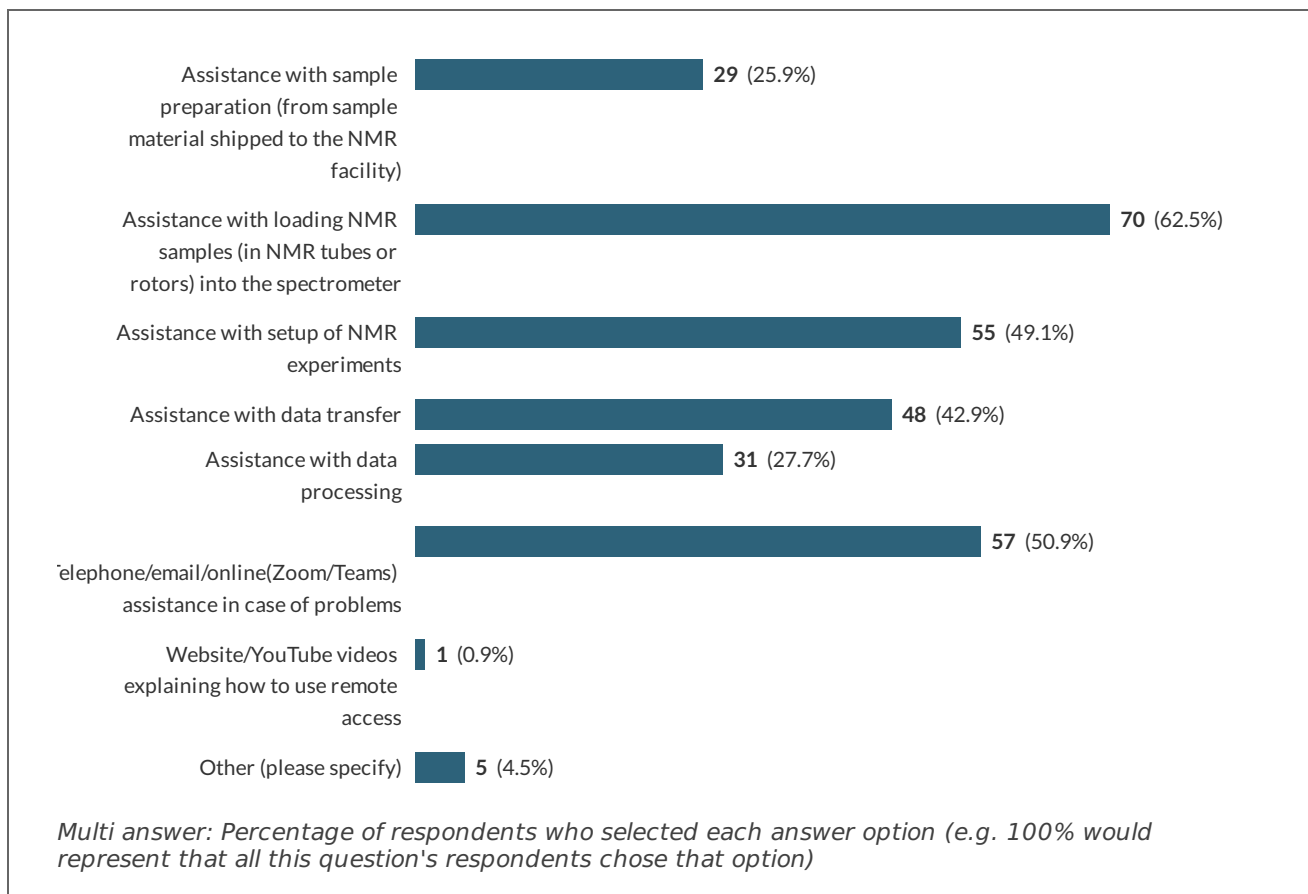
14.a If you selected Other, please specify:

Showing first 5 of 40 responses	
See previous answer for assisted remote access	987038-987020-103842897
Microsoft Remote Desktop app	987038-987020-103867866
Remote Desktop Connection	987038-987020-103875649
cisco	987038-987020-103912509
Windows remote desktop	987038-987020-103913102

15 As a remote user, were you provided with support by the NMR facility staff?



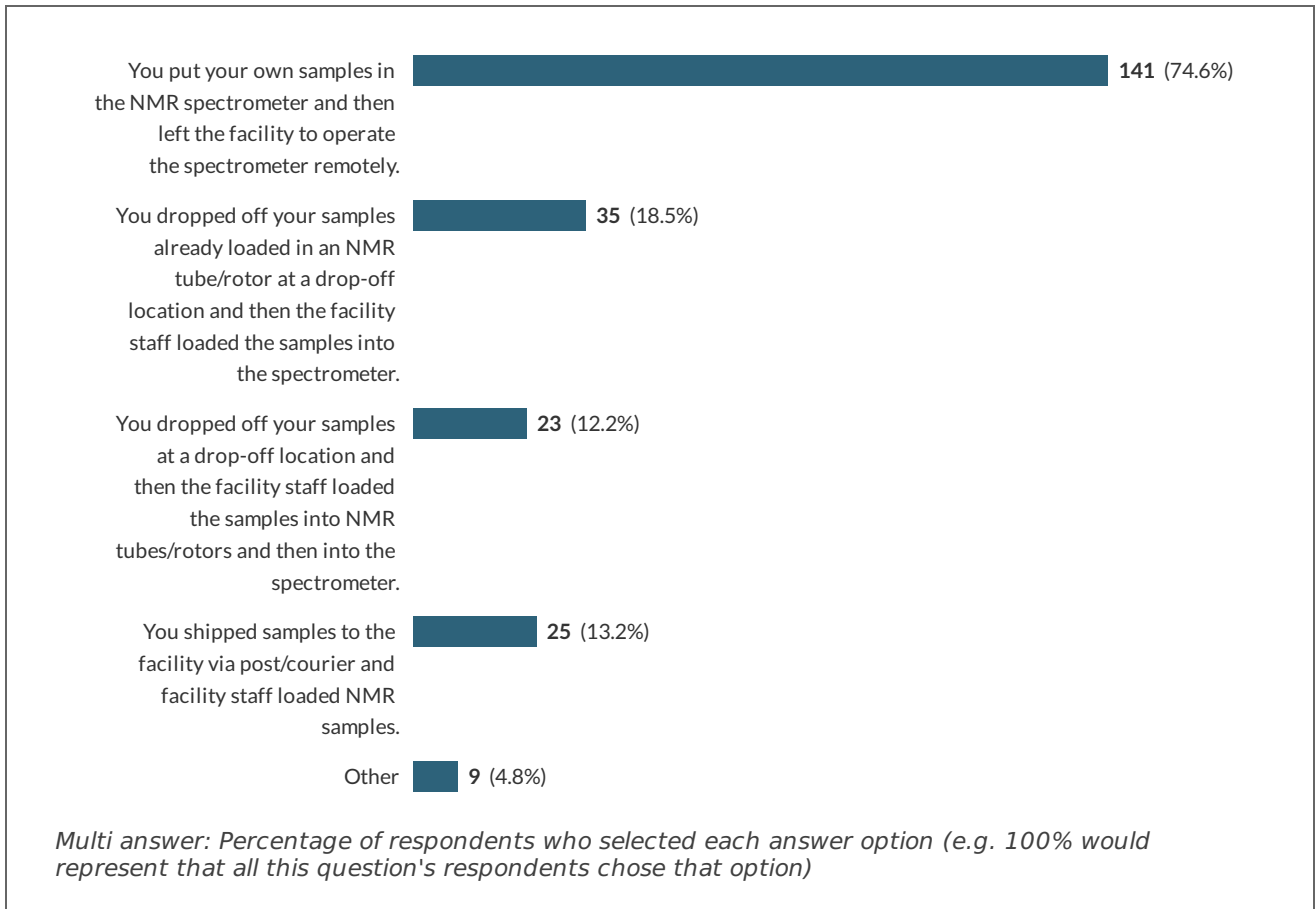
15.a If yes, what type of support was provided? (select all that apply)



15.a.i If you selected Other, please specify:

Showing all 5 responses	
Assistance with connecting to the spectrometer and assistance with data transfer via the remote connection.	987038-987020-103912490
Training in how to connect to the spectrometers from a remote location	987038-987020-104004509
Made up the samples and sent them through to the EU facility in Utrecht and in the past made up the samples and went to B'ham where they were shimmed and recorded by Sara Whittaker	987038-987020-104651420
Description of how to setup remote access on my computer	987038-987020-104737700
I am the person who bought and installed the software for remote use of the NMR spectrometers. Therefore, I was not assisted by other persons but assisted other persons.	987038-987020-104884554

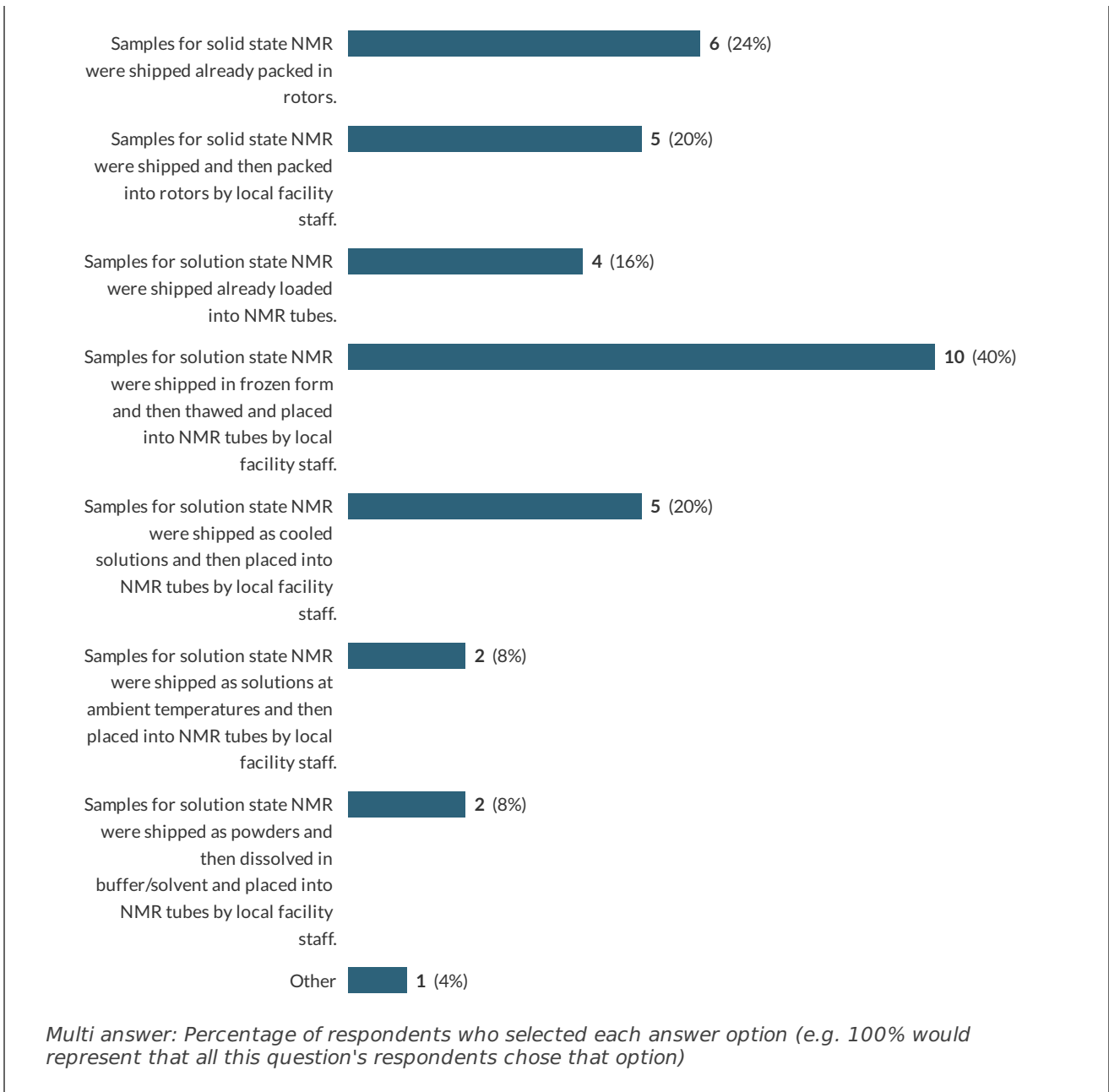
16 How were your NMR samples delivered to the NMR facility and loaded into the NMR spectrometers? (select all that apply)



