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Transforming solid-state nuclear magnetic resonance towards a chemistry-ready technique

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ABSTRACT

Solid-state nuclear magnetic resonance (solid-state NMR) is an essential tool for probing local structure and dynamics in complex materials, yet its uptake in the broader chemistry community has remained limited by technical and operational barriers. The PANACEA project established a pan-European infrastructure to transform solid-state NMR into a community-ready analytical technique by combining state-of-the-art instrumentation, coordinated user access, and targeted technological innovation. Over three years, PANACEA enabled over 90

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user projects across chemistry and materials science, while driving advances in DNP methods, probe design, ultra-fast MAS, and interoperable software platforms such as EasyNMR and CHEMeDATA. This article presents the main outcomes of the initiative, illustrating how infrastructure-driven research and guided access can broaden the impact of solid-state NMR and integrate it into mainstream chemical workflows.

1. Introduction

Solid-state nuclear magnetic resonance (solid-state NMR) spectroscopy has emerged over the last two decades as a uniquely powerful tool for characterizing atomic-level structure, dynamics, and interfaces in complex solid materials. With advances in ultrahigh magnetic fields, fast magic-angle spinning (MAS), and dynamic nuclear polarization (DNP), solid-state NMR can now deliver extremely detailed chemical insights, offering structural understanding of crystalline, disordered or heterogeneous materials, complementing information obtained from X-ray methods and electron microscopy.

Despite its significant analytical potential, the use of solid-state NMR has long remained limited to expert laboratories. The technique's complexity, coupled with the cost and specialization of the instrumentation, has posed a barrier to its broader adoption within the general chemistry community. As a result, many chemists who would benefit from solid-state NMR (those working on catalytic surfaces, battery materials, pharmaceutical formulations, biominerals, or hybrid materials) have lacked access to the methods and expertise needed to exploit it fully.

This landscape is beginning to change. A combination of technological innovations and strategic investments in access to infrastructures is making solid-state NMR more user-friendly, scalable, and scientifically impactful. In particular, efforts to standardize experimental protocols, integrate software tools for data interpretation, and offer guided access to advanced instrumentation are lowering the barriers for non-specialists.

In this article, we present a case study illustrating this shift: the large-scale, pan-European initiative PANACEA (a PAN-europeAn network for Chemistry-Enabling Access) that has enabled over 90 chemistry research projects to use state-of-the-art solid-state NMR under open access. Over a three-year period, this infrastructure, backed by coordinated research and training efforts, has demonstrated that solid-state NMR is not only scientifically transformative but also operationally viable as a service-oriented technology. We highlight here key outcomes from both instrumentation and user projects, that indicate that solid-state NMR clearly has the potential to become a more widely used structural tool in the chemistry community.

2. Solid-state NMR as an enabling technology

2.1. A rapid technological shift

Modern chemistry increasingly relies on the ability to investigate complex solids at the atomic scale, across a diverse range of applications, from catalysis and energy materials to pharmaceuticals and medical implants. A critical bottleneck in many of these areas lies in the characterization of disordered, amorphous, or composite solids for which traditional crystallographic techniques are inadequate or inapplicable, and for which XAFS (X-ray Absorption Fine Structure) techniques often provide only partial descriptions. There is thus an acute need for advanced analytical methods that can reveal atomic-scale information in structurally heterogeneous systems.

Solid-state NMR spectroscopy has emerged as a uniquely powerful technique in this context [1]. Unlike diffraction methods, solid-state NMR does not rely on long-range order and provides local, site-specific information on both structure and dynamics. Over the past 25 years, solid-state NMR has undergone a rapid transformation, driven by instrumentation and methodological breakthroughs, that now enables the characterization of molecular connectivity, dynamics, morphology, and even electronic structure in a wide variety of solid materials (see Fig. 1).

Recent breakthrough in hardware and methods developments have dramatically improved both resolution and sensitivity as follows:

- **Higher magnetic fields**, which enhance signal-to-noise and spectral dispersion. The availability of 1.2 GHz and even 1.5 GHz magnets now places solid-state NMR among the most powerful techniques for atomic-scale spectroscopy.
- **Fast MAS**, reaching spinning frequencies up to 160 kHz, allows high-resolution proton detection, even in highly paramagnetic systems.
- **DNP**, which enables up to 100-fold sensitivity enhancement by microwave-driven polarization transfer at cryogenic temperatures on a variety of samples.

These instrumental advances are complemented by new pulse sequences, numerical simulation tools, and cross-disciplinary integration with crystallography, microscopy, and modeling.

2.2. A unique and versatile solution for a variety of chemistry problems

Today, modern solid-state NMR, supported by state-of-the-art instrumentation, is deeply embedded in the discovery process across multiple branches of chemistry. Its unmatched ability to probe local structure, dynamics, and electronic environments at the atomic scale has made it indispensable in both fundamental and applied research. Over the past two decades, methodological developments have expanded the reach of solid-state NMR, making it possible to solve crystal structures of powdered solids, characterize molecular motions, analyze local morphology in disordered systems, and unravel the fine electronic details around paramagnetic centers and reactive surfaces.

This versatility stems not only from the intrinsic sensitivity of NMR to the local chemical environment, but also from the experimental creativity it enables. Spectroscopists can design tailored pulse sequences to address specific structural questions or isolate dynamic features, making solid-state NMR adaptable to a wide range of scientific challenges.

A growing number of emblematic studies illustrate the central role of solid-state NMR in tackling key chemistry problems. Some case studies are illustrated in Fig. 2, and span a broad spectrum of materials and applications (solid adsorbents, catalysts, semiconductors, construction materials, biominerals, and energy storage) demonstrating the unmatched flexibility and scientific impact of solid-state NMR across the chemical sciences. Together, these examples underscore how solid-state NMR can provide crucial insights in diverse areas of chemistry, often in systems where no other technique can deliver the same level of atomic-scale resolution under native conditions.

3. PANACEA: building a european infrastructure for solid-state NMR

3.1. From cutting-edge technology to accessible infrastructure

The recent revolution in solid-state NMR spectroscopy has been driven by major technological advances—but it has also come at a cost. A typical high-end solid-state NMR spectrometer operating at 600 MHz exceeds €1 million, while the most advanced high-field systems, equipped with fast MAS and DNP capabilities, can cost upwards of €12

million. These instruments are complex, infrastructure-intensive, and require expert personnel to operate and interpret the data effectively.

As a result, only a limited number of expert centers in Western Europe currently host such capabilities, most of which have evolved into national infrastructures. While some academic chemists are aware of the power of modern solid-state NMR, the broader chemistry community remains largely unconnected from this transformation, both due to the rarity of the equipment and the perceived complexity of the techniques.

The challenge and opportunity, therefore, is to shift advanced solid-state NMR from a tool of specialist to a community-accessible platform: one that chemists can use, understand, and trust for solving structurally complex problems across diverse fields.

3.2. Enabling access through a coordinated european network

The PANACEA project was launched to demonstrate that advanced solid-state NMR can be made broadly accessible to the wider chemistry community, not only through instrumentation, but by building an integrated, service-oriented infrastructure at the European scale. Its central aim was to support a growing multidisciplinary user base in chemistry, many of whom had little or no prior experience with solid-state NMR, by offering them access to world-leading expertise and state-of-the-art technology.

To achieve this, PANACEA brought together eight major infrastructures (Fig. 3a): seven national centers in Europe, hosted at CNRS (France), Aarhus University (Denmark), CERM-CIRMMP (Italy), Radboud University (Netherlands), University of Aveiro (Portugal), University of Gothenburg (Sweden), and University of Warwick (UK), and one complementary international partner at the National High Magnetic Field Laboratory (Florida State University, USA). All were opened to academic and industrial users from across Europe, forming a distributed but tightly coordinated network.

Crucially, the project was not limited to physical access. PANACEA built its model on three interlinked pillars: networking activities, transnational access, and joint research and development. This was reinforced by strategic partnerships with leading technology providers and research institutions: Bruker BioSpin, an SME (Small or Medium-sized Enterprise) in analytical software (Mestrelab), and top-tier academic groups at EPFL (Switzerland) and the Weizmann Institute of Science (Israel). These partners contributed to expanding methodological capabilities, streamlining user interfaces, and accelerating technology transfer across the network. Notably, including an SME in the PANACEA consortium was considered essential to foster innovation and facilitate the translation of technological developments into practical applications, aligning with EU goals.

The PANACEA infrastructure offered users access to 27 solid-state NMR spectrometers, with proton frequencies ranging from 100 to 1500 MHz. This array represents over €100 million in capital investment and included cutting-edge capabilities such as fast and ultra-fast MAS, high-resolution proton detection, paramagnetic and quadrupolar NMR, DNP-enhanced MAS, spatially resolved NMR, wide-line NMR, relaxometry, and on-site hardware modification. The sophistication and diversity of this equipment is rarely accessible even within national programs; without PANACEA, many users would simply not have had the opportunity to conduct such advanced experiments.

What truly distinguished PANACEA, however, was the depth and breadth of expertise embedded within the participating infrastructures (Fig. 3b). These were not simply access points, but laboratories with demonstrated excellence in pulse sequence development, methodological innovation, data interpretation, software development and hardware engineering. Each site brought its own strengths, but the network as a whole offered end-to-end support for designing, executing, and interpreting solid-state NMR experiments tailored to the problem of the user. In addition, the scientific reach of the infrastructure was remarkably broad. PANACEA welcomed projects across virtually the entire spectrum of chemistry: from heterogeneous catalysis and pharmaceuticals to polymers, biomaterials, battery components, photovoltaics, cement, minerals, and beyond. This diversity reflected the consortium's unique ability to respond to application-specific needs while maintaining methodological rigor and experimental excellence.

By integrating these capabilities into a coherent access platform, PANACEA laid the foundation for a sustainable community of users and practitioners. It demonstrated that solid-state NMR is no longer the preserve of experts alone, but can become an enabling tool for chemists across disciplines, provided that access is coupled with training, guidance, and collaborative innovation.

3.3. Building a community around access

PANACEA was conceived not only as a mechanism for providing access to instrumentation, but as a vehicle for structuring and promoting a user community around advanced solid-state NMR. Achieving this goal required coordination on several interdependent fronts. From the outset, the consortium focused on harmonizing access procedures across its distributed infrastructure. A unified application portal and centralized evaluation system were established to streamline the onboarding

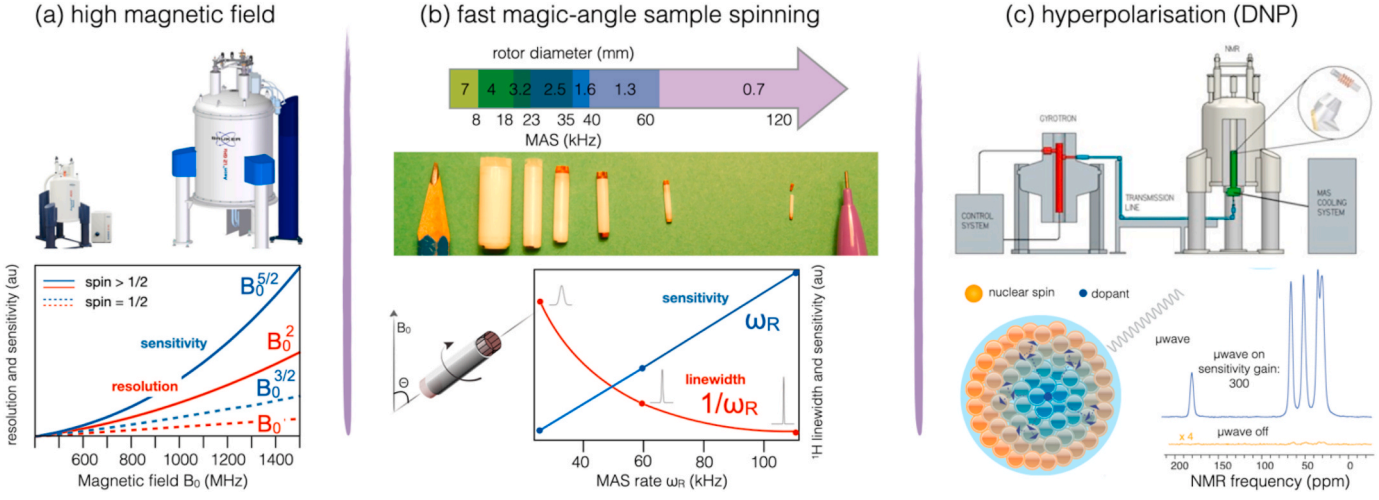

Fig. 1. Recent instrumental and methodological developments such as very high magnetic fields (a), ultra-fast MAS (b) and DNP (c), open unprecedented characterization opportunities. Fig. 1(c) is adapted from with permission from Refs. [2,3]. [2]: Copyright © 2016 Elsevier Inc [3].: Copyright © 2023 The Authors. Published by American Chemical Society. This publication is licensed under CC-BY 4.0.

process, ensuring consistency and fairness in user selection while simplifying the journey for new applicants.

