Progress in Nuclear Magnetic Resonance Spectroscopy 152–153 (2026) 101595

Contents lists available at ScienceDirect

Progress in Nuclear Magnetic Resonance Spectroscopy

journal homepage: www.elsevier.com/locate/pnmrs

Moving NMR infrastructures to remote access capabilities

James Tolchard [a], Tanguy Le Marchand [a], Ruud L.E.G. Aspers [b], Gyula Batta [c], Burkhard Bechinger [d,e], Ulrika Brath [f], Styliani A. Chasapi [g], Ana Čikoš [h], Kornél Ecsedi [c], Adrien Favier [i], Ana Sofia D. Ferreira [j], Radovan Fiala [k], Panagiota D. Georgiopoulou [g], Jennifer S. Gómez [b], Kristaps Jaudzems [l], Göran Karlsson [f], Arno P.M. Kentgens [b], Sander F.H. Lambregts [b], Francesca Morelli [m], Frans A.A. Mulder [n], Sivanandam V. Natarajan [f], Cecilia Persson [f], Roberta Pierattelli [m,o], Miquel Pons [p], Jesus Raya [d], Christina Redfield [q], Vilko Smrečki [h], Georgios A. Spyroulias [g], Julien Trébosc [r], Alicia Vallet [i], Carine van Heijenoort [s], Hugo van Ingen [t], Thomas Vosegaard [u], Julia Wirmer-Bartoschek [v,*], Harald Schwalbe [v,*], Anne Lesage [a,*], Guido Pintacuda [a,*]

[a] Ecole Normale Supérieure de Lyon, CNRS, Lyon 1 Université, Centre de RMN à Hauts Champs de Lyon (CRMN), 5 rue de la Doua, 69100 Villeurbanne, France
[b] Magnetic Resonance Research Center, Institute for Molecules and Materials, Radboud University Nijmegen, Heyendaalsweg 135, 6525, Nijmegen, the Netherlands
[c] Department of Chemistry, University of Debrecen, Egyetem sqr. 1, 4032 Debrecen, Hungary
[d] University of Strasbourg / CNRS, UMR7177 Chemistry Institute, 67000 Strasbourg, France
[e] Institut Universitaire de France, 75005 Paris, France
[f] Swedish NMR Centre, University of Gothenburg, Medicinaregatan 5C, 41390 Gothenburg, Sweden
[g] Department of Pharmacy, University of Patras, Panepistimioupoli-Rion, 26504 Patras, Greece
[h] NMR Centre, Ruđer Bošković Institute, Bijenička cesta 54, 10000 Zagreb, Croatia
[i] Université Grenoble Alpes, Commissariat à l'Énergie Atomique et aux Énergies Alternatives, CNRS, Institut de Biologie Structurale, 71 av des Martyrs, 38044 Grenoble, France
[j] Portuguese NMR Network (PTNMR), Department of Chemistry, NOVA School of Science and Technology, NOVA University of Lisbon, 2829-516 Caparica, Portugal
[k] CEITEC Masaryk University, Kamenice 753/5, 625 00 Brno, Czech Republic
[l] Department of Physical Organic Chemistry, Latvian Institute of Organic Synthesis (LIOS), Riga, Latvia
[m] Consorzio Interuniversitario Risonanze Magnetiche Metallo Proteine (CIRMMP), Via Luigi Sacconi 6, 50019 Sesto Fiorentino, Italy
[n] Institute of Biochemistry, Johannes Kepler University, Altenberger Strasse 69, 4040 Linz, Austria
[o] Department of Chemistry 'Ugo Schiff' and Magnetic Resonance Center (CERM), University of Florence, Via Luigi Sacconi 6, 50019 Sesto Fiorentino, Italy
[p] Biomolecular NMR laboratory, Department of Inorganic and Organic Chemistry, Universitat de Barcelona (UB), Baldiri Reixac, 10-12. 08028, Barcelona, Spain
[q] Department of Biochemistry, University of Oxford, South Parks Road, Oxford OX1 3QU, United Kingdom.
[r] Univ. Lille, CNRS, INRAE, Centrale Lille, Univ. Artois, FR 2638 - IMEC - Institut Michel-Eugène Chevreul, 59000 Lille, France
[s] CNRS, Institut de Chimie des Substances Naturelles (ICSN), 1 avenue de la terrasse, 91190 Gif-sur-Yvette, France
[t] Bijvoet Center for Biomolecular Research, Utrecht University, Padualaan 12, 3584 Utrecht, the Netherlands
[u] Interdisciplinary Nanoscience Center and Department of Chemistry, Aarhus University, Langelandsgade 140, 8000 Aarhus, Denmark
[v] Institut für Organische Chemie und Chemische Biologie, Johann Wolfgang Goethe-Universität Frankfurt, Max-von-Laue Str. 7, 60438 Frankfurt, Germany

ARTICLE INFO

Editor: Edited by Bradley Chmelka and David Neuhaus

Keywords:
Remote access
NMR infrastructure
Standard operating procedures (SOPs)
Workflow design
Data management and security
Sustainability

ABSTRACT

Traditionally, Nuclear Magnetic Resonance (NMR) infrastructures have relied on in-person access, requiring researchers to travel to centralized facilities to conduct experiments. However, recent advancements in remote access technologies, accelerated by the constraints imposed by the COVID-19 pandemic, have demonstrated the feasibility and strategic benefits of transitioning NMR operations toward remote accessibility. This review examines the key challenges and opportunities associated with remote access to NMR instrumentation, including standardized protocols for sample handling, secure authentication mechanisms, real-time instrument control, and data management. By establishing a unified framework for remote access, we aim to enhance the sustainability and accessibility of NMR facilities. Our findings highlight the necessity for collaborative efforts to develop best practices that ensure reproducibility, high-quality data acquisition, and equitable access to NMR infrastructure on a global scale.

* Corresponding authors.
E-mail addresses: wirmer@nmr.uni-frankfurt.de (J. Wirmer-Bartoschek), schwalbe@nmr.uni-frankfurt.de (H. Schwalbe), anne.lesage@ens-lyon.fr (A. Lesage), guido.pintacuda@ens-lyon.fr (G. Pintacuda).

https://doi.org/10.1016/j.pnmrs.2026.101595
Received 13 August 2025; Accepted 14 January 2026
Available online 20 January 2026

Contents

1. Introduction

Nuclear Magnetic Resonance (NMR) spectroscopy is a cornerstone analytical technique with far-reaching applications across multiple scientific disciplines, including chemistry, biochemistry, physics, materials science, geology, and medicine. It is a fundamental tool for quality control and structural analysis of a vast array of substances, from small organic molecules to polymers and biomacromolecules such as proteins, DNA, and RNA. Given its essential role in both academic research and industrial applications, NMR spectrometers are not only present in universities worldwide, but are also integral to the chemical, pharmaceutical, and materials industries.

Due to the high cost of instrumentation, the need for specialized expertise, and the complexity of experimental setup and data analysis, NMR facilities are typically centralized into dedicated infrastructures that provide access to a broad user base. These facilities range from small institutional platforms to large national or international infrastructures, each differing in their instrumentation, user community, and operational framework. Despite this diversity, most NMR facilities operate on a walk-in access model, where researchers conduct experiments in-person, often in close collaboration with on-site technical staff. This traditional approach was drastically disrupted by the COVID-19 pandemic, which imposed severe restrictions on user mobility. During this period, many NMR facilities transitioned toward remote access, enabling users to conduct experiments without physically traveling to the facility. This included two primary modes: *direct remote access*, where users could operate the NMR spectrometer themselves via a secure remote login to the instrument's control computer, and *assisted remote access*, where users communicated with on-site staff (via video conferencing or phone) who executed experiments based on instructions provided in real time. The success of these emergency adaptations demonstrated that remote access to NMR is not only feasible but also offers long-term strategic benefits, such as enhanced resilience of research infrastructures against future crises (e.g., pandemics, travel restrictions, institutional shutdowns), reduced environmental footprint, as minimizing user travel aligns with sustainability goals, and improved accessibility, particularly for researchers located in remote regions or without the means to travel frequently.

While remote access holds significant potential, the lack of standardized protocols, infrastructure compatibility, and user-interaction models across different facilities remains a major barrier to its full implementation. A transition toward a fully integrated and interactive remote access system requires the development of common operational frameworks, technological solutions, and best practices. Such a system must ensure that users can effectively engage with the instrumentation, monitor and modify experiments in real time, and receive adequate technical support—closely replicating the experience of on-site access.

Recognizing these challenges and opportunities, leading European NMR infrastructures have joined forces to define the key requirements for remote access and develop a set of shared protocols within the framework of *Remote-NMR* (R-NMR), a European-funded project. In the following sections, we analyze the current state of remote NMR access, identify critical areas requiring harmonization, and propose a roadmap for establishing common protocols. Specifically, we examine key aspects such as **sample shipping and handling** (best practices for packaging, regulatory compliance, and pre- and post-shipment quality control), **user training and authentication** (development of training programs and secure access protocols for remote users), **remote user interaction**

(definition of access levels, ranging from full operator control to independent remote operation), **software and hardware compatibility** (standardization of tools for remote experiment control and real-time data acquisition), **data management and security** (guidelines for data access, sharing, and compliance with local, national, and international regulations) and **quality assurance** (mechanisms to ensure sample stability, data integrity, and experimental reproducibility). By addressing these critical factors, we aim to provide a comprehensive framework for the future of remote NMR access with the objective of enhancing scientific productivity, promoting equitable access to cutting-edge infrastructure, and strengthening the global NMR community's ability to tackle pressing scientific and societal challenges.

2. Key procedural steps for remote NMR access

The implementation of remote access in NMR facilities requires a systematic approach to ensure efficiency, reliability, and user support. This section outlines the key procedural steps necessary to facilitate seamless remote access, from project submission and initial verification to sample shipment, data acquisition, and post-experiment processing.

2.1. Project submission and initial access procedures

To ensure a streamlined and efficient remote access process, all project submissions should follow a standardized initial procedure, regardless of sample type or access mode. This framework establishes a clear and transparent pathway for researchers seeking remote access to NMR facilities while maintaining operational consistency across different infrastructures.

The first step in gaining remote access is to formally submit a project proposal through an existing access route. This may involve direct contact with an NMR facility or the use of established institutional and transnational online submission platforms designed to support external users. Before initiating this process, potential users are expected to review the facility's overview (including its instrumentation, capabilities, and areas of expertise) to ensure it meets the specific requirements of their project. These platforms facilitate structured access requests and ensure that necessary project details are efficiently communicated between the user and the host facility. Once access to a platform has been granted, essential project information must be exchanged to enable smooth planning and execution of the experiments. This information may be submitted via an online access system or through direct communication with facility staff. In either case, the proposal should include the following essential details:

- **Project title and description:** A concise overview of the scientific objectives, including relevant preliminary NMR data (if available), expected experimental outcomes, and funding sources.
- **Primary contact information:** Names and contact details of the lead researcher and the principal investigator responsible for the project.
- **Instrumentation requirements:** Specifications regarding the necessary hardware, probe selection, and spectral resolution requirements.
- **User experience and training level:** A summary of the user's practical experience with NMR spectroscopy and prior facility access (see section 3 below for details).
- **Remote access level:** The degree of user interaction required (e.g., fully autonomous, guided remote access, or staff-assisted operation).
- A detailed **list of all items** to be shipped to the host facility (including samples, tubes, rotors, and any required consumables), along with information on sample quantity, concentration of relevant components, solubility in selected solvents, sensitivity to moisture, oxygen, temperature, pressure, light, or other environmental conditions, safety classifications (e.g., biohazard level), and any applicable regulatory restrictions. This information is essential to assess the feasibility and safety of the proposed experiments.