16.a If you selected Other, please specify:

Showing first 5 of 9 responses	
I work on other peoples samples. Either they or other facility staff load the sample into a sample changer and provide me with information on its location	987038-987020-104004509
I put my own sample in the NMR spectrometer, started experiment and once its started, used remote facility to check if the experiment is running fine and to access results further.	987038-987020-104130885
Nice colleagues put my samples in the spectrometer	987038-987020-104409197
That was done by my colleagues who were working in person	987038-987020-104486977
I put the samples in an autosampler next to the NMR and an automated system (roboter) is loading and processing the sample	987038-987020-104772110

16.b If you shipped samples to the NMR facility via post/courier, could you provide more information about how this was done? (select all that apply)



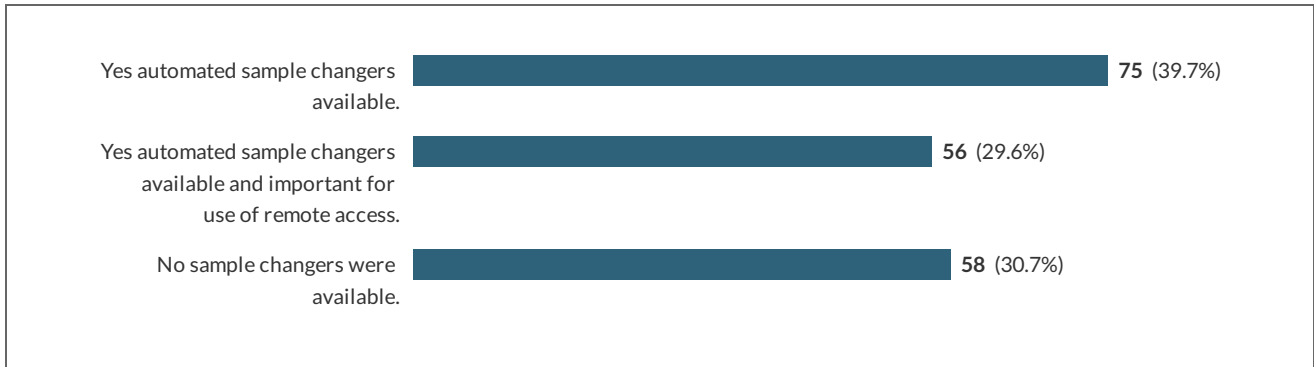
16.b.i If you selected Other, please specify:

Showing 1 response	
Metabolism of cells	987038-987020-104995202

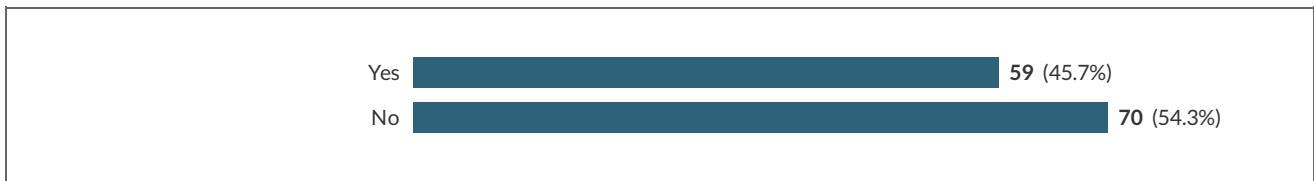
16.c In the text box below, please enter any additional information about sample shipping? (such as courier company used, special packing materials used to prevent damage to samples, any other precautions taken, procedures for transnational sample shipping etc).

Showing all 8 responses	
ample prepared self and stored in 4 C	987038-987020-104130885
standard shipping via PostNord (Postal service)	987038-987020-104382232
FEDEX The procedures for transnational sample shipping from Argentina to Italy did not work properly and the sampled thaw in the process.	987038-987020-104423415
We use FEDEX and ship samples frozen on dry ice or as lyophilized powder. We very rarely ship refrigerated solutions. We always ship samples in an eppendorf, stored inside a falcon tube to make sure it does not break during shipment. We usually ship two tubes, one of them as a backup.	987038-987020-104436599
DHL	987038-987020-104439880
TnT (reliable, but expensive), FEDEX, DHL (not recommended...)	987038-987020-104680024
Companies used were FedEx, Roadrunners (Nottingham), BioCair	987038-987020-105046974
A good hard case protecting for the already packed rotors were sent. But, there is always some problems associated with couriers in general, they never deliver thing properly and on time. So, a good protecting packing, especially air tight if needed, is always done in my case.	987038-987020-106870635

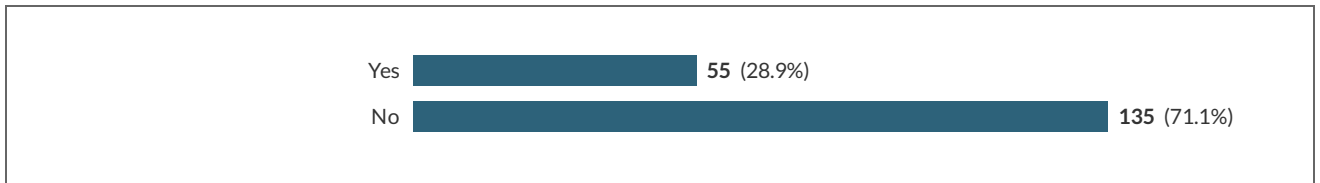
17 Are spectrometers you used for remote access equipped with automatic sample changers and were these important for your use of remote access?



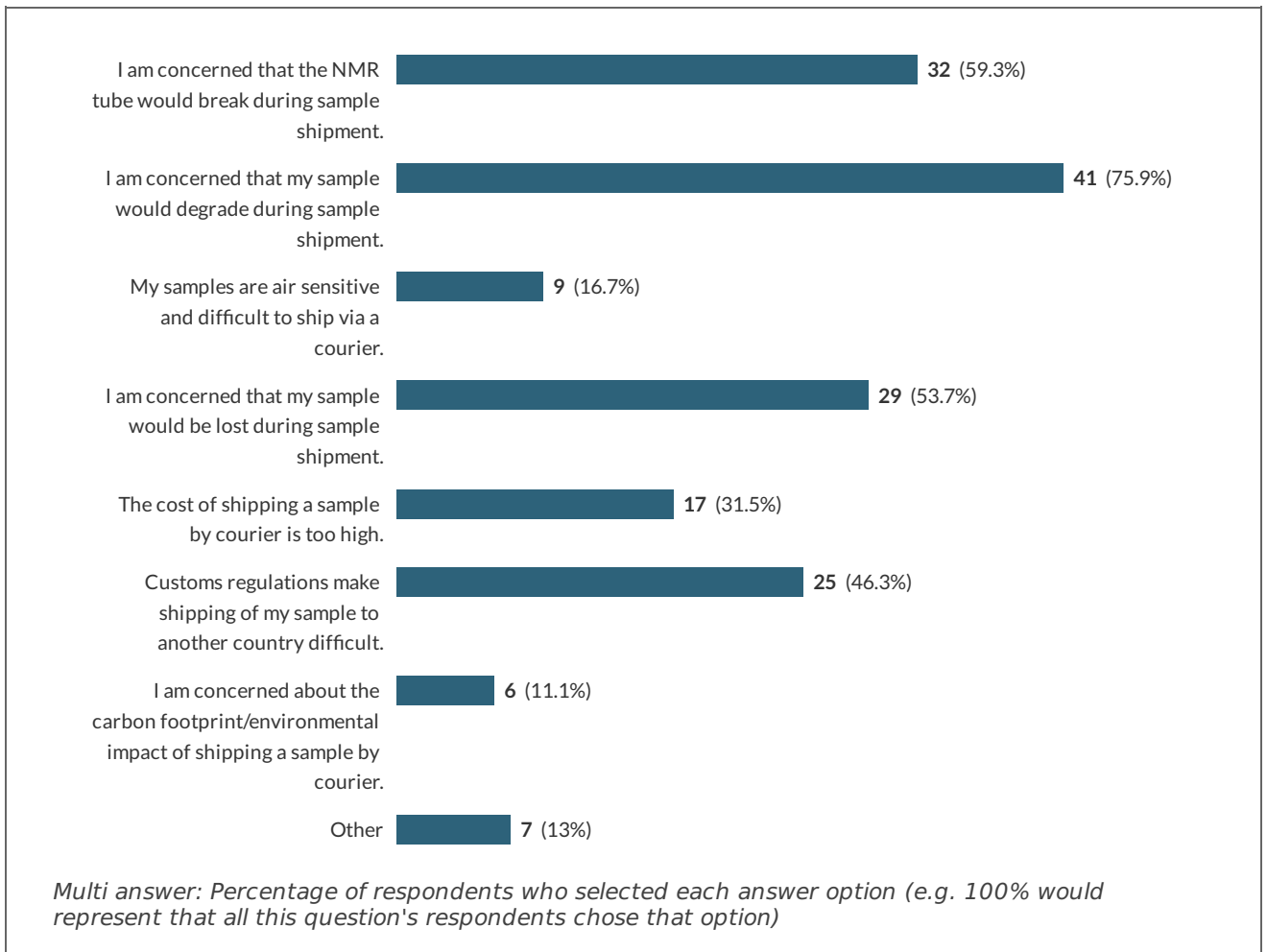
17.a If yes, was the sample changer temperature controlled (i.e. are samples stored at a specified temperature before insertion in the spectrometer)?