In parallel, PANACEA laid the groundwork for integrated data management and sharing practices, fostering a culture of openness and reproducibility. By guiding users through data curation and processing pipelines, the project helped remove one of the key barriers to broader adoption of solid-state NMR among chemists unfamiliar with the method.

Training and outreach activities played a crucial role in community-building. A wide array of initiatives (including workshops, webinars, tutorials, and in-person visits) supported the emergence of a new generation of chemists and materials scientists equipped to use and interpret solid-state NMR data. These events not only provided technical knowledge but also fostered peer connections and collaboration across disciplines.

Industry engagement was also a central priority. PANACEA partnered with private-sector actors both within and beyond the consortium to highlight how solid-state NMR can address real-world research and development challenges in fields such as catalysis, pharmaceuticals, and energy materials. These interactions influenced the design and prioritization of access projects and opened new opportunities for technology transfer and co-development.

Finally, the project took proactive steps to communicate the broader societal value of solid-state NMR research. Through targeted dissemination, ranging from scientific publications to public engagement activities, PANACEA helped bridge the gap between fundamental science and societal impact, raising awareness of how advanced analytical tools can contribute to innovation, economic development, and public well-being.

4. Scientific outcomes from platform-driven innovation

The broader adoption of solid-state NMR in chemistry depends not only on access to instrumentation but also on the ongoing expansion of its capabilities. Through coordinated development efforts across facilities and industrial partners, significant progress has been made in improving both the performance and usability of cutting-edge solid-state NMR techniques. These advances, developed as part of a joint research effort, were rapidly transferred to user-facing platforms, demonstrating that innovation in instrumentation, methods, and software can directly feed into enhanced analytical capabilities for the community.

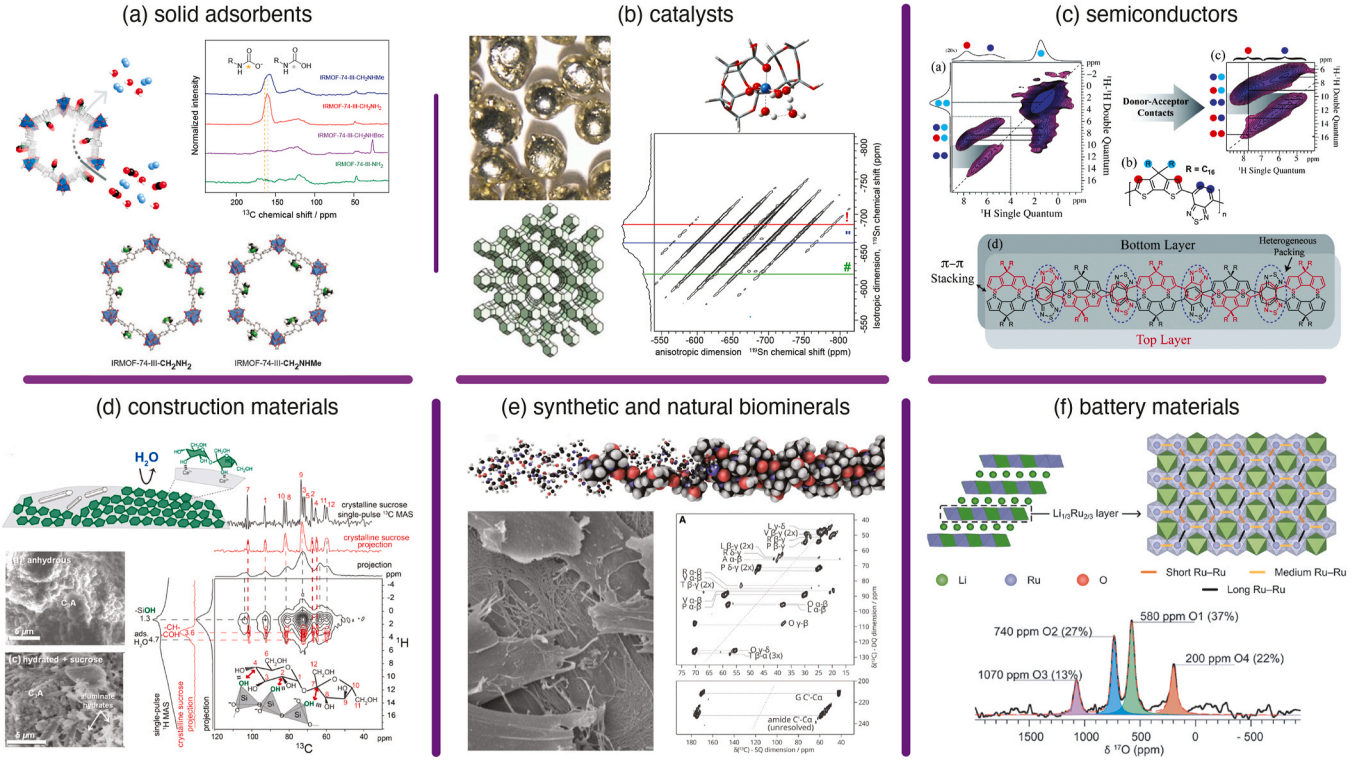

Fig. 2. Modern solid-state NMR provides landmark solutions to increasingly challenging problems at the heart of chemistry. (a) Solid adsorbents: Discovering that MOFs engineered with tailored functional groups are efficient at taking up CO_2, as well as removing CO_2 from wet nitrogen gas streams [4]. Adapted with permission from Ref. [4]. Copyright © 2014 American Chemical Society (b) Catalysts: polyethylene macromolecules are catalytically transformed by hydrogenolysis using well-dispersed Pt nanoparticles supported on $SrTiO_3$ perovskite nanocuboids: "single-use plastic bags" are thus converted into high-quality liquid products, such as lubricants and waxes, with a narrow distribution of shorter oligomeric chains [5]. Adapted with permission from Ref. [5]. Copyright © 2019 American Chemical Society. (c) Semiconductors: Developing the design paradigm for donor-acceptor copolymers toward field-effect transistors (FETs) with ultrahigh motilities, yielding polymer design principles that can lead to semiconductors exhibiting hole motilities exceeding 3 $cm^2\ V^{-1}\ s^{-1}$ [6]. Adapted with permission from Ref. [6]. Copyright © 2011 American Chemical Society. (d) Construction materials: Discovering the atomic-level structure of the interaction between saccharide adsorbates and cement materials, explaining the striking variability observed between different additives used to slow setting and alter rheological properties in cements, which are properties critical to large-scale construction projects or oil-well cementing [7]. Adapted with permission from Ref. [7] Copyright © 2011 National Academy of Sciences. (e) Synthetic and natural biominerals: Using multidimensional NMR spectra of animal and in vitro model tissues as fingerprints of their respective molecular structures, allowing the determination of the detailed atomic-level structure of developing bone [8]. Adapted with permission from Ref. [8]. Copyright © 2014 American Association for the Advancement of Science. (f) Battery materials: Showing how to elucidate the structure of pristine cathodes in Li-ion batteries and their structural evolution on cycling by ^{17}O NMR [9]. These discoveries provide a new understanding of the charge compensation mechanisms in high-capacity cathodes. Adapted with permission from Ref. [9]. Copyright © 2022 The Authors. Published by American Chemical Society. This publication is licensed under CC-BY 4.0.

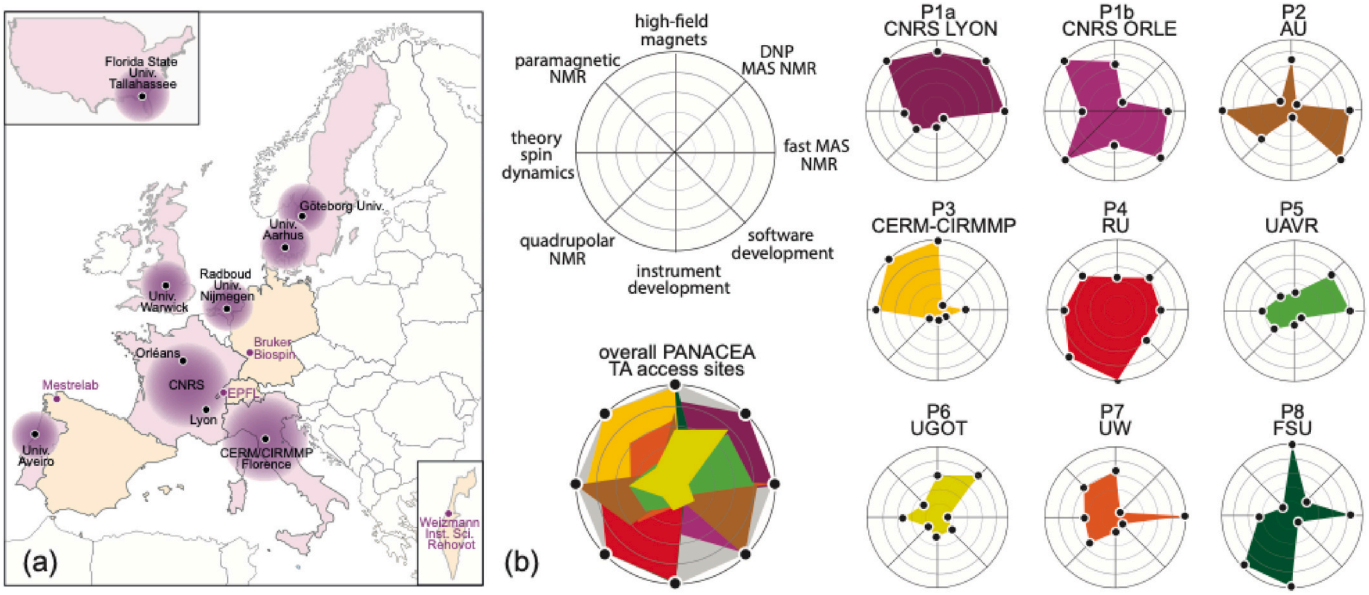

Fig. 3. (a) The PANACEA consortium (the name of the access providers is indicated in black, the technological partners are written in purple). The French infrastructure (CNRS) has two entry sites operating jointly. (b) The complementarity of technical expertise within the access sites.

4.1. Integrated software tools for solid-state NMR analysis

To broaden the accessibility of solid-state NMR and remove key obstacles that currently limit its uptake to a relatively small community of expert users (and to chemists directly collaborating with them) PANACEA focused on two main directions: (1) the development of a unified, web-based analysis platform, and (2) the creation of standards for metadata, data sharing, and interoperability.

4.1.1. A unique web-based interface for facilitated NMR data analysis and interpretation

For solid-state NMR to become a mainstream analytical tool in chemistry, its data must be as interpretable and interoperable as its hardware is powerful. Recognizing this, PANACEA launched a coordinated effort to develop a web-based platform that would simplify data analysis, promote data sharing, and facilitate the integration of solid-state NMR with complementary experimental and computational methods. The result is EasyNMR (easy.csdm.dk), a flexible, modular platform aimed at both newcomers and experienced users of solid-state NMR (Fig. 4).

The platform was conceived with two primary goals. First, it would provide a user-friendly interface to bring together many of the powerful (but often fragmented) tools already developed for solid-state NMR simulation and processing. Second, it would allow interoperability with other analytical data types, enabling joint analysis with results from techniques such as X-ray diffraction, electron microscopy, IR, EXAFS, or DFT-based chemical shift prediction. Together, these features are designed to lower the barriers that currently restrict solid-state NMR use to a small circle of expert practitioners.