Upon approval of the project proposal, the host facility should provide the user with a detailed confirmation package outlining:

- **Designated facility contact person:** A representative responsible for handling the request and guiding the user through the process.
- **Expected scientific outcomes:** Confirmation of feasibility and potential refinements to the experimental plan.
- **Proposed experimental dates:** A timeline for the planned measurements and data collection.
- **Shipping and logistics information:** Detailed instructions for sample shipment, including the facility's address, courier preferences, and any legal restrictions that might apply.
- **Remote access setup:** Confirmation of the level of remote interaction permitted and, if necessary, instructions for establishing remote access connections and secure data transfer protocols.

By implementing these standardized submission and verification procedures, NMR facilities can ensure efficient and transparent access management, allowing researchers to engage in remote experiments while maintaining high standards of data integrity, safety, and user experience.

2.2. Procedures for sample shipping

The shipment of samples between users and NMR facilities represents a critical logistical and technical challenge in the implementation of remote access workflows. While often perceived as a routine step, sample shipment is one of the major bottlenecks in ensuring seamless remote experimentation, particularly for international users. Regulatory barriers, material classification inconsistencies, and transport limitations can introduce significant delays or prevent research from being carried out. Specific challenges include customs clearance, classification of biological hazards and chemical safety, transport of frozen samples (e.g., dry ice shipments), degradation of sensitive biomolecules, and the shipment of hazardous materials (toxic, explosive, radioactive, or biohazardous samples). The experience of the Covid-19 NMR network (https://covid19-nmr.de), which involved shipping samples across multiple countries, demonstrated that inadequate preparation and regulatory discrepancies can significantly hinder time-sensitive research projects. To overcome these challenges, a clear, standardized approach to sample shipping is necessary to ensure the safe, timely, and reproducible transport of samples across different infrastructures.

Currently, most NMR facilities lack formalized standard operating procedures (SOPs) for sample shipping, and written instructions for users are often incomplete or absent. To streamline and harmonize remote access across European and international NMR infrastructures, we propose a set of best practices for shipping solution and solid-state NMR samples, developed from existing facility procedures and user surveys.

Before shipping, users should engage in pre-shipping communication with the host facility to confirm sample compatibility with on-site instrumentation and to verify the necessary information, including:

- **Sample acceptability:** Confirmation that the sample can be handled and analyzed at the host facility, considering safety classifications, biohazard levels, and any potential regulatory restrictions.
- **Required safety documentation:** Identification of necessary certifications regarding sample safety and whether they need to be submitted in advance or accompany the shipment.
- **Shipping logistics:** Clarification of the appropriate recipient for the sample at the host facility and shipment dates, taking into account whether upcoming national or local holidays, facility closures, or transport disruptions (e.g., strikes) may impact delivery timelines.

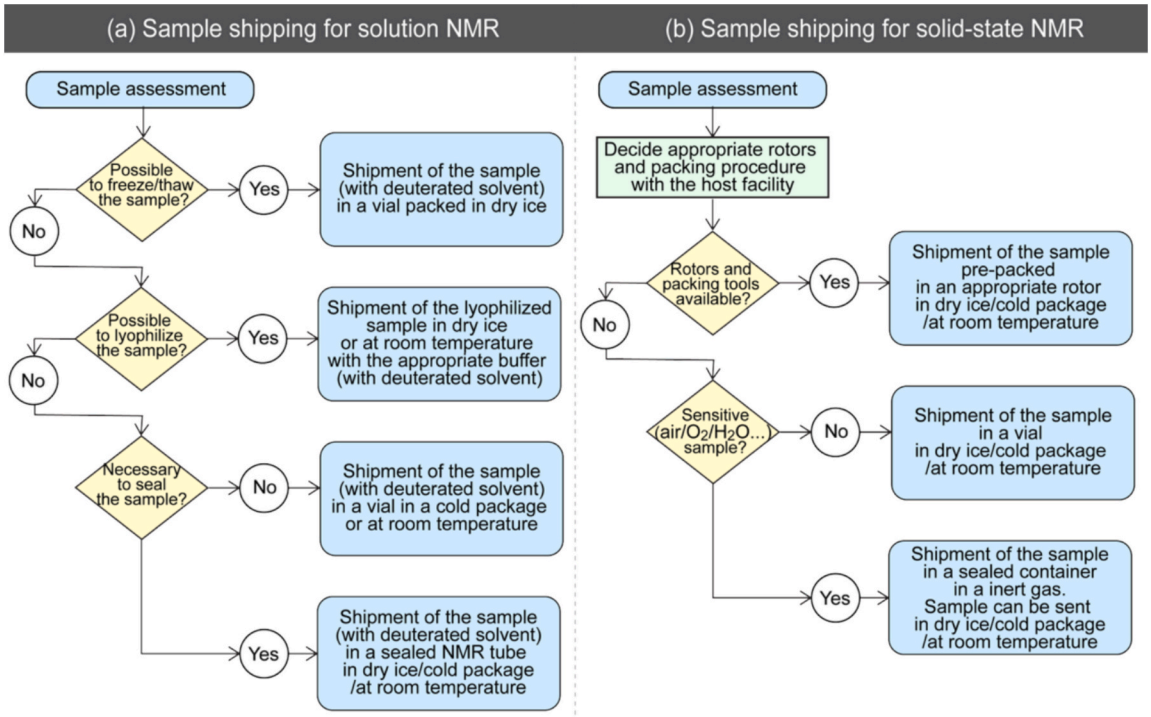

Fig. 1. Workflow chart for sample shipment. Recommended decision pathways are summarized for remote shipment of samples for (a) solution NMR and (b) solid-state NMR, covering a wide range of sample types. Although many examples derive from organic, biochemical, or biological systems, the workflows also apply to sensitive chemical and materials samples, including powders, air- or moisture-sensitive compounds, and samples requiring controlled atmosphere or temperature.

- **Storage equipment** on site at the facility (freezer, refrigerator, glovebox, etc)

Each facility should define the regulatory paperwork required for shipment, including customs declarations for international shipments, safety certifications for hazardous materials, and sample integrity forms for biological specimens. Customs formalities are primarily determined by the regulations of both the country of origin and the destination country, and may also be influenced by additional restrictions in place in transit countries. Because these requirements can vary widely and are difficult to anticipate for every route, it is recommended that users and facilities verify applicable regulations with their courier service prior to shipment. In the longer term, establishing a shared reference list summarizing procedures and documentation required for the most common countries of origin and transit would greatly facilitate compliance and reduce administrative delays.

Additionally, to minimize shipment-related delays and ensure seamless remote access, standardized specific steps should be established for solution and solid-state NMR. Corresponding guidelines are illustrated in Fig. 1 and detailed below.

2.2.1. Guidelines for sample shipment in solution NMR

Sample stability is the primary factor determining the optimal transport conditions for solution NMR experiments. Based on the properties of the sample, the following best practices should be followed:

(i) **Frozen Sample Shipment.** If the sample can be rapidly frozen and thawed without damage, shipping in a small plastic or glass vial on dry ice is the preferred method. This approach ensures sample integrity during transport and reduces the likelihood of degradation. To further minimize handling at the NMR facility, it is recommended that the sample already contain the necessary deuterated solvent. Upon arrival, facility staff can then thaw the sample and transfer it into an NMR tube.

(ii) **Lyophilized Sample Shipment**. If the sample can be lyophilized and later reconstituted without degradation, it may be shipped as a dry powder. The remote user should supply an appropriate buffer, including the necessary deuterated solvent, for reconstitution at the host facility. Depending on stability requirements, the lyophilized sample can be shipped at room temperature. This method minimizes potential degradation during transport, eliminates the need for refrigeration and reduces shipping costs.

(iii) **Powdered Sample Shipment**. Samples of small organic molecules may be shipped in powder form. Remote users should specify the required deuterated solvent for dissolution at the host facility. This method is preferred over shipping the sample already dissolved in deuterated solvent.

(iv) **Solution Shipment in Vials.** For samples that cannot be frozen or lyophilized, shipment in liquid solution is necessary. In this case, the sample should be placed in a robust vial and transported either at ambient temperature or under cooled conditions. While ambient temperature shipment is logistically simpler, it may lead to sample degradation, especially for biologically sensitive compounds. Shipping at reduced temperatures can mitigate this risk, but it requires additional coordination, particularly if transit times exceed 24 h. To simplify the workflow at the facility, it is preferable that the sample already contain the required deuterated solvent.

(v) **Shipment in NMR Tubes.** Direct shipment of samples in NMR tubes is generally discouraged due to the fragile nature of the glass, the risk of leakage, and potential bubble formation caused by liquid movement during transport. However, in cases where air-sensitive samples must be prepared under controlled conditions, shipping in sealable NMR tubes may be necessary. If this method is used, tubes should be individually secured in protective casings before transport to prevent breakage and sample loss. Specialized tube types require particular attention. Shigemi™ tubes should not be shipped with a sample inside, as vibration or mechanical shock during transit can cause the plunger insert to

shift, leading to bubble formation. When required, Shigemi™ tubes should therefore be shipped empty accompanied by the sample in a separate container. Conversely, shaped or thick-walled tubes used for high-salt or viscous samples may be shipped if properly sealed and protected.

(vi) **Metabolomic Samples.** Some samples for metabolomic studies require a fully sealed transport mode to prevent any manipulation upon arrival at the facility. For facilities equipped with automated sample changers, users may pre-load samples into 96-tube racks with protective caps to maintain sample stability. If manual handling at the remote facility is permitted, frozen shipment remains preferable, as it helps preserve sample integrity until the experiment is conducted. If the solvent cannot be frozen using dry ice (e.g. methanol-d_4, dichloromethane-d_2, ethanol-d_6), the sample should be transported vertically, as the cap-tube connection may cause potential leakage.

To facilitate sample tracking and handling, each shipment should be accompanied by a detailed sample information sheet, including the sample name, concentration, solvent composition (buffer type, pH, ionic strength, and amount of deuterated solvent), toxicity classification, and storage conditions before measurement. For proteins, other details such as the isoelectric point, sample mass, molecular weight, and the primary sequence should also be included. For particularly sensitive samples, users should include clear guidance for mitigating potential degradation during unplanned delays in transit (e.g., specifying acceptable temperature ranges, using stabilizing additives, or providing instructions for temporary storage upon arrival). While it is not always feasible to prevent degradation entirely, advance planning and communication with the host facility can substantially reduce risks associated with extended shipment or customs delays.

Upon receipt of the sample, the host facility should confirm its arrival and condition, provide an estimated timeline for experiments, and specify the return shipment process if required. Effective communication between users and facilities is critical to ensure that the entire process, from shipment to analysis to sample return, is carried out efficiently and in compliance with safety and regulatory standards. After the completion of experiments, samples should be returned to the user according to the provided shipment instructions. In certain cases, and upon user request, the host facility can arrange for the degradation or disposal of samples.