18 Do you consider sample shipment/delivery to an NMR facility to be a barrier to remote spectrometer access?



18.a If yes, what are your main concerns about sample shipment? (select all that apply)



18.a.i If you selected Other, please specify:

Showing first 5 of 7 responses	
An effective 24 h turnaround on NMR samples was very disruptive to working.	987038-987020-103842897
Some clinical samples are not allowed to be shipped.	987038-987020-104106458
I want to use my samples multiple times. Personally readjusting a sample in the magnet or shigemi if needed is not possible.	987038-987020-104673241
Safety. Many samples will be in chloroform or other controlled solvent	987038-987020-104679564
In a way, all of the above may be true, depending on sample and urgency. I would still always take the option and in most cases shipment has worked before.	987038-987020-104680024

- 19 What bottlenecks or other problems did you identify in using NMR spectrometers by remote access? Do you have any suggestions about how remote access could be improved?

Showing all 98 responses	
I think sample shipping is the biggest problem. I run experiments for external users and many/most of these would rather travel to our facility with their sample than shipping the sample.	987038-987020-103832699
None, generally it was excellent and I would be happy to do all my research remotely	987038-987020-103832964
A view of the automatic sample changer (through a webcam) is advisable.	987038-987020-103841365
absence of automated tuning&matching If something goes wrong, it is much more difficult to trouble shoot. Knowledgeable staff is required to be present by the spectrometers anyway, otherwise we may wait too long for local assistance...	987038-987020-103901122
A bottleneck is a slight delay in the connection which makes interactive phasing a bit tedious. However, taking your time/phasing slowly alleviates the problem. Other than this, no problems were identified during my use.	987038-987020-103912490
Unwanted change of samples in the sample changer by other users.	987038-987020-103914070
Clearly the position(s) of the sample(s) in the 'sample changer' is crucial and it may represent an issue during an intense and combined 'direct' and 'remote' usage of NMR spectrometers. The related problems can be avoided by people awareness, by respecting a pre-established protocol for handling the NMR samples.	987038-987020-103933631
Very time consuming.	987038-987020-103933604
no	987038-987020-103945877
The main problem, by far, was convincing our IT department to open the	987038-987020-103947685

ports necessary to access the spectrometers. It took us years to convince them that this was safe.	
Auto sampler and auto tuning would be beneficial.	987038-987020-103971664
For my home institution there were no bottlenecks.	987038-987020-103989826
I have no experience with an NMR facility outside my home institution.	
Remote access was mostly for monitoring experiments set up in person (i.e. not remote).	987038-987020-104005042
Interactive operations such as Phasing can be tricky due to the slower response. A fast internet connection is a pre-requisite.	987038-987020-104004509
No problems	987038-987020-104016821
It's time consuming.	987038-987020-104033457
I am the head of the facility. We use No Machine for remote access, protected by a VPN. It is stable and it works well. So far, we imposed no restriction of access. The main problem is the lack of control of many non expert users using the remote access to copy datasets. We are considering restricting the access.	987038-987020-104033656
Software issues that arise when no one is around to resolve	987038-987020-104036011
Lag on the internet connections was the main issue. Nice computers with good graphic cards and top quality internet connection will help.	987038-987020-104036746
Unable to perform hyperpolarization experiments remotely. Operation of hyperpolarization infrastructure is manual.	987038-987020-104036834
The critical point is regarding the internet connection, it depends from the building where the facility is located	987038-987020-104039216
data protection issue	987038-987020-104051197
The bottle neck is the sample shipment. I shipped samples under dry ice within Brazil, prices were too expensive and samples arrived at room temperature.	987038-987020-104066039
if the sample does not spin for MAS, then cannot be done anything remotely unless , we check rotors if we need to acquire reference spectra then we need to change samples manually and operate further sometimes the software freezes when you access remotely , a better and fast computer required	987038-987020-104130885
Bottleneck: Being extra careful since sometimes the active window through AnyDesk in reality stuck and the command hasn't been applied.	987038-987020-104215034
In Canada, we have national facilities in Edmonton and Montreal that have worked well for years. They have technical people who will run your requested experiments although I prefer remote access so I can ensure all my parameters are set and make adjustments in real time.	987038-987020-104377423
less bureaucracy to get a measurement time in other facilities.	987038-987020-104381797

Primary bottleneck is not software/IT but Legal - standard contracts with clear identification over who owns what available from the outset (combination of corporate legal and university legal is a big barrier)	987038-987020-104382232
The lack of fund for international remote access is a bottleneck.	987038-987020-104392826
The remote acces by AnyDesk is just fine. The bigger problem is that we have an old instrument with manual tuning and multiple probes. Remote acces is used regardless of Covid. It is a great help to check on the measurements after work or running long experiments on weekends.	987038-987020-104382711
Only the lack of an automatic sample changer	987038-987020-104402900
Alternate remote and in-person would enhance training and facilitate transport.	987038-987020-104423415
At NoMachine there is the problem of newest log-in gets access. So people are able to shut out users. This can cause problems if people want to process at spectrometer, but next one is doing experiments.	987038-987020-104425976
Some initial setup need to be performed by host facility staff.	987038-987020-104429762
If the protein behaves well and can be frozen/thawed or resuspended after lyophilization (without precipitation), there is no bottleneck for using remote NMR spectrometers in our experience. We have started using remote access before covid. It saves time and economical resources (travel, hotel...).	987038-987020-104436599
it is better if the teams at both sites have had the chance to meet and interact often.	987038-987020-104439880
--	987038-987020-104466561
accidental interference with non-self measurements	987038-987020-104477989
Actually I like our system as it saves a lot of time, even if sometimes one has to wait a bit for the available time slot, or if the queue is longer. During my PhD I ran all NMR samples myself, which in the end was very time consuming (walking to the NMR and typing in the samples into the software).	987038-987020-104487345
I am concerned that the magnet is correctly calibrated, configured and working properly when the samples are to be analyzed. I am also concerned about the conservation and/or preparation of the samples.	987038-987020-104486977
The main bottleneck is the diversity of software platforms that could possibly be used for remote access. The phasing out of the native support in the Bruker Topspin is a serious drawback, as one cannot maintain the old versions of Topspin [supporting the reemote access directly], as there is a requirement for the new versions of the acquisition software, that follows the new trnds in pulse programming, bugs correction and firmware updates. In my view, the client-server architecture of the Topspin remote access was an advantage and should be re-implemented.	987038-987020-104494482
Sample preparation: -Special conditions: buffers, salt. etc -high number of samples -Weighting samples	987038-987020-104501448

<p>Changing solid-state samples is an issue, in particular if experiments are to be run using very fast MAS. This is because of limited number of 1.3 mm rotors (price!) and also because samples have to be loaded manually into the probe.</p>	987038-987020-104504200
<p>As a user I did not perceive difficulties during times in which the spectrometer functioned normally. Using Topspin software via TeamViewer proved no problem. Some people managing the NMR computers were however concerned about misuse/ accidental deletion of data.</p> <p>However, during times when the cryoprobe we are using was defective/ in repair, automatic tuning/matching was not implemented for the replacement probe, therefore measurements of samples of different composition via the automation and remote access was no longer possible.</p>	987038-987020-104569325
<p>Lack of auto tuning and matching in solid state</p> <p>Some manual Processing e.g. Phase correction (screen lag makes it difficult to fine adjust)</p>	987038-987020-104572895
<p>I did not have problems in using remote access to NMR spectrometers, I received an excellent assistance. How feel not comfortable in performing NMR titration experiments because there is too much sample handling. I believe remote access is perfect to run long lasting experiments.</p>	987038-987020-104578649
<p>If the sample changer doesn't work anymore, remote access doesn't help, so I need to go to the spectrometer anyway.</p>	987038-987020-104606871
<p>Sample stability is a big concern. Most of my samples have to be freshly prepared and cannot stay for long periods at RT (>72h)</p>	987038-987020-104619504
<p>air bubble inside the nmr tube, somebody needs to be at the spectrometer in case having this problem</p>	987038-987020-104650540
<p>Navigating vnc port setups, ssh connections, tunnels, firewalls etc is not for the beginner!</p> <p>Equally, I'd be concerned to let inexperienced users loose remotely without supervision. The potential to get something wrong due to network lag, or a small screen size, is higher than physical presence next to the spectrometer.</p>	987038-987020-104652020
<p>I have been doing NMR for the past 42 years, at the start on 100 MHz and then during a 3 year postdoc in the Netherlands on the Groningen 360 MHz in Rob Kaptein's lab and then on the 500 MHz on the Netherlands facility in Kees Hilbers lab in Nijmegen Shimming and collecting myself. Then I used a 500MHz at Yale which was a home built spectrometer and moved to doing more crystallography due to the size and correlation time of the complex. Worked with students on the MRC NIMR spectrometers to solve several protein complexes in the HIV area where we made the samples and let the expert spectroscopists shim and record spectra as well as use the Utrecht NMR EU facility with local experts recording and the same in B'ham at 900 MHz them.</p>	987038-987020-104651420

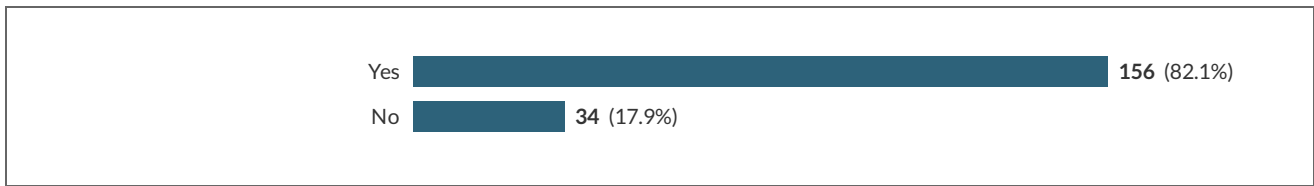
Kinetic studies almost impossible via R-NMR.	987038-987020-104652171
Sample readjusting (in the shigemi or the magnet) is not possible.	987038-987020-104673241
Perhaps engage with a specialist shipping company that would serve universities, be well versed in what these samples entailed - are simple to use as there is some form of agreement governing their use so arranging the shipment is seamless. I would like it to be as simple as ordering a takeaway but you know the sample will be delivered same day to an NMR centre.	987038-987020-104674153
for routine air/moisture/temperature stable samples i do not see any bottlenecks. However my samples are air/moisture sensitive and frequently only stable at lower temperatures and therefore i like to run samples myself, and in as shorter time as possible to get the best data. I dont think it is possible to get any quicker than the computer directly at the machine. For those that are more on the stable side, it is handy to be able to add additional experiments remotely	987038-987020-104678345
Samples being removed from sample changer carousel by other users and/or technical staff If spectrometer does not have, or if sample is unstable or time critical, clearly user must be physically present at spectrometer	987038-987020-104679564
-Stability of connection (most likely at the own end) -sometimes incompatibility of typing languages/keyboard settings	987038-987020-104680024
Over time, Topspin slows down and becomes impossible to use with Remote Desktop for the spectrometer running Topspin 3.6 and Windows 7. No problem with Topspin 4.2 and Windows 10.	987038-987020-104679345
I believe remote access removes bottlenecks rather than creates them and would not want to go back to pre-covid days when we did not have remote access to our spectrometers.	987038-987020-104700377
Overall, it's OK and possible to do for an experience user. it's very useful to have a facility manager on the site in case any network/hardware problems. tuning could be quite painful and slow sometime. it's relatively easy to do a standard setup but it's difficult to do anything more complicated (e.g., a new pulse-sequence setup, etc). big screen on home computer is definitely a benefit.	987038-987020-104731960
Occasional drop outs which require being in the facility to reset the remote access software.	987038-987020-104737700
the reactivity of the graphical interface and mouse sensitivity can be slow or badly controlled in remote accesses.	987038-987020-104742070
Bandwidth to download the data	987038-987020-104844176
At my non-home facility, remote access was indeed not available then. Fortunately, covid restrictions were already lifted and I could go to the	987038-987020-104858892

