Remote-NMR: NMR Facility Manager Survey

1 You are invited to complete this online survey aimed at NMR facility managers. We will ask questions about your NMR facility, your experiences with providing remote access to NMR spectrometers and for your views on how remote access can be improved in the future. The survey can 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. There will be the option to provide more detailed information via a one-to-one online interview; in this case you will be asked to provide your name/email address so that you can be contacted directly. 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; however this information will not be associated with your name or your email address. 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). An anonymised version of the survey (without any name/email information) will be created for longer-term storage. We intend to keep this version for 3 years after publication of the outcome of the project. Please confirm below: That you have read this information, and if you require further detailed information, that you have read the Participant Information Sheet. That you understand who will have access to any personal data that you provide, how data will be stored and what will happen to data at the end of the project. That you understand how to raise a concern or make a complaint. That you are willing to continue with the survey.

Yes　　**20** (100%)

No　　**0**

2 Please confirm that you are the manager of an NMR facility. (Please try to ensure that the survey is only completed by one person involved in the management of your NMR facility).

Yes　　**20** (100%)

No　　**0**

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

Country	Value
Austria	0
Belgium	0
Bulgaria	0
Croatia	0
Cyprus	0
Czech Republic	0
Denmark	0
Estonia	0
Finland	0
France	0
Germany	0
Greece	0
Hungary	0
Iceland	0
Ireland	0
Israel	0
Italy	0
Latvia	0
Lithuania	0
Luxembourg	0
Malta	0
Netherlands	0
Norway	0
Poland	0
Portugal	0
Romania	0
Serbia	0
Slovakia	0
Slovenia	0
Spain	0
Sweden	0
Switzerland	0
United Kingdom	20 (100%)
Ukraine	0
Other	0

3.a If you selected Other, please specify:

No responses

4 Is your NMR facility part of a national infrastructure?

Yes	**4** (20%)
No	**16** (80%)
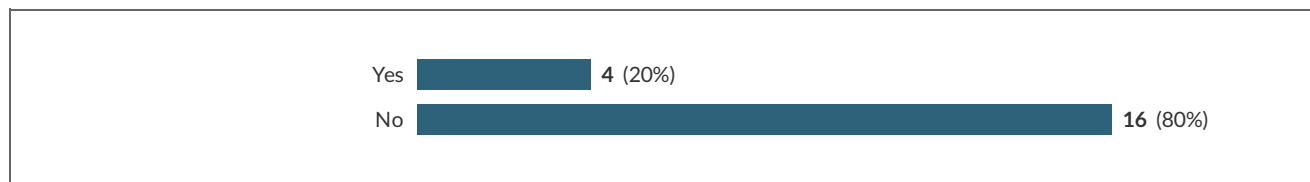
5 How many spectrometers do you have in your NMR facility?

1	**3** (15%)
2	**1** (5%)
3	**5** (25%)
4	**4** (20%)
5	**0**
6-9	**5** (25%)
10-15	**2** (10%)
>15	**0**
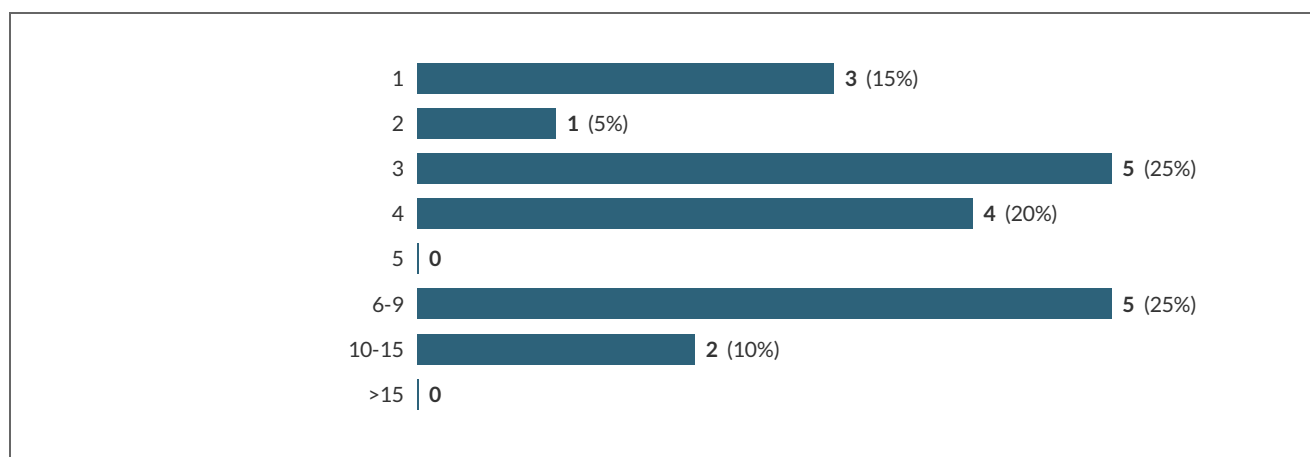
6 At what 1H frequencies do your spectrometers operate? (select all that apply)
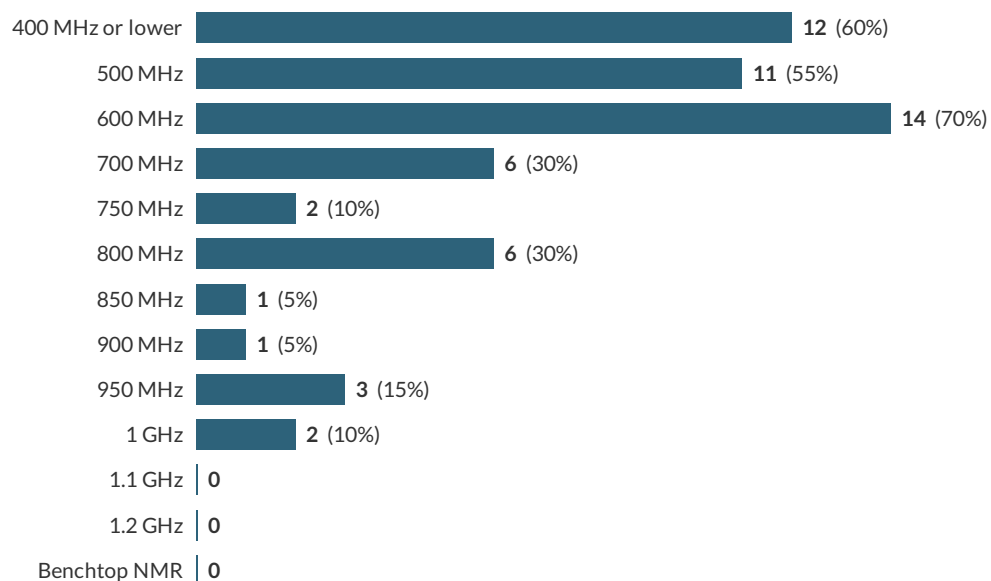
400 MHz or lower — **12** (60%)
500 MHz — **11** (55%)
600 MHz — **14** (70%)
700 MHz — **6** (30%)
750 MHz — **2** (10%)
800 MHz — **6** (30%)
850 MHz — **1** (5%)
900 MHz — **1** (5%)
950 MHz — **3** (15%)
1 GHz — **2** (10%)
1.1 GHz — **0**
1.2 GHz — **0**
Benchtop NMR — **0**

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

7 What type of spectrometers do you have in your facility? (select all that apply)
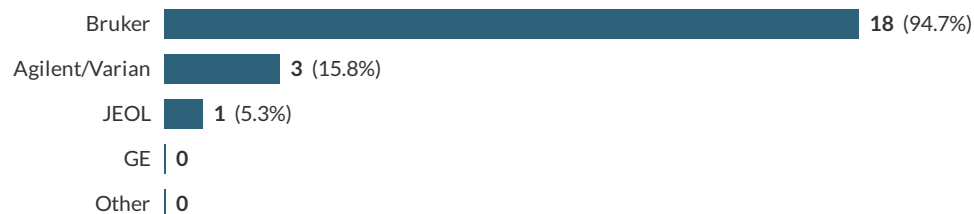
Bruker — **18** (94.7%)
Agilent/Varian — **3** (15.8%)
JEOL — **1** (5.3%)
GE — **0**
Other — **0**

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

7.a If you selected Other, please specify:

No responses

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

Bruker TopSpin **19** (95%)

Bruker IconNMR **8** (40%)

Agilent VnmrJ **2** (10%)

JEOL Delta **1** (5%)
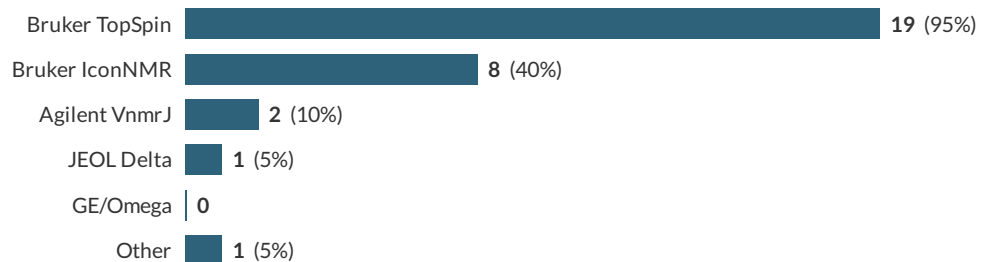
GE/Omega **0**

Other **1** (5%)

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

8.a If you selected Bruker TopSpin, please specify the version (if more than one version is used please enter versions on separate lines).