2.2.2. Guidelines for sample shipment in solid-state NMR

Solid-state NMR samples vary significantly in composition, ranging from powdered materials to biological aggregates such as membrane proteins, sedimented cells, or tissue samples. Depending on stability requirements, samples may be transported on dry ice, under refrigeration, or at ambient temperature. The following best practices should ensure optimal transport conditions for solid-state NMR samples:

(i) **Pre-Packed Rotors**. When possible, users should pre-pack the sample into a solid-state NMR rotor before shipping. Pre-packing minimizes the amount of sample manipulation required at the facility and reduces the workload for local staff, provided that packing quality and rotor balance are adequate. To ensure compatibility and proper packing procedures, the user should consult with the host facility in advance. Experience in filling solid-state rotors is required, as irregular packing can lead to uneven spinning of the rotor, potentially resulting in a rotor crash. Ideally, the rotor should be tested on spinning at the required spinning speed before shipping. If there are any doubts about the packing, it is advisable to proceed to (ii).

(ii) **Shipment in Raw Form.** If rotor packing is not feasible at the user's site, the sample has to be shipped in its raw form and packed into the appropriate rotor at the host facility. This approach allows for visual inspection of the material before loading, ensuring sample integrity. Facilities may provide appropriate rotors on loan upon request, especially when users lack experience in solid-state NMR sample preparation. In such cases, prior agreement on handling responsibilities and possible compensation for damage to consumable rotor components (e.g., caps or drive tips) is recommended.

(iii) **Air-Sensitive Sample Shipment.** Air-sensitive materials require special handling to prevent exposure to oxygen or moisture. These samples should be sealed under an inert atmosphere, such as nitrogen or argon, before shipment. The receiving facility must be equipped with a glovebox or an equivalent containment system for unpacking and transferring the sample into an NMR rotor. Alternatively, pre-packed rotors sealed in containers can be shipped directly to the NMR facility, ensuring that the sample remains protected during transit.

To facilitate handling and minimize errors, users must provide a detailed sample information sheet with each shipment, specifying the sample name, quantity, composition, toxicity classification, and required storage conditions. Upon receipt of the sample, the host facility should confirm its arrival and condition, provide an estimated timeline for experiments, and specify the return shipment process if required. Effective communication between users and facilities is critical to ensure that the entire process, from shipment to analysis to sample return, is carried out efficiently and in compliance with safety and regulatory standards. For all shipments, users are responsible for arranging prepaid return shipping at the time their samples are sent to the facility. This ensures timely return of materials once experiments are completed. Alternatively, upon explicit written request, the host facility may arrange for sample disposal in compliance with local safety and environmental regulations.

2.3. Work flowcharts for remote access

The diversity of operational modes across NMR facilities necessitates the development of a standardized workflow for remote access that accommodates different sample types, instrumentation setups, and experimental conditions. Remote users may work with a broad range of materials, from solutions and biofluids to powders, hydrated crystals, sediments, and air-sensitive compounds, requiring distinct handling procedures. Likewise, the facilities cater to various NMR techniques, including solution-state and solid-state experiments, dynamic nuclear polarisation (DNP), and the detection of both common (^{1}H, ^{13}C, ^{15}N, ^{31}P) and less abundant nuclei (^{27}Al, ^{17}O, ^{43}Ca, ^{89}Y, ^{95}Mo, ^{47}Ti, etc.).

To ensure compatibility across disciplines, two standardized workflows are proposed, one for solution NMR and one for solid-state NMR. These workflows map out the full remote experimental process, from sample admission to post-experiment data handling, while identifying bottlenecks where on-site intervention remains essential. They also highlight the steps where remote users can have direct control, thereby optimizing efficiency while preserving data integrity.

2.3.1. Standardized workflow design

The workflows for remote solution and solid-state NMR are divided into four key operational phases:

(i) **Sample Admission**. Once a sample arrives at the facility, the first step is the evaluation of its physical integrity, and its storage under appropriate conditions, as indicated by the user, which typically includes temperature-controlled storage (−80 °C, −20 °C, 4 °C, room temperature) or an inert atmosphere (glovebox for air-sensitive samples). The facility team evaluates degradation risks and labelling accuracy before scheduling experiments in coordination with the user. If degradation or inconsistencies are detected, the remote user is immediately consulted before proceeding further.

(ii) **Pre-Acquisition Settings**. Before data collection begins, sample preparation and spectrometer setup must be finalized. In solution NMR, this involves preparing NMR tubes with the correct solvent composition, verifying sample concentration and temperature, as well as ensuring compatibility with the designated probe. Compatibility includes both physical and experimental aspects, such as tube geometry and volume, solvent and salt content, and the probe's operational frequency range and temperature limits. In solid-state NMR, rotors must be packed appropriately, with visual inspections conducted for powdered materials and biological aggregates to confirm homogeneity. Spectrometer setup includes probe installation and configuration, and quality assessment of the instrumentation on standard samples as defined in section 5, before user sample insertion.

(iii) **User Communication.** A remote communication channel is established between the facility and the user to allow real-time monitoring and feedback. Depending on the user's preference, this step may also be carried out prior to configuring the pre-acquisition settings.

(iv) **Data Collection**. Once the experiment is ready to begin, the NMR facility performs final instrument optimizations, including setting the working temperature, adjusting the probe tuning and shimming, locking the magnetic field, and calibrating radiofrequency (RF) pulses. Following these adjustments, the required one-dimensional (1D) or multi-dimensional (nD) NMR experiments are executed. Remote users may have the ability to adjust parameters in real-time and fully control the spectrometer, depending on the level of access permitted by the facility. (see section 3)

Post-Acquisition Operations. Upon completion of data collection, the facility ensures secure data transfer to the user and assists in data processing if required. Samples may either be stored for future experiments or shipped back to the user, following agreed-upon practices, or disposed of according to the established security procedures. Facilities must establish clear storage policies to prevent excessive sample accumulation unless future experiments are explicitly planned. Data integrity is maintained by ensuring proper metadata labelling and

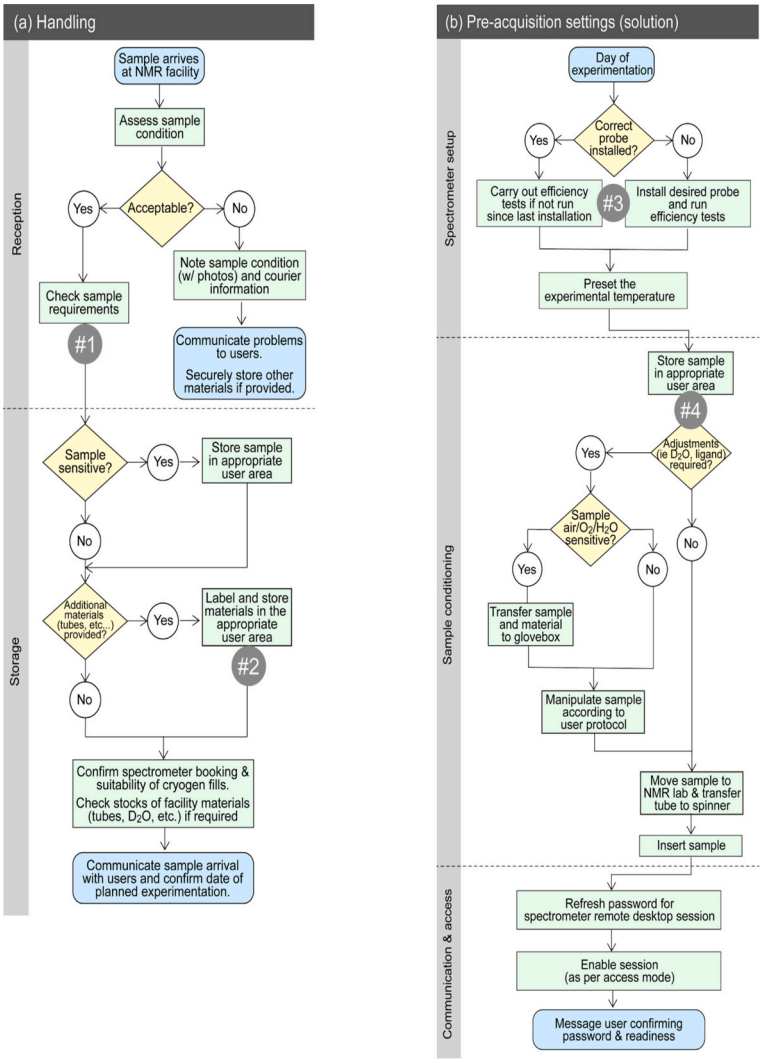

Fig. 2. Workflow chart for solution and solid-state NMR experiments. The end-to-end process for remote NMR is illustrated, covering all operational stages from handling (a: sample submission, shipping, and admission), to spectrometer setup (b-c), data acquisition (d), and post-acquisition operations (e: data transfer and sample storage or disposal). Specific provisions are made for the handling of air-sensitive or temperature-dependent materials, as well as for safety and reproducibility checks. Red-highlighted steps identify operations that can be fully controlled by remote users without local assistance. Numbered items (#1-#7) correspond to general implementation recommendations summarized in Table 1. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

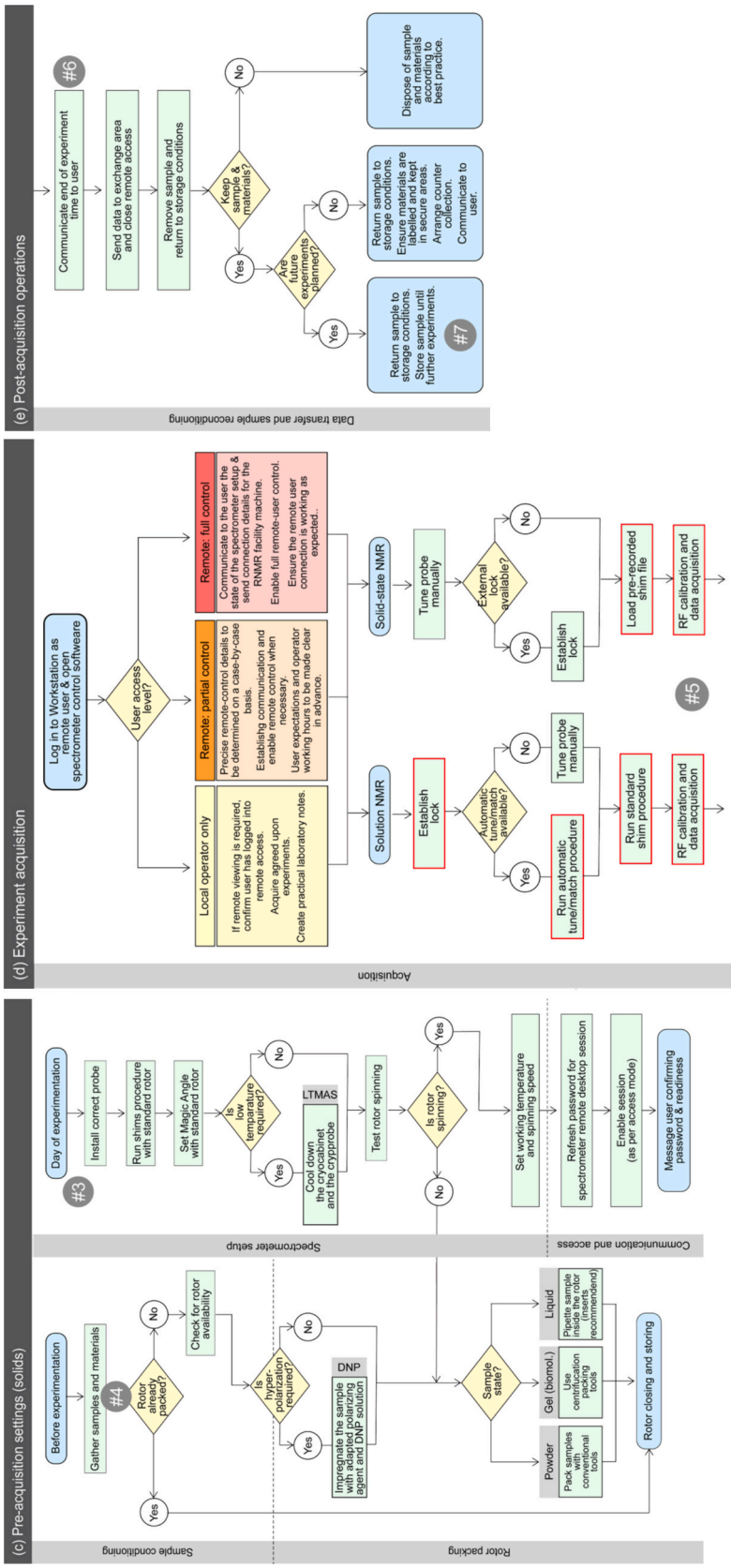

Fig. 2. (*continued*).

standardized documentation of all steps performed during the experiment.

