Deliverable 2.2

REMOTE-NMR LANDSCAPE INCLUDING TABLE OF CRITICALITIES

of Remote NMR (R-NMR):

Moving NMR infrastructures to remote access capabilities

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CONTENTS

1. Executive Summary

Deliverable D2.2 within Work Package 2 (WP2) summarizes the overall findings of WP2. Each section of the report focusses on one of the five Work Package tasks. During the first 18 months of the R-NMR project, information on current practices relating to remote NMR access was collected from the NMR community using online surveys. This information has been used to define the Remote NMR Landscape in Europe as it existed in 2022 and to identify critical factors that should be considered in defining a common procedure for remote NMR access. This information has been and will be of use in informing the work of other aspects of the Remote-NMR project (WP3 and WP4). Considerations which are thought to be important for the common protocol are summarized at the end of the report in the Table of Criticalities.

2. Background

Work package 2 (WP2) involved the collection of information from the NMR community in order to provide a definition of and a better understanding of the 'Remote NMR Landscape' which developed during the Covid 19 pandemic. WP2 is defined by five main objectives:

- O2.1 – Providing a detailed picture of the operation of NMR facilities in Europe during the pandemic
- O2.2 – Understanding the user perception of remote access and stratification of users
- O2.3 – Mapping data protection and security needs
- O2.4 – Identifying issues and solutions regarding sample shipments
- O2.5 – Monitoring the carbon footprint

These objectives have been addressed through the work carried out in the five tasks within WP2. Much of the information was gathered from the NMR community via online surveys. Each of the five tasks are summarized individually in the following sections and the main outcomes of each task are discussed. The insights gained during WP2 have allowed us to identify important factors to consider in a common protocol for Remote Access; these are summarized in the Table of Criticalities for Remote NMR in the final section.

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

An online survey of NMR facility managers was carried out in November 2022 in order to provide a detailed picture of the operation of NMR facilities in Europe during the pandemic (O2.1). A copy of the survey and the detailed analysis of the survey results are presented in the Milestone 2.1 report that is available on the Outcome page on the R-NMR website (https://r-nmr.eu/results-of-facility-survey-wp2-ms2-1/). Some of the additional insights gained via the survey from a subsequent more detailed analysis of free-text responses to the survey are outlined in this section.

Overall, responses to the survey were collected from 142 facility managers from 29 countries; 41.5% of the responses were from national NMR infrastructures. The detailed responses to a range of questions about instrumentation, software, userbase, mode of remote access and reasons for not providing remote access have provided important insights into how the NMR community responded to the pandemic and have proved to be a valuable resource in the development of remote access protocols within WP 3 and 4. The survey indicated that 83 of the 142 facilities responding (58%) had provided some form of remote access during the Covid pandemic while 59 facilities (42%) had not. It is encouraging that 70% of the sites not providing remote access indicated that they would be interested in implementing 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.

The first part of the survey included questions about the instrumentation and software used in NMR facilities. More than 95% of the NMR facilities (135 of 142) were equipped with Bruker spectrometers but as many as 39 facilities also have spectrometers from other manufacturers (Agilent, JEOL, and Magritek). Facilities providing remote access indicated that 97% did this with Bruker and 9.5% with Agilent spectrometers. The large proportion of Bruker spectrometers in the NMR community justifies the majority of effort in R-NMR in the implementation of remote access to these Bruker systems. However, if time allows in the project, protocols for remote access to other NMR systems, particularly Agilent ones, should be discussed with relevant stakeholders.

The Bruker spectrometers operate various versions of TopSpin ranging from 1.3 to 4. The majority (64%) of facilities run TopSpin 3 (versions 3.1 to 3.6) while the remaining facilities run an earlier version (17%, versions 1 or 2) or a later version (19%, version 4). IconNMR is also widely used on Bruker spectrometers for automation; again, a range of versions are in use (5% using version 3, 33% using version 4 and 62% using version 5). Linux is the most common operating system for spectrometers (65% of facilities use Linux). The most common Linux implementation is CentOS (a range of versions 2, 3, 5, 6, 7 and 8 in use with CentOS 7 the most common implementation). It should be noted that CentOS will reach its end-of-life on 30 June 2024 and will no longer be supported. Bruker is suggesting Alma Linux as a replacement for CentOS and more information about this should be available from Bruker during 2024. Windows is also a widely used operating system (53% of facilities use Windows) with versions including XP, 7, 9, 10 and 11 in use; Windows 10 is the most commonly used version. The widespread use of both Linux and Windows and the large range of operating system versions in use may represent a challenge for the implementation of a common protocol for remote access in WP 3 and 4.

The survey also addressed topics including: user login procedures, NMR data security, and levels of user expertise and spectrometer access. The most common user login mode (59%) is via a shared account and 94% of these accounts have open access to other users' files. This 'open access' login mode can put data at risk so an automated backup of data to a server, an approach used by many facilities, is an important option. While shared accounts and open access to data may be appropriate for local users within a single department or institution, care must be taken to ensure data security when an NMR facility provides access to a wider national or transnational userbase or when experiments involving 'sensitive personal data' are collected (see section 5). By contrast, 37% of facilities have a more 'secure' system of individual login accounts and 81% of these accounts have no access to other users' files.

The majority of facilities providing remote access (81%) used the same user login procedures for remote and on-site users. In many cases, some level of spectrometer and data security is provided by local IT staff who imposed restrictions on network access for remote users. Around half of facilities providing remote access required a VPN (virtual private network) account and/or required registration for a local computer account. One aspect of security that was not considered in the survey, but is important, is the security of the spectrometer software installation (i.e. Bruker TopSpin); it is generally not desirable for most users to be able to modify pulse programs or parameter files that other users may depend on.

The majority of NMR facilities (74%) provide different levels of spectrometer access for users with different levels of expertise. There is a balance of non-expert (25%), standard (34%) and expert (32%) NMR facility users. The most common assessment of expertise is, to some extent, 'subjective', based on a range of factors including: status and experience (PhD student, postdoc, established researcher), and previous interactions with facility staff. Other facilities required users to undergo some form of in-person training and/or supervision (without formal assessment). A smaller number of facilities had dedicated training courses or relied on training from within individual users' research groups. The majority of facilities providing remote access to spectrometers (84%) did apply access restrictions on the basis of user expertise; 73% of facilities only provided remote access to 'expert users', 17% of facilities provide access only after specific remote-access training, and 10% only provided remote access to 'local users'.