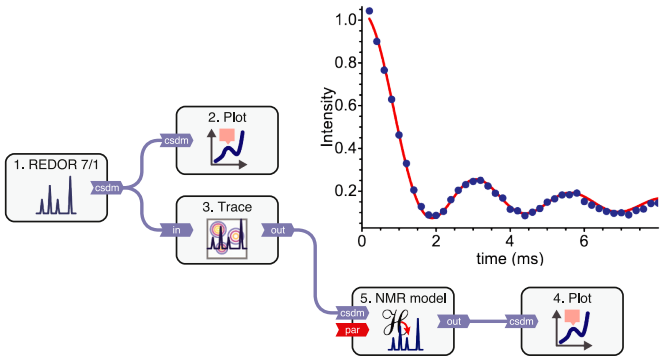

Fig. 4. EasyNMR is an online web-based platform to control the workflows involved in the processing, analysis and visualisation of NMR data. The figure shows the workflow for analysis of a REDOR dataset, providing internuclear distance information, with the data plotted in the inset, experimental data points as blue circles, the fit as a red line.

Developed primarily at Aarhus University (AU) in collaboration with CNRS-Orléans, EasyNMR was opened to users in the first year of the project and has since undergone continuous enrichment. It now integrates a wide range of established tools (including NMRGlue [10], SIMPSON [11,12], MRSimulator [13], ^{2}H dynamics [14], DNPSoup [15], ssNake [16], and EasySpin [17]) as well as links to predictive resources such as NMRShiftDB [18] and ShiftML [19]. To support workflows involving molecular structures, EasyNMR includes RDKit and OpenBabel, enabling streamlined management of geometry files and NMR assignment. Computational power for more extensive computations is provided by NMRbox [20]. Interactive tutorials and example workflows have been published on easynmr.readthedocs.io, making it easy for visiting users to continue analysing their data independently after an access visit.

The versatility of the platform has already enabled advanced research. A milestone example involved the determination of the molecular structure of verinurad, a pharmaceutical compound with a previously unknown crystal structure. 1D and 2D ^{1}H and ^{13}C MAS NMR spectra were recorded within the consortium, processed and simulated via EasyNMR, and analysed using the ShiftML module for chemical shift prediction. Among a set of candidate geometries, the structure best matching experimental shifts was selected, yielding a molecular model consistent with both NMR and DFT data [21]. This workflow (experiment, simulation, prediction, and validation) represents a new standard in what is now termed NMR crystallography, a growing field supported by international efforts such as the IUCr Commission on NMR Crystallography and Related Methods.

PANACEA also contributed to interoperability with other major European data initiatives. In particular, the project engaged with the Collaborative Computational Project for NMR Crystallography (CCPNC, www.ccpnc.ac.uk) and the magres database, which hosts computed NMR parameters for crystalline solids. Partner institutions (notably UW)

have worked to integrate PANACEA workflows with DFT-based predictions hosted on platforms such as NOVAD (NOvel MAterials Discovery, nomad-lab. eu) and PSDI (Physical Sciences Data Infrastructure, www.psdi.ac.uk), thereby ensuring long-term reusability and cross-validation of structural data.

To date, EasyNMR has attracted 346 registered users, including over 110 active contributors who have helped guide new features based on real-world use cases. It is becoming a reference platform for solid-state NMR analysis, with strong uptake from both academic and industrial users, particularly those working in multi-technique environments.

4.1.2. *Metadata, data sharing and interoperability*

A key innovation of the platform lies in its support for metadata and data sharing, developed in collaboration with the R-NMR EUproject (www.r-nmr.eu). While existing spectral formats (e.g., JCAMP [22], CSDM [23]) provide partial solutions, PANACEA team identified the need for more chemically descriptive, domain-specific metadata. This led to the introduction of CHEMeDATA object definitions for spectra, molecules and related objects with illustration examples. CHEMeDATA [24], is a flexible and lightweight schema-based framework for storing and visualizing chemical data, ranging from spectra and assignments to molecular structures and simulation results. These JSON-based objects ensure human-readability, interoperability across software, and robust long-term data accessibility.

CHEMeDATA objects are designed to be both extensible and visual. A single NMR spectrum, for example, can be linked directly to assignment tables, coupling constants (J-graphs), or 3D molecular structures. Synchronizing views across these representations facilitates exploratory analysis and educational use (Fig. 5). Mestrelab's Mnova software now supports JSON export compatible with CHEMeDATA (from version 15.1 onward), bridging the gap between proprietary analysis tools and open data platforms. Additionally, compatibility with external formats like. mol, .sdf, or. jcamp ensures smooth data exchange with the broader chemical informatics community (see Fig. 6).

From a data management perspective, a prototype NextCloud-based repository has been deployed to allow embargoed data sharing between PANACEA users and access providers, with secure login via ORCID and minimal installation effort. This system, already in testing at AU, aligns with European open science mandates while respecting data ownership and confidentiality requirements.

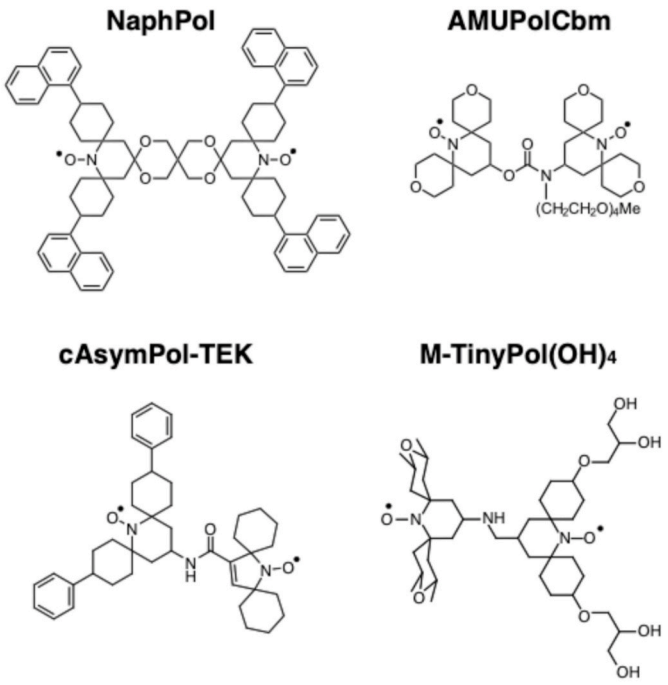

Fig. 6. Some of the new binitroxides introduced during PANACEA suitable for exogenous DNP NMR.

4.2. *Expanding the applicability of DNP-enhanced solid-state NMR through polarizing agent design and formulation development*

As mentioned in Section 2, DNP has recently emerged as a transformative technique in solid-state NMR spectroscopy, offering signal

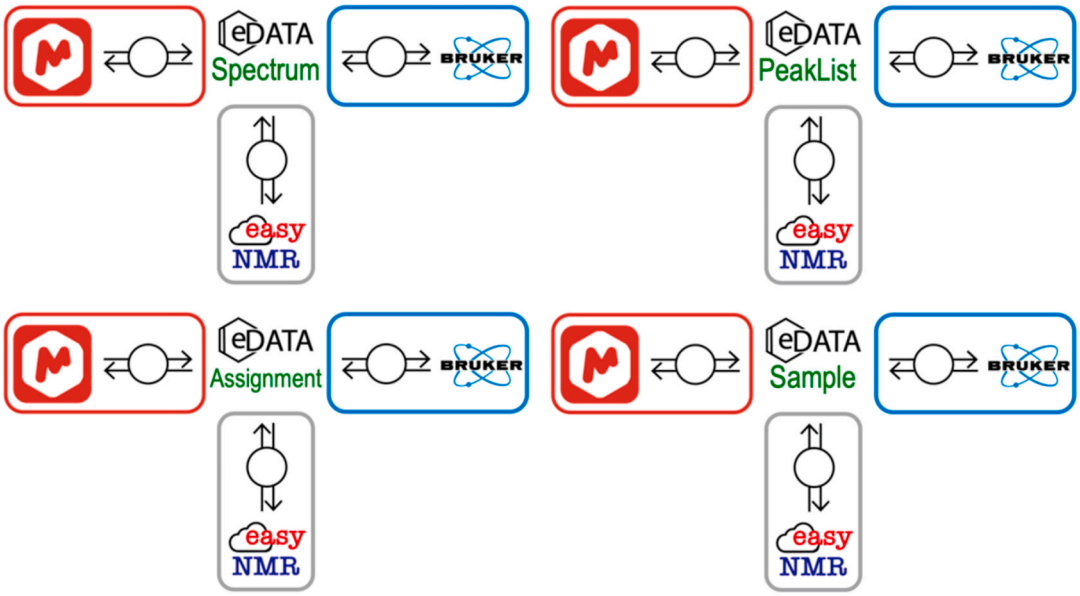

Fig. 5. The CHEMeDATA initiative provides a standardized framework for the solid-state NMR community, enabling interoperability across software platforms. Within this framework, key data elements (such as spectrum, sample, peak list, and others, shown in green) are defined as distinct, well-scoped objects. Each object encapsulates specific information: for example, the sample object includes system-specific parameters, while the experiment object captures details such as dimensionality, correlation types, and decoupling schemes. Additional objects describe processing steps (e.g. line broadening, peak picking) and extracted results (e.g. J couplings, anisotropy tensors, assignments). Developers can independently build tools that read and write these objects according to their needs, facilitating seamless data exchange between programs such as Mnova, Bruker TopSpin, EasyNMR, and others.

enhancements exceeding two orders of magnitude. A key objective of the joint research efforts within PANACEA has been to broaden the applicability of this method to a wider range of samples and experimental conditions, thereby increasing its accessibility and impact within the chemistry community. One central challenge in the broader application of DNP-enhanced NMR is the limited availability of efficient polarizing agents (PAs) and optimized sample formulations. To address this, the consortium pursued two main strategies: the design and evaluation of new families of polarizing agents, and the expansion of the portfolio of sample formulations compatible with DNP.

4.2.1. New polarizing agents for exogenous DNP

First, a series of deuterated TEKPol derivatives was investigated to probe the effect of deprotonation on MAS DNP at 9.4 T. Experimental investigations, supported by numerical simulations, revealed that strong hyperfine couplings with proximal protons facilitate efficient polarization transfer across the spin diffusion barrier, resulting in short build-up times and high enhancements. Notably, the presence of protons on the phenyl rings was shown to be critical for polarization transfer to the bulk, as evidenced by longer build-up times in more extensively deuterated isotopologues. Building on this insight, a new biradical, NaphPol, was designed, which outperforms previously reported agents in organic solvents in terms of overall sensitivity enhancement [25]. Additional polarizing agents suitable for a variety of solvents were developed. By investigating a series of 18 biradicals for solid-state DNP NMR at 9.4 T and 100 K, including eight newly synthesized compounds, Venkatesh et al. later demonstrated that the key parameters contributing to overall DNP sensitivity (namely, enhancement factor, polarization build-up time, and the contribution factor) often counterbalance one another, resulting in comparable overall sensitivity across the series. Among the tested PAs, NaphPol and HydroPol were shown to deliver the highest overall sensitivity in organic and aqueous solvents, respectively. Notably, one of the new biradicals, AMU-PolCbm, showed consistently high performance across all three solvent systems, making it a promising candidate as a "universal" polarizing agent [26].