2.3.2. *Workflow flowcharts for solution and solid-state NMR*

The workflows for remote solution NMR and solid-state NMR are presented in Figs. 2. These flowcharts provide a structured view of the experimental process, detailing each step from sample admission to data transfer and return shipment. They are designed to accommodate various access levels, from fully automated measurements to remote-controlled experiments with user intervention.

Key highlights of the flowcharts include:

(i) **Predefined secure storage areas** are identified for different sample types, ensuring proper handling conditions for sensitive materials.
(ii) **Standardized quality control procedures** are outlined for probe calibration, sample integrity checks, and instrument performance validation before running experiments.
(iii) **User interaction points** are explicitly marked, ensuring clear communication between the facility and remote users throughout the workflow.
(iv) **Red-highlighted steps** indicate the parts of the process where remote users can have **full control** without the need for local assistance.

These workflows are designed to streamline remote access, reduce operational variability between facilities, and improve overall efficiency in performing NMR experiments remotely.

By implementing and refining these workflows, NMR facilities can expand remote access capabilities while maintaining the precision and reliability required for high-quality research. The integration of user feedback and continuous adaptation of these procedures will further enhance the effectiveness and accessibility of remote NMR experimentation.

To provide a concise operational summary of the elements discussed in sections 2.1–2.3, Fig. 2 is accompanied by a harmonized checklist of key implementation points (#1-#7). These recommendations serve as a bridge between the textual procedures and the visual workflows, allowing users and facility managers to quickly identify critical steps and responsibilities common to both solution- and solid-state NMR remote-access operations. They are summarized below in Table 1.

Table 1
Cross-facility implementation checklist for remote-access NMR workflows. Numbered items correspond to the labels (#1-#7) in Fig. 2 and summarize operational best practices described in sections 2.1–2.3.

Item	Topic / title	Best-practice checklist
#1	Sample requirements and safety	Users provide full information on sample composition, preparation, and safety during project submission; any unusual requirements or hazards are discussed in advance (see §2.1, §2.2).
#2	Secure storage, labelling, handling	Facilities maintain clearly designated storage by temperature or atmosphere (−80 °C, −20 °C, 4 °C, room temperature, glovebox) with standardized labelling and traceable inventory (see §2.3.1 (i)). Facilities communicate the availability of specialized equipment (e.g., gloveboxes for air-sensitive samples) and request that users provide non-standard accessories where needed.
#3	Instrument verification and facility capabilities	Routine probe checks, calibrations, and performance tests are performed before user experiments (see §2.3.1 (ii)).
#4	Handling protocols and reagents	Users supply detailed manipulation and preparation protocols, shipping any required reagents or buffers. For solid-state NMR, this includes rotor-packing procedures and air-sensitive handling details (see §2.2.1–2.2.2).
#5	Metadata and experiment labelling	Consistent metadata documentation distinguishes standard, optimisation, and test measurements, recording sample identifiers, preparation stages, and instrumental parameters (see §2.3.1 post-acquisition operations).
#6	Data exchange and communication	The preferred secure data-transfer mechanism is agreed in advance. Continuous communication between users and facilities ensures efficient execution and data integrity (see §2.1 and §2.3.1 (iii)).
#7	Sample storage policy	Facilities avoid long-term storage of user samples; retention occurs only when follow-up experiments are planned, with clear timelines for return or disposal (see §2.3.1 post-acquisition operations).

3. User access levels and support strategies

A survey conducted among facility managers and users has highlighted a wide range of instrumentation, user expertise, and operational practices across different NMR infrastructures. Given this diversity, establishing a universal metric for assessing user competency and determining access levels proves to be challenging. Consequently, the decision regarding user access is entrusted to facility managers and local operators, who will make an informed assessment based on their prior exchanges with the users during the sample admission and pre-acquisition stages.

To ensure consistency and safety across facilities, users, facility managers and local operators should undergo standardized training in remote-access procedures and risk management. For users, this may take the form of on-line or in-person modules addressing spectrometer operation, data security, and remote-safety protocols. For facility managers and technical staff, periodic workshops and shared best-practice exchanges (organized at national or European levels) would help maintain up-to-date knowledge of evolving standards in cybersecurity, quality assurance, and user support. Such training not only harmonizes practice across infrastructures but also fosters mutual understanding between users and operators, improving communication and minimizing operational errors during remote sessions.

To provide a structured approach to user evaluation, a standardized questionnaire has been developed to guide facility managers in assessing a user's formal NMR training, familiarity with specific spectrometer brands, experience handling various sample types, expertise in pulse programming, and ability to perform calibration tasks. An example of this questionnaire is illustrated in Fig. 3 and may be adapted and integrated into local, national, or European NMR infrastructure submission portals.

Based on these assessments, three distinct remote access levels have been defined, ranging from full operator control to fully autonomous user operation (Fig. 4). These access levels ensure that users are provided with an appropriate degree of control and supervision based on their expertise, while also maintaining the security and integrity of the NMR facility operations.

3.1. *Level 1: Monitoring-only mode*

In Level 1 remote access, all aspects of the experimental workflow are performed by the local operators, with the user solely observing the process. This access level is intended for users with minimal NMR expertise. Users at this level may be granted the ability to remotely observe the spectrometer control screen, though without direct control capabilities. This observational mode can serve an educational purpose, allowing users to gain familiarity with instrument operation and experimental setup. Users may additionally opt to monitor ongoing experiments to provide real-time input in case of unexpected deviations from the expected results. For Level 1 access, clear communication between users and local operators is essential. Prior to data acquisition,

1. NMR User Level:

☐ Beginner/Basic ☐ Advanced ☐ Expert

2. Formal Training:

☐ Yes ☐ No If yes, specify (courses, workshops, etc.): _____

3. Spectrometer Experience (check all):

☐ Bruker ☐ Varian/Agilent ☐ JEOL ☐ Other: _____

4. Sample Experience:

Class: ☐ Liquids ☐ Solids ☐ Both

Type: ☐ Organic ☐ Inorganic ☐ Biomolecular

5. Relevant Experiment Experience:

☐ Yes ☐ No If yes, details: _____

6. Pulse Sequence Modification:

☐ Yes ☐ No If yes, brief description: _____

7. Independent Task Proficiency (✓ = Yes / ✗ = No)

Task	✓/✗
Manual sample insertion	
Auto sample insertion (e.g., SampleJet)	
Lock (auto/manual)	
Probe tuning (auto/manual)	
Magnet shimming (auto/manual)	
Calibrate ^{1}H pulses (auto/manual)	
Calibrate indirect pulses (^{13}C, ^{15}N, etc.)	
Set receiver gain (auto/manual)	
Choose method (e.g., couplings, relaxation)	
Select pulse sequence from standard library	
Optimize parameters (e.g., SW, power, acquisition time)	
Solvent suppression setup + optimization	

Fig. 3. Example of a standardized questionnaire designed to evaluate user expertise and training during the sample admission process.

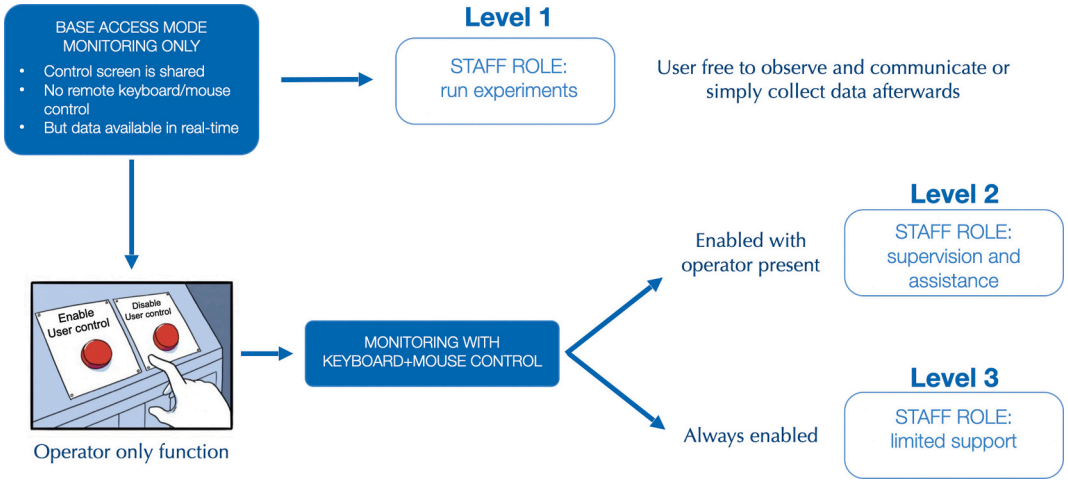

Fig. 4. Overview of the three remote access levels. This diagram illustrates the degree of user control, facility intervention, and required supervision across Levels 1, 2, and 3. By implementing a standardized framework for user access allocation, NMR facilities can ensure efficient resource utilization, maintain high data quality, and support a diverse community of researchers across varying levels of expertise.

users should define their experimental expectations and ensure that any critical adjustments are discussed in advance. In the absence of direct communication during the experiment, operators may make informed decisions (e.g., optimizing signal-to-noise ratios) without requiring additional user input.

3.2. *Level 2: Staff supervision mode*

At Level 2 access, users are granted limited remote-control capabilities, typically under the supervision of local facility staff. In practice, this means that users may connect to the spectrometer computer via remote desktop access, but direct control is only permitted when the local operator is present or aware of the session. In most cases, remote users at this level will be restricted to controlling specific experimental parameters, such as sample queuing or initiating predefined experiments. For example, with Bruker spectrometers, users may be limited to interacting with the IconNMR module while more advanced instrument settings remain restricted to local operators. Because Level 2 users have partial control over the experiment, it is critical that local staff remain available for assistance and troubleshooting when required. This mode is particularly beneficial for users with some prior NMR experience who require an intermediate level of support while refining their data collection process.