Around 58% of the facilities provided some type of remote access to NMR spectrometers during the pandemic. These facilities were asked further questions relating to their provision of remote access. During the preparation of the R-NMR grant application, the project partners had identified AnyDesk, NoMachine (NX) and TeamViewer as software they had used for remote access. These three software packages were used by many NMR facilities (Team Viewer 42%, Any Desk 23% and No Machine 12%) but, interestingly, the survey showed that a number of other packages were also used to provide remote access by 57% of facilities. A short description of each of the 16 software packages mentioned in the NMR Facility Manager survey is included in Appendix 1 along with the criteria used in the drafting of these descriptions and a list of desirable features for a remote-access software package. This information will be of interest to R-NMR partners and will be useful in WP4.

The survey indicated that remote users were provided with support from local staff at 70% of NMR facilities. Most support (~80%) involved telephone/email assistance in case of problems and assistance with loading NMR samples into spectrometers. Around 73% of facilities allowed local users to insert NMR samples themselves and then to operate the spectrometer remotely. Around 52% of facilities had a local drop-off point for samples which were then loaded into the spectrometer by facility staff. In the case of national NMR infrastructures, 50% indicated that samples were shipped via post/courier and then loaded into the spectrometer by facility staff, often after that samples had been placed in appropriate NMR tubes or rotors.

Support was also frequently needed (>50%) for setting up experiments, data transfer and sample preparation. Here, the user expertise level and familiarity with the local facility would certainly affect the degree of support needed for experiment setup. With the development of a common protocol for remote access and the availability of online training materials (introduction to the NMR facility, YouTube videos, SOPs for sample shipment/handling, remote connection and data transfer, and other documentation), it can be expected that, in future, remote users will require less assistance with experiment setup and data transfer.

Finally, facility managers were asked about bottlenecks that they encountered in provision of remote NMR. Many of the perceived bottlenecks related to the need to develop, at short notice in response to the Covid pandemic, a remote access procedure at their facility in the absence of information and advice on how to do this. Many of the problems encountered related to identifying appropriate software, security considerations (user accounts, data, hardware, samples) and the increased burden on facility staff. The development of a common remote-access protocol within the R-NMR project and the robust testing that this protocol will undergo during the project should remove many of the bottlenecks encountered by facility managers. However, the increased burden on already busy NMR facility staff needs to be considered when implementing a remote access protocol.

The high level of responses to the NMR Facility Manager survey demonstrated a widespread interest in remote access to NMR spectrometers. To engage further with the wider NMR community, three online workshops focussing on different aspects of remote access provision were organised in June, November and December 2023; a list of symposia topics and speakers is included in Appendix 2. These symposia were well attended with up to 100 participants. Recordings of most of the talks given at the June and November symposia are available on the Training page of the R-NMR website (https://r-nmr.eu/category/training/). The talks from the December symposium will be available in due course.

4. Users' needs and stratification of users (Task 2.2)

An online survey of 'hands-on' users of NMR facilities was launched in January 2023 in order to gain as understanding of user perceptions of remote access and the stratification of users (O2.2). A copy of the survey and the detailed analysis of the survey results are presented in the Milestone 2.2 report that is available on the Outcome page on the R-NMR website (https://r-nmr.eu/m2-2-user-survey-report/). Responses were collected from 401 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 have provided important insights into the user experience and have been a valuable resource in the development of remote access protocols within WP 3 and 4. Encouragingly, 82% of the respondents using remote access have continued to do so post-pandemic.

The survey, targeting NMR facility users, was focused on the user experience aspects, such as the type of NMR research being done, 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.

Solution-state NMR is the primary type of NMR being carried out by the respondents (77%). Only 7% of respondents primarily use solid-state NMR and 16% use both solution and solid state NMR. The NMR users were asked about the types of NMR experiments they carry out; the responses cover all areas of biological and physical sciences. Biomolecular NMR and routine small molecule characterisation supporting organic chemistry were the most common responses. The NMR users were asked to categorize their level of expertise in operating NMR spectrometers. 15% are 'non-expert' users who select from a limited list of experiments and parameters. 50% are 'standard' users who select from a wider list of experiments but cannot run their own pulse sequences. 33% 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. This information has been useful in Task 3.2 (defining user access levels).

There were 201 NMR users who did collect NMR data via remote access; they represent 23 European countries and 4 other countries. The majority of users were provided with support by NMR facility staff (59%). 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. This is consistent with the information provided by NMR facility managers. The majority of users put their own samples into the spectrometer and then left the NMR facility to operate the spectrometer remotely. Some respondents 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; 71% of respondents did not consider it to be a barrier. The 29% 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. These responses relating to sample shipment have also been considered in Task 2.4 and have been used to draft the guidelines on sample shipment included in WP 3 Deliverable 3.1.

There were 200 NMR users who did not collect NMR data via remote access; they represent 19 European countries and 5 other countries. Several reasons were given by the users in this group for not using remote access. The most common reasons were 1) remote access not available at the NMR facility (52%) and 2) there were no restrictions during the pandemic restricting in-person access (39%). Encouragingly, 72% of the respondents not using remote access 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.

5. Review of GDPR (General Data Protection Requirement) aspects (Task 2.3)

The General Data Protection Requirement (GDPR) is a regulation in EU law that governs data protection and privacy. GDPR applies to the processing of personal data. Personal data is any information that refers to an identified or identifiable natural person. Certain personal data is by its nature particularly sensitive and therefore has stronger protection. It is essential that defining a common procedure for remote access to NMR spectrometers meets GDPR requirements with respect to the data that is collected and stored at each NMR facility, and how that data is shared with users. In order to assess this, and to address Objective 2.3, 79 NMR facilities completed an online survey in June 2023 describing their current GDPR procedures and any other data privacy requirements in place locally. A copy of the survey and the detailed analysis of the survey results are presented in the Deliverable 2.1 report that is available on the R-NMR website (https://r-nmr.eu/deliverable_2_1_gdpr_security_shipment/).

The general awareness of the GDPR is relatively well established among the 79 facilities participating in the survey; only 5% of facility managers were unsure whether GDPR applied in the country where their facility was located. However, some responses reflected an uncertainty about what personal data actually includes and how GDPR relates to this information. For sensitive personal data, the more detailed written comments in the survey responses also reflect an uncertainty about whether the handled data is truly anonymous, and thus outside the scope of the GDPR, or not. The focus seemed to be whether data and person could be matched at the *facility* (it could not), not whether data and person could be matched *at all* (it could). This reasoning points to a confusion and uncertainty about proper guidelines and procedures.

In the Deliverable 2.1 report, it was suggested that a 'Fact Sheet and Guidelines on GDPR as it relates to NMR Facilities' would be beneficial to the NMR community. This document has now been drafted and is included here as Appendix 3; it has also been uploaded to the Outcome page of the R-NMR website where it is accessible to all NMR facilities. This can serve as a starting point for facilities to ensure that their procedures are complying with GDPR.