Fortunately, covid restrictions were already lifted and I could go to the spectrometer to further set up experiments.	
operating lagtime during the remote connexion	987038-987020-104858091
Assistance needed for changing rotors and starting the spinning for newly packed rotors (all rotors should be spun before running experiments to ensure good spinning)	987038-987020-104874197
Remote access could be improved by the availability of automatic sample changers for all kinds of NMR tubes and MAS rotors. Furthermore, as many NMR probes as possible should contain motors to have to possibility for remote or automatic tuning and matching.	987038-987020-104884554
Some equipment problems cannot be solved remotely. Sometimes the network can be unstable.	987038-987020-104890370
In our lab, the fragile VPN connection makes things a bit more complex. At the remote IR-RMN Lille site, the engineer was there to help.	987038-987020-104929943
Sometimes you dont have access to the probe especifications when you operate the spectrometer remotely. It would help to have access to the safe limits values to operate the probe.	987038-987020-104987098
The already discussed ones	987038-987020-104995386
Internet connection might be unstable or might cause some lag causing issues (also quite dangerous) in the set-up	987038-987020-105004542
Complicated in terms of secure access. Vnc gives best performance but must be run via a vpn.	987038-987020-104995202
Verification of sample state (optical check for precipitate, color) Network reliability, in particular from home and if high network load on campus due to live streaming of lectures during the pandemic remedy: reserved bandwidth, network separation from streaming network	987038-987020-105024523
The main thing is that you do not see the things going on in the lab. So when people walk close to the magnet, activities going on, temperature drop etc etc. Of course a camera can help but this is not workable on all systems. Systems need to be up to date. For example, we work with an attached apparatus to our Bruker 600 which does not (yet) allow upgrade of the CentOS 5.9 operating system. This means that old web browser won't work, anydesk is not operational at this version and teamviewer can handle older systems connect to newer ones. Same is true for an inova500 system. The NMR part works perfectly providing high ranked papers but the operating system is old ... very old	987038-987020-105024937
Automatic sample changers should be present in all the spectrometers with the possibility to store the sample refrigerated.	987038-987020-105005282
At the moment the system used required a physical login to the spectrometer computer. This require a site visit or passing on login details to a staff member which compromises security. A method of securely logging in from a remote location would greatly aid the utility of the remote access whilst retaining security.	987038-987020-105046974
Anydesk on the spectrometer (linux OS) sometimes stops working and	987038-987020-105055804

nas to be manually restarted by someone with superuser privileges.	
Based on my experience with a remote desktop, I do not need any improvement	987038-987020-105056889
Poor performance of the remote connection apps. Sometimes, the console or PC should be restarted and, consequently, the remote connection is lost.	987038-987020-105087822
Issues with "only" seeing the computers interface with the instrument. For example He and N2-Levels are not part of the software, air-flow rates for cooling are sometimes inaccurate, samples have been stuck in the sample changer. Maybe the addition of webcams might help (at least for some issues).	987038-987020-105197740
I am happy to run all my own experiments, however I would prefer if all our NMR spectrometers had Teamviewer.	987038-987020-105235641
The quality of remote access to research infrastructures heavily depends on the quality of the person who supports the access locally (staff/facility manager). I have mixed experience with access in Lyon (little support) and good experience in Grenoble. Making sure that a person locally feels in charge of the experiment is really crucial. Moreover, I find it really important that a good library of experiments is available. For example, NMRLib (solution and solids) is a good basis, in my opinion.	987038-987020-105235200
The biggest bottleneck is of course a spectrometer that is not able to auto tune and match. And if you're not measuring via automation with a sample changer, you have to put the sample into the spectrometer at least. There are no further suggestions in these cases.	987038-987020-105359436
Hardware changes (VT, tuning/matching, MAS control) were either not possible remotely or considered too risky (no-one around if something goes wrong). Remote sample loading/removing is due to special sample handling requirements not an option.	987038-987020-105428768
No bottlenecks, what it would we nice to have a autosampler in other instruments	987038-987020-105433478
The limitation comes from the fact that the network must be opened to external users.	987038-987020-105704489
A stable connection was not always guaranteed in my own experience. I used VNC. Then I had to pop into the lab and re-establish the connection.	987038-987020-106138336
When spinning the sample, it is nice to be able to hear the spinning.	987038-987020-106146312
None for the present low-field applications, for high-field solid-state NMR experiments it is important to have video monitoring to avoid physical problems with sample spinning etc.	987038-987020-106148495

<p>The bottlenecks are connected with the use of old instruments and the lack of autosample changers. Moreover, beside the optimization of the remote access, one technician should be around for every "strange" possible situation</p>	987038-987020-106373721
<p>Sometimes, lags made it impossible or at least very difficult to work. Small laptop screen size was a nuisance and kids on top of my head provided a new layer of difficulty.</p>	987038-987020-106588677
<p>Software issues, Remote Desktop Connection does not work well with IconNMR, it freezes and crashes.</p>	987038-987020-106803889
<p>loss of flexibility. You usually have to write a proposal, wait to get it approved (even if that is rather unbureaucratic), send a sample, get the data. It is OK for routine stuff, but you cannot quickly try something.</p>	987038-987020-106835847
<p>A good, simple and efficient shipping procedure should be developed for scientific samples delivery. And a good guidance at the facility by staff is always appreciated/needed for remote users. A dedicated (experimental) experienced staff should be hired at each university/ facility, the work should not be given to existing PhD students or postdocs with non-direct experience, wherever the remote access is allowed for external users. This, otherwise, will result in time experimental wasting or non-conclusive NMR research, especially for non-NMR experts, which is currently mostly the case when measuring at different facilities, as per my personal experience.</p> <p>Otherwise, I am in very favor of remote NMR. It is exceptionally useful for the researchers especially from the developing countries, who does not have a in-person access to high tech NMR instrumentation.</p>	987038-987020-106870635
<p>Insertion of samples if no autosampler. Tuning and matching probehead if no automatic device present</p>	987038-987020-106968186
<p>normally you see only the desktop of the spectrometer computer but if samples are not correctly lifted into the magnet or you have other issues with the sample case you are lost if possible some kind of video control to see the sample case or magnet could improve trouble shooting</p>	987038-987020-107009335
<p>If problems come up with the sample changer (that happens quite often with our nmr) you are not able to eliminate the defects on a remote way. You would need a camera to supervise the operation of the sample changer but that is a problem in Germany because of forbidden work control/surveillance and you can't help a sample which is sticking in the tube anyway if you are at home.</p>	987038-987020-107339769

20 Are you continuing to use remote access to NMR spectrometers now that some/many/all 'pandemic' restrictions have been lifted?



21 If you have further information that you would like to provide, please enter this in the text box below.

Showing all 20 responses	
Remote access is an excellent option. Works great with liquids where ATM and sample changers are available. For solids, usefull for long studies (multiple experiments) with a single sample.	987038-987020-103901122
Remote NMR access is a great thing, even if it is more or less a by-product of the COVID-19 pandemic. It simplifies both office/lab work and work-from-home. However, I think that sooner or later, users will run into problems with either the hardware or experiment setup. Good troubleshooting support is therefore necessary.	987038-987020-103912490
no	987038-987020-103945877
R-NMR is a great idea, specially since less time is wasted for travel so you can be more efficient. But for newbies in the field it might be less educative.	987038-987020-103971664
For me Remote working is now the norm.	987038-987020-104004509
None	987038-987020-104016821
There should be a visible indicator of the queue line that you should expect if you submit a project to a given NMR facility. Like that you could chose the facility in function not only of the field and experiments that you want to perform, but also control better the time-window to have the experiments done.	987038-987020-104036746
The 700 MHz that I use is on the 4th floor and my lab is on the 3rd floor. If my sample is already in the magnet, I will use remote access every time from the comfort of my own office!	987038-987020-104377423
--	987038-987020-104466561
Another advantage of the remote access only-one-person-is-in-charge procedure in my opinion is the limited access of less-frequent NMR users, which limits poential problems by wrong usage of the machines. Only experienced users, who regulary go to the NMR, should really use it.	987038-987020-104487345
It would be good if quality control and process traceability protocols were integrated and standardized. Including for example things such as the naming of the experiments, names assigned to the samples, file formats, etc.	987038-987020-104486977
no	987038-987020-104578649
There are two problems that I would like to use the highest fields at 1 GHz to solve or I need the dispersion for those NMR systems	987038-987020-104651420

<p>at 1 GHz to solve as I need the dispersion for these DNA systems. They are part of a DNA-protein complex for which we wish to study the DNA component in solution as so far we have not been able to crystallise them - and anyway we would like to see them independent of the crystal lattice</p>	
<p>Remote access in our facility in Leeds, UK was initiated during the pandemic, but has since proven extremely useful. In particular, the ability to set up and run experiments/change samples at anti-social hours from home has been very helpful.</p>	987038-987020-104737700
<p>Independent of pandemic restrictions, I regard remote-NMR as a very helpful possibility for an effective use of working time. It is possible to work with (more than one) spectrometer with the own workstation in the office or at home and simultaneously deal with other work. We used remote-NMR already before Covid-19.</p>	987038-987020-104884554
<p>Reference spectra help for less experienced users - just copy the directory, and adjust p1 and spectral widths.</p> <p>Changing samples is always a bit of a worry - if problems with the SampleJet, you are stuck.</p> <p>Don't leave the guacamole on in your office - you can only log in once!</p>	987038-987020-104929943
<p>Remote access is great for monitoring and setting up simple sequences, but the physical presence has a huge benefit when it involves hardware-related things and troubleshooting.</p>	987038-987020-105428768
<p>Remote access is important for national, transnational instrumentation, but also a potential asset locally to ensure optimal use of time</p>	987038-987020-106148495
<p>Remote access is great, difficulties can be overcome.</p>	987038-987020-106588677
<p>Direct remote access is like being there yourself. However, it is often prohibited due to IT-security concerns (and those concerns are of course justified). Access through others is not like being there yourself, the possibility of experimenting with the spectrometer is lost. Then, remote NMR (outside my own university) is good for larger routine measurements (e.g. running all experiments necessary for protein assignment), but not for trying something new.</p> <p>Remote NMR does not replace a local NMR, but the local NMR can be of lower field strength, and the remote NMR of higher field strength.</p> <p>Remote NMR must be free of charge, otherwise no one will use it.</p>	987038-987020-106835847

APPENDIX 4

Remote-NMR (R-NMR): Moving NMR infrastructures to remote access capabilities

NMR USER SURVEY (8 January -29 March 2023)

Univ. of Oxford Central University Research Ethics Committee Approval Reference: [R77838/RE002]

SUMMARY OF RESPONSES FROM NMR USERS NOT COLLECTING DATA

WITH REMOTE ACCESS

Introduction

Lockdown restrictions in many countries during 2020-2021 Covid19 pandemic resulted in the implementation of remote access to NMR spectrometers as a way of enabling the continuation of important research. The experiences of several European NMR facilities during the pandemic have shown that this access mode can work well within the field of NMR spectroscopy. It is the aim of the Remote-NMR project to develop and exploit remote access to NMR facilities. Work Package 2 within R-NMR focusses on the "Remote NMR Landscape". Task 2.2 within WP2 is a review of NMR users' need with respect to remote access to NMR facilities; this includes aspects such as facilities used during the pandemic, level of assistance provided by facilities/would additional assistance have been useful; is confidentiality of samples/experiments important; how were samples sent; likelihood of using remote access even when there are no travel restrictions; suggestions for improvement. This information has been collected via an online survey of NMR users.