3.3. *Level 3: Limited-support mode*

Level 3 access is reserved for expert users who are trusted to operate the spectrometer independently. At this level, local operators intervene only for tasks requiring physical on-site execution, such as sample handling, probe exchange, or hardware adjustments. Users have full remote access, including full desktop control of the spectrometer, and may perform advanced operations such as modifying pulse sequences, adjusting RF parameters, and executing custom acquisition workflows. However, even at Level 3, certain critical hardware-related actions (such as rebooting the spectrometer or modifying hardware configurations) are subject to prior approval from the local operator. This ensures that any modifications do not compromise instrument stability or interfere with other scheduled experiments.

Because of the autonomy involved, Level 3 access is typically limited to users who are part of the host facility or have undergone formal qualification procedures. Clear communication with local operators is required prior to the experiment to define the division of responsibilities

and outline any expected on-site support (adjusting sample positioning, calibrating the magic angle in MAS NMR, or reconfiguring the instrument for specific nuclei). Facilities should also systematically communicate the relevant technical specifications of the probe(s) used (e.g., RF power limits, duty-cycle constraints, supported nuclei, temperature limits). As these parameters can vary between probe models and generations, their explicit transmission is essential for safe and responsible autonomous remote operation. To mitigate risk, especially in the case of high-value instrumentation (e.g., cryoprobes, MAS probes, amplifiers), users may be asked to formally acknowledge and accept liability for any damage resulting from operator error during remote use. This requirement is essential to ensure safe operation and protect facility resources, and may include the signing of a usage agreement or training certification.

In some infrastructures, liability management is complemented by dedicated insurance or service-contract clauses. Certain manufacturers or institutions include accidental-damage coverage within their maintenance contracts, although this practice is not yet widespread and terms vary considerably between countries and suppliers. Where no such coverage exists, facilities may consider introducing a nominal insurance fee or requiring that external users provide proof of institutional coverage as part of their access agreement. Importantly, these measures are not unique to remote operation but extend existing in-person risk-management practices to digital contexts. For facilities where insurance coverage cannot be implemented, Level 3 access should be restricted to users who are institutionally affiliated or otherwise covered by the host organization's internal policies.

4. Technical requirements for remote access

The implementation of standardized remote access to NMR facilities requires a clear understanding of the technical requirements necessary to support remote spectrometer control, data retrieval, and communication. Based on the findings from facility manager and user surveys, it is evident that there is no universal "one-size-fits-all" solution due to the technical, financial, and administrative heterogeneity of the institutions involved. While in some cases, remote access may not be feasible due to infrastructure limitations, for most facilities, a viable solution can be achieved by using available software and hardware configurations. A key challenge in this respect is that NMR spectrometers are often operated by computers with operating systems that are not up to date. While this did not pose significant problems in the past, today's massive need for IT safety and security conflicts with such operation. Here, *safety* refers to the reliable and controlled operation of the spectrometer hardware, while *security* relates to the protection of networked systems and user data from unauthorized access or cyber threats. Both aspects are increasingly interdependent, as secure IT infrastructures are essential to ensure safe instrument operation and prevent system disruptions. We foresee that future versions of the spectrometer software must be compatible with state-of-the-art computer hardware that fulfils all security requirements of the hosting institution.

The following sections outline the essential technical requirements for remote NMR access, covering aspects such as user workspace management, data storage, persistent access, and communication tools. By identifying key needs and potential implementation strategies, we aim to provide facility managers with the necessary framework to develop practical remote access solutions that align with both institutional policies and user expectations.

4.1. Core technical requirements

A fully functional remote NMR access system should fulfill several key criteria, including:

- **Dedicated storage and user workspaces** for experiment control and data retrieval.
- **Cross-platform connectivity**, ensuring compatibility across different operating systems and devices.
- **Remote desktop capabilities** to allow users to interact with the spectrometer in real-time.
- **Screen sharing**, enabling facility staff to assist users during experiments.
- **Direct messaging tools** for real-time communication between users and facility operators.
- **Video conferencing support** for troubleshooting, discussions, and collaborative decision-making.
- **A fast and reliable user experience**, ensuring smooth data processing and remote interaction.
- **Secure connections** with end-to-end encryption to protect user data and privacy, with continuous monitoring and updates to maintain state-of-the-art cybersecurity.
- **Compliance with institutional and regulatory policies**, including General Data Protection Regulations (GDPR) and local data security requirements.

These requirements aim to balance operational flexibility with security and data integrity, ensuring that both users and facility managers can efficiently conduct and oversee remote NMR experiments.

4.2. User workspaces and access management

The implementation of dedicated user workspaces is a fundamental requirement for remote spectrometer access. Ideally, each remote user should have a personalized digital workspace, allowing them to securely access the spectrometer control interface and manage their experimental data. In most cases, this involves remote access to a user account on the spectrometer workstation. The creation of such accounts may be handled by local NMR operators or may require administrator privileges at the institutional level. Regardless of the method, accounts must be created individually for each remote user, with well-defined permissions and access rights to ensure compliance with data protection regulations. To meet GDPR and institutional security requirements, no element of remote-user data (including user credentials, project descriptions, or experimental data) should be accessible to non-authorized local users (i.e., members of the host institution who are not part of the facility's operational or technical staff). Authorized facility staff, who are responsible for instrument setup, maintenance, and supervision, may retain limited access as required for safety and operational oversight.

Similarly, remote users should not have access to data outside their personal home directory. They may, however, modify or create new pulse programs or parameter sets within this private workspace. These files remain confidential to the user unless explicitly shared, although facility staff must retain the technical ability to review them when necessary to ensure safe spectrometer operation (for instance, to verify RF power limits or pulse-sequence safety). This controlled oversight may appear in tension with GDPR data protection; however, it falls within the scope of legitimate operational interest, as it ensures compliance with institutional safety policies and prevents hardware damage.

One challenge that arises from this strict data compartmentalization is how facility staff can access standard reference data (e.g., pulse programs, parameter sets) on behalf of remote users. Potential solutions include creating user accounts based on a default template, preloaded with necessary reference files, or setting up a read-only shared directory containing essential experimental parameters. Maintaining and updating these shared reference datasets (along with software and methodological standards) should be a core responsibility of the local facility staff, ensuring that instruments and workflows remain aligned with the state of the art. Facilities that typically operate with shared workstation accounts may need to modify their standard operating procedures to accommodate these security constraints.

Additionally, it emerged that the automatic metadata collection in the Bruker TopSpin™ software could lead to unauthorized access to

experimental data. This highlights the importance of using individual workstation accounts as a safeguard to prevent violation of the GDPR regulations.

4.3. Data storage and retrieval

The storage and management of experimental data must be clearly defined at the time of project submission. Facilities and users should agree on key aspects such as:

- **Storage location** (local workstations vs. institutional servers).
- **Data retention policies**, including the duration for which the facility will retain data.
- **Volume limitations**, ensuring that large datasets do not exceed facility storage capacities.
- **User access rights**, specifying whether remote users can retrieve data independently.

Data management and protection policies must also comply with regional and international regulations. In cross-border collaborations, facilities may need to navigate overlapping or conflicting governmental frameworks (e.g., GDPR in Europe versus differing standards in North America or Asia). While such issues can be complex at the global scale, they are generally more manageable within regions sharing comparable legal and policy environments.

NMR facilities may implement institution-specific data retention policies, but users should be encouraged to retrieve their experimental data promptly and take responsibility for long-term storage. While it may be useful to keep user data temporarily on the spectrometer workstation, facilities should be cautious about offering long-term storage guarantees, as this could lead to excessive accumulation of unclaimed data.

In addition, data retention policies should explicitly address the long-term reliability of storage infrastructures. Reliance on a single storage medium (e.g., a dedicated workstation or local server) carries an inherent risk of irreversible data loss in the event of hardware failure or unforeseen incidents occurring years after data acquisition. To mitigate this risk, we recommend implementing redundant data-storage strategies, ideally involving duplication of datasets across at least two physically distinct locations. Such measures, which are already standard practice in many institutional IT environments, significantly enhance data resilience against catastrophic events (e.g., hardware failure, fire, flooding, and ransomware attacks) and should be considered an integral component of sustainable remote-access NMR infrastructures.

Given that NMR datasets can be too large for email transfer (often exceeding 20 MB per dataset), each facility should predefine its preferred data transfer method. Data security and encryption should be of paramount concern, with regular system updates to guard against hacking, ransomware, and other cyber threats. Several viable options exist:

- **Command-line interface (CLI) tools** such as scp or rsync for experienced users.
- **Graphical user interface (GUI) tools** such as TeamViewer™, AnyDesk™, or a VNC-based connection, which allow users to download data through the remote desktop session.
- **Institutional file transfer services**, such as *filesender.renater.fr* (France) or university-managed cloud solutions.
- **Commercial cloud services**, including Google Drive™, OneDrive™, or WeTransfer™, though data privacy and intellectual-property protection concerns should be carefully considered when using third-party providers.
- **Non-commercial cloud services**, including institutionally managed NextCloud™ installations, i.e., open-source software typically deployed on local servers and maintained by institutional IT teams, though different hosting configurations may exist.

Facilities should focus on implementing existing, secure, and scalable solutions that meet institutional compliance requirements.

4.4. Persistent user access for data processing

A key limitation of many remote desktop software solutions is that they do not create separate graphical user sessions for each remote login. To provide computational access for data processing *after* a user's allocated experiment time, facilities may therefore wish to explore external solutions for persistent user workspaces. One widely-used approach is NMRBox, a web-based service developed at the University of Connecticut and the University of Wisconsin (https://nmrbox.nmrhub.org/) [1]. NMRBox provides:

- **Secure virtual Linux machines**, preloaded with over 260 supported NMR software tools for data analysis.
- **Persistent user accounts**, allowing remote users to access and process data even after their experimental session has ended.
- **Easy integration with standard NMR data formats**, supporting TopSpin and other common software tools.

For remote users (especially those from institutions with limited IT resources) NMRBox offers a practical and accessible solution to continue data analysis after their experimental session.

4.5. Communication tools for remote access

Effective communication between remote users and facility operators is critical for smooth remote NMR operation. While email remains an option for non-urgent inquiries, facilities should adopt real-time communication tools for time-sensitive interactions. However, the availability of support outside standard working hours (e.g., evenings, weekends, or holidays) depends on local facility policies and staff resources. Most facilities do not provide continuous technical coverage, and remote assistance during off-hours can only occur on a voluntary basis. Users should therefore clarify expected support hours in advance and plan experiments accordingly to avoid interruptions requiring out-of-hours intervention.

These may include:

- **Video conferencing platforms** such as Zoom™, Microsoft Teams™, or Webex™, allowing users to discuss experimental settings and troubleshooting in real-time.
- **Direct messaging applications** like Slack™, Microsoft Teams™, or integrated chat functions in remote desktop software, enabling quick exchanges.
- **Secure document-sharing platforms** for transmitting sensitive information such as sample formulations, access credentials, or experiment metadata.

At the start of the remote access process, users and facility staff should agree on which platforms will be used for communication and ensure that all parties have access to the necessary tools. Since communication may involve confidential data, best practices for secure information exchange should be followed to prevent unauthorized access.

4.6. Practical examples of remote access implementation

There are two primary approaches for implementing remote NMR access while preserving security, usability, and functionality within modern institutional networks. The first relies on commercial software solutions that utilize third-party servers to establish web-based connections, effectively bypassing institutional firewalls. This approach, while convenient, introduces additional security concerns, as external data routing increases exposure to potential breaches. The trade-off

Table 2
Summary of Remote Access Methods. Each approach offers a different balance of security, ease of use, and institutional compliance. Facilities must assess their internal IT policies and available resources to determine the most suitable remote access solution for their needs.