6. Transnational sample shipment (Task 2.4)

Although NMR spectrometers can be accessed remotely, the samples need to be transported to the NMR facility and inserted into the NMR spectrometer. This can be an important factor in determining whether users are able/willing to use remote access. Users may be unwilling to send valuable samples via a courier because of concerns about sample damage. The requirements will be different for solution and solid-state NMR and will also depend on the type of material being studied. The importance to users of having samples returned to them after data collection must also be considered.

In order to collect data pertaining to sample shipment, and to address Objective 2.4, an internal survey involving all R-NMR partners was carried out. The R-NMR consortium's NMR facilities were asked about how NMR samples were handled, how sample shipments were made, and the standard operating procedures that were followed (a copy of the survey and the detailed analysis of the survey results are presented in the Deliverable 2.1 report that is available on the Outcome page on the R-NMR website (https://r-nmr.eu/deliverable_2_1_gdpr_security_shipment/). Additional information, specifically about the NMR users' attitudes to and experiences with sample shipment, was obtained from questions included in the NMR Users' Survey (Task 2.2) conducted earlier in 2023 (M2.2 User Survey Report https://r-nmr.eu/category/outcome/).

These survey results have provided useful insights into current practices relating to sample shipment. There are several areas related to sample shipment with an apparent lack of standard operating procedures in place at NMR facilities and/or a lack of information readily available to NMR users. This includes a lack of defined procedures for sample shipment and handling of samples upon arrival at a facility, a lack of written instructions on how to package samples for shipment, a lack of standard procedures for sample quality control upon delivery to a facility. The lack of these standard procedures may be creating a bottleneck for sample shipment that deters some users or NMR facilities from widening remote NMR access. In order to address this shortcoming, a standard operating procedure (SOP) for sample shipment has been written and this is included in WP 3 Deliverable 3.1 which will be available from the R-NMR Outcome web page. The SOP provides guidelines for the shipment of samples for both solution-state and solid-state NMR and includes a flowchart for determining the best procedure to be adopted by NMR users.

7. Monitoring the carbon footprint (Task 2.5)

In Task 2.5, a set of tools for the calculation of carbon footprint that are suitable to cover the range of impacts caused by the operation of NMR infrastructures were selected and made available to R-NMR partners. This addresses Objective 2.5 to allow NMR facilities to start to consider the carbon footprint of their facilities and their provision of NMR access. Within this task, all R-NMR partners adopt a common approach to the calculation of the footprint of their users' travel. In addition, tools that can capture the footprint of equipment usage will be investigated. A detailed report on monitoring the carbon footprint of NMR facilities is included in Appendix 4. Some of the main conclusions from the report are highlighted here.

Travel can be a carbon intensive activity. An increased use of remote access to NMR facilities can limit the carbon footprint associated with this travel. In the report in Appendix 4, two tools are selected to calculate the carbon footprint associated with air and with train travel (https://www.icao.int/environmental-protection/Carbonoffset/ , https://www.raileurope.com/). The recommendation is that, when possible, train travel is preferable.

Sample shipment, which is often essential for remote NMR access, also has an associated carbon footprint. This depends on how the sample is shipped (by air or land) and how the sample is packaged (i.e. does it require dry ice for cooling). The report references a web-based calculator from the courier DHL that allows estimation of the carbon footprint associated with the shipment of small parcels.

Most NMR related activities are dependent on electricity. The report in Appendix 4 shows that the carbon footprint of these activities is closely tied to the type of power generation plants used in specific countries; hydro, nuclear and renewable power generation has a much smaller carbon footprint than gas or coal power generation. As a result, there is a roughly hundred-fold difference in the carbon footprint of electricity generation (g CO_2 e/kWh) across Europe. This means that the carbon footprint of NMR spectrometers varies widely from country to country.

The report in Appendix 4 considers the carbon footprint of the various components of the NMR instrumentation and that associated with operation of the spectrometer. Cryoprobes, and the associated helium compressor and chiller units, represent by far the largest power consumption of an NMR system. However, cryoprobes offer a huge advantage in sensitivity and have become the norm for biomolecular NMR. Most NMR spectrometers are equipped with superconducting magnets that require liquid nitrogen and liquid helium. The annual consumption of these cryogens by a variety of magnet types and the associated carbon footprint resulting from the extraction/liquefaction and transport of the cryogens is outlined in the report. Finally, the carbon footprint of air conditioning of NMR facilities, which is required due to the temperature sensitivity of NMR consoles, is also discussed.

A tool for estimating the carbon footprint associated with a particular spectrometer configuration (magnet type/strength, spectrometer components, country in which spectrometer is located) has been developed. This is only able to give a rough estimate of the carbon footprint of a spectrometer but it allows NMR facilities to begin to consider the environmental impact of their spectrometers. During the R-NMR project, the project partners are encouraged to use this tool and to engage in discussion about possible ways in which to minimize their carbon footprint. The carbon footprint estimation tool will be made more widely available before the end of the R-NMR project.

8. Summary - Table of Criticalities

The five tasks within Work Package 2 have been completed. The results of these provide a good picture of the Remote NMR Landscape as it existed at the start of the project in July 2022. In addition, the tasks have highlighted the importance of considering data protection and security needs, all aspects of sample shipment and sample handling and the environmental impact of activities associated with providing NMR access. The results of these five tasks have allowed the R-NMR partners to identify a number of critical factors that must be taken into account in the design of a common protocol for remote NMR access; these are outlined on the next page in the Table of Criticalities.