Showing all 18 responses	
3.6.2	951912-951894-101360820
4.1.1	951912-951894-101372382
3.6.5	951912-951894-101397499
3.2.6 3.5.6	951912-951894-101411307
3.6.3 and 4.1.4	951912-951894-101445018
3.5pl7	951912-951894-101603924
TopSpin 3.1.7, 3.2.1, 3.2.6 and 3.6.1	951912-951894-101359111
3.2pl15; 4.0.2; 4.0.8; 4.0.9; 4.1.8	951912-951894-101737673
3.5.6 3.6.2 3.6.4	951912-951894-101745973
TS3.2.6 (600 AVANCE III) TS3.5.6 (500 AVANCE III) TS3.6.2 (600 AVANCE III) TS3.6.4 (600 & 900 AVANCE III HD) TS4.0.5 (800 NEO) TS 4.1.4 (1000 NEO)	951912-951894-101849988
2.1 4.1.4 4.0.9	951912-951894-101889996
Topspin 3.6.3	951912-951894-101890829
3.6, 3.2, 2.1	951912-951894-101890690
Topspin 3.5 patch level 6 (600MHz & 700MHz) Topspin 4.0 patch level 7 (800MHz)	951912-951894-101891636
TopSpin3.5 & TopSpin4.1 (on 800)	951912-951894-101953004
3.2 3.5pl6	951912-951894-101966822
4.1 3.6 2.1	951912-951894-102043034
3.2pl7 (W10, maximum supported by Fourier 300) 3.6.5 (W10) 3.2pl7 (solids, CentOS 5.5) 3.2pl7/3.5pl6 (solids, CentOS 5.5)	951912-951894-102051473

8.b If you selected Bruker IconNMR, please specify the version (if more than one version is used

please enter versions on separate lines).

Showing all 7 responses	
5	951912-951894-101397499
5.0.11 and 5.2.4	951912-951894-101445018
4.2.2 5.2.4 5.1.9	951912-951894-101889996
not known	951912-951894-101890829
IconNMR 5.0 patch level 6 (600MHz & 700MHz) IconNMR 5.1 patch level 7 (800MHz)	951912-951894-101891636
3.6.4	951912-951894-102043034
5.0.12 build 7 (as per TopSpin 3.6.5) 4.7.7 build 20 (as per TopSpin 3.2pl7)	951912-951894-102051473

8.c   If you selected Agilent VnmrJ, please specify the version (if more than one version is used please enter versions on separate lines).

Showing all 2 responses	
4	951912-951894-102043034
VNMRJ 3.2	951912-951894-102078028

8.d   If you selected JEOL Delta, please specify the version (if more than one version is used please enter versions on separate lines).

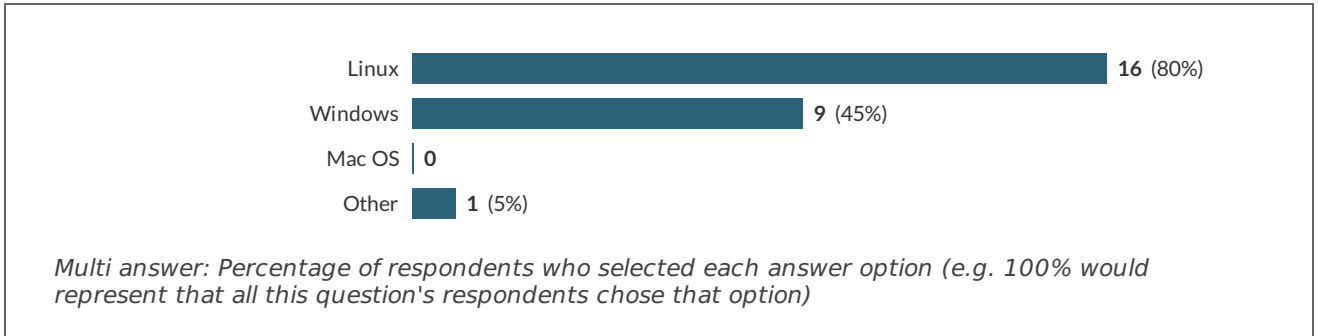| Showing 1 response	
5.3.1	951912-951894-101411307

8.e   If you selected GE/Omega, please specify the version (if more than one version is used please enter versions on separate lines).

No responses

8.f   If you selected Other, please specify the software name and version (if more than one version is used please enter versions on separate lines).

Showing 1 response	
SpinSight	951912-951894-101737673

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

Linux	**16** (80%)
Windows	**9** (45%)
Mac OS	**0**
Other	**1** (5%)

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 Linux, please specify the distribution (Debian, Fedora etc) and version.

Showing all 16 responses	
CentOS 7.9	951912-951894-101376176
Centos 7	951912-951894-101397499
Centos 5.11	951912-951894-101411307
CentOS 7	951912-951894-101445018
CentOS 7	951912-951894-101603924
Centos 7.9, 5.11 and 5.8	951912-951894-101359111
CentOS 10	951912-951894-101737673
Centos	951912-951894-101745973
CentOS 5 CenOS 7	951912-951894-101849988
Win10 & CentOS	951912-951894-101890690
CentOS7 (only linux distribution supported by Bruker)	951912-951894-101891636
Centos 5 & Centos 7	951912-951894-101953004
Centos	951912-951894-101966822
CentOS7	951912-951894-102043034
CentOS 5.5	951912-951894-102051473
CentOS 2.28	951912-951894-102078028

9.b If you selected Windows, please specify the version.

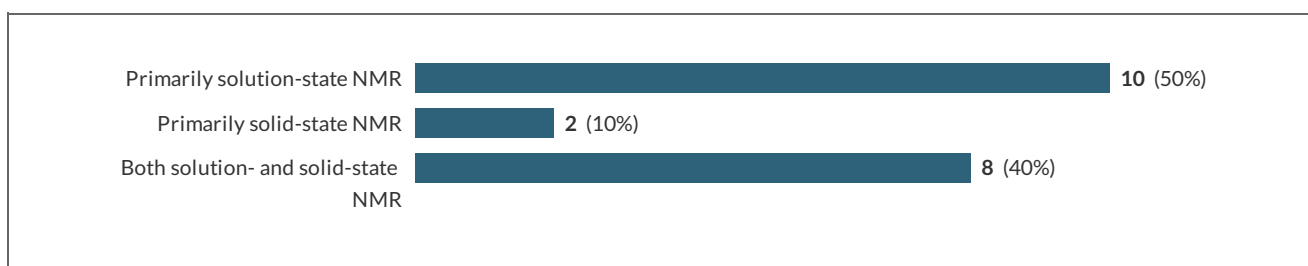| Showing all 8 responses	
10	951912-951894-101360820
10	951912-951894-101372382
Win10 pro 21H1	951912-951894-101376176
windows 7	951912-951894-101411307
10 pro	951912-951894-101745973
Windows 10 Pro	951912-951894-101889996
Windows 10	951912-951894-101890829
10	951912-951894-102051473

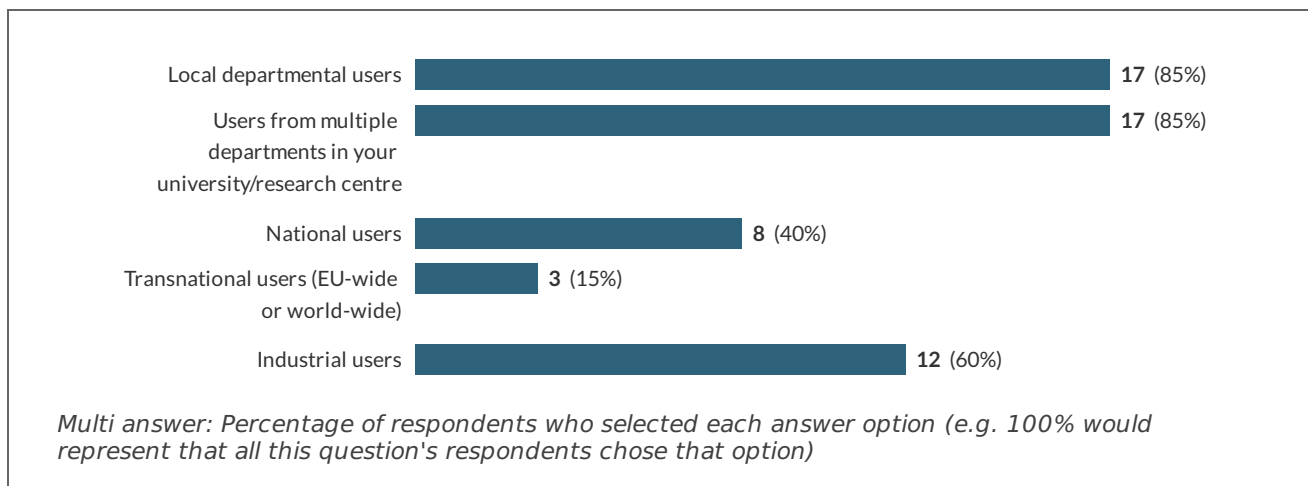9.c If you selected Mac OS, please specify the version.

No responses

9.d If you selected Other, please specify the operating system and version.