Method	Technical expertise required	Cost	Security	Flexibility	IT policy risks
Commercial remote desktop (TeamViewer™, AnyDesk™)	Low	Medium	Moderate	High	High (can be blocked by institutional policies)
VPN-based remote desktop (RealVNC™, apache guacamole)	Medium	Low	High	Moderate	Low (requires institutional IT support)
Custom network bridge (bastion machine)	High	Low	Very high	Moderate	Low (managed entirely by facility staff)

between convenience and security must therefore be carefully evaluated at each facility. Developing standardized protocols, as proposed in this framework, can help define best practices for achieving a balanced compromise between operational flexibility, interconnectivity, and data protection. The second approach involves direct integration into institutional networks via VPN credentials or custom network bridges, allowing users to securely access spectrometer-controlling machines through a local-area network (LAN). The feasibility of each approach depends on the network policies of the hosting institution, the available IT infrastructure, financial constraints, and security requirements. While some facilities may opt for commercial software due to its ease of deployment, others may prefer institutional VPN or custom network solutions to maintain direct control over data security and user access. The advantages and limitations of each method are outlined below (Table 2).

4.6.1. Commercial remote desktop software (minimal technical resources, medium cost, moderate security risks)

Commercial remote desktop software offers a simple and widely adopted solution for remote spectrometer access. Among the available options, TeamViewer™ and AnyDesk™ are the most commonly used tools, as identified in the R-NMR user and facility manager surveys. These platforms enable secure, cross-platform remote access, requiring only an ID code and password provided by the software for users to establish a connection. A key advantage of TeamViewer™ is its preinstallation on Bruker-provided workstations, simplifying deployment in NMR facilities already using Bruker instruments. Additionally, both TeamViewer™ and AnyDesk™ provide free versions for personal and student use, although academic institutions with high traffic and multiple users may require a professional license. Industrial users must obtain commercial licenses, and in some cases, TeamViewer™'s licensing may be version-bound, requiring attention when managing software updates.

For remote access control, both TeamViewer™ and AnyDesk™ allow facility managers to restrict user permissions, ensuring that monitoring-only and staff-supervised modes can be enforced when necessary. This flexibility makes them viable for institutions needing to support different levels of remote access. However, commercial remote desktop solutions introduce potential security concerns. Since these services route connections through third-party servers, all transmitted data may be accessible to the service provider, necessitating robust encryption measures to protect sensitive information. Additionally, these platforms rely on centralized authentication mechanisms, meaning that weak access credential management (e.g., failure to update passwords regularly) could expose institutions to unauthorized access risks. Similarly, while both TeamViewer™ and AnyDesk™ offer security features such as allowlists to restrict access to authorized accounts or devices, these measures are only effective if properly configured and maintained. Occasionally, these commercial tools may experience temporary service interruptions due to provider-side maintenance or upgrades, though such downtime is rare and typically announced in advance. Nevertheless, facilities relying on these services should plan for possible short connection outages and have fallback access options available.

4.6.2. Remote desktop via institutional VPN (medium technical resources, low cost, high security)

For institutions that do not permit commercial third-party remote desktop solutions, a more secure approach is to enable remote access via an institutional Virtual Private Network (VPN). In this setup, remote users first authenticate with the host institute's VPN, granting them temporary access to the local-area network (LAN), where the spectrometer-controlling workstation is located. Many institutions already have VPN infrastructure in place, making this a low-cost and administratively manageable option. Common VPN solutions include: Cisco AnyConnect™, F5 Access™, Tunnelblick™ (for macOS).

Once a VPN connection is established, the remote user can directly connect to the spectrometer workstation using remote desktop software such as RealVNC™ or Apache Guacamole. A key benefit of Apache Guacamole is that it enables web browser-based remote access, eliminating the need for additional software installation on the user's machine. This client-less approach simplifies access while maintaining institutional security policies. While this method minimizes security risks and avoids reliance on third-party services, one limitation is that open-source remote desktop tools lack built-in access control mechanisms. As a result, facility staff may need to implement separate security measures to enforce monitoring-only or staff-supervised access levels, depending on the expertise of the remote user.

Despite this minor limitation, VPN-based remote access is considered one of the most robust solutions for institutions that prioritize data security and compliance with IT policies while providing remote users with direct control over NMR experiments.

4.6.3. Custom network bridge (high technical resources, low cost, high security)

In cases where commercial solutions are blocked by institutional firewalls and temporary VPN credentials cannot be issued, facilities may create a custom network bridge using a dedicated "bastion machine" (Fig. 5). This approach involves setting up a Linux server with dual network interfaces, one facing the external internet and the other connected to the internal NMR facility network. When properly configured, a bastion machine would function as a secure gateway, enabling remote users to access internal resources without exposing spectrometer workstations directly to the internet. Because this setup offers complete local control over authentication and security policies, it represents the most desirable and sustainable solution where institutional IT resources permit its deployment. It can be envisaged that this type of solution would be fully managed by the local facility staff or IT team, allowing

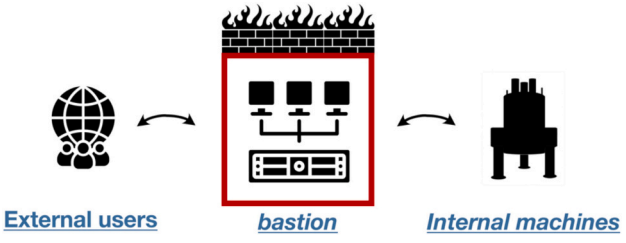

Fig. 5. The concept of bastion machines provides a network bridge, from the outside world, to internal LAN, over institutional firewalls.

complete control over security policies, authentication mechanisms, and access permissions. In some cases, institutions may already operate a central bastion server for all staff (not limited to NMR), and NMR facilities may integrate into this wider system if compatible with the required access and security constraints. Both facility-specific and institute-wide configurations are possible, though institutional systems typically impose stricter access conditions.

After a remote user connects to the bastion machine, they can establish a remote session using standard desktop-sharing tools such as RealVNC™ or Apache Guacamole, as described in the VPN approach. User authentication and IP whitelisting can further enhance security, ensuring that only approved users from pre-registered locations can establish connections. Although this method requires significant IT expertise for initial setup and ongoing maintenance, it offers the highest level of security and complete control over institutional policies. Regular system administration, including software updates, firewall configuration, and intrusion monitoring, should be considered an essential and recurring operational expense, no less critical than cryogen, maintenance, or power costs. Despite this, for institutions that can support it, custom network bridges provide a sustainable, high-security remote access solution for long-term use.

5. Quality assessment of the instrumentation

Ensuring the optimal performance and reliability of NMR spectrometers is essential for both on-site and remote access. The quality of instrumentation is assessed through standardized experiments, focusing on three key parameters:

(i) **Experimental Sensitivity** – Measuring the signal-to-noise ratio (SNR) to ensure that spectrometers are operating at their expected performance levels.
(ii) **Spectral Resolution** – Evaluating line shape and peak broadening to verify that sample and hardware conditions do not compromise spectral quality.
(iii) **Radiofrequency (RF) Pulse Efficiency** – Determining the accuracy and effectiveness of pulse calibrations across different NMR channels.

To achieve consistent and comparable results, we have defined a set of standard reference samples used for hardware validation and experimental quality control. These reference samples are largely based on existing standards provided by manufacturers, ensuring broad compatibility across different facilities. While a comprehensive, universally maintained list of standard reference samples lies beyond the scope of this review, the development of such a shared resource would be highly valuable to the community. Establishing a "living" online repository (regularly updated with validated reference materials and calibration protocols) could greatly promote harmonization and transparency across NMR infrastructures. Such an initiative could, in the future, be coordinated under the auspices of international organizations such as Ampere or ISMAR, or through collaborations among national NMR networks. The reference samples and experiments described in the following sections have been selected to assess solution and solid-state NMR instrumentation, serving as representative examples rather than a comprehensive catalogue.

Table 3
Standard reference samples and experiments for routine calibration and quality control in solution NMR.

Test	Sample	Experiment
Shimming	0.3% chloroform ($CHCl_3$) in acetone-d_6	^{1}H single pulse
^{1}H sensitivity	0.1% ethylbenzene (EB) in chloroform-d	^{1}H single pulse
Water suppression	2 mM sucrose 0.5 mM DSS 2 mM NaN_3 in H_2O/D_2O 90/10	^{1}H single pulse
^{15}N & ^{13}C pulse calibration	100 mM ^{15}N-enriched urea 100 mM ^{13}C-enriched methanol in DMSO-d_6	^{15}N & ^{13}C single pulse or detection via inverse ^{1}H excitation
^{13}C sensitivity & resolution	40% dioxane in benzene-d_6 (ASTM)	^{13}C single pulse
^{15}N sensitivity & resolution	90% formamide in DMSO-d_6	^{15}N single pulse
Gradient recovery	0.1 mg $GdCl_3$/ml D_2O with 1% H_2O + 0.1% CH_3OH ^{13}C	^{1}H gradient echo
Temperature	Neat ethylene glycol (for range 300-380 K) or methanol-d_4 (for range 180-300 K)	^{1}H shift
Spectrometer stability over time	Quinine in DMSO-d_6 ^{13}C–^{15}N-labeled ubiquitin pH 6.0 99.8% ^{2}H-methanol / 2 mM sucrose in 90:10 H_2O/D_2O	^{1}H single pulse 2D ^{1}H,^{15}N-HSQC ^{1}H single pulse

5.1. Standardized tests for solution NMR

For solution NMR, routine performance tests are used to verify the proper functioning of spectrometer components, including probe tuning and matching, shimming, sensitivity and resolution tests, gradient performance, and temperature calibration (Table 3). The standard evaluation focuses on the ^{1}H, ^{13}C, and ^{15}N channels, as these represent the most commonly studied nuclei. For less common nuclei, dedicated reference materials and experiment setups should be defined on a case-by-case basis (once defined, such reference protocols should ideally be shared through coordinated infrastructure networks or international working groups, ensuring that new standards are easily accessible and periodically reviewed as instrumentation evolves). Temperature calibration should be performed using standard samples, such as ethylene glycol or methanol-d_4, to ensure reliable thermal regulation. Additionally, spectrometer stability and performance should be periodically validated using representative samples from major application domains, covering a range of spectral complexity. For each domain, a community-approved reference sample has been selected to enable reproducible preparation and direct comparability across facilities. These standards allow both on-site and remote users to assess the quality of their experiments against a known benchmark. The following reference samples and conditions are currently recommended:

- **Small organic molecules (structure determination and characterization):** *Sample:* 0.6 mg quinine in 600 µL DMSO-d_6 (99.9% D), containing 0.03% (*v*/v) tetramethylsilane (TMS), recommended for instruments equipped with cryoprobes. For measurements with a room-temperature probe, the quinine concentration should be increased tenfold (i.e., 6 mg in 600 µL). *Tube:* 7-in. Bruker NMR sealed glass tube, 5 mm outer diameter.
- **Biopolymers and oligomers (proteins, DNA, RNA, peptides, oligosaccharides):** *Sample:* ~250 µM uniformly ^{13}C,^{15}N-labeled ubiquitin in 180 µL of 15 mM potassium phosphate buffer, 50 mM NaCl, pH 6.0, supplemented with 10 µM DSS (sodium trimethylsilylpropane-sulfonate, more precisely sodium 2,2-dimethyl-2-silapentane-5-sulfonate, historically abbreviated DSS to distinguish it from TSP, trimethylsilylpropionic acid) and protease inhibitors. *Tube:* 7-in. Bruker NMR sealed glass tube, 3 mm outer diameter.
- **Special applications (metabolomics, food science, quantitative NMR):** *Sample:* 99.8% ^{2}H-methanol and 2 mM sucrose in 90:10 H_2O/D_2O containing either TSP-d_4 or DSS-d_6 as internal standards.