Table of Criticalities for Remote Access to NMR

Software	Any software used in a remote access protocol must be compatible with both Windows and Linux operating systems; both are used on NMR spectrometer consoles.
	Any software used in a remote access protocol must be compatible with older versions of Windows and Linux operating systems since these may not be upgradeable.
	Any software used in a remote access protocol must be compatible with older versions of spectrometer software (i.e. older versions of TopSpin or IconNMR) because upgrading this is often not possible without costly spectrometer hardware upgrades.
	Any software used in a remote access protocol should be compatible with different types of spectrometers. Although Bruker is the main type used in European NMR facilities, there are many facilities also using Varian/Agilent, JEOL and other types of spectrometers.
	It is desirable that any software used in a remote access protocol is free of charge to academic users or that an alternative free software option is available and supported.
Security/privacy aspects	NMR spectrometers are usually part of a network that is controlled by departmental and/or university IT staff who may impose strict security requirements. It is essential that a remote access solution is flexible enough to be able to work in a range of IT security scenarios.
	It is essential that the privacy/confidentiality of user samples/experiments/data is maintained during remote access. This means that a remote user must be confident that information about their data collection is not available to others but also that remote users do not have access to the data collected by other users. This privacy/confidentiality can be implemented at the level of individual users or within research teams.
	It is essential that NMR facilities providing remote access are familiar with the General Data Protection Regulation (GDPR) as it pertains to NMR and that the facility operates in accordance with GDPR.
User aspects	It is essential that a remote access system is set up in a way that is suitable for a range of user expertise. This means that access is controlled in a way that protects the NMR spectrometer (i.e. an inexperienced user should not be allowed to implement new pulse sequences) but also that remote users are provided with a suitable level of assistance which could be via onsite NMR facility staff or via online training materials.
Sample shipment	A robust and reliable system for sample shipment to/from NMR facilities in both a national and transnational context is essential. Sample shipment must ensure that samples arrive in good condition and in a timely manner at the NMR facility. It is also desirable for the NMR facility to have a quality control procedure in place to assess samples shipped to them.
	In cases where shipment of samples containing ‘sensitive materials’ is concerned, ethical, legal, and social implications (ELSI) must be considered.
NMR facility	NMR facilities must be familiar with the carbon footprint of various aspects of their facility operation.
	It is important that the implementation of a remote access protocol does not create a substantial additional workload for NMR facility staff who may already be overworked.
	It is important that a remote access protocol is attractive to NMR facilities not currently providing remote access so that they are able to adopt the protocol in future.
	It is important that in the early stages of a remote access protocol, advice for trouble shooting is available to NMR facilities implementing the protocol.

APPENDIX 1

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

Short descriptions of software used by NMR facilities for remote access

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Introduction

In the survey conducted as part of Task 2.1, NMR Facility managers were asked about the software that they had used for remote access. During the preparation of the R-NMR grant application, the project partners had identified AnyDesk, NoMachine (NX) and TeamViewer as software they had used for remote access. These three software packages were used by many NMR facilities (Team Viewer 42%, Any Desk 23% and No Machine 12%) but a number of other packages were also used to provide remote access by 57% of facilities.

Within Task 2.1, a more detailed analysis of the responses relating to remote access software was undertaken. A brief description of features of each software package mentioned by facility managers is outlined below (in alphabetical order). This is followed by a list of the criteria used to describe each of these software packages and some of factors (or the 'wish list') that might be of importance to NMR facilities in the selection of a suitable software package.

- **AnyDesk**

  A popular and effective remote desktop solution with file transfer functionality. It uses a proprietary protocol. As it is cloud based it can provide access to clients behind a firewall. If direct access is possible between hosts then traffic is not routed through the cloud. No local user assistance needed when its unattended access feature is activated.

- **Bastion**

  Azure Bastion can be used to access only virtual machines in the cloud. No free version exists. Not available globally, only available in specific regions.

- **Bomgar Remote Support (BeyondTrust)**

  This is a complete commercial remote support solution (remote desktop, file access, etc.). No free version exists. It has much broader scope than we need for remote NMR access.

- **Bruker IconNMR/IconWeb**

  IconNMR is a larger software suite, not a general remote desktop solution, that is used for spectrometer control and automation, in particular. Requires license but usually available on Bruker spectrometers.

- **DWService**

  Cloud-based remote access using open source local agents. Both Linux and Windows are supported. Registration is needed on the DWService portal. No client needed to access the remote computer, only an HTML5 capable browser. Free up to a 6 Mbps bandwidth limit.

- **FastViewer**

  It is a complete solution for teamwork, conferences, support and maintenance. Requires a license. Its scope is much broader than a mere remote desktop access.

- **Google sharing software**

  Chrome Remote Desktop allows a permanent, pre-authorized connection to a remote computer while Remote Assistance is designed for short-lived remote connections, and requires an operator on the remote computer to participate in authentication. Requires an agent on the remote computer. Supports both Linux and Windows.

- **Guacamole**

  Apache Guacamole is a free and open-source cross-platform Remote Desktop Gateway (RDP, VNC, SSH, but no X11 support). A server must be set up inside the company network where remote desktops are located. The server is Linux based. No need to install an agent on the remote computers. Clients can connect with any modern browser. Direct file transfer between the local and remote computers is not possible.

- **NoMachine (NX)**

  Allows RDP, VNC and XDM connections beside its own fast proprietary protocol. Free to use non-commercially. There is no server for the basic version: computers must be able to connect directly to each other (possibly using VPN) and both ends must install the NX client software. Users must have local accounts on the remote computer. Commercial versions of the NoMachine product family have more advanced features.

- **PulseSecure**
- Ivanti has a complete product portfolio of unified endpoint management tools. License needed. It has a much broader scope than needed, but very powerful indeed.
- **Remote Utilities**

  Free for up to 10 endpoints per organization. Uses a proprietary protocol. It requires a host agent on the remote computer and a viewer on the local machine. Only the Windows version is fully functional, Linux and Mac versions implemented the viewer but not the host component.

- **Splashtop**

  Uses proprietary protocol for fast remote desktop access. Needs license. Mostly Windows-centric. Wider scope than needed.

- **TeamViewer**

  Free for non-commercial use, but very soon detects frequent use and demands a license anyway. Uses a proprietary protocol. Runs on Windows, Linux and Mac.

- **VNC**

  Mainly screen sharing, limited file transfer support. Because of its weak security additional secure channel is recommended (e.g. VPN). Direct connections only, cannot access remote computers behind a firewall.

- **Windows Remote Desktop**

  Native desktop sharing in Windows, but supports Linux and Mac as well. Uses proprietary protocol. Free. File transfer possible. Direct connections only, cannot access remote computers behind a firewall (VPN needed). Only a single session is permitted. Windows Home version does not have this feature.

- **X2go**

  Open source, but the server runs only on Linux and not all desktop environments are compatible with it. Does not seem to be mature enough.