In parallel, PANACEA partners successfully functionalized the Tinypol scaffold [27] with hydroxypropyl chains, creating new polarizing agents with significantly improved DNP efficiency at high field and fast MAS. One radical in this series, M-TinyPol $(OH)_4$ achieved a record DNP enhancement (>200) at 18.8 T and 65 kHz MAS in aqueous solution, thus matching the best performance of dinitroxides at much lower fields (9.4 T). EPR, molecular dynamics, and quantum mechanical simulations revealed that hydroxypropyl chains in the new TinyPol series enhance polarization transfer from the biradical to the bulk solution, identifying them as key structural features for increasing DNP performance at high-field DNP and in the fast MAS regime [28]. Two new polarizing agents of the AsymPol family, AsymPol-TEK and cAsymPol-TEK were introduced for MAS-DNP applications in non-aqueous solvents [29]. They exhibit significantly shorter DNP build-up times than TEKPol in 1,1,2,2-tetrachloroethane (TCE) at 100 K and 9.4 T, thanks to their significant electron-electron coupling. This was showed to be, with AsymPol-POK and cAsymPol-POK to be advantageous to polarize proton-dense matrices [30,31]. Those biradicals appear to have distinct polarization pathway and may not rely on the protons on the structure to generate the bulk nuclear hyperpolarization [32,33]. Finally, a new family of trityl-nitroxide polarizing agents, PyrroTriPol, was introduced based on a piperazine linker for use in both aqueous and organic media. This hybrid radical offers an improved control of the spin-spin interactions via a rigid bridge, leading to superior DNP performance across various fields and MAS rates, while requiring less microwave power than bis-nitroxides. Its efficiency, surpassing that of TEMTriPols, was demonstrated at 9.4, 14.1, and 18.8 T, in bulk solutions as well as on γ-Al_2O_3 [34].

4.2.2. Formulations for endogenous DNP

Paramagnetic metal ions represent a unique route as DNP polarizing agents as they provide sensitivity in the bulk of inorganic solids where proton concentration is low, and the hyperpolarization produced by exogenous biradical can hardly penetrate inside the material. A practical guide was published to assist chemists interested in applying Metal Ion DNP (MIDNP). The guide thoroughly outlines all essential steps, including the selection of suitable metal ion dopants, characterization of their concentration and spatial distribution, and the setup and comprehensive evaluation of the DNP experiment, from the optimisation of field position to the accurate determination of enhancement factors [35]. The application field of MIDNP was also extended. Leskes and co-workers notably showed that this approach could also be implemented in porous materials, such as metal organic frameworks (MOFs) (Fig. 7). In this case, MIDNP is advantageous compared to organic radical-based formulations as it provides sensitivity gains while leaving the pores of the MOFs empty for potential guests. For example, the authors showed how Gd(III) ions doped into the MOF structure, LaBTB (BTB = 4,4′,4″-benzene-1,3,5-triyl-trisbenzoate), could be exploited as efficient PAs, providing up to 30-fold ^{13}C signal enhancement for the organic linkers, while leaving the pores empty for potential guests. Protocols to address the challenges associated with the framework mobility and residual oxygen trapped within the pores at 100 K were also described [36]. In parallel, the effect of spin diffusion on the DNP enhancement and buildup time in MIDNP was investigated, in a regime where spin diffusion and direct DNP rates are similar, as is the case in metal-ion doped inorganic solids, providing new insight into endogenous DNP mechanisms [37]. Finally, PANACEA researchers demonstrated that both exogenous and endogenous DNP sources could be used to reveal the chemical composition of the solid electrolyte interphase (SEI) in sodium-ion batteries (SIBs), as well as the spatial distribution its constituent phases. This innovative approach represents a new avenue for investigating SEIs and optimizing battery design [38].

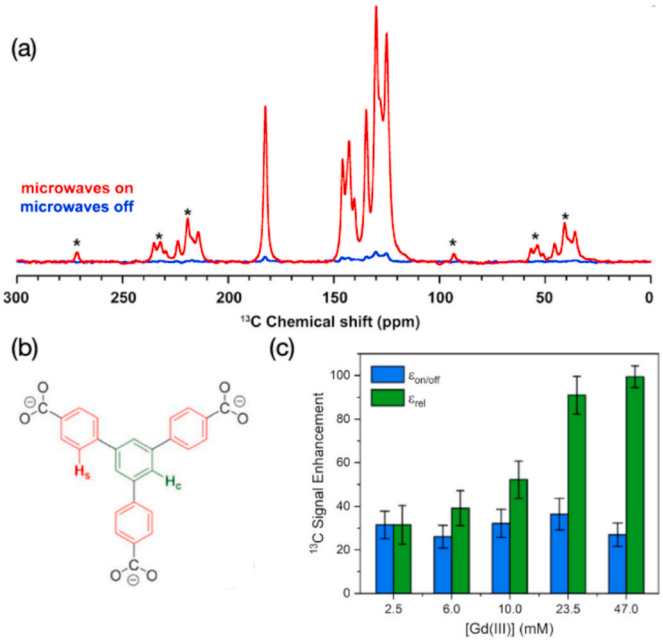

Fig. 7. ^{13}C MAS NMR spectra acquired for 10 mM Gd-doped LaBTB at 100 K with (red) or without (blue) microwaves at the optimal field position. The structure of LaBTB is shown in (b). (c) Enhancement factors for ^{13}C nuclei as a function of Gd(III) concentration in Gd-LaBTB. $\varepsilon_{on/off}$ (blue) is determined as the ratio between integrated microwave-on and microwave-off signals at steady-state conditions. ε_{rel} (green) is the enhancement $\varepsilon_{on/off}$ normalized by the paramagnetic quenching and the change in the build-time. Adapted with permission from Ref. [36]. © The Royal Society of Chemistry 2023. This article is licensed under a Creative Commons Attribution 3.0 Unported Licence.

4.2.3. Photochemically induced DNP

In the quest for even larger signal enhancements, a novel strategy based on optically-generated hyperpolarization has also been explored. In particular, Emsley and co-workers put attention on photochemically induced DNP (photo-CIDNP) in solid samples, an NMR hyperpolarization technique where light is used to excite a suitable donor-acceptor system, creating a spin-correlated radical pair whose evolution drives nuclear hyperpolarization. Systems that exhibit photo-CIDNP in solids are not particularly common, and this effect has, up to now, only been observed for ^{13}C and ^{15}N nuclei. In this context, the authors have reported the first example of optically enhanced solid-state ^{1}H NMR spectroscopy in the high-field regime, achieved via photo-CIDNP of a donor-chromophore-acceptor synthetic molecule in a frozen solution at 0.3 T and 85 K. Spontaneous spin diffusion among the abundant strongly coupled ^{1}H nuclei relayed the polarization through the whole sample, yielding a 16-fold bulk ^{1}H signal enhancement under continuous laser irradiation. These findings enabled a new strategy for hyperpolarized NMR beyond the current limits of conventional microwave-driven DNP [39]. More recently, this approach has been also verified at higher magnetic fields, from 9.4 T to 21.4 T [40]. Site-selective deuteration of PhotoPol was used to understand the mechanism behind the generation of spin polarization in donor-chromophore-acceptor systems and identify key protons in the molecule [41].

4.3. Innovations in DNP MAS NMR probe technology

DNP instrumentation is currently limited to wide-bore magnets and restricted to certain subsets of nuclei combinations. These bottlenecks were tackled during PANACEA by building DNP MAS probes for standard-bore magnets to extend the number of spectrometers with DNP capabilities, and developing triple resonance MAS probes for allowing ^{1}H/^{19}F/X tuning so that ^{19}F nuclei become fully amenable to DNP NMR, with a substantial impact in the characterization of pharmaceutically relevant preparations and advanced materials.

4.3.1. Triple resonance DNP MAS probes for ^{1}H/^{19}F/X experiments

Within the PANACEA project, a 3.2 mm triple-resonance MAS DNP probe prototype with simultaneous ^{1}H-^{19}F tuning capability was developed by Bruker Biospin. The probe features a unique coil design with separate radiofrequency channels for ^{1}H excitation and ^{13}C or ^{19}F detection, enabling a versatile range of experiments (Fig. 8a). These include ^{1}H–^{19}F cross-polarization (CP) MAS, direct ^{19}F detection with proton decoupling, ^{13}C acquisition with simultaneous double decoupling on the ^{1}H and ^{19}F channels, and ^{1}H–^{19}F–^{13}C double-CP experiments, all performed under low-temperature MAS DNP conditions. The probe was used to study AZD2811, an active pharmaceutical ingredient (API) from Astra-Zeneca, both in its pure form and formulated form. ^{1}H–^{19}F CP MAS experiments performed with the new HFX probe offer a significant advantage over conventional direct-detection ^{19}F methods (Fig. 8b). For the pure API impregnated with DNP solution, an indirect ^{19}F DNP enhancement of 26 was achieved via ^{1}H–^{19}F CP, resulting in an overall 30-fold increase in sensitivity compared to direct ^{19}F detection under similar conditions [42]. Indirect enhancement by ^{1}H–^{19}F CP was instrumental for the analysis of the API encapsulated in functionalized polymeric nanoparticles, where a direct enhancement was not detected.

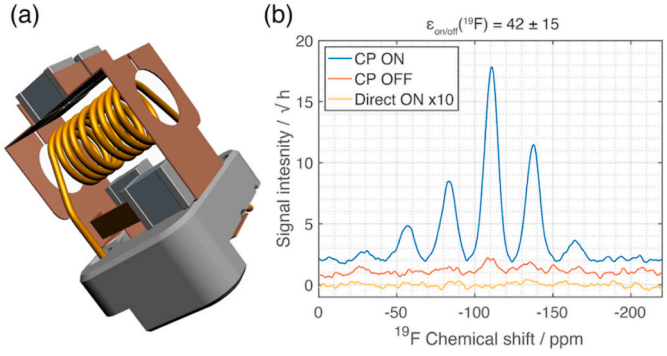

Fig. 8. (a) Radiofrequency coil setup of the HXF solid-state MAS DNP probe. The setup utilizes two distinct coils: a solenoid coil doubly tuned to ^{19}F and X-nuclei, and a capacitively tuned cage coil dedicated to ^{1}H. The cage coil features a unique low electric field (low-E) design that minimizes sample heating during high-power cross-polarization and decoupling pulses. Crosstalk between the closely spaced resonance frequencies of ^{1}H and ^{19}F is effectively avoided by orienting the RF fields of the solenoid and cage coils perpendicular to one another. (b) Solid-state ^{19}F spectra of AZD2811 nanoparticle suspension with (blue) and without (orange) microwaves together with a direct-detected ^{19}F spectrum (yellow) measured at 100 K, 9.4 T, and 10 kHz MAS. Adapted from Ref. [42] with permission. Copyright © 2025 Elsevier. This is an open access article under the CC BY 4.0 license.

4.3.2. Standard-bore DNP probe

Developing solid-state MAS DNP probes for standard-bore (SB) NMR magnets poses significant challenges due to spatial constraints and the necessity to design specific dewars to achieve and maintain cryogenic temperatures. Nevertheless, in the course of PANACEA, Bruker Biospin successfully developed DNP MAS probes for standard-bore magnets. Initial tests showed that enhancements of up to 70 could be obtained with a 1.3 mm probe operating at 18.8 T, using 10 mM AMUPol in water/glycerol at 17 kHz MAS frequency.

4.4. Advances in ultra-high field and ultra-fast MAS NMR for chemistry and materials science

The introduction of ultra-high magnetic field NMR instruments and ultra-fast MAS technology opens new frontiers for solid-state NMR. Within PANACEA, the consortium aimed to develop NMR solutions that are only feasible at these extreme performance regimes, solutions that would unlock structural and physico-chemical information previously inaccessible. By capitalizing on the exceptional instrumentation available within the consortium, the project achieved substantial improvements in resolution, coherence lifetimes, and overall spectral interpretability. These advances have broadened the analytical power of NMR for key classes of quadrupolar nuclei and paramagnetic systems, as well as for protons in pharmaceutical powders or biomolecular systems.

4.4.1. Approaches at ultra-high field

One notable achievement in this area was the development of steadyDFS, a new technique to improve the sensitivity of quadrupolar NMR experiments at high magnetic fields [43]. Quadrupolar nuclei, such as ^{39}K, ^{43}Ca, ^{17}O, or ^{49}Ti, are present in many important materials but are notoriously difficult to observe due to their broad and weak signals. The steadyDFS method offers a simple yet powerful way to overcome this, by repeating specific radiofrequency pulses (double frequency sweeps, DFS) and readout pulses in a steady-state regime, dramatically boosting excitation efficiency for half-integer quadrupolar spins (I = 3/2, 5/2, 7/2, and 9/2). In practice, this approach led to dramatic improvements in signal strength (up to 46-fold for e.g. ^{39}K and ^{17}O, corresponding to a 20-fold increase in sensitivity per unit time) making it much easier to study chemically and industrially relevant systems. Importantly, the method is versatile and can be readily adapted to a range of materials, helping to establish quadrupolar NMR as a more accessible and routine tool for solid-state analysis at high fields.