5.2. Standardized tests for solid-state NMR

For solid-state NMR, calibration protocols differ depending on the nature of the sample (organic or inorganic) and on the spinning regime used, with additional distinctions between slow MAS, employing rotors in the 7 mm to 2.5 mm range, and fast MAS using 1.9 mm to 0.4 mm

Table 4
Standard reference samples and experiments for routine calibration and quality control in organic/biomolecular solid-state NMR, both in the slow and fast spinning regimes.

MAS rates	Test	Sample	Experiment
Slow-intermediate (<60 kHz)	Shimming	Adamantane	^{13}C single pulse with decoupling
	^{1}H pulse calibration	Adamantane L-alanine	^{1}H single pulse
	^{15}N & ^{13}C pulse calibration	^{15}N, ^{13}C-labeled L-alanine	Direct: ^{15}N & ^{13}C single pulse with decoupling Indirect: ^{15}N & ^{13}C cross polarisation with decoupling
	^{13}C sensitivity	^{13}Cα-labeled L-alanine	Direct: ^{13}C single pulse with decoupling Indirect: ^{13}C cross polarisation with decoupling
	Magic angle	KBr	^{79}Br single pulse
	Temperature	Water (protein samples; 250–320 K) / $Sm_2Sn_2O_7$ (>85 K) / $PbNO_3$ (100–423 K) / KBr (20−300 *K*) / CsI (<10*K*)	Single pulse (^{1}H/ ^{119}Sn/ ^{207}Pb), R_1 (^{79}Br/ ^{127}I)
Fast (>60 kHz)	Shimming	Adamantane Tetrakis(trimethylsilyl) silane	^{13}C single pulse with decoupling ^{1}H single pulse
	^{1}H pulse calibration	Adamantane L-alanine	^{1}H single pulse
	^{15}N & ^{13}C pulse calibration	^{15}N, ^{13}C-labeled L-alanine	^{1}H,^{15}N & ^{1}H,^{13}C cross polarisation experiments with ^{1}H decoupling
	^{13}C sensitivity	^{13}Cα-labeled L-alanine	^{1}H,^{13}C cross polarisation experiments with ^{1}H decoupling
	Magic angle	L-alanine Tetrakis(trimethylsilyl) silane	^{1}H spin echo
	Temperature	Water (protein samples; 250–320 K) / $Sm_2Sn_2O_7$ (>85 K) / $PbNO_3$ (100–423 K) / KBr (20–300 K) / CsI (<10 K)	Single pulse (^{1}H/ ^{119}Sn/ ^{207}Pb), R_1 (^{79}Br/ ^{127}I)

rotors (Tables 4 and 5). The following samples and conditions are currently recommended:

- **Organic and biomolecular samples at slow spinning**: Shimming is typically performed using crystalline adamantane to optimize magnetic field homogeneity. MAS calibration is verified using potassium bromide (KBr) [2], which serves to assess rotor alignment and minimize spinning sidebands. To streamline the procedure, a single reference sample combining adamantane and KBr can be used, allowing both shimming and MAS calibration to be performed in the same measurement without compromising accuracy. RF pulse calibrations and sensitivity benchmarks are obtained by using adamantane and ^{13}C- or ^{15}N-enriched L-alanine, either in direct excitation or cross-polarisation (CPMAS) experiments. These tests offer reliable indicators of probe performance, RF efficiency, and sensitivity on ^{13}C/^{15}N channels. Alternatively, ^{15}N- and ^{13}C-enriched N-formyl-L-methionyl-L-leucyl-*L*-phenylalanine-OMe (MLF) tripeptide can be used for ^{15}N /^{13}C/^{1}H pulse calibration [3]. Glycine should be avoided due to occurence of a polymorphic transition over time. Temperature calibration is typically performed using a range of compounds suitable for different regimes, from aqueous protein samples (to verify accurate temperature control under physiological conditions) to inorganic materials such as $Pb(NO_3)_2$, KBr, or CsI, which are stable over broader thermal ranges [4].
- **Organic and biomolecular samples at fast spinning**: Under fast MAS conditions, shimming is performed either on the ^{13}C signals of adamantane or on the ^{1}H signals of tetrakis(trimethylsilyl)silane (TTMSS), also called tetrakis-silane (TKS) [5], which offer higher sensitivity in smaller rotors. MAS calibration is also performed on KBr, although the setting is usually repeated directly on the sample of interest based on the observation of ^{1}H T_2' via (H)NH or (H)CH sequences [6] or by optimizing the H–N (or H–C) *J* coupling full spin echo [7]. These same (H)NH or (H)CH sequences are also used for pulse calibration of ^{15}N and ^{13}C, as well as for qualitative assessments of heteronuclear sensitivity under fast MAS.

- **Materials science:** Solid-state NMR spectroscopy applied to materials science typically involves a wide range of nuclei. These include spin-½ nuclei such as ^{1}H, ^{13}C, and ^{29}Si, as well as quadrupolar nuclei with spin greater than ½, such as ^{23}Na ($I = 3/2$), ^{27}Al ($I = 5/2$), and ^{14}N ($I = 1$). Because of this diversity and the varying physical properties of the nuclei involved, a range of different types of probes, calibration strategies, and standard reference compounds are required. The optimal standard sample depends on the nucleus of interest, the magnetic field strength, and the probe configuration (notably low-γ versus high-γ design). Although IUPAC-recommended chemical-shift standards are available for most NMR-active nuclei [8] it is often practical on solid-state instruments to rely on secondary solid standards that are stable, inexpensive, and easy to pack reproducibly. For exemple, for spin-½ nuclei, adamantane and L-alanine are typically used for ^{13}C and ^{1}H calibration, while tetramethylsilane (TMS) or kaolinite may be used for ^{29}Si. For quadrupolar nuclei, typical reference materials include NaCl for ^{23}Na calibration, aluminum nitrate or aluminum oxide solutions for ^{27}Al, water (10% enrichment) or $SrTiO_3$ for ^{17}O, and ammonium nitrate (NH_4NO_3) or glycine for ^{14}N. These standards also provide a means to assess line shapes, radiofrequency field strengths, and B_1 field homogeneity, which is particularly important when dealing with broad quadrupolar patterns. While the examples above cover the most commonly studied nuclei, solid-state NMR in materials and geosciences routinely involves many additional isotopes across the periodic table (e.g., ^{43}Ca, ^{89}Y, ^{95}Mo, ^{99}Ru, ^{183}W, among others). Comprehensive compilations of recommended reference materials and chemical-shift conventions for these nuclei can be found in the IUPAC guidelines [8] and in the extensive review by Smith [9].
Finally, we note that for experiments involving quadrupolar nuclei, accurate setting of the magic-angle is crucial. While KBr is commonly used for this purpose, a more precise adjustment, especially for wide, anisotropic patterns, can be achieved using ^{23}Na single-pulse spectra of $NaNO_3$, significantly improving the fidelity of quadrupolar lineshapes and the reproducibility of derived parameters.

Together, these standardized procedures provide a consistent and reproducible framework to assess the performance of solid-state NMR

Table 5
Standard reference samples and experiments for routine calibration and quality control in inorganic solid-state NMR.

Test	Probe specs	Sample	Experiment
Shimming	Standard probes	Adamantane	^{13}C single pulse with ^{1}H decoupling
		Silicon rubber	^{1}H single pulse
		Teflon (polytetrafluoroethylene, PTFE)	^{19}F single pulse
	Low-γ probes	^{15}N-labeled glycine	^{15}N single pulse with ^{1}H decoupling
		KBr or KCl solution	^{39}K single pulse
		LiCl solution	^{6}Li single pulse
		NaCl solution	^{37}Cl single pulse
Magic angle	Standard probes	KBr	^{79}Br single pulse
		KI	^{127}I single pulse
		$NaNO_3$	^{23}Na single pulse
		Sapphire rotor [7]	^{27}Al single pulse
	Low-γ probes	Poly(methylmethacrylate)-d_8 (dPMMA)	^{17}O single pulse
		3-(Trimethylsilyl)propionic-2,2,3,3-d_4 acid sodium salt (TSP-d_4)/oxalic acid-d_6 /L-alanine-2-d_1	^{2}H single pulse
		KNO_3	^{14}N single pulse
RF pulse calibration	Direct calibration	**Spin $I = 1/2$**	
		Adamantane	^{1}H and ^{13}C single pulse
		Teflon (PTFE)/CaF_2	^{19}F single pulse
		^{15}N-labeled glycine	^{15}N single pulse with decoupling
		Zeolite A / Octakis(trimethylsiloxy) silsesquioxane (Q8M8)	^{29}Si CPMAS
		Spin $I > 1/2$ | sample with a $C_Q = 0$	
		$AlCl_3$ / $AlNO_3$ solution	^{27}Al single pulse
		H_2O	^{17}O single pulse
		NH_4Cl	^{14}N single pulse
		NaCl	^{23}Na single pulse
		Spin $I > 1/2$ | sample with a $C_Q > 0$ (large)	
		Effective nutation frequency $(I + 1/2)\ \omega_1$	
	Indirect calibration	Silicon rubber	^{1}H Bloch-Siegert [15]
		U–^{15}N, ^{13}C-labeled L-alanine	
		Glycine	

instrumentation across different laboratories and application domains.

5.3. Chemical shift calibration

Standards for chemical shift calibration in biomolecular NMR are well-established and summarized by Wishart et al. [10] and Harris et al. [11], while additional practical guidance for the solid state is provided by Morcombe and Zilm [12]. For ^{1}H NMR, the primary reference compound is DSS (set at 0 ppm), which can either be added directly to the sample or used indirectly by referencing the water resonance via the temperature-dependent relation: $\delta(^{1}H) = 7.83 - K:\ T(K)\ /\ 96.9$ ppm [13]. ^{13}C and ^{15}N chemical shifts are then usually referenced indirectly from the ^{1}H scale by using the IUPAC-recommended gyromagnetic-ratio (γ) conversion, which requires γ values known to at least nine significant figures to ensure consistency across laboratories. IUPAC recommends ^{13}C shifts to be reported relative to TMS rather than DSS. When ^{13}C shifts are indirectly referenced via ^{1}H signals calibrated on DSS, this leads to an apparent offset of approximately +2.72 ppm relative to the IUPAC (TMS-based) scale.

In solid-state NMR, particularly at low MAS rates, adamantane is widely used as an external ^{13}C reference. The low-field (higher ppm) adamantane signal is set at 37.77 ppm relative to TMS (or 40.49 ppm on a DSS-consistent scale). With adamantane as a reference, ^{1}H and ^{15}N chemical shifts are again obtained indirectly through gyromagnetic ratios.