The main criteria used in drafting the descriptions of the software packages included:

1. Licensing: completely free, free with restrictions, commercial only.
2. Technology: based on open or proprietary protocols. Proprietary protocols are usually faster and more effective on lower bandwidths. Open protocols are more future-proof.
3. Server side: whether a central server is required to build up the connection between computers. This can mean the provider's servers (usually in the cloud) or the institute's own servers inside the organizational network. Some solutions can provide only direct connections between local and remote computers without a server.
4. Remote client agent required or not. Most solutions need a special agent program on the remote side. Guacamole is an exception because it is a protocol gateway.
5. Local client program required or just an HTML5 browser. Some solutions can be used only with their special client programs, some provide a more universal HTML5 interface which just needs a browser.
6. Platform support: at least Linux, Windows and Mac must be supported by the solution both on the local (viewer/controller) side and the remote (controlled desktop) side. It is an advantage if the viewer can be a mobile device, too.
7. Firewall penetration: as most spectrometers are located behind firewall, it is important that an external client can access remote desktops inside the organizational network. Solutions providing only direct access need a VPN connection or an SSH tunnel to get behind a firewall.
8. Multiple users: sometimes more than one user has to access the remote desktop at the same time, or the local and remote user must work together on the same desktop. For example, Windows remote desktop forbids this (purely out of licensing considerations, the software could do it otherwise).
9. User authentication: strong authentication is an important aspect. Some solutions use only a password, others can do username/password logins, private keys, kerberos, or two factor authentication.
10. Connection security: it's crucial to have strong end-to-end encryption between local and remote computers. VNC implementations sometimes lack an acceptable encrytion, and need a VPN or SSH channel to provide proper security.

11. Remote assistance: it is an advantage if a user operating a spectrometer can ask for remote help. The most popular programs are AnyDesk and TeamViewer, but in a Linux environment x11vnc can also provide a simple solution.
12. Ease of use: a good remote desktop solution must be user friendly. All of the examined programs are more or less satisfy this requirement.
13. Extra services: remote desktop programs usually have a wide range of other services beside desktop sharing. In this survey the most important was file transfer capability.

A 'wish list' for an ideal or optimal solution for remote access might have the following criteria:

- every component is freely available,
- actively maintained and open source,
- multi-platform: every component runs on Linux, Windows and Mac, and the viewer component also runs on mobile devices (e.g. uses HTML5),
- can penetrate firewalls, in which case it needs a central server component inside the organizational network or private cloud (does not rely on an external service provider),
- can build direct connections without a central server (e.g. when the computers are on the same LAN),
- has strong end-to-end connection security,
- uses strong user authentication with optional 2FA and can handle multiple users,
- capable of managing multiple parallel sessions to the same desktop (e.g. for remote assistance),
- provides at least easy file transfer in addition to desktop sharing.

APPENDIX 2

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

Online Workshops on the topic of Remote Access organized in 2023

Online workshops on the topic of Remote Access organized in 2023

of Remote NMR (R-NMR):

Moving NMR infrastructures to remote access capabilities

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

Workshop 1: R-NMR Remote Access Workshop
Tuesday June 6th 10am-12pm CET

10-10:15am Christina Redfield (Oxford) - Brief Introduction to the Remote-NMR project and an update on the results of the NMR Facility Manager and NMR User surveys.

10:15-10:30am W Trent Franks (Warwick, UK) - Remote Access NMR: Experiences from a National Solid-State NMR Facility.

10:30-10:45am Hugo van Ingen (Utrecht NL) - Remote NMR experiences @ Utrecht University.

10:45-11am Goran Karlsson (Gothenburg SE) - GDPR in NMR – what does it mean?

11-11:15am Jarl Underhaug (Bergen NO) - Remote access at University of Bergen.

11:15-11:30am Jennifer Gomez Badillo & Jop Wolffs (Radboud University NL) - Tuning and Matching remotely: applications and demonstration.

11:30-11:45am Daniel Mathieu (Bruker) - Simplifying NMR experiments for entry level users.

11:45am-12pm. Final Questions & Discussion

Workshop 2: R-NMR IconNMR Workshop
Friday November 10th 10am-12pm CET

The topic is IconNMR, a Bruker automation package that may be of use in implementations of remote NMR access. R-NMR partners, especially those running an NMR service and/or using a sample changer, may already be familiar with some aspects of IconNMR. This symposium will provide an introduction to IconNMR and how it can be used both on newer and older Bruker NMR spectrometers for a variety of applications.

10-10:30am Benjamin Goerling (Bruker Applications Team Karlsruhe) - Live IconNMR Dem

10:30-11am Christian Richter (BMRZ Frankfurt) - Screening Using IconNMR

11am-11:30am Ana Cikos (Zagreb) - IconNMR for Elderly NMR Spectrometers

11:30am-12pm Final Questions & Discussion

Workshop 3: R-NMR Apache GuacamoleWorkshop
Monday December 11th 2pm-4pm CET

Online workshop focussing on experiences with remote access using the Apache Guacamole software (one of the options for remote access).

14h CET Goran Karlsson (Goteborg) - Remote access, servers and clients?

14:30h CET Kornel Ecsedi (UniDeb) How to survive a building reconstruction?

15:00h CET Jonathan Farjon & Stephane Guerin (CEISAM, Nantes) - Remote access with Apache Guacamole at CEISAM lab in Nantes University

APPENDIX 3

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

Fact Sheet and Guidelines on GDPR as it relates to NMR Facilities

Fact Sheet and Guidelines on GDPR as it relates to NMR Facilities

of Remote NMR (R-NMR):

Moving NMR infrastructures to remote access capabilities

Authors: Göran Karlsson *(UGOT), Anders Bay Nord (UGOT) and Christina Redfield (UOXF)*

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

What is GDPR?

GDPR is a regulation in EU law that governs data protection and privacy. It is essential that defining a common procedure for remote access to NMR spectrometers meets GDPR requirements with respect to the data that is collected and stored at each NMR facility, and how that data is shared with users. GDPR applies to the processing of personal data. Personal data is any information that refers to an identified or identifiable natural person. What is crucial is that the information on its own or in combination with other information can be linked to a living person. Typical personal data includes:

- a person's personal identity number,
- name,
- address,
- email address.

In the context of NMR facilities, personal data collected/stored is likely to refer to users of the NMR facility. GDPR stipulates that a person can request to be informed about their registered data and to have their registered personal data deleted.

Certain personal data is by its nature particularly **sensitive** and therefore has stronger protection. This type of data is called *sensitive personal data*. Processing of sensitive personal data is as a rule prohibited but there are certain exceptions. Sensitive personal data is data concerning:

- ethnic origin,
- political opinions,
- religious or philosophical beliefs,
- membership of a trade union,
- health,
- a person's sex life or sexual orientation,
- genetic data,
- biometric data that is being used to uniquely identify a person.

From an NMR perspective, analysis of human biomaterial (biofluids, tissue, extracts from tissue, *etc.*) can generate information, for example, on health or drug abuse, that is considered to be sensitive personal data, if that data can be traced to a person. It is important to note that a coded sample can still be traced through a pseudo-anonymized coding list. Only truly anonymized samples, which cannot be traced to a person, are not subject to the GDPR.