Showing 1 response	
Sun Microsystems	951912-951894-101737673

10 What type of NMR are the spectrometers in your facility equipped for? (select one)

Primarily solution-state NMR	**10** (50%)
Primarily solid-state NMR	**2** (10%)
Both solution- and solid-state NMR	**8** (40%)

11 Tell us about the users of your NMR facility. (select all that apply)

Local departmental users **17** (85%)

Users from multiple departments in your university/research centre **17** (85%)

National users **8** (40%)

Transnational users (EU-wide or world-wide) **3** (15%)

Industrial users **12** (60%)

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

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

NMR associated with undergraduate/graduate teaching **13** (65%)

Routine small molecule characterization supporting organic chemistry **15** (75%)

Biomolecular NMR research **15** (75%)

Metabolomics research **8** (40%)

Micro-imaging research **1** (5%)

Materials Science NMR research **6** (30%)

Other Physical Sciences NMR research **8** (40%)

Other **3** (15%)

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

12.a If you selected Other, please specify:

Showing all 3 responses	
Work that would fall under the NERC remit (soils, mineralogical samples, etc.).	951912-951894-101360820
Metabolic tracing research	951912-951894-101849988
complex mixtures	951912-951894-101953004

13 On average, how many users does your facility have in a year?

1-25	**3** (15.8%)
26-50	**9** (47.4%)
51-100	**3** (15.8%)
>100	**4** (21.1%)
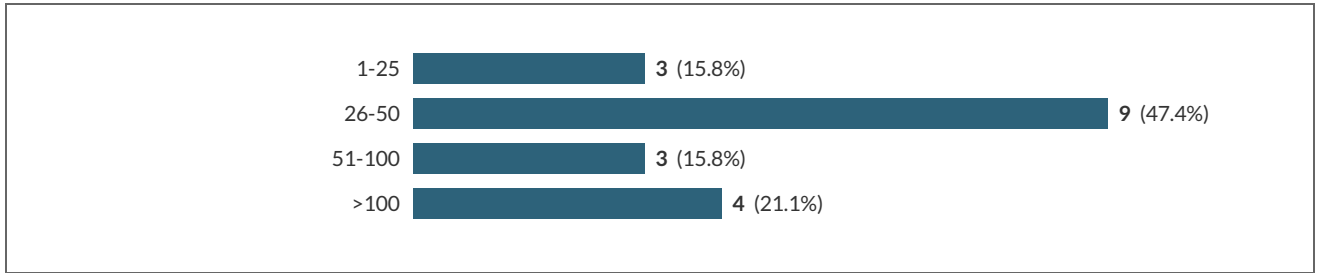
14 Local users

Showing all 19 responses	
5 PIs	951912-951894-101360820
30	951912-951894-101372382
<50	951912-951894-101376176
300	951912-951894-101397499
40	951912-951894-101411307
20	951912-951894-101445018
8	951912-951894-101603924
20	951912-951894-101359111
25	951912-951894-101737673
20	951912-951894-101745973
20	951912-951894-101889996
26-50	951912-951894-101890829
400	951912-951894-101890690
53	951912-951894-101891636
>100	951912-951894-101953004
26	951912-951894-101966822
50 (research groups, 600 individuals including UG teaching)	951912-951894-102043034
60-70	951912-951894-102051473
35	951912-951894-102078028

15 National users

Showing all 16 responses	
3 Pls	951912-951894-101360820
5	951912-951894-101372382
0	951912-951894-101376176
1	951912-951894-101411307
1	951912-951894-101445018
1	951912-951894-101603924
10	951912-951894-101359111
40	951912-951894-101737673
20	951912-951894-101745973
0	951912-951894-101890829
0	951912-951894-101890690
8	951912-951894-101891636
>10	951912-951894-101953004
1	951912-951894-101966822
15	951912-951894-102043034
1	951912-951894-102051473

16 Transnational users (EU-wide and world-wide)

Showing all 10 responses	
1-2 Pls	951912-951894-101360820
0	951912-951894-101372382
0	951912-951894-101376176
0	951912-951894-101603924
0	951912-951894-101359111
15	951912-951894-101737673
0	951912-951894-101890829
0	951912-951894-101890690
0	951912-951894-101966822
0	951912-951894-102051473

17 Industrial users

Showing all 17 responses	
0-1 Organisations	951912-951894-101360820
0	951912-951894-101372382
0	951912-951894-101376176
5	951912-951894-101397499
2	951912-951894-101411307
4	951912-951894-101445018
1	951912-951894-101603924
2	951912-951894-101359111
5	951912-951894-101737673
15	951912-951894-101745973
0	951912-951894-101890829
2	951912-951894-101890690
2	951912-951894-101891636
>5	951912-951894-101953004
1	951912-951894-101966822
15	951912-951894-102043034
4 (as a service)	951912-951894-102051473

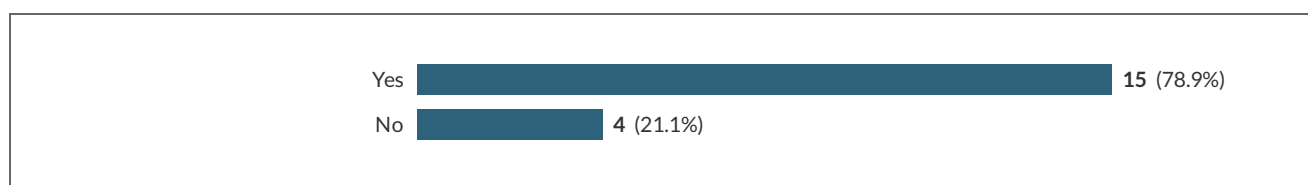**18** How do users of your NMR facility login to the spectrometers and do they have access to other users' data? (select all that apply)
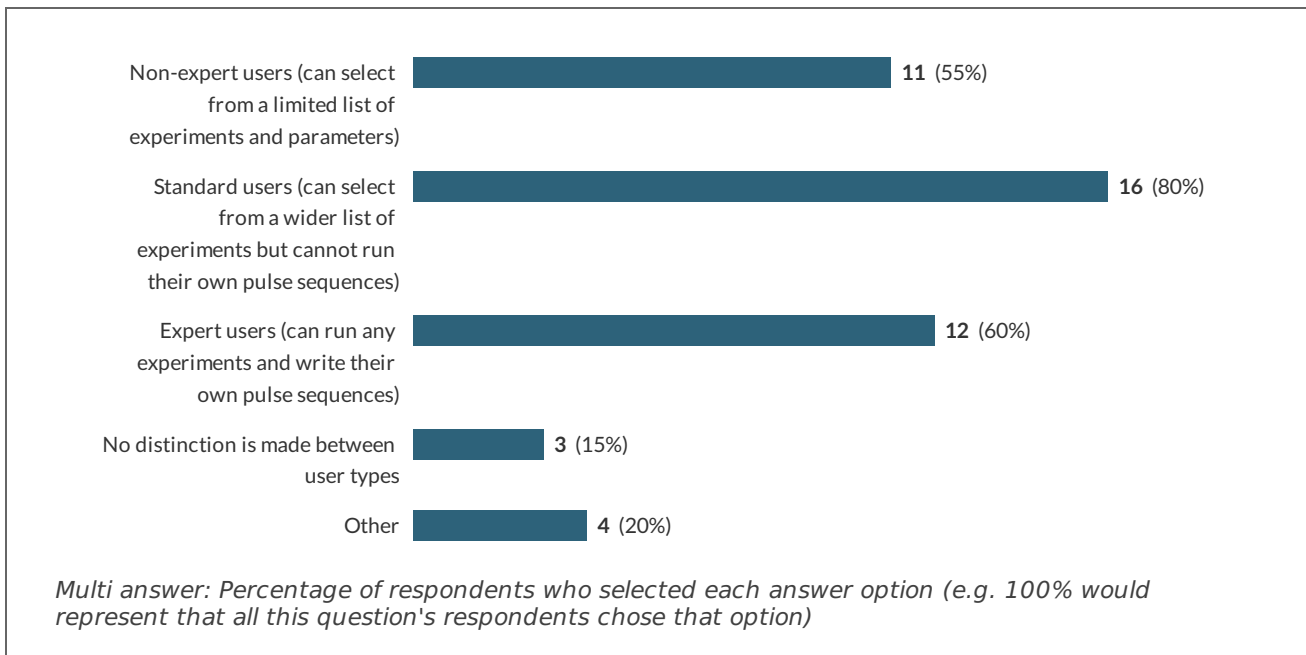
Individual accounts with no access to other users' files	5 (25%)
Shared account with open access to other users' files	11 (55%)
Short-term login account with no access to other users' files (usernames are recycled)	0
Other	8 (40%)

Multi answer: Percentage of respondents who selected each answer option (e.g. 100% would represent that all this question's respondents chose that option)
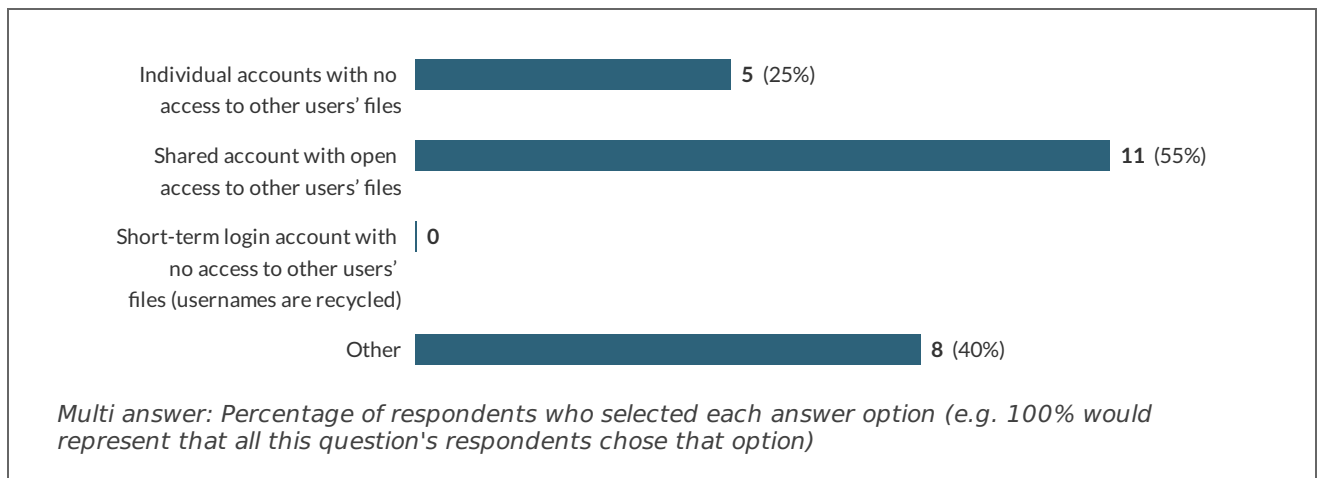
18.a If you selected Other, please specify:

Showing all 8 responses	
Solid-state NMR research group users can access the shared login for running experiments and viewing data. Other users submit samples which are run by the facility manager, who then emails out a link to their data in a zip file on Dropbox.	951912-951894-101360820
Individual accounts with access to other users' files	951912-951894-101376176
Individual accounts with access to others files controlled by UNIX permissions	951912-951894-101603924
Individual Accounts with access to other's files with an option for a sequestered environment if needed.	951912-951894-101737673
Individual accounts with limited access to other users' files	951912-951894-101745973
Individual accounts with possible access to other users' files depending on permissions set by account owners. Users can share data/files if they choose to. Account holders can belong to specific groups and decide who they share files with.	951912-951894-101849988
We use in house developed NMR data management system. https://www.nomad-nmr.uk/	951912-951894-101890690
Solution state: open access with shared Windows perma-login, but individual accounts in IconNMR. Users can see other users' files. Solids: individual Linux accounts, and users cannot access other users' files	951912-951894-102051473

19 Are different levels of spectrometer access provided for users with different levels of expertise?

Yes	15 (78.9%)
No	4 (21.1%)

20 Which of the following describe categories of users in your facility? (select all that apply)

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

20.a If you selected Other, please specify:

Showing all 4 responses	
Non-expert users discuss experiments and science with the facility manager, who then decides on the experiments to run.	951912-951894-101360820
In reality, it's not the list of experiments available to users that describes their category of expertise, rather the amount of supervision provided/required. Non-expert users will naturally require full supervision, until they have proved and developed their abilities at the spectrometer.	951912-951894-101849988
supervised users - access with direct supervision only service users - spectra acquired by facility staff	951912-951894-101891636
Solution state: all users have access to "Edit all acquisition parameters..." option in IconNMR, but in practice no-one uses it, and the only thing routinely changed by users is the number of scans within IconNMR. Solid state: no guardrails!	951912-951894-102051473

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21 If your facility has different categories of users, how is user expertise level assessed? (Please specify)

Showing first 5 of 15 responses	
Experts come from within the solid-state NMR research group. Everyone else is a non-expert in the technique but probably knows roughly what their materials are and what questions they want answered.	951912-951894-101360820
Structured training levels	951912-951894-101376176
We have specialist users, who are able to run their own experiments in TopSpin without the support of NMR staff. These users must: i) Convince NMR staff that they will be regular users of our NMR instrumentation; ii) Be running experiments that are not normally available on open-access instrumentation; and iii) Once trained/during training display a sufficient level of competence to run and NMR experiment with the assistance of NMR staff.	951912-951894-101397499
most users are standard users. Only a couple of main users here are expert users - no specific assessment is done, but user experience and time on machine are considered.	951912-951894-101411307
Users ability is assessed on a case-by-case basis	951912-951894-101445018

22 How is user NMR data kept secure and how do users access their data? (Please specify).

Showing all 19 responses	
No particular security although industrial data is removed from the spectrometer PCs' hard drives and stored on a separate machine. Non-expert users can only access their data via email link.	951912-951894-101360820
All data is copied onto a local server, which acts both as a backup and a method of access for local users. Access to data for less local users is still done on a more ad-hoc basis (email/teamviewer/FTP etc.) as appropriate for the user and data in question.	951912-951894-101372382
Copied to archive server (after acquisition). Read only access to data shares.	951912-951894-101376176
all data are backed up. access is through data server or directly from the spectrometer computer	951912-951894-101411307
Encrypted Hard drives with password protection. Data is accessed based on login credentials.	951912-951894-101445018
No special security above Unix permissions. Data backed up nightly. Data transfers by SSH or file drop website.	951912-951894-101603924
Only registered users are allowed access to the spectrometers. Remote access requires VPN account. Data is accessed either via USB or via sftp/ssh. For external users data is sometimes sent via a secure data transfer system operated by the university.	951912-951894-101359111
Industrial Users have an isolated file tree that is not accessible to anyone but the Local Managers and the Industrial users. This data is deleted upon	951912-951894-101737673

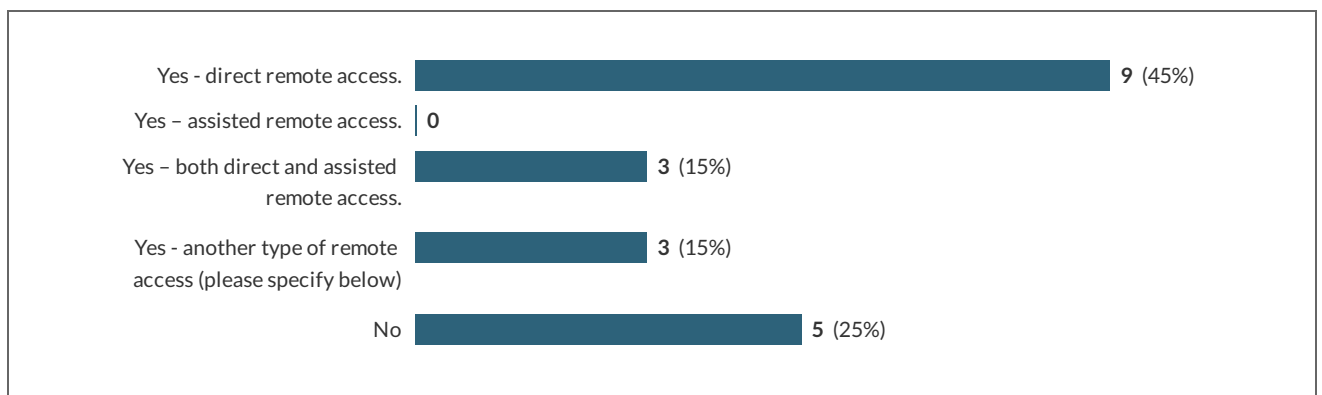|	
request, or after a set amount of time. "Normal" users have access to their data through TeamViewer file transfer, through a user account provided by the university IT services, or through email file drop. Users are held to the honor system to only access their own data.	
Data are backed up to two remote locations. User's own data are available for download from a file server	951912-951894-101745973
Data are stored on the facility firewall-protected data server, which sits behind the University firewall. While visiting the facility, users can access the data server via available workstations (PC and spectrometer-based) which are linked by the facility local subnet. Remote access to the data server and spectrometers (via the data server) is possible by ssh, for remote transfer of data.	951912-951894-101849988
Spectrometer PCs manually backed up approx. monthly to secure cloud storage. User access to data typically by exporting from spectrometer PC to external removable media	951912-951894-101889996
Data are stored locally in the NMR magnet PC and copied on a backup shared drive where end users can access. In principle all the folders are accessible by all end users with an account. We are trying to restrict that with our IT team so it is a "read only" mode.	951912-951894-101890829
All data acquired under automation are stored by our NOMAD system (https://www.nomad-nmr.uk/). Current version of NOMAD does not handle data acquired manually yet. We use spectrometers in manual mode only very occasionally and therefore need for development of that part of system is not that big. However, the feature is definitely on the road map.	951912-951894-101890690
Access to spectrometer logins (and physical access to spectrometer PCs) is restricted - once access is granted all data on that spectrometer is open / can be viewed. The facility keeps confidentiality mainly by anonymity of the dataset name / details (rather than permission structure) but this is something we wish to review. Linux allows for periodic backups (direct to specific users password protected accounts) and removal of sensitive data from the spectrometer PC in a timely manner. Approved users can access data on the spectrometer direct from linux using secure shell (ssh) or facility staff will send datasets to external users via wetransfer.com	951912-951894-101891636
external (mostly industrial) users data are kept in password protected folders	951912-951894-101953004
Users copy data onto their own university accounts for further analysis and are themselves responsible for keeping it secure and backed up.	951912-951894-101966822
data is stored on a secure server. users have read only access. data is segregated into research group mount points.	951912-951894-102043034
Solution state: automated archiving to university fileserver, access to which requires authentication using university credentials (VPN if off-	951912-951894-102051473

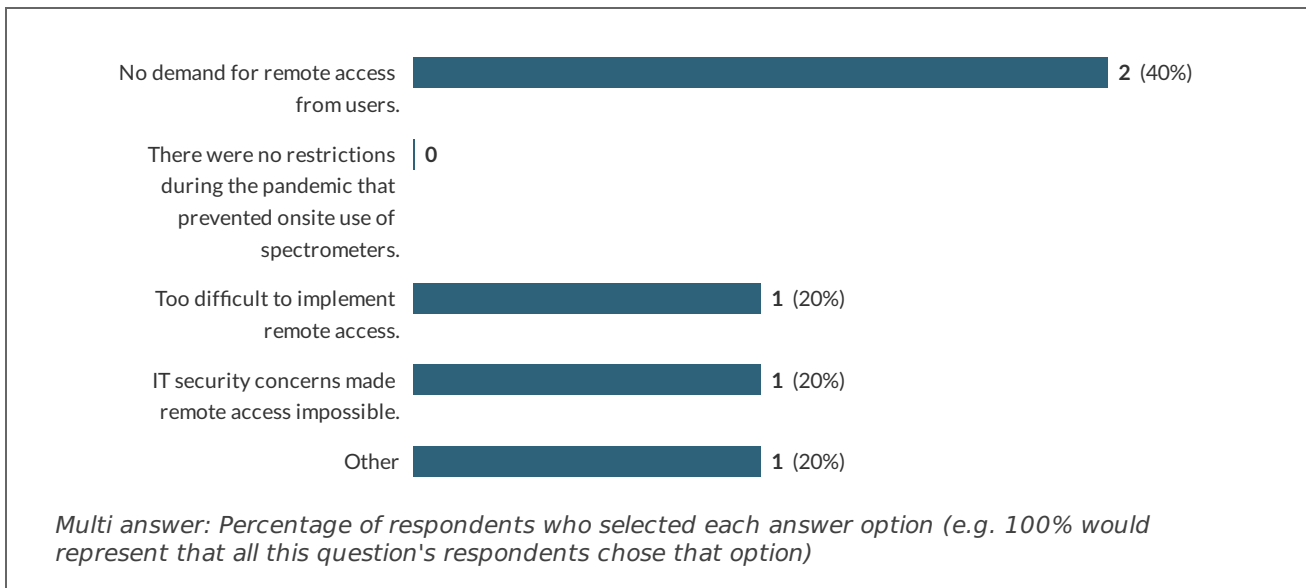|	
campus). Physical access to NMR lab controlled using university ID cards, and USB drives disabled for Windows machines. Solids: physical access to NMR lab controlled using university ID cards, ad hoc arrangements with USB drives	
Data is located on a shared network drive	951912-951894-102078028