This document is a summary of the responses from the subset of 200 NMR users who completed the survey and indicated that they had not used remote access for NMR data collection.

Remote-NMR: User Survey

Showing 200 of 401 responses

Showing **all** responses

Hiding **9** questions

With filter **q11-is-no** applied

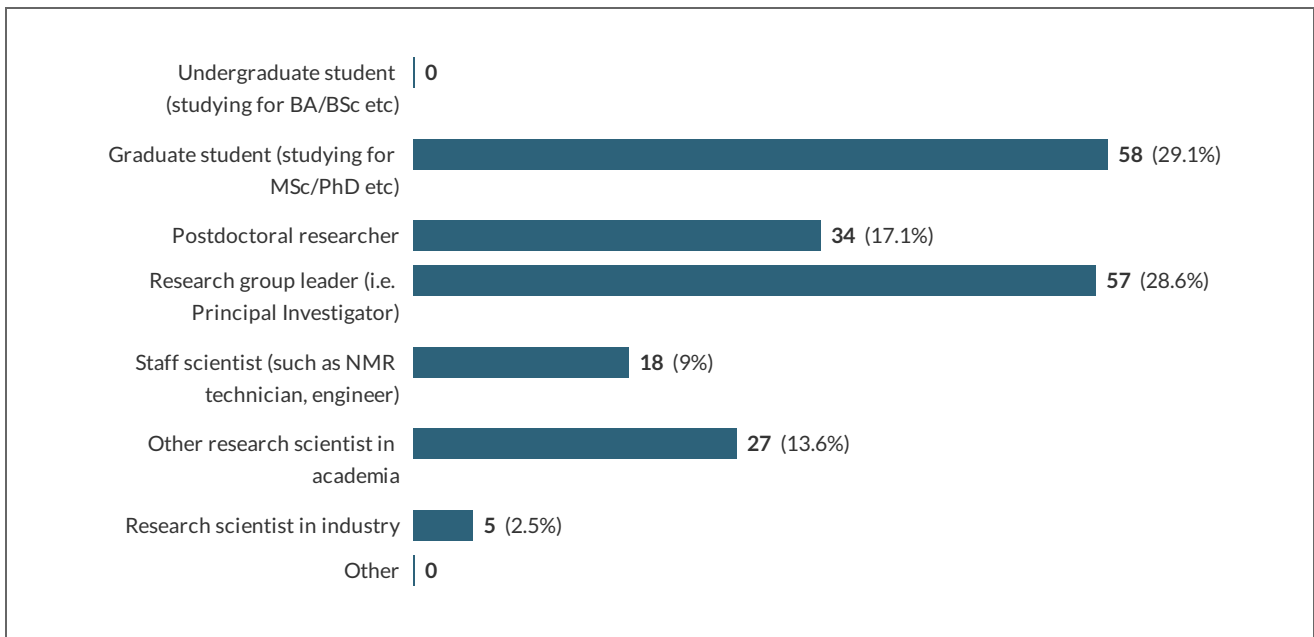
- 1** You are invited to complete this online survey aimed at users of NMR facilities. We will ask questions about the NMR facility(ies) that you use, about your experiences (if any) with remote access to NMR spectrometers and for your views on how remote access can be improved in the future. The survey will be completed anonymously (you will not be asked for your name or email address) but you will be asked to indicate in which country your NMR facility is located. Information that you provide about your experiences with remote access will be included in discussions with other R-NMR project participants and in project reports. All survey data will be stored at the University of Oxford on a secure computer (password protected and behind a firewall) during the duration of the R-NMR project (until 30 June 2025). A version of the survey will also be created for longer-term storage; we intend to keep this version for 3 years beyond the end date of the project. Please confirm that you have read this information and that you are willing to continue with the survey.

Yes  200 (100%)
No | 0

- 2** Please confirm that you are a user of an NMR facility. By user, we mean someone who actively collects NMR data. (Please only complete the survey once even if you have received the link from multiple sources.)

Yes  200 (100%)
No | 0

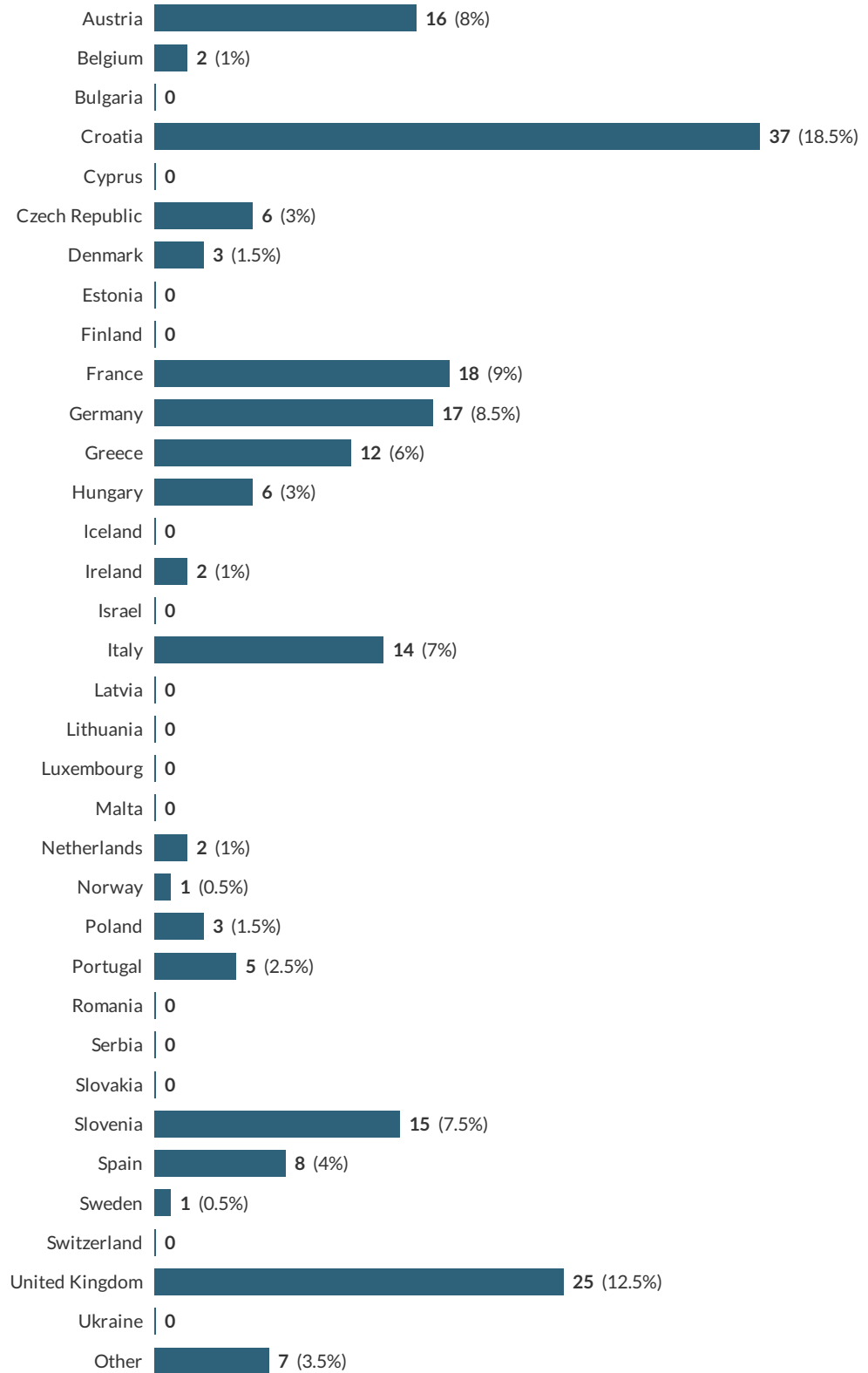
- 3** Please select the option that best describes you?



3.a If you selected Other, please specify:

No responses

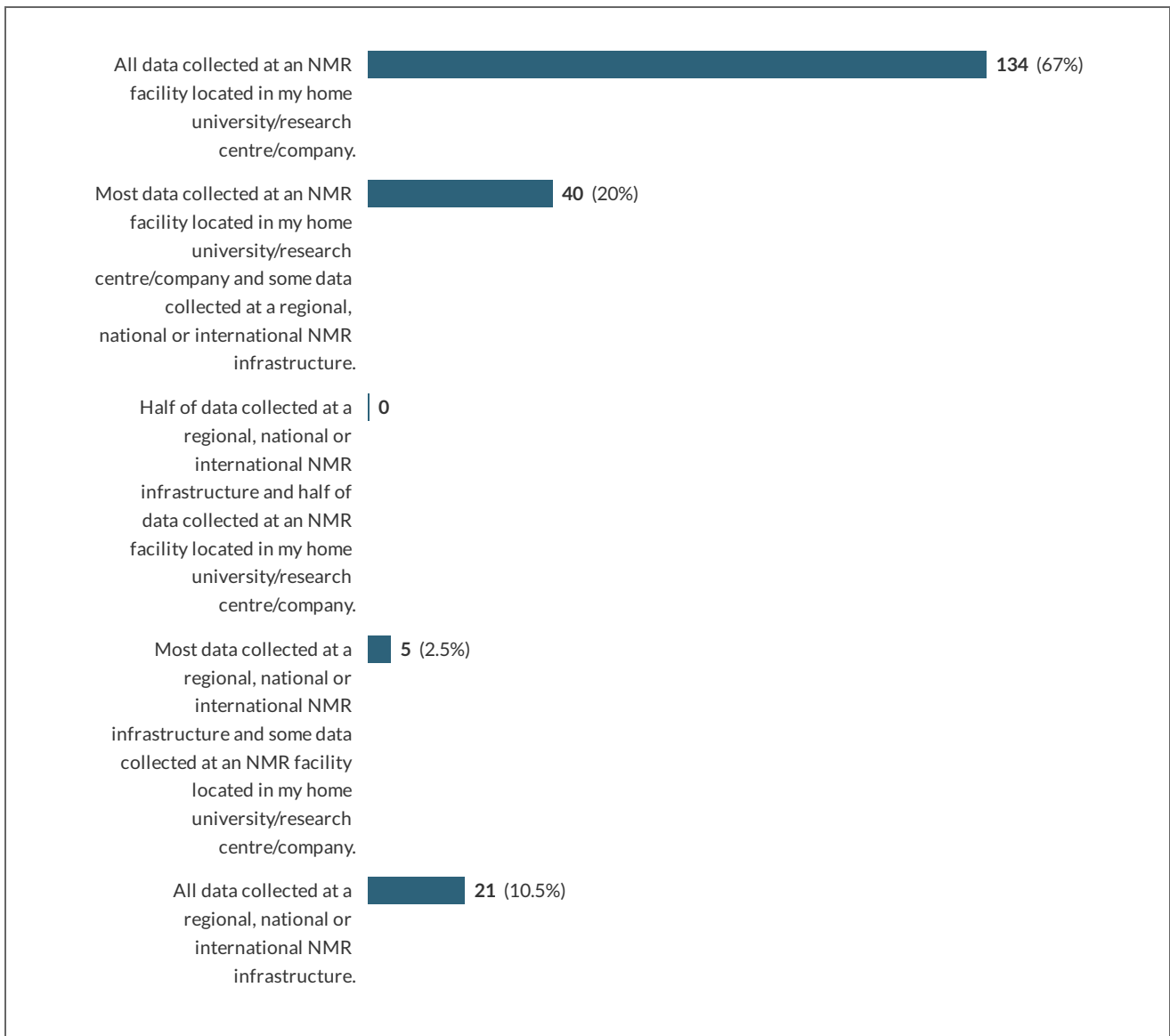
4 In which country do you carry out your NMR research? This is most likely to be the country in which you live. If you also use an NMR facility in another country you will be able to indicate that later in the survey. Select one:



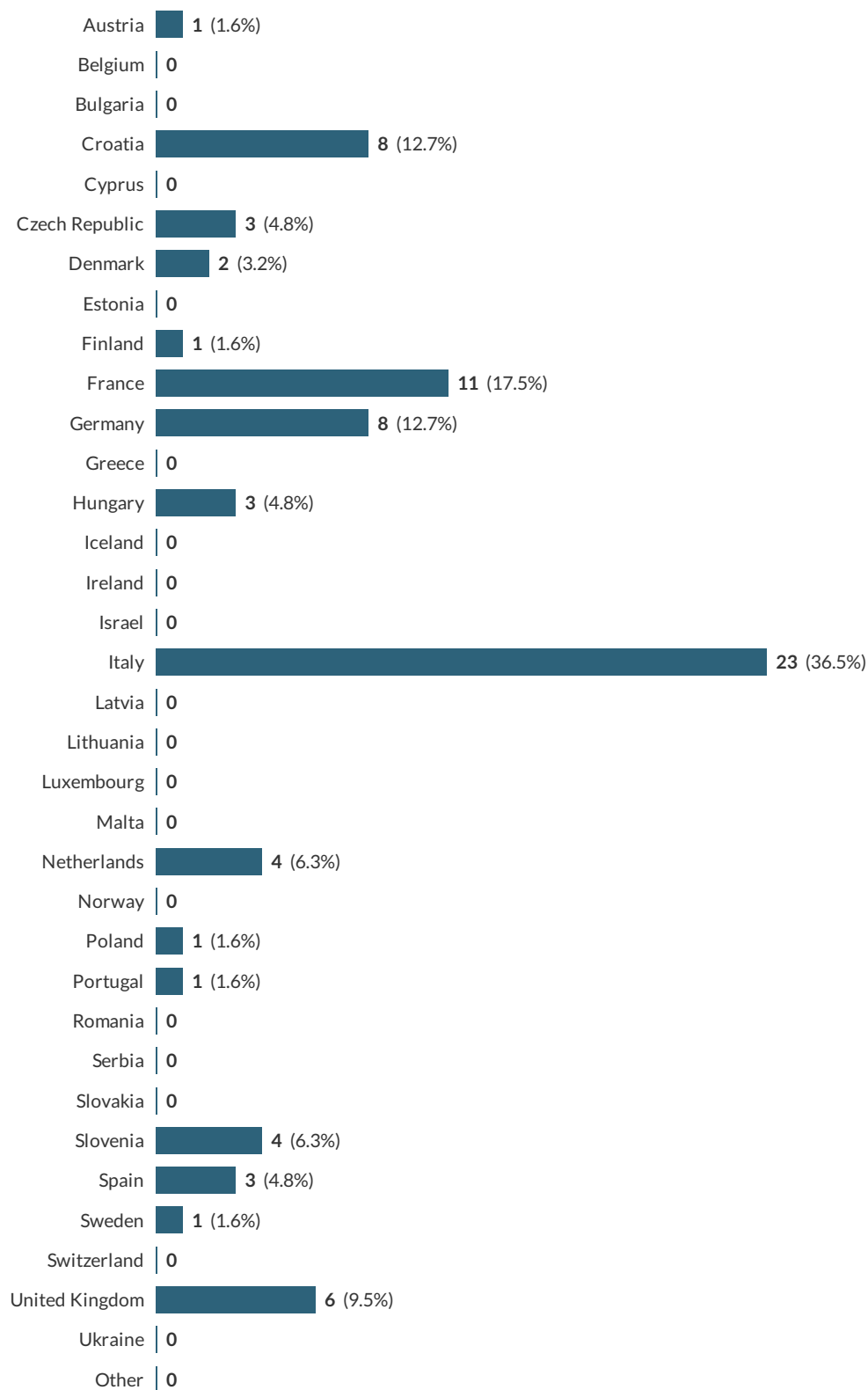
4.a If you selected Other, please specify:

Showing all 7 responses	
Russia	987038-987020-104378805
Turkey	987038-987020-104397267
Mexico	987038-987020-104418281
United States of America	987038-987020-104421282
USA	987038-987020-104467387
Argentina	987038-987020-104756491
Argentina	987038-987020-104840209

5 Where do you collect your NMR data? (select one option)



5.a If some or all of your NMR data are collected at one or more national or international NMR infrastructures, instead of your local NMR facility, please specify in which country(ies) these NMR infrastructures are located. Select all that apply:

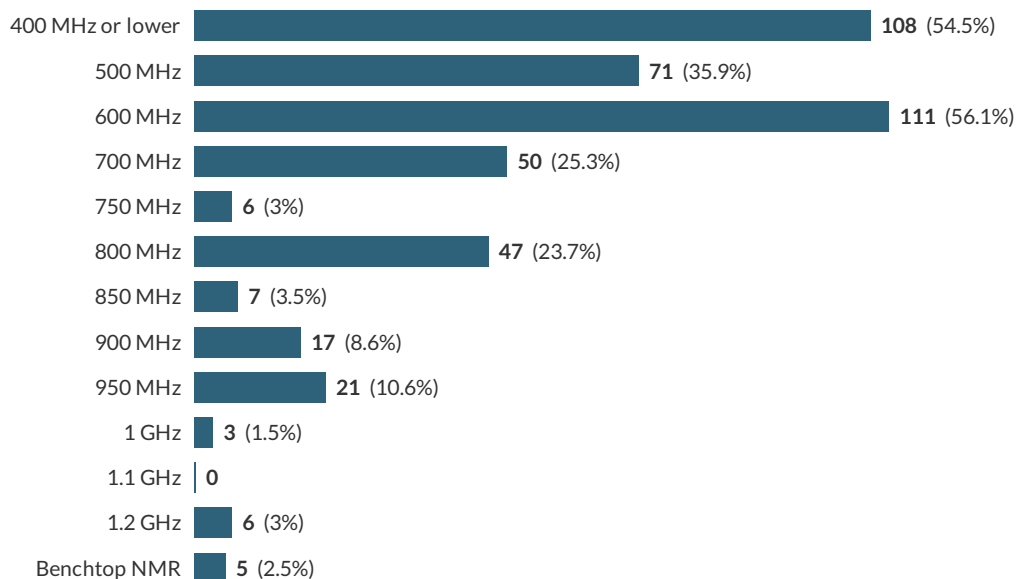


Multi answer: Percentage of respondents who selected each answer option (e.g. 100% would represent that all this question's respondents chose that option)

5.a.i If you selected Other, please specify:

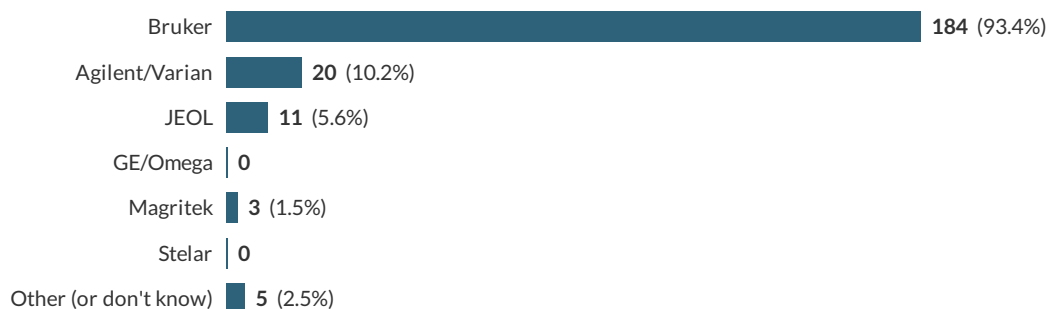
No responses

6 At what 1H frequencies do you collect NMR data? (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)

7 What type of spectrometers do you use for data collection? (select all that apply)

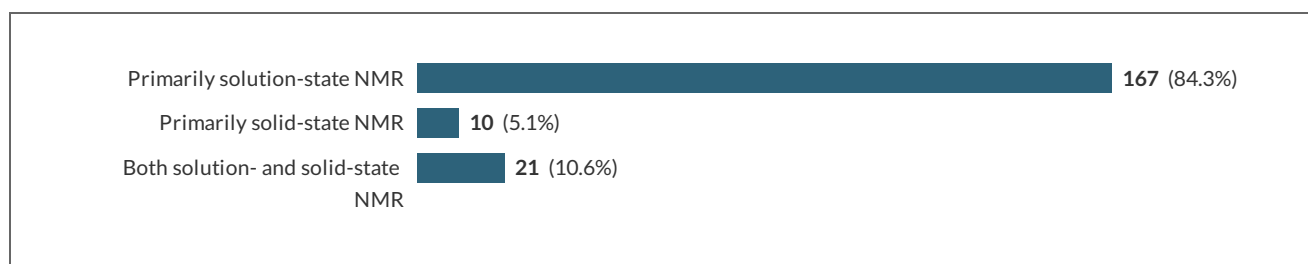


Multi answer: Percentage of respondents who selected each answer option (e.g. 100% would represent that all this question's respondents chose that option)