Guidelines

1) Personal data collected/stored at NMR Facilities

Most NMR facilities keep a register of their users in some form (list of users' names/email addresses, LIMS/electronic notebook, Excel spreadsheet, *etc*). NMR facilities must be able to provide all information about a user if requested to do so by that user and to delete that personal data upon request by that user. Personal data relating to NMR users is similar to the information kept by department/university IT services about users of their IT facilities. It is the overarching responsibility of the universities and specifically university administrations, or other legal entities, hosting the NMR facilities to have procedures in place relating to GPDR and the handling of personal data. This is the ultimate source from which proper guidelines and information on operating procedures under the GDPR must be obtained. This should not have to be re-invented at the NMR facility level.

2) Sensitive personal data collected/stored at NMR Facilities

From an NMR Facility perspective, metabolomic studies involving human biomaterial are the most likely source of sensitive personal data (if that data can be traced to a person). It is important to note that a coded sample can usually still be traced through a pseudo-anonymized coding list. The data are considered sensitive even if the pseudo-anonymized coding list is not available at the NMR Facility. Only truly anonymized samples, which cannot be traced to a person, are not subject to the GDPR. NMR studies involving human biomaterials will normally have been granted ethical approval via an appropriate institutional committee and the NMR Facility should confirm that such approval is in place.

If the NMR Facility is involved in the collection or processing of sensitive personal data, then this must comply with a number of requirements imposed by GDPR. These are:

- Data and meta-data (during the statistical analysis of metabolomics data) should be F.A.I.R. (Findable, Accessible, Interoperable, Reusable) and minimal.
- The sending/receiving of meta-data should be secure (*e.g.* not via regular e-mail).
- Acquired data should not be left on spectrometer hard drives for general access.
- Access to stored data should be secure (*e.g.* MFA, multi-factor authorization) and traceable.
- Analysis of data should be in a secure environment (*e.g.* using MFA, access events should be logged).
- Transfer of data should follow the same principles (e.g. MFS, secure, logged, traceable).
- Data and meta-data should routinely be deleted after a fixed period of time unless permission is obtained to keep the data for an extended period.

When carrying out NMR studies involving sensitive personal data, NMR Facilities must ensure that the acquisition of NMR data, the storage of acquired NMR data, the analysis of stored

NMR data, the handling of meta-data, and the transfer of stored NMR data (including meta-data, analysis results, *etc*) comply with the above GDPR requirements.

The NMR Facility must be able to identify the personal data controller and the personal data processor. The data controller is defined as the natural or legal person, public authority, agency or other body which, alone or jointly with others, determines the purposes and means of the processing of personal data. The data processor is defined as a natural or legal person, public authority, agency or other body which processes personal data on behalf of the controller. The personal data controller or processor do not need to be individuals working within the NMR Facility but the Facility Manager must know who they are within the institution.

Again, it is the overarching responsibility of the universities and specifically university administrations, or other legal entities, hosting the NMR facilities to have procedures in place relating to GPDR and the handling of sensitive personal data. This is the ultimate source from which proper guidelines and information on operating procedures under the GDPR must be obtained. This should not have to be re-invented at the NMR facility level.

APPENDIX 4

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

Monitoring the carbon footprint

Monitoring the carbon footprint

of Remote NMR (R-NMR):

Moving NMR infrastructures to remote access capabilities

Authors: Peter Podbevsek (NIC), Janez Plavec (NIC), Thomas Vosegaard (AU), Sara Whittaker (HWB-NMR) and Daniel Matthieu (Bruker)

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

Introduction

Description of work: In task 2.5, we will select a set of tools for the calculation of carbon footprint that are suitable to cover the range of impacts caused by the operation of NMR infrastructures. All partners will adopt a common approach to the calculation of the footprint of their users' travel. In addition, we will look into tools that can capture the footprint of equipment usage. The results of these analyses will be communicated to the relevant stakeholders.

Virtually all our activities leave a carbon footprint and NMR is no different. Some activities are directly related to burning fossil fuels. These include transport (sea, air, road and, to an extent, rail) and heating (excluding heat pumps). However, most NMR related activities are dependent on electricity and here the carbon footprint is closely tied to the type of power generation plants used in a specific country. Countries with many hydro, nuclear and renewable power generating plants will generate a smaller carbon footprint per unit of electric power. On the other hand, countries with mostly coal or gas powered plants will leave a much larger carbon footprint. When considering EU member states, the difference can be on the order of a hundredfold (Figure 1). The EU-27 average of 275 g CO_2e equivalents per kWh will be used in all calculations.

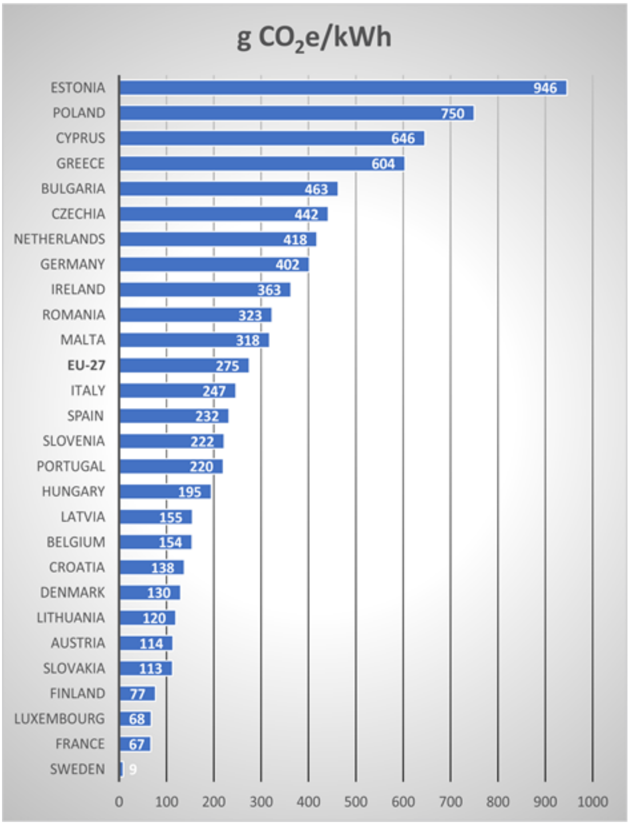

Figure 1 - CO_2 equivalents per kWh of electricity produced in different member states (Source: EEA). For completeness, the value for the UK is 269 CO_2 equivalents per kWh.

In the sections that follow, the carbon footprint of various aspects of the operation of an NMR facility will be discussed. These include: transport of people and of samples, the electricity consumption associated with various hardware components of NMR spectrometers, air conditioning of NMR facilities, liquid helium, and liquid nitrogen.