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

Yes - direct remote access.   **9** (45%)
Yes – assisted remote access.   **0**
Yes – both direct and assisted remote access.   **3** (15%)
Yes - another type of remote access (please specify below)   **3** (15%)
No   **5** (25%)

23.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 12 responses	
Initially allowed expert users to use TeamViewer but now use DWService. Non-expert users have no remote access (and don't need it) because the facility manager runs experiments for them.	951912-951894-101360820
Bruker IconWeb	951912-951894-101376176
the option is only open to expert users. they can connect via teamviewer or vnc	951912-951894-101411307
Direct remote access was provided via the software NoMachine	951912-951894-101445018
secure VNC connection over VPN	951912-951894-101603924
We provided access through TeamViewer or through X2go. The local managers would either use the built-in chat features of teamviewer, or open a teams or zoom session on a personal device (laptop, iPad, etc.)	951912-951894-101737673
SSH tunnel and VNC	951912-951894-101745973
Anydesk and Zoom were most successful for direct and assisted access respectively.	951912-951894-101891636
remote access t o spectrometers is provided via TeamViewer just for experienced users. All other users can acess their data on demand remotely on shared platforms e.g Microsoft OneDrive.	951912-951894-101953004
Using the program Pulsesecure supplied and installed by our IT. In addition Teams or Zoom can then be used.	951912-951894-101966822
vnc over ssh has always been available to advanced users. Remote http access to IconNMR queues was enabled during the pandemic but is now disabled again.	951912-951894-102043034
Solution state: remote access to Windows machines. In principle could be shared with users, but currently only used by the facility manager for maintenance and method development.	951912-951894-102051473

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

No demand for remote access from users.	2 (40%)
There were no restrictions during the pandemic that prevented onsite use of spectrometers.	0
Too difficult to implement remote access.	1 (20%)
IT security concerns made remote access impossible.	1 (20%)
Other	1 (20%)

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

**23.b.i** If you selected Other, please specify:

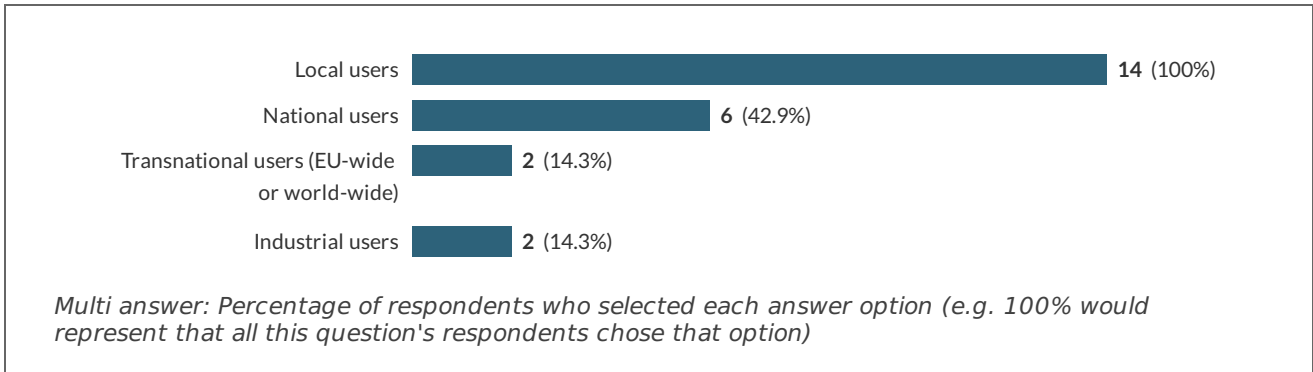| **Showing 1 response**	
The lack of expertise of our end users made it impossible. We cannot trust them. They just know how to operate the instrument in automatic mode. Past experiences taught us they cannot have admin rights or autonomy to operate the magnet themselves for troubleshooting or anything outside the standard experiments in IconNMR. Also, there is a high turnover of students every year, so there is a small number of people who becomes confident to use the instrument. If anything, we would implement remote access for a selected group of people with different levels of access.	951912-951894-101890829

23.c The aim of the Remote-NMR project is to develop a common framework for remote spectrometer access taking into account best practice across the EU/UK. Standardized training for remote access will also be put in place. Once this has been completed, would your NMR facility be interested in implementing remote spectrometer access?
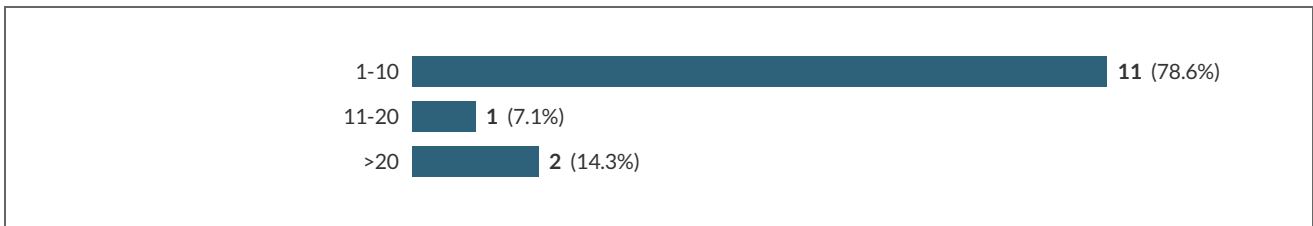
| Yes | 2 (50%) |
| No | 2 (50%) |

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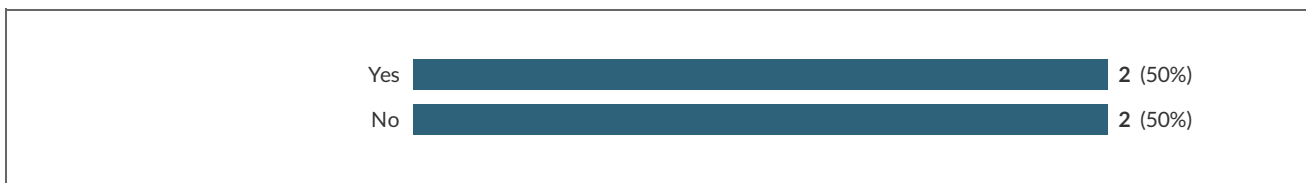
24 If your facility has provided any type of remote access then select 'Yes' to proceed to further questions about your implementation of remote access. If your facility has not provided any type of remote access then select 'No' to proceed to the end of the survey.

Yes	**14** (70%)
No	**6** (30%)
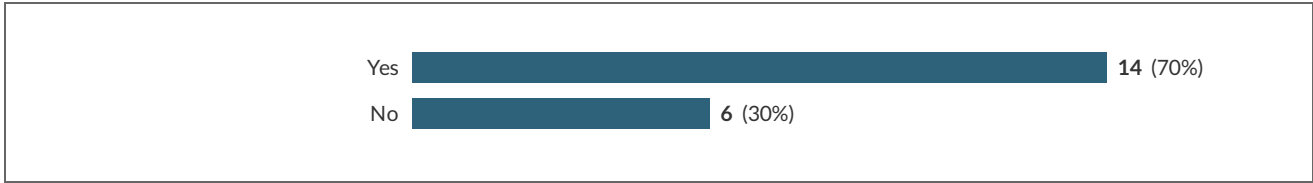
25 If you have provided remote access, what categories of users had remote access. (please select all that apply)

Local users	**14** (100%)
National users	**6** (42.9%)
Transnational users (EU-wide or world-wide)	**2** (14.3%)
Industrial users	**2** (14.3%)

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

26 Overall, how many remote users has your facility had in the last 2-3 years?

1-10	**11** (78.6%)
11-20	**1** (7.1%)
>20	**2** (14.3%)

27 Local users

Showing all 14 responses	
8 individuals from one group	951912-951894-101360820
1	951912-951894-101372382
<10	951912-951894-101376176
2	951912-951894-101411307
12	951912-951894-101445018
10	951912-951894-101359111
20	951912-951894-101737673
4	951912-951894-101745973
2	951912-951894-101849988
7	951912-951894-101891636
5-10	951912-951894-101953004
6	951912-951894-101966822
30	951912-951894-102043034
1	951912-951894-102051473

28 National users

Showing all 12 responses	
0	951912-951894-101360820
3	951912-951894-101372382
0	951912-951894-101376176
2	951912-951894-101359111
40	951912-951894-101737673
4	951912-951894-101745973
4	951912-951894-101849988
2	951912-951894-101891636
1-5	951912-951894-101953004
0	951912-951894-101966822
0	951912-951894-102043034
0	951912-951894-102051473

29 Transnational users (EU-wide and world-wide)

	Showing all 9 responses
0	951912-951894-101360820
0	951912-951894-101372382
0	951912-951894-101376176
0	951912-951894-101359111
10	951912-951894-101737673
1	951912-951894-101849988
0	951912-951894-101966822
0	951912-951894-102043034
0	951912-951894-102051473

30 Industrial users

	Showing all 9 responses
0	951912-951894-101360820
0	951912-951894-101372382
0	951912-951894-101376176
0	951912-951894-101359111
5	951912-951894-101737673
1	951912-951894-101849988
0	951912-951894-101966822
0	951912-951894-102043034
0	951912-951894-102051473