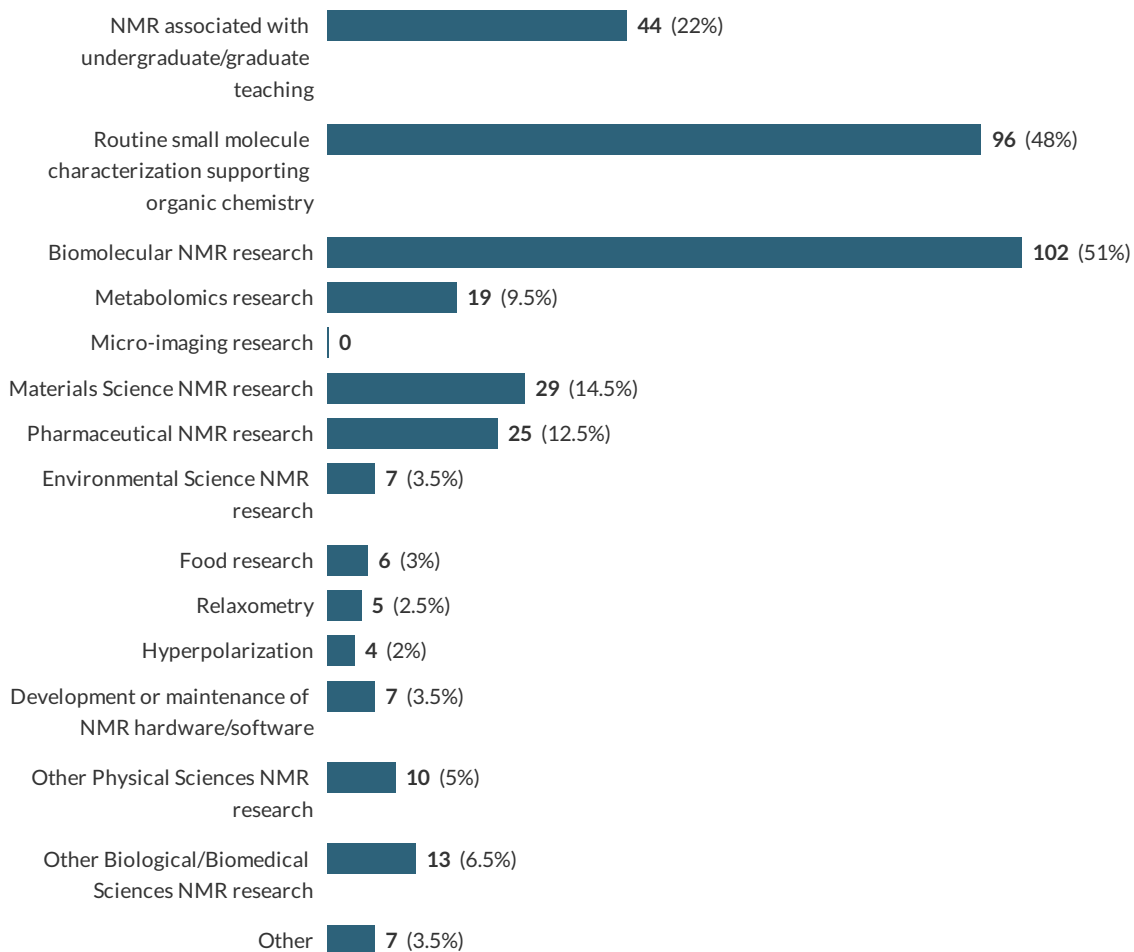
7.a If you selected Other, please specify:

Showing all 3 responses	
Tecmag	987038-987020-104037885
QuOne	987038-987020-104378805
Oxford	987038-987020-106173927

8 What type of NMR data do you typically collect? (select one)



9 What types of NMR experiments do you carry out? (select all that apply)

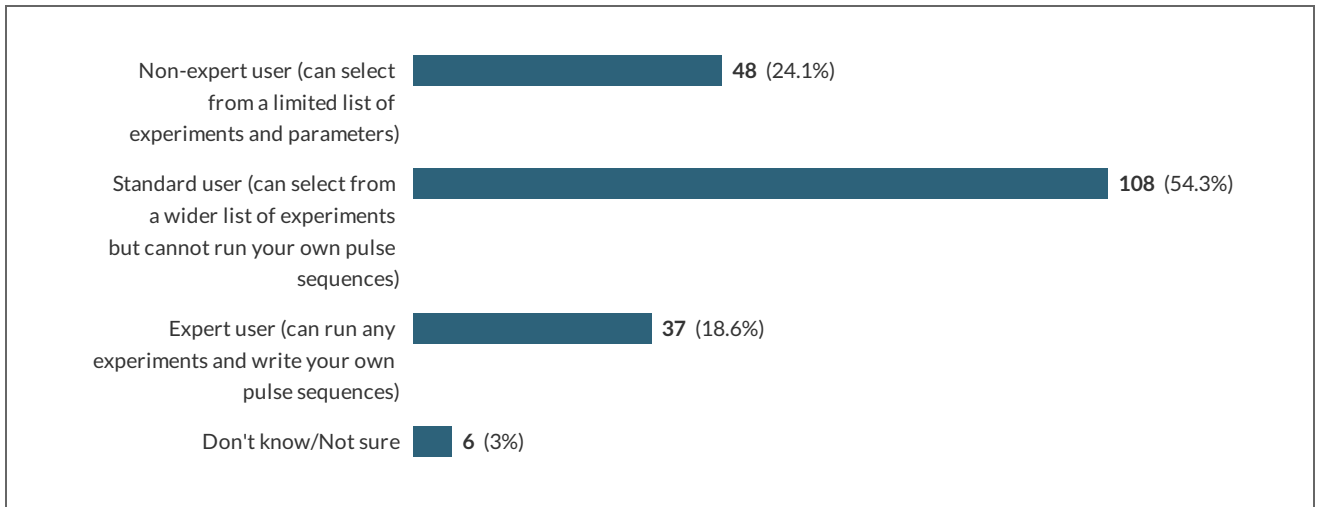


Multi answer: Percentage of respondents who selected each answer option (e.g. 100% would represent that all this question's respondents chose that option)

9.a If you selected Other, please specify:

Showing all 7 responses	
Organometallics research	987038-987020-104039591
NMR on colloidal quantum dots	987038-987020-104382331
Reaction monitoring	987038-987020-104677232
Reaction monitoring and kinetics Molecular Dynamics	987038-987020-104712621
molecular synthesis	987038-987020-104851393
NMR on polymers	987038-987020-105022810
qNMR	987038-987020-106586217

10 How would you categorize your level of expertise in operating NMR spectrometers? (select one)



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.a If you would like to provide more detailed information about your mode of remote spectrometer access then please fill in the text box.

No responses

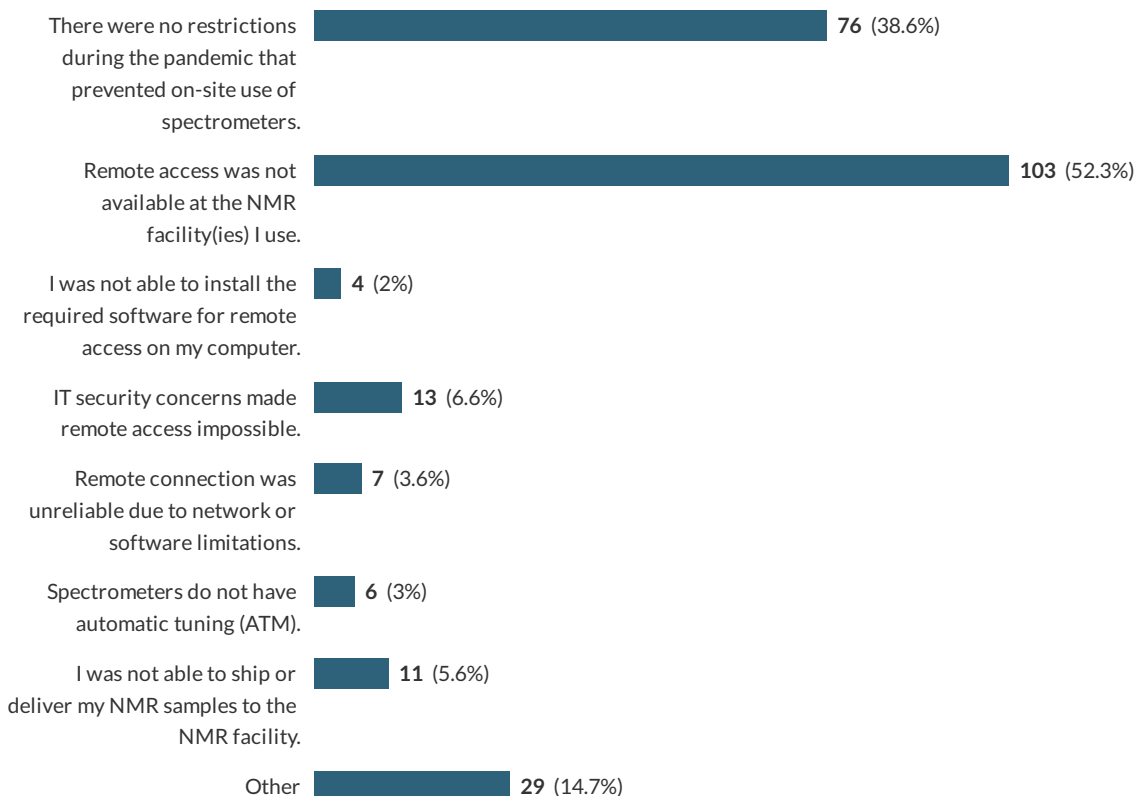
11.b Where has remote access been provided? (select one)

At an NMR facility located in your home university/research centre/company. | 0

At a regional, national or international NMR infrastructure. | 0

At both an NMR facility located in your home university/research centre/company and at a regional, national or international NMR infrastructure. | 0

11.c Why have you not used remote access to NMR spectrometers? (select any that apply)



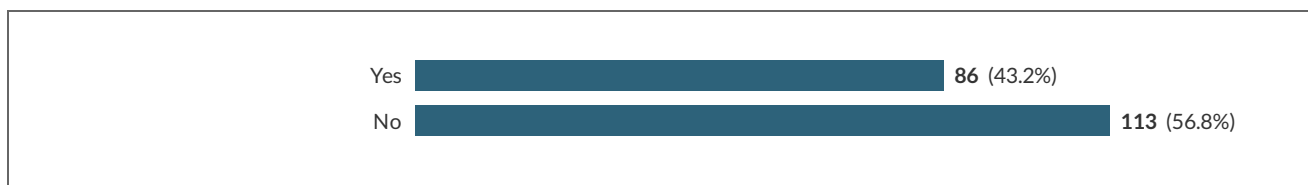
Multi answer: Percentage of respondents who selected each answer option (e.g. 100% would represent that all this question's respondents chose that option)