Transport

Personnel (scientists):

Travelling is a carbon intensive activity, especially when air travel is involved. When work cannot be done remotely or samples cannot easily be shipped, travelling scientists can estimate their carbon footprint using an air or train travel calculator:

ICAO - International Civil Aviation Organization
https://www.icao.int/environmental-protection/Carbonoffset/

Rail Europe
https://www.raileurope.com/

Air travel produces considerably (an order of magnitude) more carbon emissions compared to rail travel. However, over large distances or some destinations travelling over land (even within continental Europe) can take days and flying is the only reasonable option. On the other hand, where high-speed (direct) rail connections exist between destinations flying should be avoided.

Example 1: Paris to Ljubljana is a 2 hour flight compared to an 18 hour train trip one-way. Prices of air and train tickets on this route are comparable. However, flying releases around 140 kg CO_2e, while the train produces less than 10 kg CO_2e.

Example 2: Paris to Marseille is a 1.5 hour flight compared to a 3.5 hour train ride. Transfers to and from the airport as well as waiting at check-in makes the travel time comparable. So is the price. Flying releases around 90 kg CO_2e, while the train accounts for less than 5 kg CO_2e.

Cargo (sample shipment):

Shipping samples is again least environmentally friendly when using air freight. Shipping stable samples at ambient temperature can be done with standard parcel delivery methods with a negligible carbon footprint. On the other hand, sensitive samples are usually shipped on dry ice with parcel sizes between 0.1 and 0.2 m^3 weighing between 10 and 20 kg. Furthermore, most of the parcel weight is frozen CO_2, which should be added directly to the carbon footprint.

The carbon footprint of shipping larger packages with samples can be estimated using an online calculator. However, most web calculators deal with tonnes of cargo or standard shipping container units, which are not suitable for NMR samples weighing a few grams or kilograms. DHL offers a web-based calculator where the carbon footprint of smaller parcels can be estimated.

https://www.dhl-carboncalculator.com/

The calculator is based on the EN 16258 standard, which establishes a common methodology for the calculation and declaration of energy consumption and greenhouse gas emissions related to any transport service.

A summary of carbon emissions associated with different modes of sample transport is presented in Table 1.

Transport mode	Emissions ($g\ CO_2e$ / tonne·km)
Road	62
Rail	22
Short sea	16
Intermodal road/rail	26
Intermodal road/short sea	21
Deep-sea container	8
Air-freight	602

Table 1 – Emissions associated with different modes of transport. (Source: McKinnon et al., Measuring and Managing CO_2 Emissions of European Chemical Transport, Heriot-Watt University, 2011).

Electricity

A typical modern solution-state NMR spectrometer equipped with a cryo-probe has a number of components including the NMR console, the PC and display screen, an air cooler (BCU) for temperature control of the sample, a cryo-cooling unit, a helium compressor and a water chiller. The typical power consumption associated with each of these components is summarized in Table 2.

System Component	Power consumption (kW)
NMR console (NEO OneBay)	1.3
PC and display	0.2
Air cooler (BCU)	0.6
Cryo cooling unit	0.5
Helium compressor	7.5
Water chiller	3.6

Table 2 – Summary of power consumption associated with NMR spectrometer components (Source: Bruker Site planning guide).

In total that is 13.7 kW of continuous power draw and 120 MWh in a year. Using the EU-27 average this produces 33 tonnes of CO_2e per year. Interestingly, most of the power draw is associated with components related to the cryo-probe (Cryo cooling unit, helium compressor and water chiller). An NMR spectrometer with a room temperature probe would draw only 2.1 kW and produce 5 tonnes of CO_2e. Spectrometers optimised for solids also do not require these 'cryo' components. However, they do use higher power amplifiers and a typical solids console will draw an additional 1.7 kW.

Superconducting magnets do not draw electrical power during their operation. However, pumped (2K) magnets do require constant operation of vacuum pumps, which use on average 0.5 kW and thus produce 1.2 tonnes of CO_2e per year.

Modern fluorescent or even LED lighting is relatively efficient. Nevertheless, lighting can be turned off, while the spectrometer is operated remotely for a modest energy saving. Modern PCs, which control the spectrometer, use between 150 and 200 W and need to be turned on at all times.

Air conditioning

Boards in NMR consoles are particularly sensitive to temperature and require a constant flow of cool air. Rooms where consoles are located need tight temperature regulation (cooling). Therefore, air conditioning units run continuously. However, cooling power requirements can vary considerably depending on room size and configuration as well as the climate and season.

On the other hand, if the magnet is not in the same room as the consoles, the magnet room may not need as tight temperature regulation. The same goes for some auxiliary components.

The room where the operator sits can also be cooled less, especially when the spectrometer is operated remotely. Nevertheless, it will be assumed that all electrical power used by different components of NMR systems is converted to heat, which needs to be removed. A typical modern air conditioning unit has a seasonal energy efficiency ratio of around 6 (W/W), which means that an additional ⅙ of the carbon footprint caused by usage of electricity is produced due to heat removal.

Liquid helium

Helium (He) is found as a trace gas in natural gas wells and regenerates very slowly as a by-product of uranium decay. While all natural gas deposits contain some helium it is often not separated and sold commercially. Currently the only significant suppliers are the United States, Algeria and Qatar. Therefore, helium needs to be shipped to Europe from overseas.

Newly extracted helium is normally liquified on site (overseas) and then transported by sea and road to a filling plant in Europe. The final leg to individual NMR facilities is by road. However, compared to the high carbon footprint of He liquefaction transport carbon footprint is negligible even if importing from the USA. Nevertheless, small scale helium liquefiers are available and relatively pure captured helium gas can be reliquefied on site, which eliminates any carbon emissions related to long distance transport. Around 10-20% of helium gas is lost during the process. Considerable amounts of helium are also lost with handling when transferring the liquid gas to smaller containers and finally into the NMR magnet.

Once helium is vented into the atmosphere it is uneconomical to recover and slowly diffuses into space. Current estimates suggest helium supplies on Earth will be depleted within a century. Some sort of helium recovery is therefore necessary for its long-term use as a cryogenic gas. Unfortunately, helium recycling is not widely used. This is mostly related to the additional cost of capture and/or liquefaction equipment as well as the high energy demand and consequently the carbon footprint.