31 What type of spectrometers were available for remote access? (select all that apply)
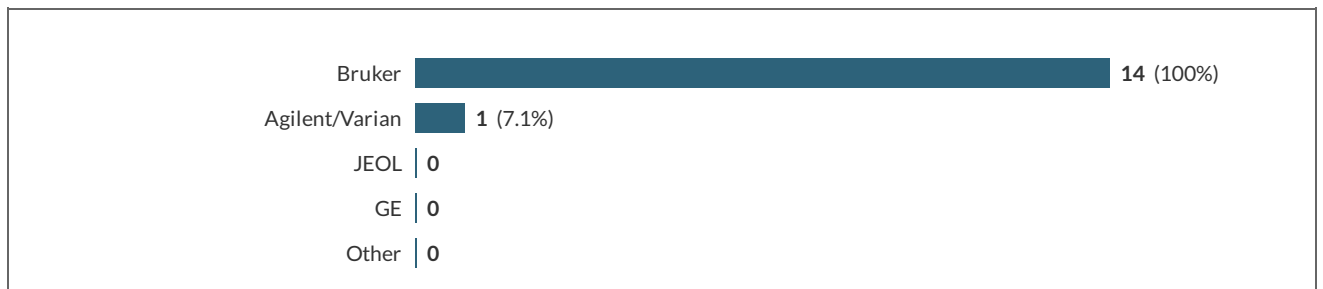
Bruker	14 (100%)
Agilent/Varian	1 (7.1%)
JEOL	0
GE	0
Other	0

31.a If you selected Other, please specify:

No responses

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

AnyDesk — **2** (14.3%)
NoMachine (NX) — **4** (28.6%)
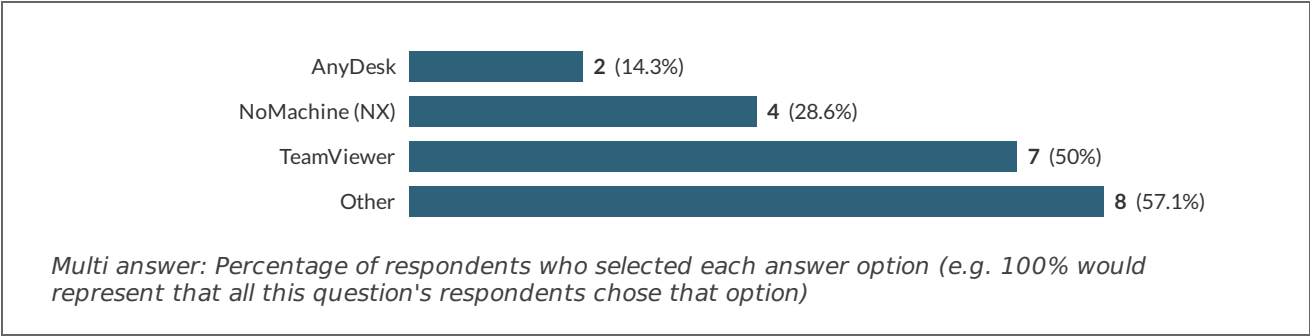TeamViewer — **7** (50%)
Other — **8** (57.1%)

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

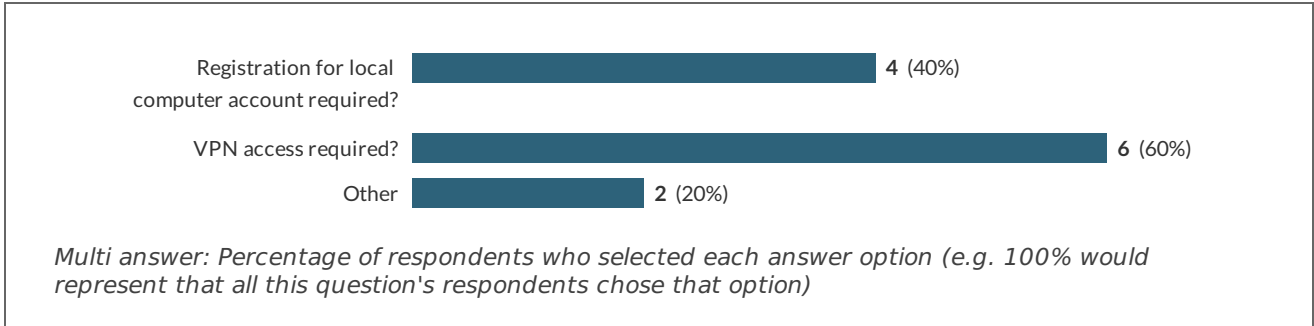
32.a If you selected Other, please specify:

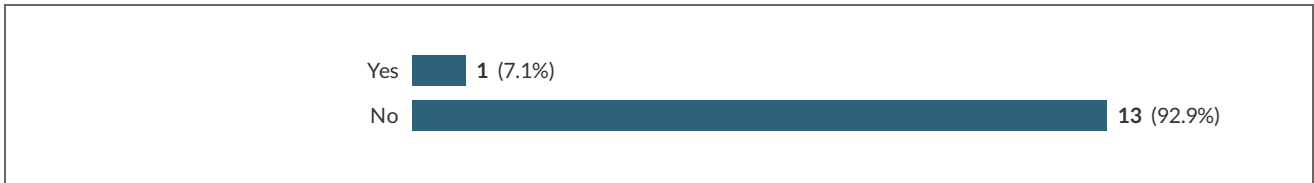| Showing all 8 responses	
DWService	951912-951894-101360820
Bruker IconWeb or MS remote desktop	951912-951894-101376176
vnc	951912-951894-101411307
SSH tunnel and VNC	951912-951894-101745973
vnc	951912-951894-101849988
PulseSecure	951912-951894-101966822
vnc (tunnelled over ssh)	951912-951894-102043034
Formerly using TeamViewer, then Remote Utilities, then AnyDesk, and now currently on NoMachine in combination with TailScale to punch through the university firewall.	951912-951894-102051473

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33 Did local IT staff place any restrictions on remote user access to ensure network security (select all that apply)?
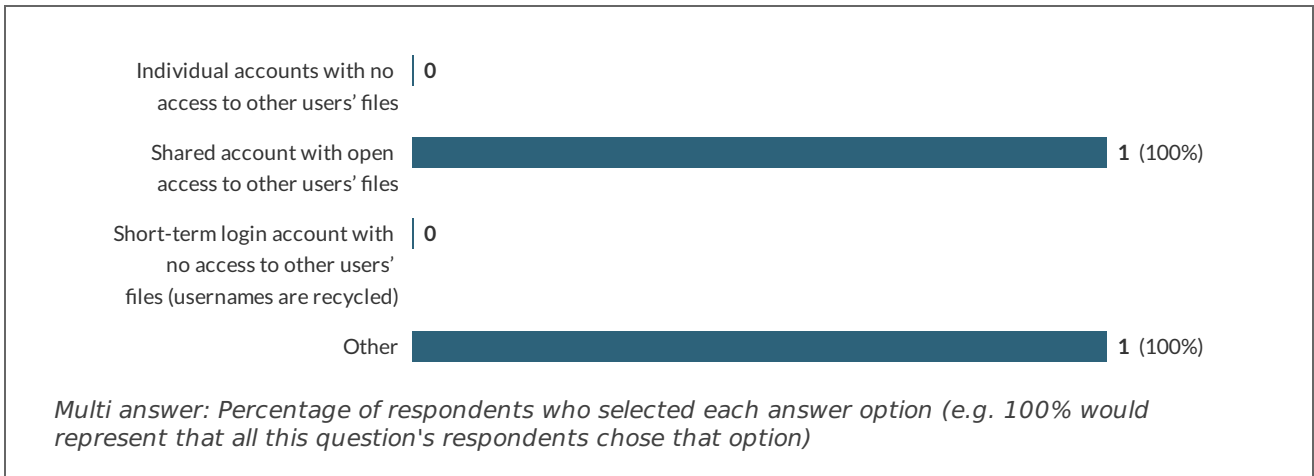
Registration for local computer account required? **4** (40%)
VPN access required? **6** (60%)
Other **2** (20%)

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

33.a If you selected Other, please specify:

Showing all 2 responses	
What they don't know won't harm them...	951912-951894-101360820
TailScale requires authentication, and setup to use university MS/O365 credentials.	951912-951894-102051473

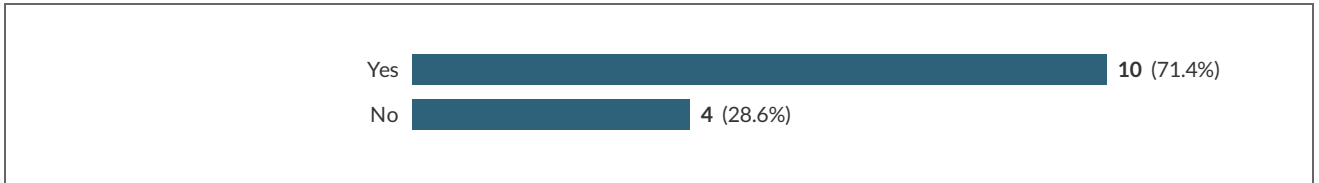**34** Did login procedures for remote users differ from those for on-site users?

Yes **1** (7.1%)
No **13** (92.9%)

34.a If yes, how did remote users login?