Ultra-high magnetic fields were also applied to benchmark surface characterization problems in heterogeneous catalysis. In one study, 2D ^{1}H-^{27}Al correlation spectroscopy at 28.2 T and 50 kHz MAS enabled the resolution and assignment of four distinct families of Al–OH surface sites in γ-Al_2O_3. By comparing experimental quadrupolar and proton chemical shift parameters to DFT-calculated values from a wide range of surface models, the study identified both edge and facet sites, including a highly deshielded Al_{IV}–OH group with an unprecedented C_Q of 18

MHz. This level of site-specific resolution illustrates the transformative power of ultra-high field solid-state NMR for addressing longstanding questions in catalyst surface chemistry [44]. Finally, the consortium additionally demonstrated that a combination of ^{13}C and ^{15}N CPMAS NMR and fast-MAS ^{1}H NMR at high magnetic field was a reliable and efficient technique for characterizing polyurethanes for biomedical applications in their native state [45].

4.4.2. *Paramagnetic NMR*

In parallel, PANACEA tackled the enduring challenge of studying highly paramagnetic solids using MAS. These systems (including supported catalysts, battery electrodes, and rare-earth phosphors) often exhibit extremely large paramagnetic shift anisotropies that result in broad, overlapping spectral features. Fast spinning alone had traditionally been insufficient to resolve such signals. However, through improvements in rotor technology and sample preparation, PANACEA demonstrated that 100 kHz MAS could dramatically enhance spectral resolution even for materials exhibiting extremely large anisotropy [46]. A new generation of 0.7 mm zirconia rotors with improved flexural strength, tighter caps, and higher manufacturing precision was introduced. These rotors, now robust enough for routine handling, in combination with tailored RF irradiation schemes, allowed high-throughput analysis of series of air- and moisture-sensitive paramagnetic samples (Fig. 9). The improved averaging of the large shift anisotropies at these higher MAS rates enabled the observation of signals that had been previously invisible at lower rates of 60 kHz, even when multi-dimensional experiments were employed. This enables routine structure elucidation of materials once deemed intractable by NMR. Overall, these advances will result in new analytical opportunities in the fields of catalysis and battery science, both of which frequently involve air-sensitive paramagnetic materials.

4.4.3. *^{1}H-aided structure determination of amorphous pharmaceuticals*

Resolved ^{1}H shifts measured at 100 kHz MAS have played a central role in the field of NMR crystallography, where PANACEA researchers have pioneered and progressively refined a general framework for atomic-level structure determination of amorphous molecular solids. The method integrates advanced solid-state NMR with large-scale molecular modeling and machine-learned chemical shift predictions. In a first demonstration, the approach was used to predict chemical shifts for hundreds of thousands of configurations. This enabled identification of key hydrogen-bonding motifs, especially drug-water interactions, that stabilize the amorphous form [47]. The method was then generalized to AZD4625, where matching full $^{1}H/^{13}C$ shift distributions to over a million simulated local environments revealed preferred conformations, specific hydrogen bonds, and energetically favorable packing [48]. Most recently, the method was used for a large glucagon-like peptide-1 receptor agonist, showing promoted carboxylic acid hydrogen bonding, distinct aromatic ring orientations, and water-driven stabilization [49]. Together, these works provide the first direct, experimentally anchored 3D ensemble descriptions of disordered pharmaceuticals, linking local structure to stability.

4.4.4. *Beyond boundaries: ultra-fast 160 kHz magic-angle spinning*

Going further, PANACEA partners explored the next generation of spinning technology with the deployment of a 0.4 mm MAS probe operating at 160 kHz. This ultra-fast MAS setup was applied to both small-molecule materials and biomolecules, with remarkable results. Benchmark measurements were conducted on the amorphous pharmaceutical solid verinurad [21]. The ^{1}H spectrum acquired at 160 kHz MAS displayed unprecedented resolution, far exceeding what is achievable at 100 kHz, and enabled detailed peak assignment and chemical shift analysis. To capitalize on this, PIPNet was developed, a machine-learning framework that extrapolates a “pure isotropic” spectrum by analysing ^{1}H data acquired at multiple MAS rates [50,51]. The analysis of the verinurad spectra with PIPNet significantly narrowed the resonances, improving spectral deconvolution and enabling direct structure determination via NMR crystallography. This work culminated in the successful structure assignment of verinurad from NMR data alone.

The same ultra-fast MAS system was also applied to biomolecular systems, including crystalline GB1 and the membrane protein aquaporin Z embedded in lipid bilayers [52]. By optimizing rotor design, sample handling tools, and temperature control, researchers overcame the fragility and low sample volume typically associated with sub-millimeter rotors. The 160 kHz MAS conditions substantially

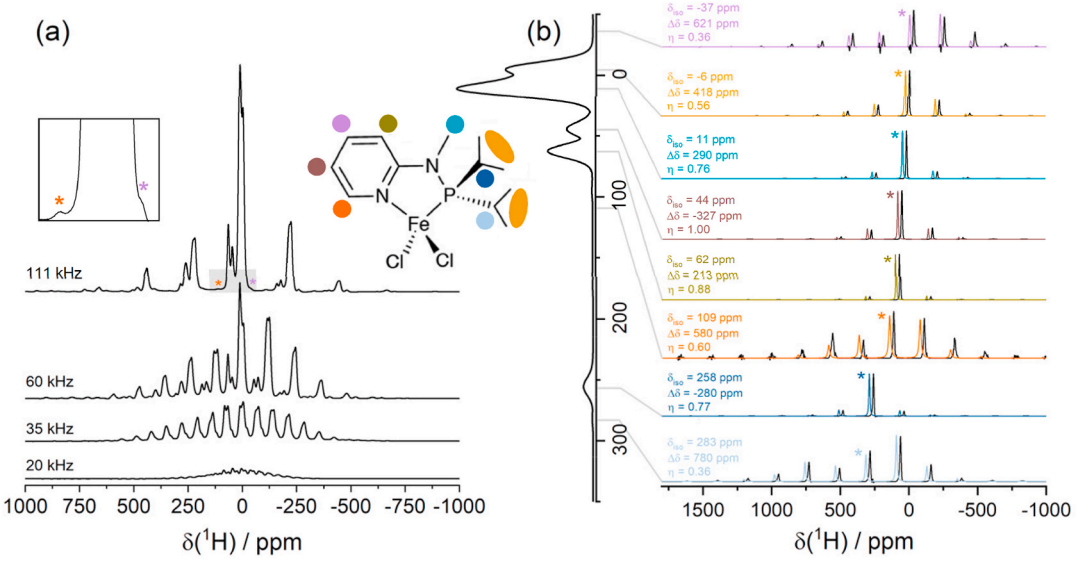

Fig. 9. Increase in resolution and consequent characterization of the ^{1}H NMR spectra of a microcrystalline organometallic catalyst at faster MAS. (a) Structure and 1D ^{1}H MAS NMR spectra of Fe (py-NMe-PiPr$_2$)Cl$_2$ obtained at 11.75 T, using spinning frequencies increasing from 20 to 111 kHz. Asterisks denote signals that are only visible at 111 kHz MAS. (b) Signal traces extracted from the 2D adiabatic Magic-Angle Turning (aMAT) experiment at 111 kHz MAS and fitted to obtain the shift tensor parameters. Asterisks denote the isotropic peaks and the color code refers to the molecular structure in (a). Also shown vertically in (b) is the “infinite-MAS” spectrum obtained from the projection of the 2D aMAT spectrum. Adapted with permission from Ref. [46].

enhanced coherence lifetimes and spectral resolution, enabling the acquisition of high-quality 1D and 2D datasets from sub-milligram quantities of protein. These results open new opportunities for studying membrane proteins, peptide formulations, and molecular assemblies under native-like conditions.

Importantly, ultra-fast MAS also enabled new developements: for the first time, ^{1}H–^{1}H J-couplings were resolved in the solid state using INADEQUATE-type experiments on camphor plastic crystals. These observations, made possible by the long coherence lifetimes at 160 kHz, pave the way for bond-resolved proton NMR in solids, a long-standing goal of structural NMR [53].

5. Scientific impact through user access: highlights across chemistry

5.1. Widening and simplifying access to advanced solid-state NMR

A core objective of the PANACEA initiative was to make high-end solid-state NMR instrumentation and expertise available to a much broader community than previously possible. This involved creating a truly open and user-friendly infrastructure that could serve academic and industrial researchers across Europe, regardless of their institutional background, geographic location, or level of experience in NMR.

Solid-state NMR is still underrepresented in chemistry departments, and very few research groups have the critical mass or resources to acquire or operate these advanced instruments. PANACEA addressed this structural barrier by integrating leading national infrastructures into a transnational platform that exceeded the sum of its parts, offering coordinated access to a comprehensive and complementary inventory of cutting-edge instrumentation and expertise. In doing so, it offered chemists across Europe (and beyond) a way to conduct research projects that would otherwise have been out of reach.

A key success factor of PANACEA was its ability to engage non-expert users and guide them through the process of project design, data collection, and interpretation. Among the 77 project leaders, 65 % had little to no prior experience with solid-state NMR of which 43 % were “familiar” but non-specialists, and 22 % were complete newcomers. Only 35 % were established experts. This distribution (Fig. 10a) illustrates the project’s inclusive model and confirms that the infrastructure, together with expert support, was effective in lowering entry barriers.

Solid-state NMR is increasingly relevant across many areas of chemistry, and the PANACEA access statistics reflect this diversity (Fig. 10b). 71 % of the user projects addressed topics central to chemical research, such as energy materials, pharmaceuticals, biomaterials, and heterogeneous catalysis. Additional demand came from polymers, environmental science, and emerging interdisciplinary applications.

Thus, through the PANACEA infrastructure, a broad community of researchers, including many with little prior experience in solid-state NMR, has produced high-quality publications across diverse fields of chemistry. These studies demonstrate not only the accessibility of advanced instrumentation, but also the added scientific value that solid-state NMR brings when embedded in broader research workflows. The following examples illustrate how solid-state NMR, enabled by guided access and tailored support, has contributed to key insights in functional materials, catalysis, pharmaceutical science, and nature-inspired chemistry.

5.2. Functional materials and energy

Advanced materials for energy applications are increasingly defined by subtle, nanoscale structure–property relationships that require local analytical techniques to resolve. Solid-state NMR has proven essential in characterizing these systems under real conditions, revealing local dynamics, electronic environments, and interface structures that are critical to function. In the field of photovoltaics, Luo et al. investigated a new class of hybrid perovskites incorporating sulphur-rich organic spacers (Fig. 11a). These chalcogen-containing molecules were designed to introduce S-π interactions and chalcogen bonding, improving charge transport and stabilizing the structure. Solid-state NMR, combined with diffraction and DFT, was used to characterize the local environments of the organic spacers and revealed how these interactions tune the optoelectronic properties of the material. The study marked a significant step forward in the design of more durable and efficient perovskite solar cells [54].

Similarly, Greve et al. examined the role of ionic liquids in halide migration within mixed-halide perovskites (Fig. 11b). By applying ^{1}H, ^{19}F, and ^{207}Pb solid-state NMR under variable temperature conditions, they demonstrated that the butyl methyl imidazolium cation ($BMIM^{+}$) facilitates bromide transport by acting as a dynamic shuttle. This work provided a molecular-level understanding of halide mixing, relevant for tuning phase stability in next-generation tandem solar devices [55]. In the area of solid electrolytes, Šimko et al. used high-field solid-state NMR to investigate cesium oxo-fluoro-aluminate compounds in the CsF-Al_2O_3 system. Their work revealed unexpected phase behavior and led to the first MAS NMR characterization of Cs_3AlF_6 and related compounds. These materials showed promising ionic conductivity and charge distribution features, relevant for next-generation energy production and storage [56].