11.c.i If you selected Other, please specify:

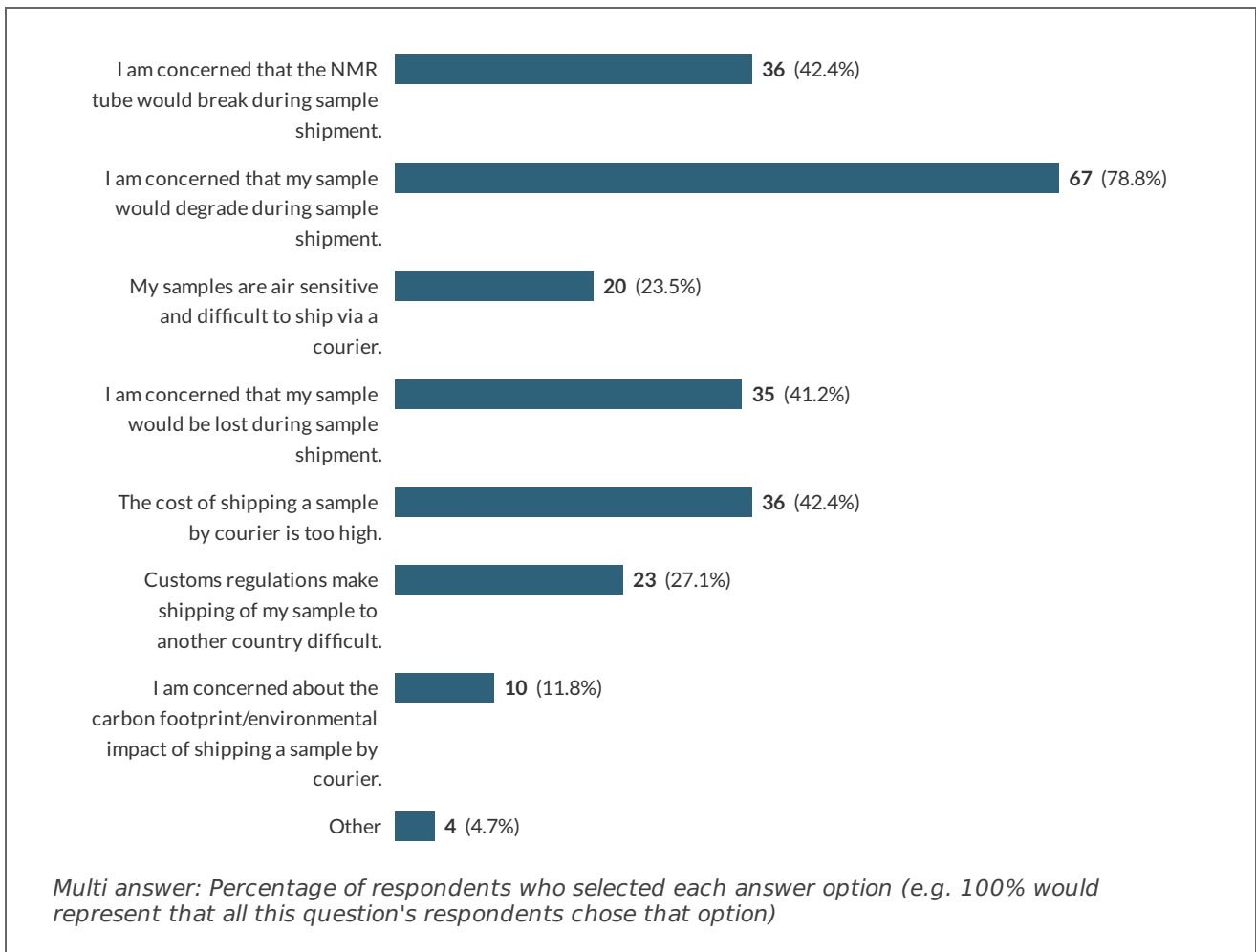
Showing all 28 responses	
I wasn't working with NMR yet.	987038-987020-103912338
I started working after the pandemic, so no restrictions that prevented on-site use of spectrometers.	987038-987020-103913260
I started after the restrictions were lifted	987038-987020-103933811
I did not need NMR data collection during the strict restriction time	987038-987020-103992982
Have not started my PhD until September 2020 and my masters project was stopped in March 2020	987038-987020-104004894
I do not need them for now	987038-987020-104013928
I have not been an NMR user for very long and so have not encountered any restrictions during my time - however my research facility was under restrictions for much of the early pandemic preventing on-site work.	987038-987020-104024542
Someone else is operating NMR spectrimeter, I send samples and get spectra by e-mail or server.	987038-987020-104036086
I did not perform any experiment during Covid-19 pandemic: restrictions to people mobility and restrictions to access to working places avoided any experiment at that time. Since Covid-19 pandemic, I had normal access to the nearest facility, so I did not need remote access.	987038-987020-104198359
I didn't start my NMR research by then and now everything can be done on campus.	987038-987020-104382331
I was not able to prepare the samples for the NMR experiments.	987038-987020-104454070
Since remote access is generally restricted, my on-site collaborating partner recorded the experiments during the pandemic.	987038-987020-104485771
I won a fellowship (Instruct ERIC) that allowed me to be physically present during data collection and analysis.	987038-987020-104545870
Staff at the facility accessed and elaborated data	987038-987020-104611593
Most of the time we are not actively operating the spectrometers at these facilities, (e.g. the actual measurements are performed by the experts there) although this via some kind of remote access could be a great option for us in the future.	987038-987020-104673945
I haven't needed to measure yet.	987038-987020-104770560
I had no need of NMR during lockdown and then the spectrometer were accessible.	987038-987020-104833479
Need to be present for titrations	987038-987020-104843071
Project had not started	987038-987020-104850009
NMR experiments that require presence (change of samples and titration experiments)	987038-987020-104864015

I did not need it, I use it only occasionally	987038-987020-104903762
During the first months of hard restrictions I had no samples to measure, later there were no restrictions anymore and i could measure on-site.	987038-987020-105233734
The consoles have been turned off for fear of power outages	987038-987020-105496764
I have waited the end of the restrictions during the pandemic period	987038-987020-106623404
I am not an expert in NMR.	987038-987020-107026866
I was not running any experiments during this period because I was an undergraduate student.	987038-987020-107385393
i was an undergraduate student	987038-987020-107385171
this was not possible / offered	987038-987020-107492647

11.d Do you consider sample shipment/delivery to an NMR facility to be a barrier to remote spectrometer access?



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

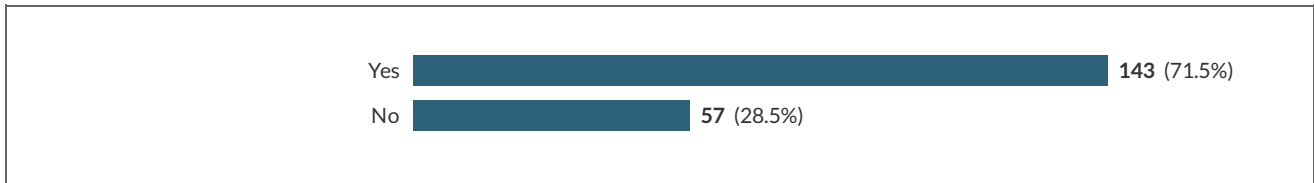


11.d.i.a If you selected Other, please specify:

Showing all 4 responses	
I like to have my results as quickly as possible	987038-987020-104042865
Clinical samples of IP sensitive samples can often not been shipped or measured outside	987038-987020-104437506
I am concerned that it is a lot of work. If I'm on site, I feel like I'm more flexible and can get my results as fast as possible. Or possibly adjust my sample.	987038-987020-104478118
Many of my samples are for kinetic studies and so need to be prepared immediately before analysis.	987038-987020-104677759

11.e 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 you be interested in remote access

to the spectrometers you use?



21 If you have further information that you would like to provide, please enter this in the text box below.

Showing all 22 responses	
Although I don't have much experience working remote I think that it's beneficial in many ways and should be encouraged.	987038-987020-103912338
It would be better to have possibility to take NMR spectra ourselves then to use the service, which is currently the only option	987038-987020-103949594
pointless survey	987038-987020-104008044
High time remote access for NMR users is sorted. So well done for doing this survey and thinking about remote access NMR. Good luck with your initiative.	987038-987020-104030135
/	987038-987020-104042865
I think remote access is a good idea and I would be keen to see this installed in my working institute.	987038-987020-104069999
Looking forward to have remote acces to the NMR spectrometers of my facility. This project is really needed.	987038-987020-104237975
Thanks a lot for presenting such a facility.	987038-987020-104397267
Would this be internationally available?	987038-987020-104421282
some of my 'remote access' occurs through the shipment of sample+student	987038-987020-104424796
I am aware of remote control software but never used in NMR. The idea of remote-NMR is wise.	987038-987020-104437114
My group also does X-ray crystallography or SAXS at synchrotron facilites.. remote access is a very good option once it is properly set-up. It is, however, still crucial, to have a contact person on-site - often to get started or in case there are some truly mechanical issues that require human intervention.	987038-987020-104467387
I would prefer to use remote access most of the time.	987038-987020-104485771
In fact, we are currently not routinely run our own experiments but we are very much interested to do so in the future. Currently, we send the samples to our partners and get back the spectra for further analysis. Some of our lab members, however, have some experience in the setup of biomolecular NMR measurements and we would welcome any future possibility of remote use.	987038-987020-104673945

I mostly use NMR for synthesis reaction/purity control, so most of the time I measure samples immediately parallel to working in the lab, therefore remote measuring is not really necessary for the workflow (as we can't work anyway if we don't get results fast). What we have is remote access to all NMR-results which is really great.	987038-987020-104673898
The remote option of NMR device would be better for my studies, even if I did not used in-person. I am encouracing to build an infrastructure about R-NMR. Cheers.	987038-987020-104682518
The choice of "remote access" has nothing to do with Covid-19 but is bare convenience because it is possible to fill waiting times (inevitably with NMR) with other work	987038-987020-104712621
I believe that remote access will solve some or probably a lot of problems. This approach is fine for NMR users. But, R-NMR should not stop the ability of NMR experts to visit European Infrastructures. This process gives the opportunity to the NMR experts to meet and exchange their thoughts on problem solving.	987038-987020-104737415
The spectrometers that I have used have been piloted by the local team, my input in the experiments performed has been limited to discussing the type of results desired and debating the advantages or disadvantages of different techniques and the required samples.	987038-987020-104850009
for basic science one should allow the access with the expert technician	987038-987020-104903762
The closest I got to remote access was receiving data via e-mail. But I guess that does not count.	987038-987020-105575669
None	987038-987020-105582613