Individual accounts with no access to other users' files **0**
Shared account with open access to other users' files **1** (100%)
Short-term login account with no access to other users' files (usernames are recycled) **0**
Other **1** (100%)

Multi answer: Percentage of respondents who selected each answer option (e.g. 100% would represent that all this question's respondents chose that option)
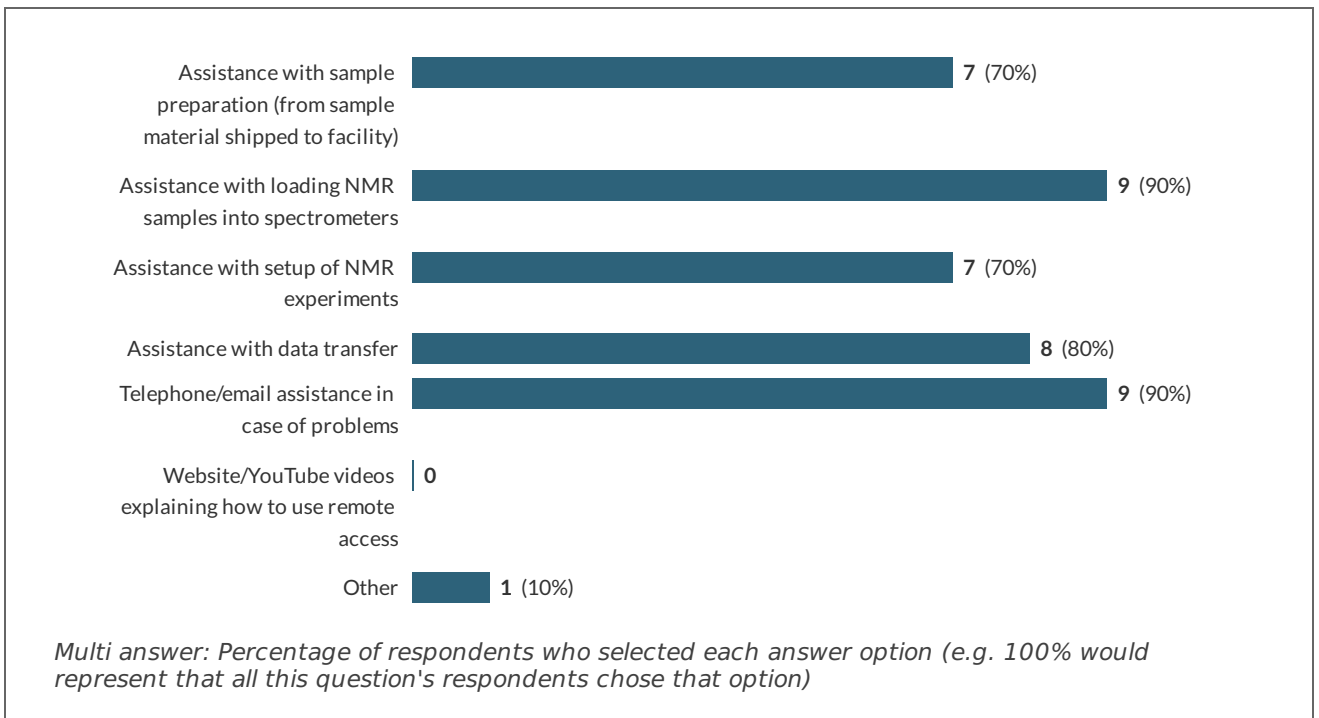
34.a.i If you selected Other, please specify:

Showing 1 response	
Remote users required VPN account while on-site users do not.	951912-951894-101359111

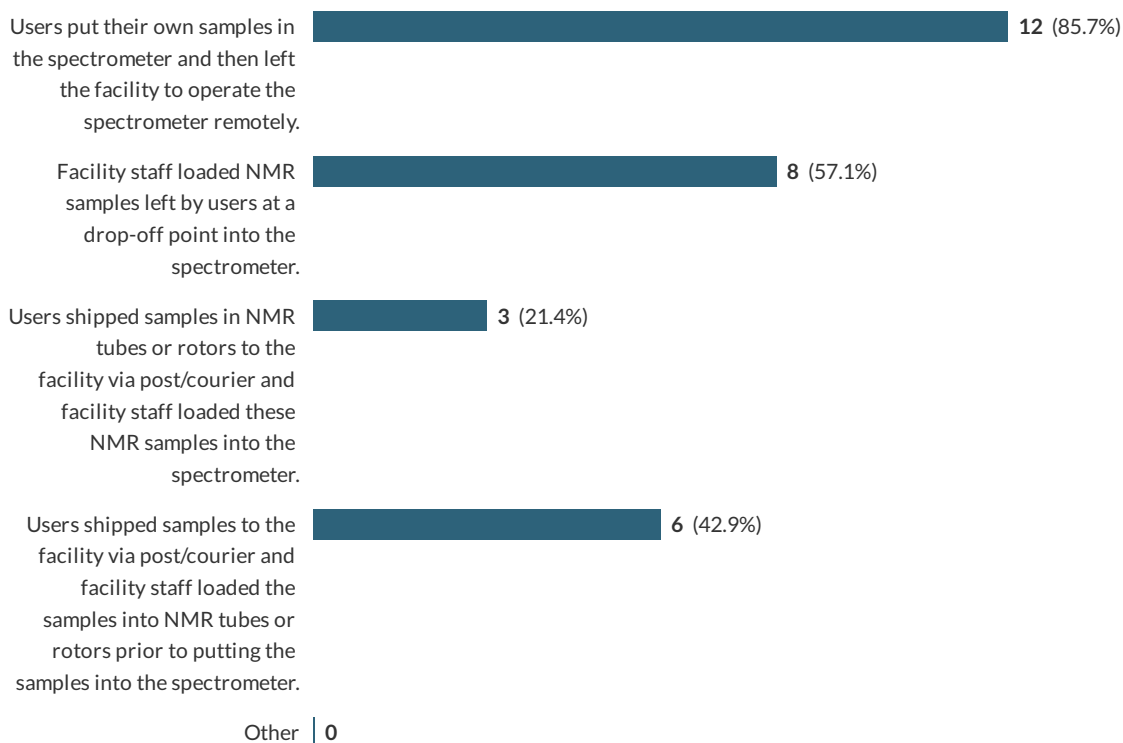**35** Were remote users provided with support by local NMR facility staff?

Yes — **10** (71.4%)
No — **4** (28.6%)

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

Assistance with sample preparation (from sample material shipped to facility) — **7** (70%)
Assistance with loading NMR samples into spectrometers — **9** (90%)
Assistance with setup of NMR experiments — **7** (70%)
Assistance with data transfer — **8** (80%)
Telephone/email assistance in case of problems — **9** (90%)
Website/YouTube videos explaining how to use remote access — **0**
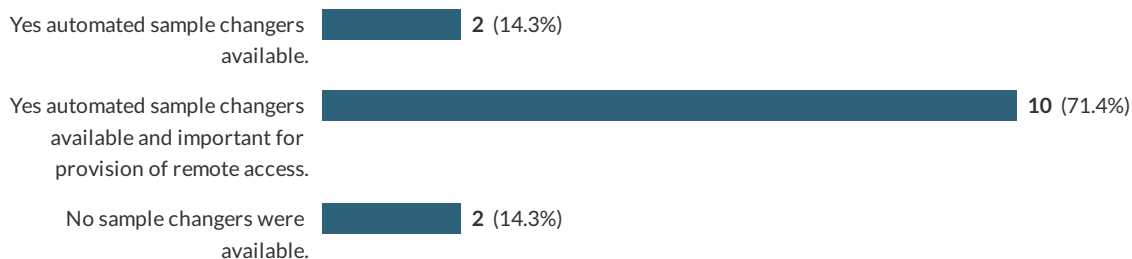Other — **1** (10%)

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

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

Showing 1 response	
Zoom support - a live session between two national users and facility staff for example	951912-951894-101891636

36 How were users' NMR samples loaded into spectrometers? (select all that apply)

Users put their own samples in the spectrometer and then left the facility to operate the spectrometer remotely. — **12** (85.7%)

Facility staff loaded NMR samples left by users at a drop-off point into the spectrometer. — **8** (57.1%)

Users shipped samples in NMR tubes or rotors to the facility via post/courier and facility staff loaded these NMR samples into the spectrometer. — **3** (21.4%)

Users shipped samples to the facility via post/courier and facility staff loaded the samples into NMR tubes or rotors prior to putting the samples into the spectrometer. — **6** (42.9%)

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)

**36.a** If you selected Other, please specify:

No responses

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37 Are spectrometers available for remote access equipped with automatic sample changers and were these important for provision of remote access?
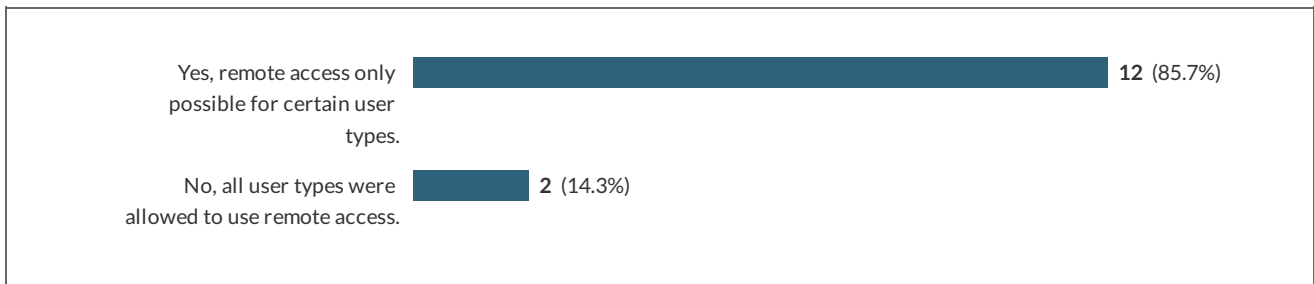

Yes automated sample changers available. — **2** (14.3%)

Yes automated sample changers available and important for provision of remote access. — **10** (71.4%)

No sample changers were available. — **2** (14.3%)

37.a If yes, please indicate the make/model of sample changer.