Membrane-based energy materials also benefited from solid-state NMR characterization. Martínez-López et al. developed a new class of mechanically robust and thermally stable polymer membranes derived from trifluorinated bis(catechol) and tetrafluoro-nitrile linkers. Designed for lithium-ion separation, these polymers were probed using ^{1}H-^{13}C cross-polarization MAS and ^{7}Li solid-state NMR, which revealed two dynamically exchanging lithium populations (mobile ions in pores and less mobile ions coordinated to carboxyl groups). NMR also captured subtle structural rearrangements induced by lithium transport, highlighting the technique’s ability to interrogate functional processes in dense, insoluble materials [57].

In another direction, Perego et al. explored molecular motion within

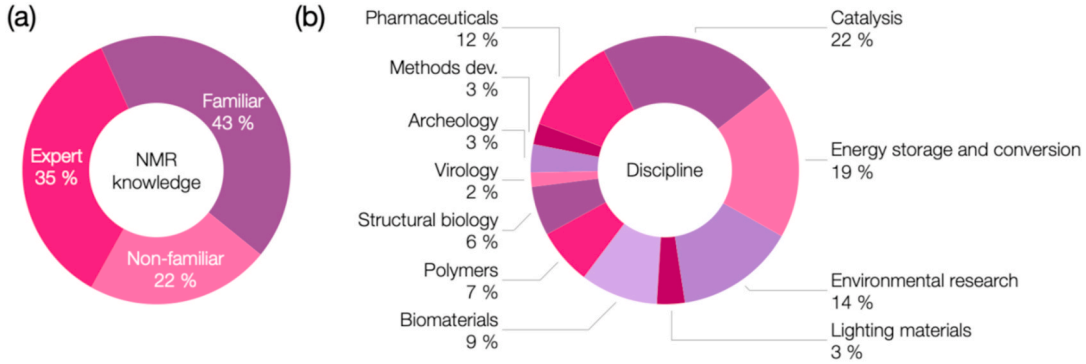

Fig. 10. (a) Knowledge distribution of users and (b) diversity of scientific fields for projects submitted during the first three years of PANACEA.

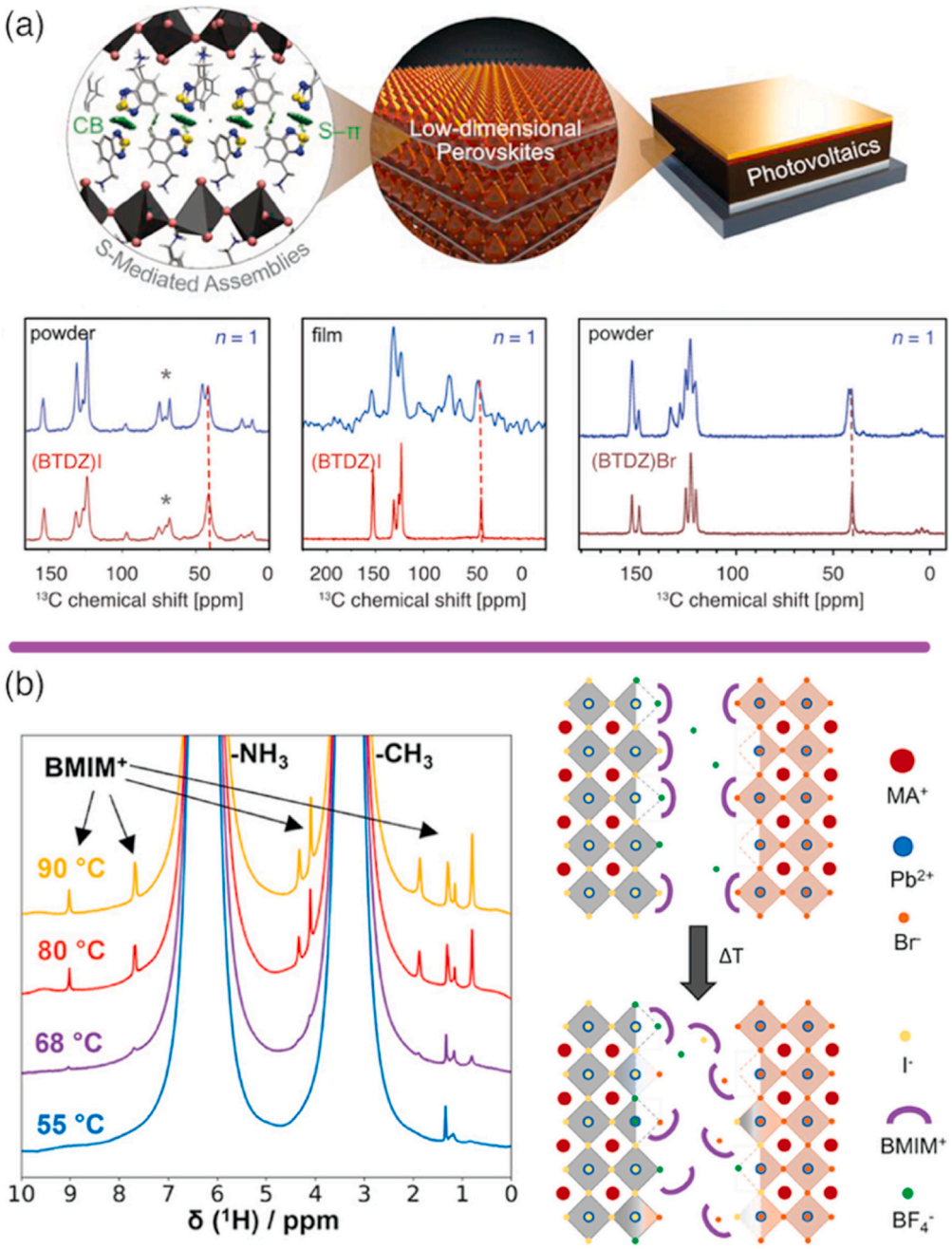

Fig. 11. (a) Solid-state NMR insights into S-bridged hybrid perovskites, offering new opportunities for hybrid materials in optoelectronics. The lower panels illustrate ^{13}C CP MAS NMR spectra of powder and thin-film hybrid perovskites with nominal (BTDZ)X and $(BTDZ)_2PbX_4$ (n = 1) compositions. Adapted with permission from Ref. [54]. © 2025 The Author(s). Advanced Energy Materials published by Wiley-VCH GmbH. This is an open access article under the CC BY license CC BY 4.0. (b) Ionic liquid-assisted halide mixing in hybrid perovskites. (left) ^{1}H MAS NMR spectra showing changes in the ionic liquid ($BMIMBF_4$) mixed with a 1:1 blend of $MAPbI_3$ and $MAPbBr_3$ at different temperatures; (right) schematic showing how the ionic liquid enhances halide exchange during heating by passivating grain boundaries and promoting ion mobility. Adapted with permission from Ref. [55]. Copyright © 2011 American Chemical Society.

flexible metal-organic frameworks (MOFs). Their study revealed how multiple dynamic elements (including pyridyl and bicyclopentane rotors) coordinate piston-like responses to external chemical stimuli. Solid-state NMR spectroscopy captured these cooperative motions down to cryogenic temperatures, offering insights into low-temperature responsiveness and potential applications in gas separation or actuation [58].

Finally, in a different approach to energy storage, Rossin and coworkers explored the possibility to generate new materials for hydrogen storage by nanoconfinement of hydrogen rich inorganic hydrides. In particular, they employed multinuclear solid-state NMR to probe the hydride incorporation and hydrogen release from boron–nitrogen hydrides (amino borane and hydrazine bis borane) confined within zirconium-based MOFs (Fig. 12). The NMR data (^{1}H, ^{11}B, ^{13}C, and ^{15}N) uncovered partial dehydrogenation within the pores and formation of B–O and boryl-amine species anchored to the MOF metallic nodes. These findings, guided by X-ray and PDF analysis allowed to determine the structure of the nanoconfined species and evidenced an interaction between these species and the organic MOF linker. This interaction and the nanoconfinement alter the decomposition pathways and lower hydrogen release temperatures, pointing to new directions for MOF-based hydrogen storage materials [59].

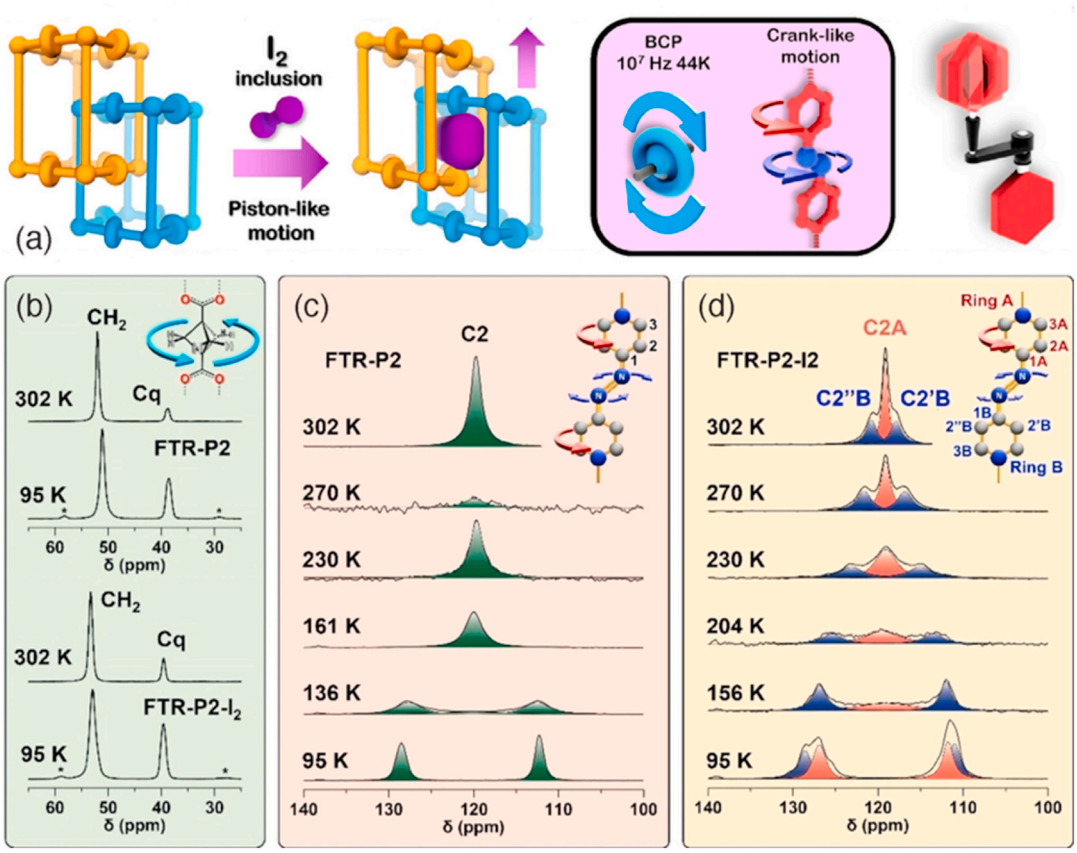

Fig. 12. Stimuli-responsive dynamics in a flexible pillared MOF. (a) Rotational motion of bicyclopentane (BCP), bipyridyl, and azopyridine (Azpy) units is triggered by external stimuli such as I_2 vapors and pressurized CO_2, enabling molecular-level motion within a pillared framework. (b–d) Variable-temperature ^{13}C CP MAS NMR spectra highlighting local dynamics: (b) BCP CH_2 and quaternary carbon signals in FTR-P2 (top) and FTR-P2-I_2 (bottom); (c) Azpy C2 signal in FTR-P2; (d) Azpy C2 signal in FTR-P2-I_2. Adapted with permission from Ref. [58]. © 2024 Wiley-VCH GmbH.