Efficiency of a helium liquefaction plant depends amongst other things on the percentage of helium in the natural gas mixture (Figure 2). It is very costly to exploit wells with less than 3% helium and the carbon footprint is consequently also very large. The optimistic value of 200 kWh/kmol can be converted to 50 kWh/kg He or 6.25 kWh/L He for liquefaction alone. Using the EU-27 average CO_2 equivalents per kWh of electricity this corresponds to more than 1.7 kg CO_2 equivalents per 1 L of liquid helium. This does not include the carbon footprint and other environmental impacts related to exploiting a natural gas well. However, these can be eliminated if helium is captured on site from magnet boil off. Helium capture equipment is readily available and does not produce a large carbon footprint since at this stage the gas is only compressed into storage cylinders ready for transport to the liquefaction plant.

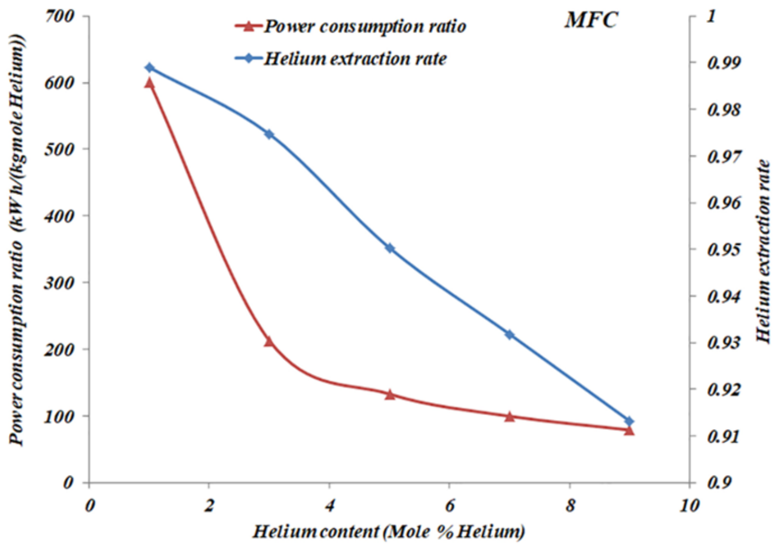

Figure 2 - Power consumption and extraction rates for different fractions of He in natural gas wells. (Source: Zaitsev et al., Int. J. Energy Res. 2020.)

Magnet	Helium consumption (ml / h)	(L / year)	Liquefaction cost (MWh / year)	CO2 emissions (kg CO_2e / year)
400 MHz	13	114	0.7	196
500 MHz	13	114	0.7	196
600 MHz	16	140	0.9	241
700 MHz	26	228	1.4	392
800 MHz	47	412	2.6	708
1.0 GHz (2K)	< 250	< 2190	< 13.7	< 3765
1.2 GHz (2K)	< 250	< 2190	< 13.7	< 3765

Table 3 - Helium consumption of modern (current generation) NMR magnets

Due to scarcity of and recent price increases for liquid helium, manufacturers are trying to decrease helium consumption of NMR magnets. Modern lower field conventional 4K superconducting magnets consume relatively small volumes of liquid helium (Tables 3, 4 and 5). On the other hand, the highest field NMR spectrometers (1.0 and 1.2 GHz) use pumped 2K superconducting magnets. These use evaporative cooling to maintain superconductivity of coil and joint material at high magnetic fields. Since this is achieved by a pumping process, which actively removes helium from the upper bath, helium consumption greatly increases. Advances in NMR magnet design allow the latest generation of 800 MHz magnets to switch from a pumped 2K to a conventional 4K magnet design greatly reducing its helium consumption (Table 5).

Magnet 600 MHz	Helium consumption (ml / h)	(L / year)	Liquefaction cost (MWh / year)	CO2 emissions (kg CO_2e / year)
early gen.	40	350	2,2	602
last gen.	26	228	1,4	392
current gen.	16	140	0,9	241

Table 4 - Helium consumption of different generations of 600 MHz NMR magnets.

Magnet 800 MHz	Helium consumption (ml / h)	(L / year)	Liquefaction cost (MWh / year)	CO2 emissions (kg CO_2e / year)
last gen. (2K)	140	1226	7,7	2108
current gen. (4K)	47	412	2,6	708

Table 5 - Helium consumption of different generations of 800 MHz NMR magnets.

Liquid nitrogen

In contrast to helium, nitrogen is the major component of Earth's atmosphere and can be liquified anywhere on the planet. This eliminates long distance transport of the liquified gas (LN2). However, nitrogen liquefaction is still moderately energy demanding. A typical plant can liquefy nitrogen with an energy cost of 0.5 kWh/L LN2, which corresponds to 0.14 kg CO_2 equivalents per 1 L of LN2. A modern 600 MHz NMR magnet will use around 2600 L of LN2 per year, which corresponds to 364 kg CO_2e. On the other hand, an early generation pumped 800 MHz magnet uses around 7800 L of LN2, which is responsible for 1092 kg CO_2e per year.

Nitrogen gas can be also recycled on site via an accessory nitrogen liquefier, which greatly reduces the number of nitrogen refills each year. This also reduces the need to transport LN2 over large distances. If the NMR system is already equipped with a cryo platform (for a cryo-probe) the nitrogen liquefier simply uses the extra cooling capacity of the cryo platform.

Summary

It is evident that (by far) the largest sources of carbon emissions are the power-hungry components related to cryoprobe operation. However, cryoprobes offer a huge advantage in sensitivity and have become the norm for biomolecular NMR. Since most of the carbon footprint is a consequence of electrical power generation the total carbon footprint of an NMR system can depend dramatically on the country where the spectrometer is operated or even the source of electricity purchased by the institution where the spectrometer is located.

With older NMR systems using pumped magnets large quantities of cryogenic gases are also a considerable source of carbon emissions. Upgrading to a non-pumped magnet can save a few tonnes of CO_2e per year. Even smaller systems (600 MHz or less) can benefit greatly from a magnet upgrade and cut the usage of cryogenic gases in half. However, there is a considerable financial cost associated with the purchase of a new magnet. Currently all magnets offering gigahertz field strengths still require pumping and are (environmentally) more expensive to run. A summary of the carbon footprint associated with some typical spectrometer configurations is shown in Table 6. This information will be useful to NMR facilities in their calculation of the carbon footprint associated with operation of their NMR spectrometers.

Tonnes of CO_2e per year	**current gen. 600 MHz (4K, RT probe)**	**current gen. 600 MHz (4K, cryoprobe)**	**early gen. 800 MHz (2K, cryoprobe)**
Electricity	5.1	33.0	34.2
Air conditioning	0.9	5.5	5.7
He	0.2	0.2	2.1
LN2	0.4	0.4	1.1
Total	**6.6**	**39.1**	**45.1**

Table 6 - Carbon footprint breakdown for some typical spectrometer configurations.