Showing all 12 responses	
Samplejet (with cooling option)	951912-951894-101372382
Bruker SampleJet or BACS-60	951912-951894-101376176
SampleJet	951912-951894-101411307
SampleCase and BACS	951912-951894-101445018
SampleJet with temp controlled racks accommodating 3mm or 5mm tubes.	951912-951894-101359111
samplejet and samplecase	951912-951894-101745973
Bruker SampleJet (cooling only versions to +6c, and latest variable temperature versions, depending on spectrometer)	951912-951894-101849988
Room temperature SampleJet (Bruker) c. 2015 (600MHz) Chilled SampleJet (Bruker) c. 2013 (700MHz) Chilled SampleJet (Bruker) c. 2018 (800MHz)	951912-951894-101891636
Bruker SampleXpress & SampleCase	951912-951894-101953004
SampleCase cooled	951912-951894-101966822
BACS 60 SampleXpress SampleCase+	951912-951894-102043034
SampleXpress	951912-951894-102051473

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

Yes **8** (66.7%)
No **4** (33.3%)
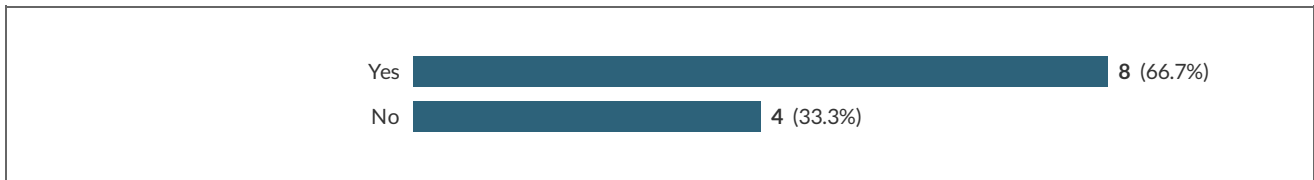
38 Was remote access restricted to users with specific levels of expertise or were all user categories able to access spectrometers remotely?

Yes, remote access only possible for certain user types. **12** (85.7%)
No, all user types were allowed to use remote access. **2** (14.3%)

38.a If remote access was restricted to users with specific levels of expertise then please specify which caterogy(ies) of users?

Showing all 12 responses	
Expert users only (i.e. the ones who use the machines themselves anyway and who can now just login from home to check it's all ticking over nicely).	951912-951894-101360820
This was done on an ad-hoc basis, based on an assessment of user skill, rather than any formalised category.	951912-951894-101372382
Advanced users with training	951912-951894-101376176
expert	951912-951894-101411307
Post-doctoral workers or equivalent and academic members of staff	951912-951894-101445018
There was generally an experienced user who took control of the spectrometer. It was generally self-regulating.	951912-951894-101737673
Those who wanted it, and requested info about the SSH/VNC route	951912-951894-101745973
Expert users only.	951912-951894-101849988
Independent users who had been trained in remote operation and could not access the spectrometers on-site	951912-951894-101891636
experienced users	951912-951894-101953004
Expert level users that can operate the spectrometer unaided	951912-951894-101966822
Facility manager	951912-951894-102051473

39 How was the NMR data collected by remote users protected and/or kept secure and did the procedures differ from those in place for on-site users? (please specify)

Showing all 14 responses	
No difference at all.	951912-951894-101360820
Data backup and security process was identical for on-site users. Access procedure differed.	951912-951894-101372382
Same as non remote acquisitions	951912-951894-101376176
retrieve data from server or ask facility manager to send data over	951912-951894-101411307
No difference to on-site users	951912-951894-101445018
Procedures the same for all users. Login to the spectrometers from outside our department network requires a local VPN account. In person access to the NMR facility is limited to people with a keycard to enter the building.	951912-951894-101359111
The access password was supposed to change for each user (but did not due to issues with permissions on TeamViewers side) The security was the same for all users.	951912-951894-101737673
No	951912-951894-101745973
Same procedure as for on-site users. Data transferred across to user's local workstation using ssh, and/or stored on the local secure facility data server.	951912-951894-101849988
Same procedures as for on-site users	951912-951894-101891636
remote users data been transfer on OneDrive folders available just to defined users.	951912-951894-101953004
Same procedure, the user is responsible for the data.	951912-951894-101966822
ICON did all the data handling for the majority of users. other users had only access to certain drives for data storage, based on their account credentials.	951912-951894-102043034
All interaction via IconNMR as normal - no difference.	951912-951894-102051473

40 What bottlenecks or other problems did you identify in providing remote spectrometer access?

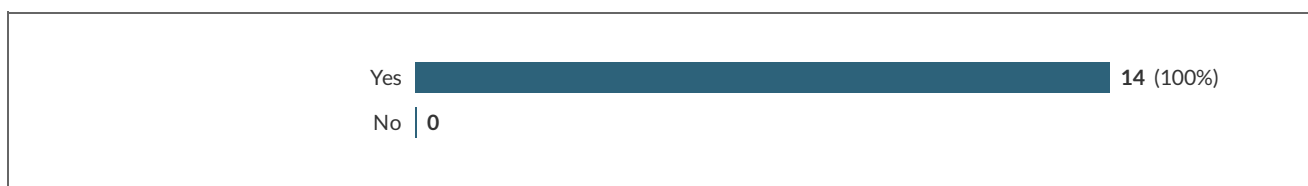| Showing all 13 responses	
The same one I always have for non-expert users: I'm only one person and part of my job involves teaching so at some times of the year it can take me months to get round to running a sample. The expert users are also a lot more reluctant to come into the building in person if they aren't changing a sample, which means they're not around to mop up spare machine time when it arises.	951912-951894-101360820
If something went wrong, difficult to diagnose. Someone had to be on site. Bugs with IconWeb software.	951912-951894-101376176

the main concern is that when something went wrong the remote user may not realise it quick enough.	951912-951894-101411307
Not all probes are ATM therefore some local manual intervention is required	951912-951894-101445018
Most of the remote users were locally based so were able to put their own samples into the spectrometer or to drop them off in the building. We offer remote access to users at other universities. They overwhelmingly prefer to travel to our site with their samples rather than risking sending the samples via courier. For shorter trips it is probably cheaper to travel by train than to send samples by courier.	951912-951894-101359111
TeamViewer passwords are not always set properly in Linux. The availability of the local operator was a bottleneck. Sample changes and spinning up samples could be a burden on the local operator since many users expectations are possible when in person, but not for someone running multiple spectrometers. There is also an underestimation of the work that a local operator may be putting in when troubles appear, as it all happens "off-camera". Shipping of the samples also did not always line up with the expectations of one party or another.	951912-951894-101737673
Our route is a bit laboured, but quite secure to satisfy local IT	951912-951894-101745973
Remote users not always remembering to advise facility staff when they've finished measuring/completed their booking, so that staff can log users out of the spectrometer. NMR time is charged based on login time. We advise users not to log out remotely unless they are 100% sure the sample has been removed from the magnet successfully. In practice, this means relying on facility staff to check sample removal/log users out.	951912-951894-101849988
Anydesk not terribly secure - only used sparingly as we really need to avoid multiple users connecting remotely simultaneously. It became clear that local users would attempt to use anydesk to view spectr outside their booked slot - creating issues fro users who were trying to operate the spectrometer at the same time. Our current solution/workaround is to change the Anydesk password frequently (weekly) to ensure only booked remote users can access. We do not have explicit permission from the universities IT services (Anydesk avoids the need for VPN etc so no formal IT support from University is not required).	951912-951894-101891636
Not everything is possible to do remotely without being familiar with the system - particularly high field spectrometers. From my point of view on one side is great to give access to 800 MHz spectrometer to wide nmr community but on other side it's still quite a time consuming for me as not all of the users are enough experienced to use the spectrometer (Bruker Neo console with TS4.1) on their own.	951912-951894-101953004
Attempts to teach about NMR remotely using both PulseSecure from a laptop to control the spectrometer host and Teams/Zoom to interact with a group of users generally suffered from the interactive controls being too slow to use in any meaningful way	951912-951894-101966822

slow to use in any meaningful way.	
Clashes between remote users and local users. Samples being removed. Software bugs making entire queues get lost.	951912-951894-102043034
User expertise Rack space to accommodate more samples	951912-951894-102051473

41 If your facility has a webpage with information about remote access please enter the URL below.

Showing all 4 responses	
N/A	951912-951894-101360820
N/A	951912-951894-101376176
https://warwick.ac.uk/fac/sci/physics/research/condensedmatt/nmr/	951912-951894-101737673
Anydesk use is not promoted	951912-951894-101891636

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

Yes	**14** (100%)
No	**0**

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

Showing all 3 responses	
Equality Inclusion and Diversity is the main reason we wish to keep remote access as an option. We have researchers with childcare issue (and indeed immunocompromised facility users) where remote access may be more appropriate. Ideally we need a solution that can be locked to a specific user for a specific account before we can roll out remote access more widely. In particular we are somewhat hamstrung by restrictions that the universities IT services impose (although we appreciate the need for secure systems we have chosen Anydesk not as it is most fit for purpose but because it circumvents university IT restrictions)	951912-951894-101891636
We are running national Scottish High Field NMR Facility under SNUG initiative already for about 3 years giving local & remote access to other places in Scotland (https://www.snug.ac.uk/). These institutions are getting 50% of 800 spectrometer time between them. I believe it makes a big impact to these institutions to have access to high resolution & sensitivity spectrometer. They can run their experiments either by themself locally or remotely or use the automation. Data are archived by the end on Microsoft OneDrive with access limited just to defined users. As mentioned before from my point of view on one side is great to give access to 800 to wide Scottish nmr community but on other side it's still quite a time consuming for me as not all of the users are enough experienced to use the spectrometer (Bruker Neo console with TS4.1) on their own.	951912-951894-101953004
It at least added versatility to our expert users who could monitor and adjust experiments remotely. Attempts to teach using remote access were mostly unsuccessful, but this could be improved by a more direct form of remote control. Our IT department however blocked the use of software like Teamviewer and similar direct remote access applications.	951912-951894-101966822