5.3. Catalysis and inorganic chemistry

Catalysis research benefits significantly from the ability of solid-state NMR to probe the structure and dynamics of active sites in complex and often disordered materials. Several user projects have used PANACEA access to uncover mechanistic insights and support the rational design of heterogeneous catalysts. Chen et al. focused on gallium-based propane dehydrogenation catalysts as sustainable alternatives to PtSn systems. Using DNP-enhanced NMR, they identified the formation and transformation of Ga species on silica surfaces. Their results highlighted the reversible formation of isolated [4]$Ga_{(4Si)}$ sites, which were correlated with high propene selectivity. This study exemplifies how surface-sensitive NMR can contribute to greener catalytic technologies [60]. Jabbour et al. explored porous polymer supports for organometallic Rh catalysts (Fig. 13a–c). Using a combination of ^{129}Xe NMR and DNP-enhanced spectroscopy, they resolved the structure of the catalyst environment within amorphous pores. This work shed light on how pore size and polymer functionalization affect substrate accessibility, enabling the design of more efficient supported catalysts [61].

Beyond catalysis, solid-state NMR has also enabled significant advances in materials synthesis and phase characterization. Korenko and co-workers investigated the molten Na_3AlF6-Y_2O_3 system as a low-temperature route for synthesizing YAG and Nd:YAG materials. Through a combination of thermal analysis and multinuclear solid-state NMR (^{19}F, ^{23}Na, ^{27}Al), the team elucidated the eutectic behavior of the system and tracked phase evolution across a wide composition range. These insights facilitated the synthesis of YAG at unprecedentedly low temperatures (as low as 630 °C), offering new possibilities for energy-efficient preparation of functional ceramics [63]. Expanding further into nanostructured materials, Gabbani et al. employed solid-state NMR to study charge carrier dynamics in plasmonic indium tin oxide (ITO) nanocrystals. NMR spectroscopy enabled the direct identification of surface-associated Sn sites, shedding light on the depletion layer and its effect on carrier density and mobility (Fig. 13d). These results offer key insights for tailoring the electronic properties of ITO nanostructures, with broad implications for optoelectronic and energy applications [62].

5.4. Pharmaceuticals and biomolecular systems

Solid-state NMR plays a crucial role in pharmaceutical research, particularly in the characterization of polymorphs, formulation stability, and molecular interactions in amorphous or heterogeneous systems. Through PANACEA, multiple users applied high-resolution MAS and DNP methods to understand structural properties relevant to drug efficacy and mechanism of action.

Jekhmane et al. investigated the action mechanism of the antimicrobial peptide plectasin, showing that it targets the bacterial membrane interacting with lipid II (Fig. 14), a peptidoglycan precursor of the bacterial cell-wall. The antimicrobial activity is strongly calcium-sensitive and significantly increases in the presence of Ca^{2+} ions. ^{43}Ca and ^{13}C solid-state NMR spectra revealed that plectasin forms fibrillar assemblies sequestering lipid-II and that calcium modulates its binding mode. Additionally, it was shown that the plectasin supramolecular structures lie onto the bacterial membrane surface possibly compromising its stability. These findings deepen our understanding of antimicrobial resistance and support the design of new host-defense peptides [64]. In another study, Shukla et al. examined clovibactin, a recently discovered antibiotic from an uncultured bacterium [65]. Their

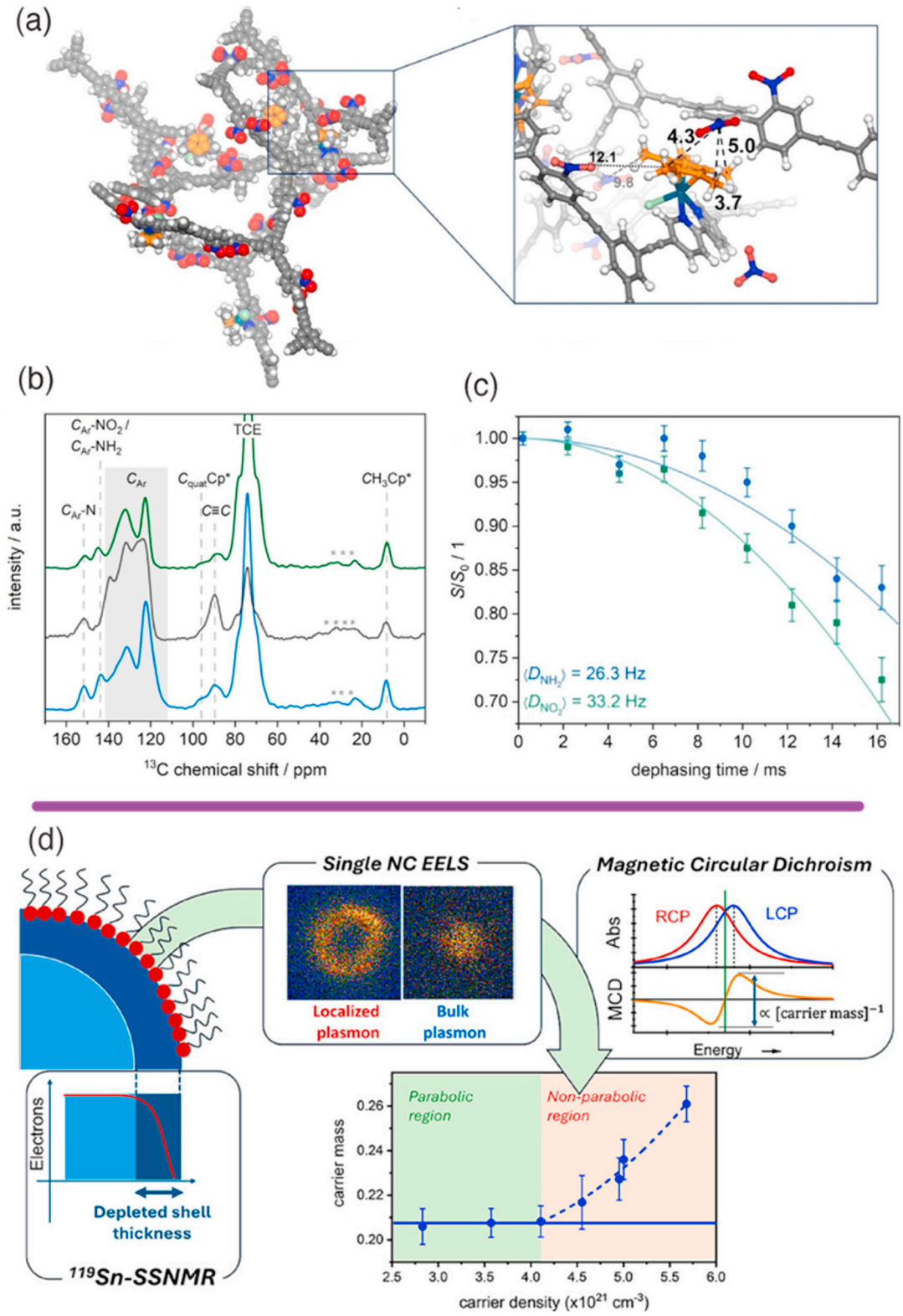

Fig. 13. (a–c) Advanced NMR methods combined with pair distribution function analysis and computational modeling reveal the coordination environment of $CpRh^{III}$ complexes grafted on functionalized porous organic polymers. (a) Representative structural models for CpRh@IV(NO_2); (b) DNP-enhanced ^{13}C CP MAS spectra of CpRh@V(NH_2) (blue), CpRh@BpyMP-1 (black), and CpRh@V(NO_2) (green); (c) Experimental $^{13}C\{^{15}N\}$ REDOR dephasing curves for CpRh@IV(NO_2) (green dots) and Cp*Rh@V(NH_2) (blue dots), overlaid with theoretical fits based on dipolar couplings from structural models. Adapted with permission from Ref. [61]. © 2023 The Authors. Angewandte Chemie International Edition published by Wiley-VCH GmbH. This is an open access article under the terms of the Creative Commons Attribution-NonCommercial License CC BY-NC 4.0. (d) A multimodal investigation combining solid-state NMR (^{119}Sn), electron energy loss spectroscopy (EELS), and magnetic circular dichroism (MCD) clarifies the charge carrier behavior in plasmonic indium tin oxide nanocrystals. Reproduced with permission from Ref. [62]. Copyright © 2024 American Chemical Society.

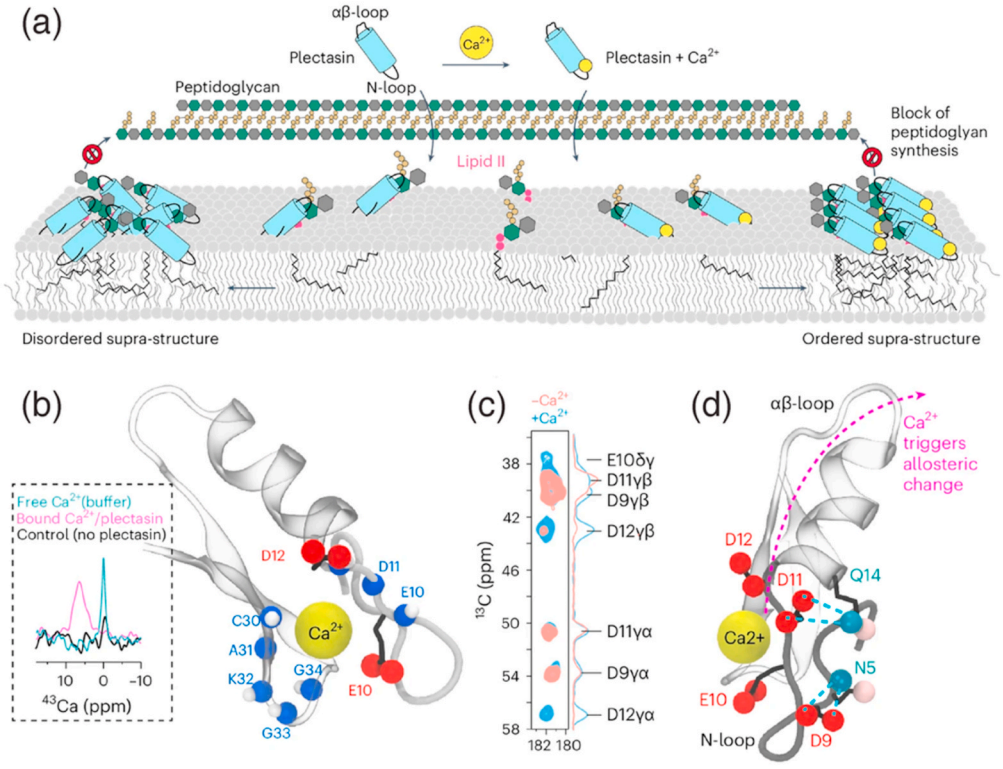

Fig. 14. Calcium-mediated binding mode of plectasin to lipid II. (a) Model of the Ca^{2+}-sensitive mode of action of plectasin. (b) Illustration of the ion-binding site with a ^{43}Ca solid-state NMR spectrum (magenta) of Ca^{2+} bound to the plectasin–lipid II complex in DOPG membranes. Control spectrum without plectasin (black) and spectrum of free Ca^{2+} in buffer (cyan) are shown for comparison. (c) Dipolar solid-state NMR data reveal rigidification of the anionic side chains E10 and D12 upon Ca^{2+} binding, supporting interaction of divalent ions with the complex. (d) Residues D9 and D11 define the conformation of the N-loop, while E10 and D12 coordinate Ca^{2+}. Adapted with permission from Ref. [64].

solid-state NMR experiments revealed that clovibactin, similarly to plectasin [64] and teixobactin [66], irreversibly binds the pyrophosphate group in lipid-II, blocking cell wall formation and forming fibrillar structures on the bacterial membrane. The pyrophosphate unit in lipid II is highly conserved throughout evolution, playing a crucial role in its stability. Unlike the amino acid–based portion of lipid II, it is not directly affected by mutations in the bacterial genetic code. Consequently, antibiotics targeting this immutable site show no detectable resistance, underscoring clovibactin's strong potential for new antibiotic development.