Direct, nucleus-specific standards may also be used when appropriate. Examples include ^{15}N-glycine at 33.4 ppm for ^{15}N [14], and for ^{29}Si, TMS (set at 0 ppm), Zeolite A (set at −89.7 ppm with respect to TMS), or octakis(trimethylsiloxy)silsesquioxane (Q8M8) (set at 11.5 ppm with respect to TMS). Additional recommended reference compounds for less common nuclei, including quadrupolar isotopes, are described extensively in the IUPAC guidelines [8] and in dedicated reviews on referencing conventions in solid-state NMR (see for example reference [9]).

5.4. Implementation of quality control measures

NMR facilities can ensure reliable experimental conditions for both local and remote users, improving data consistency, reproducibility, and inter-laboratory benchmarking by implementing the following measures:

1. **Routine Performance Testing**: Facilities should conduct these standardized tests regularly (e.g., weekly or monthly) to ensure consistent spectrometer performance.
2. **Automated Logging & Trend Analysis**: Instrument performance data should be logged and analyzed over time to detect long-term drifts or inconsistencies.
3. **Benchmarking Across Facilities**: Results from standard reference samples should be shared among remote-access partners to enable comparisons and identify potential sources of variation.
4. **Remote Quality Monitoring**: Remote users should be provided with access to performance logs to verify instrument calibration before initiating their experiments.

6. Conclusions and future perspectives

The outcomes of this analysis establish the foundation for more integrated and resilient NMR infrastructures, ensuring their long-term sustainability and continued advancements in methodology. The implementation of remote access to NMR facilities through standardized protocols and methodologies will significantly enhance the accessibility and impact of NMR spectroscopy across multiple scientific fields. Of course, some advantages of in-house facilities, for instance the ability to schedule spectrometer access flexibly to accommodate unstable or short-lived samples, cannot easily be replicated by external facilities, whether accessed remotely or in person. Nonetheless, by enabling researchers to perform remote measurements, data analysis, and processing, this access modality removes most barriers for scientists who lack direct access to high-end instrumentation, allowing them to more fully exploit the capabilities of advanced NMR techniques.

Looking ahead, continuous refinement of remote access models will integrate new hardware, software improvements, and automation strategies, further optimizing usability and efficiency. Advances in robotic hardware, such as automated sample changers, probe exchangers, and future self-tuning systems leveraging artificial intelligence, promise to increase throughput and reproducibility, while reducing the need for manual intervention. In parallel, stronger inter-facility collaboration will foster the exchange of resources, expertise, and best practices, reinforcing global scientific cooperation and further establishing NMR as a cornerstone technology in analytical research.

Sustainable operation will also depend on well-defined funding and cost-sharing mechanisms. Remote access inherently involves additional personnel time, data management resources, and instrument wear, as well as ongoing costs for cryogens and maintenance. While government support remains essential for maintaining baseline infrastructure, clear user-fee models (potentially differentiated for academic and industrial clients) could help ensure equitable and financially viable access. Transparent accounting of such operational costs will be critical to sustaining long-term remote access services.

Beyond academic settings, standardized methodologies will also expand industrial engagement, making NMR a more attractive and accessible tool for commercial applications. This will promote closer collaboration between academia and industry, driving innovations in biomedicine, materials science, and pharmaceutical development. Ultimately, the broad adoption of remote NMR workflows and standardized experimental protocols will not only enhance scientific productivity and infrastructure efficiency, but will also position NMR as a key analytical tool for addressing global challenges in health, energy, and materials research. By reducing barriers to access and fostering a more interconnected research landscape, this initiative will contribute to the continued evolution of NMR spectroscopy as a powerful and universally accessible scientific method. Importantly, the overall procedures and standardized protocols described in this review could be readily transposed to other analytical techniques, such as EPR spectroscopy or mass spectrometry, broadening their reach and impact across the analytical sciences.

CRediT authorship contribution statement

James Tolchard: Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Tanguy Le Marchand:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Ruud L.E.G. Aspers:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Gyula Batta:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Burkhard Bechinger:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Ulrika Brath:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Styliani A. Chasapi:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Ana Čikoš:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Kornél Ecsedi:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Adrien Favier:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Ana Sofia D. Ferreira:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Radovan Fiala:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Panagiota D. Georgiopoulou:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Jennifer S. Gómez:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Kristaps Jaudzems:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Göran Karlsson:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Arno P.M. Kentgens:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Sander F.H. Lambregts:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Francesca Morelli:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Frans A.A. Mulder:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Sivanandam V. Natarajan:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Cecilia Persson:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Roberta Pierattelli:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Miquel Pons:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Jesus Raya:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Christina Redfield:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Vilko Smrečki:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Georgios A. Spyroulias:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Julien Trébosc:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Alicia Vallet:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Carine van Heijenoort:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Hugo van Ingen:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Thomas Vosegaard:** Conceptualization, Investigation, Writing – original draft, Writing – review & editing. **Julia Wirmer-Bartoschek:** Writing – original draft, Writing – review & editing, Conceptualization, Investigation. **Harald Schwalbe:** Writing – original draft, Writing – review & editing, Conceptualization, Investigation. **Anne Lesage:** Writing – original draft, Writing – review & editing, Conceptualization, Investigation. **Guido Pintacuda:** Writing – original draft, Writing – review & editing, Conceptualization, Investigation.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

This work was carried out within the framework of the European Remote-NMR (R-NMR) network gathering major European NMR infrastructures to promote remote NMR measurements across Europe. R-NMR has received funding from the European Union's Horizon Europe research and innovation programme (2021-2027), under grant agreement No 101058595. Work at BMRZ Frankfurt, an Instruct-ERIC center, is supported by the state of Hesse. The participation of the Lyon,

Grenoble, Gif and Lille laboratories was further supported by Infranalytics (FR2054), while the University of Oxford's contribution was additionally funded through Innovate UK (UKRI), project No. 1004096, and the participation of NOVA-FCT was supported by UCIBIO (proj. UIDB/04378/ 2020) and LAQV (proj. UIDB/50006/2020). Participation of LIOS was also supported by the European Union's HORIZON-WIDERA-2023-ACCESS-02 Twinning programme (GA 101160091 "MR LATVIA"). The support by the Italian Ministry for University and Research (FOE funding) to the CERM/CIRMMP Italian Centre of Instruct-ERIC in gratefully acknowledged. The 1 GHz instrument and major upgrades to other high field instruments at University of Barcelona that are currently an Instruct-ERIC facility have been financed by grants ICT2021-006875 and ICT2022-7829 from the Ministry of Science, Innovation and Universities with funds from the European Union Next Generation EU/PRTR. Additional resources and outputs of the project (including a GDPR Factsheet, a comparative overview of remote access software, and standardized protocols and methodologies) are available on the project website: www.r-nmr.eu.

Data availability

No data was used for the research described in the article.

References

[1] M.W. Maciejewski, A.D. Schuyler, M.R. Gryk Moraru II, P.R. Romero, E.L. Ulrich, H. R. Eghbalnia, M. Livny, F. Delaglio, J.C. Hoch, NMRbox: a resource for biomolecular NMR computation, Biophys. J. 112 (2017) 1529–1534.

[2] J.S. Frye, G.E. Maciel, Seting the magic angle using a quadrupolar nuclide, J. Magn. Reson. 48 (1982) 125–131.

[3] C.M. Rienstra, M. Hohwy, L.J. Mueller, C.P. Jaroniec, B. Reif, R.G. Griffin, Determination of multiple torsion-angle constraints in U-^{13}C,^{15}N-labeled peptides: 3D ^{1}H-^{15}N-^{13}C-^{1}H dipolar chemical shift NMR spectroscopy in rotating solids, J. Am. Chem. Soc. 124 (2002) 11908–11922.

[4] (a) T. Takahashi, H. Kawashima, H. Sugisawa, T. Baba, ^{207}Pb chemical shift thermometer at high temperature for magic angle spinning experiments, Solid State Nucl. Magn. Reson. 15 (1999) 119–123;
(b) K.R. Thurber, R. Tycko, Measurement of sample temperatures under magic-angle spinning from the chemical shift and spin-lattice relaxation rate of ^{79}Br in KBr powder, J. Magn. Reson. 196 (2009) 84–87;
(c) R. Sarkar, M. Concistrè, O.G. Johannessen, P. Beckett, M. Denning, M. Carravetta, M. al-Mosawi, C. Beduz, Y.F. Yang, M.H. Levitt, An NMR thermometer for cryogenic magic-angle spinning NMR: the spin-lattice relaxation of ^{127}I in cesium iodide, J. Magn. Reson. 212 (2011) 460–463.

[5] R.X. Han, A.L. Paterson, M.H. Milchberg, Y.C. Pang, B.H. Vanderloop, C.M. Rienstra, Tetrakis(trimethylsilyl)silane as a standard compound for fast spinning solid-state NMR experiments, J. Magn. Reson. 367 (2024) 107747.

[6] E. Nimerovsky, K.T. Movellan, X.C. Zhang, M.C. Forster, E. Najbauer, K. Xue, R. Dervisoglu, K. Giller, C. Griesinger, S. Becker, L.B. Andreas, Proton detected solid-state NMR of membrane proteins at 28 tesla (1.2 GHz) and 100 kHz magic-angle spinning, Biomolecules 11 (2021) 752.

[7] S. Penzel, A.A. Smith, M. Ernst, B.H. Meier, Setting the magic angle for fast magic-angle spinning probes, J. Magn. Reson. 293 (2018) 115–122.

[8] R.K. Harris, E.D. Becker, S.M. Cabral de Menezes, R. Goodfellow, P. Granger, NMR nomenclature. nuclear spin properties and conventions for chemical shifts (IUPAC Recommendations 2001), Pure Appl. Chem. 73 (2001) 1795–1818.

[9] M.E. Smith, Recent progress in solid-state nuclear magnetic resonance of half-integer spin low-γ quadrupolar nuclei applied to inorganic materials, Magn. Reson. Chem. 59 (2021) 864–907.

[10] D.S. Wishart, C.G. Bigam, J. Yao, F. Abildgaard, H.J. Dyson, E. Oldfield, J. L. Markley, B.D. Sykes, ^{1}H, ^{13}C and ^{15}N chemical-shift referencing in biomolecular NMR, J. Biomol. NMR 6 (1995) 135–140.

[11] R.K. Harris, E.D. Becker, S.M.C. De Menezes, P. Granger, R.E. Hoffman, K.W. Zilm, Further conventions for NMR shielding and chemical shifts (IUPAC recommendations 2008), Pure Appl. Chem. 80 (2008) 59–84.

[12] C.R. Morcombe, K.W. Zilm, Chemical shift referencing in MAS solid state NMR, J. Magn. Reson. 162 (2003) 479–486.

[13] A. Lesage, C. Gardiennet, A. Loquet, R. Verel, G. Pintacuda, L. Emsley, B.H. Meier, A. Böckmann, Polarization transfer over the water-protein interface in solids, Angew. Chem. Int. Ed. 47 (2008) 5851–5854.

[14] P. Bertani, J. Raya, B. Bechinger, ^{15}N chemical shift referencing in solid state NMR, Solid State Nucl. Magn. Reson. 61-62 (2014) 15–18.

[15] I. Hung, P. Gor'kov, Z. Gan, Using the heteronuclear Bloch-Siegert shift of protons for B_1 calibrarion of insensitive nuclei not present in the sample, J. Magn. Reson. 310 (2020) 106636.