Solid-state NMR also holds great potential for studying biological drugs, particularly multispecific biologics that combine monoclonal antibodies with other protein fragments to enhance efficacy. Epitope mapping is essential for optimizing binding, production, and stability, yet traditional techniques like X-ray or cryo-EM struggle with the flexibility of these proteins. Fragai and co-workers demonstrated that solid-state NMR can overcome these limitations by mapping residue interactions in PD-L1 complex, highlighting its suitability for analyzing large, flexible biologics [67]. Advanced solid-state NMR methods were also applied to probe protein–drug conjugates, widely used in cancer therapy, consisting of cytotoxic molecules linked to carrier proteins through covalent or non-covalent interactions. Ligand-induced structural and dynamic changes that impact the stability of such assemblies were revealed by 2D ^{13}C–^{13}C and ^{13}C-^{15}N correlation experiments [68]. Another emerging area is protein frameworks—porous protein-based biomaterials with applications in medicine and technology. While typically characterized by X-ray techniques, solid-state NMR has shown promise for studying systems with low crystallinity, such as protein–macrocycle frameworks. Finally, unprecedented insight could be gained into the structure of porous protein-based biomaterials with applications in medicine and technology [69]. These examples demonstrate the routine applicability of modern solid-state NMR methods in pharmaceutical development, even for non-expert users.

5.5. *Nature-inspired and sustainable materials*

Nature-derived systems often pose structural challenges due to their heterogeneity and complex macromolecular architectures. Solid-state NMR is uniquely suited to probe such systems, offering chemical resolution without the need for crystallinity or labeling.

Poulhazan et al. investigated the molecular composition of velvet worm slime, a natural adhesive secreted by Onychophorans (Fig. 15a). Using DNP-enhanced solid-state NMR, they discovered that the slime contains phosphonate-rich glycoproteins, with conserved 2-aminoethyl phosphonate motifs. This finding not only challenges previous assumptions about protein phosphorylation but also provides inspiration for the design of recyclable bio-adhesives [70]. In a study related to environmental chemistry, Casey et al. used solid-state NMR to characterize Fe_2O_3 nanoparticles functionalized with amines for catalytic PET recycling. ^{13}C and ^{29}Si NMR confirmed ligand attachment and catalytic performance, demonstrating that molecular-level design of the catalyst surface directly improves depolymerization efficiency (Fig. 15b–e) [71]. Bravetti et al. took on the challenge of elucidating the structure of leucopterin, the white pigment in butterfly wings. By combining solid-state NMR, diffraction, and computational modeling, they resolved its solid-state packing and showed how its nanostructure contributes to optical properties, offering new insights into bioinspired photonic materials [72]. Finally, Bastos et al. explored the complex restructuring of yeast cell walls during beer brewing, focusing on the covalent connectivity between glycogen and other cell wall polysaccharides (Fig. 16). By combining DNP-enhanced solid-state NMR with selective enzymatic hydrolysis, they demonstrated that glycogen becomes covalently linked

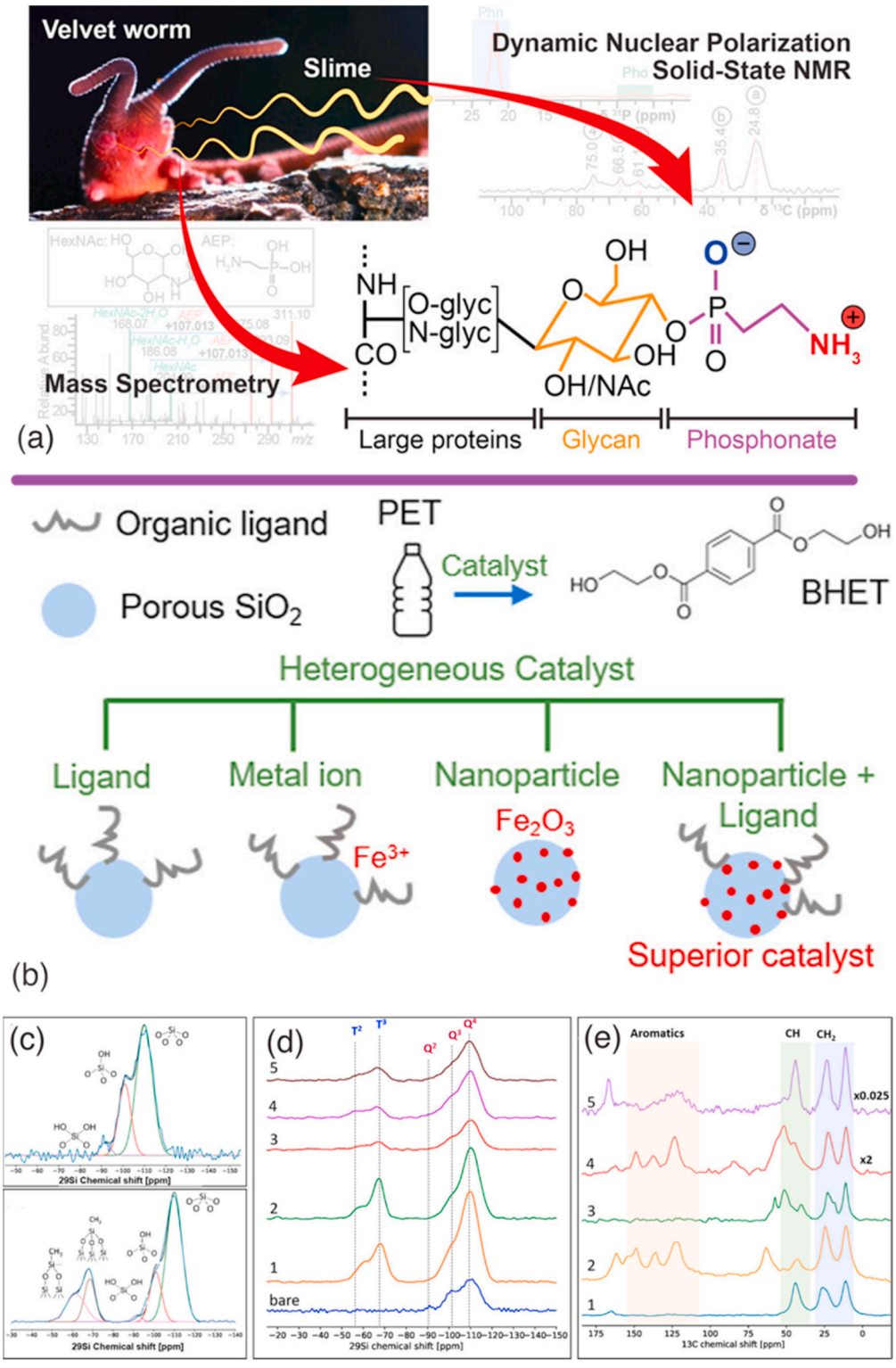

Fig. 15. (a) Analysis of velvet worm slime by solid-state NMR DNP offers insights into recyclable material design and highlights a unique, conserved protein. Reproduced with permission from Ref. [70]. Copyright © 2023 The Authors. Published by American Chemical Society. This publication is licensed under CC-BY 4.0. (b–e) NMR characterization of amine-functionalized Fe_2O_3/silica catalysts for enhanced PET recycling: (b) Fe_2O_3 nanoparticles functionalized with amine ligands significantly improve PET depolymerization efficiency compared to other catalysts; (c) 1D ^{29}Si MAS NMR spectra and their deconvolution for bare silica and SiO_2-NH_2 (1); (d) Stacked ^{29}Si MAS NMR spectra of all samples: bare silica, SiO_2-NH_2 (1), SiO_2-NH_2-SB (2), SiO_2-NH-NH_3 (3), SiO_2-NH-NH_2-SB (4), and SiO_2-pincer (5); (e) ^{13}C CP MAS NMR spectra of the functionalized silica with ligands (1) to (5). Adapted with permission from Ref. [71]. Copyright © 2023 The Authors. Published by American Chemical Society. This publication is licensed under CC-BY 4.0.

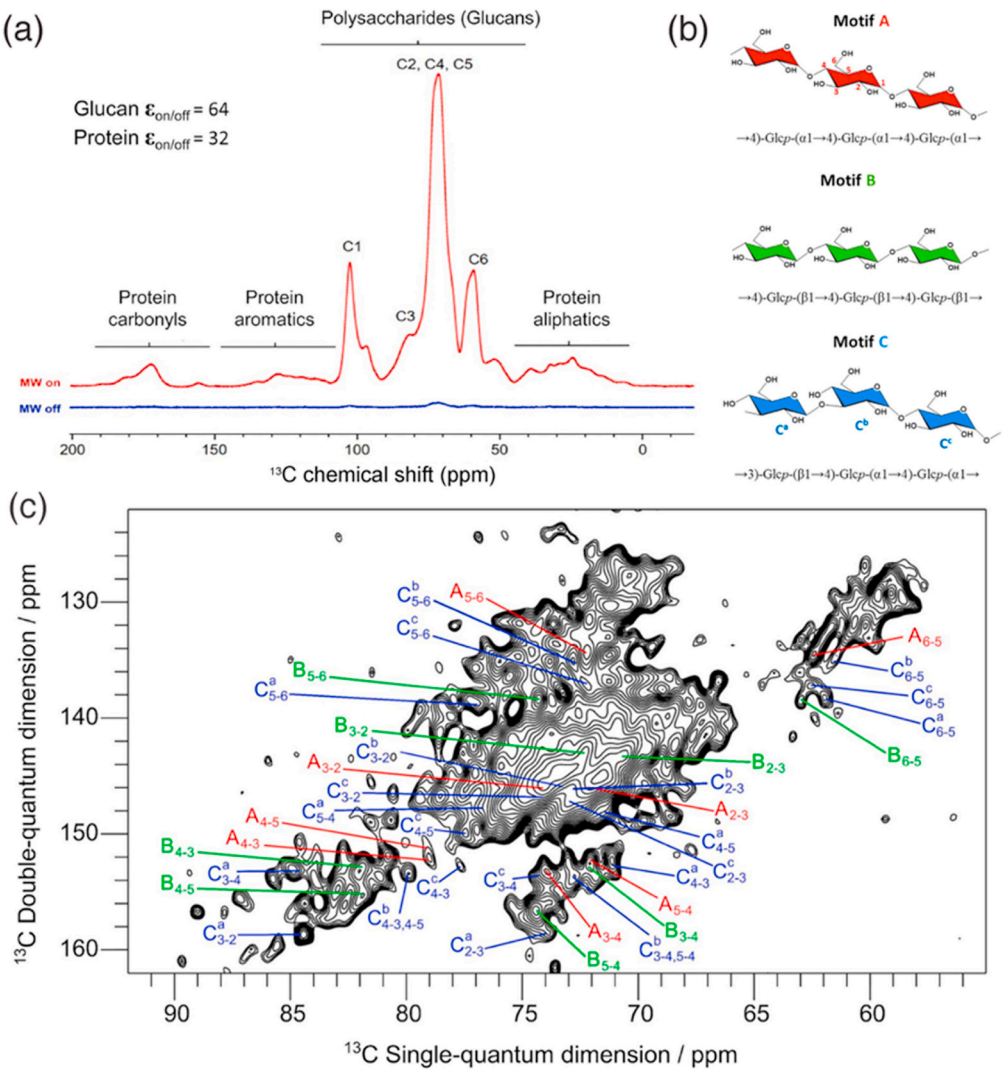

Fig. 16. MAS-DNP analysis of the alkali-insoluble glucan fraction from *S. pastorianus* and proposed structural motifs. a) ^{13}C CP spectra recorded with microwave irradiation ON (red) and OFF (blue); b) ^{13}C DQ dipolar INADEQUATE showing through-space correlations between dipolar-coupled carbons; c) glucan structural motifs identified in the fraction. Adapted with permission from Ref. [73]. © 2024 The Author(s). This article is licensed under a Creative Commons CC-BY-NC-ND license.

to (β1→3)-, (β1→4)-, and (β1→6)-glucans through multiple glycosidic motifs. These structural insights shed light on the molecular remodelling of yeast cell walls during fermentation and may inform the valorization of brewing by-products in bio-based materials [73].

6. Conclusions and outlook

PANACEA has demonstrated that solid-state NMR, once considered a specialist technique, can be transformed into a powerful, accessible tool for a wide chemistry community. By combining advanced instrumentation with coordinated access, user support, and targeted innovation, the project enabled impactful research across diverse fields. Looking ahead, sustaining and expanding this integrated infrastructure will be key to embedding solid-state NMR more deeply into chemical discovery, fostering cross-disciplinary applications, and advancing toward routine, open-access structural analysis in the solid state.

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.

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Data availability

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

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