

Review

Artificial Intelligence-Assisted Low-Field Benchtop NMR Spectroscopy: Analytical Applications, Challenges, and Perspectives

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Abstract

Low-field benchtop nuclear magnetic resonance (NMR) spectroscopy has emerged as an accessible analytical platform for rapid, routine, and application-oriented analysis. However, its broader analytical adoption remains constrained by intrinsic limitations, including reduced spectral resolution, severe signal overlap, and lower sensitivity compared with conventional high-field instruments. To address these limitations, artificial intelligence (AI), including machine learning and deep learning approaches, has increasingly been explored alongside conventional chemometric strategies to enhance information extraction from low-field spectral data. This review examines recent developments in AI-assisted benchtop NMR across three major application domains: classification and authentication, quantitative analysis, and spectral processing or automated interpretation. Current evidence suggests that classification and authentication currently represent the most mature application area, whereas quantitative analysis shows promising but often condition-dependent performance. In contrast, spectral reconstruction and automated interpretation remain comparatively early-stage and exploratory, despite their potential long-term relevance for addressing intrinsic information limitations. Key challenges, including limited dataset diversity, poor model transferability, validation pitfalls, limited interpretability, and the lack of benchmarking and standardized workflows, are critically discussed. Future progress will likely depend not only on advances in AI algorithms, but also on the development of robust, reproducible, and analytically meaningful workflows. Overall, AI-assisted benchtop NMR is evolving from proof-of-concept applications toward a more structured analytical framework for extracting chemically meaningful information from spectrally constrained low-field data.

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1. Introduction

Nuclear magnetic resonance (NMR) spectroscopy is a cornerstone analytical technique for molecular identification, structural elucidation, and quantitative analysis across chemistry, biology, and materials science. Conventional high-field NMR systems provide excellent spectral resolution and sensitivity, but their high cost, infrastructure requirements, and operational complexity generally restrict their use to specialized laboratories [1–4].

In contrast, low-field benchtop NMR spectrometers based on permanent magnets have substantially improved the accessibility of NMR spectroscopy by reducing instrument size, cost, and maintenance demands. Over the past decade, benchtop NMR has evolved from a niche alternative into a practical analytical platform for applications including food analysis, pharmaceuticals, process monitoring, metabolomics, and materials research [2–5]. These developments have positioned benchtop NMR as an attractive tool for rapid, routine, and application-oriented analysis.

Despite these practical advantages, the broader analytical utility of low-field benchtop NMR remains constrained by intrinsic spectral limitations. Reduced magnetic field strength leads to lower chemical-shift dispersion, more severe peak overlap, and lower sensitivity than in high-field instruments, making the interpretation of complex mixtures and the discrimination or quantification of chemically similar components more difficult [1–3,6]. As a result, the central analytical challenge in low-field NMR is often not spectrum acquisition itself, but the reliable extraction of chemically meaningful information from spectrally crowded and information-limited datasets.

To address these limitations, benchtop NMR has increasingly been combined with multivariate analysis and chemometric approaches capable of extracting latent information from complex spectral fingerprints. More recently, artificial intelligence (AI), including machine learning (ML) and deep learning (DL), has emerged as a complementary extension of these data-driven strategies. Unlike conventional peak-centered interpretation [2,7,8], AI-based approaches can exploit distributed spectral information and identify subtle patterns embedded within overlapping signals, making them particularly relevant for low-field NMR applications where analytically useful information is often not confined to well-resolved resonances.

This methodological shift is becoming increasingly evident in practical benchtop NMR applications. Recent studies have shown that low-field benchtop ^1H NMR combined with machine learning (ML) can support both classification and quantitative prediction tasks, including applications such as fatty acid profiling in meat products and compositional analysis of dairy samples [9,10]. These findings suggest that AI-based approaches may extend the analytical utility of low-field NMR beyond conventional limitations associated with reduced spectral resolution.

Recent reviews have highlighted broader developments in AI-enabled NMR spectroscopy, including biomolecular NMR, AI-assisted spectral reconstruction, and comprehensive perspectives on AI-enabled NMR methodologies, implementations, quality assessment, and prospects [11–13]. However, many of these discussions are based on high-field NMR or general method-development contexts, where richer spectral information and more established workflows provide favorable conditions for automated interpretation and reconstruction. Although these advances provide important methodological references for the future development of AI-assisted NMR, their direct translation to low-field benchtop NMR is not straightforward, because reduced spectral dispersion, stronger peak overlap, and lower information density impose distinct analytical constraints. Therefore, the role of AI in the specific analytical setting of low-field benchtop NMR remains less systematically discussed.

Accordingly, this review provides a structured overview of recent developments in AI-assisted low-field benchtop NMR, with emphasis on methodological foundations, representative analytical applications, current limitations, and future perspectives. Particular attention is given to how AI-based approaches may help address the intrinsic information constraints of low-field NMR, while critically considering challenges related to validation, interpretability, transferability, and analytical robustness. A conceptual overview of this framework is presented in Figure 1.

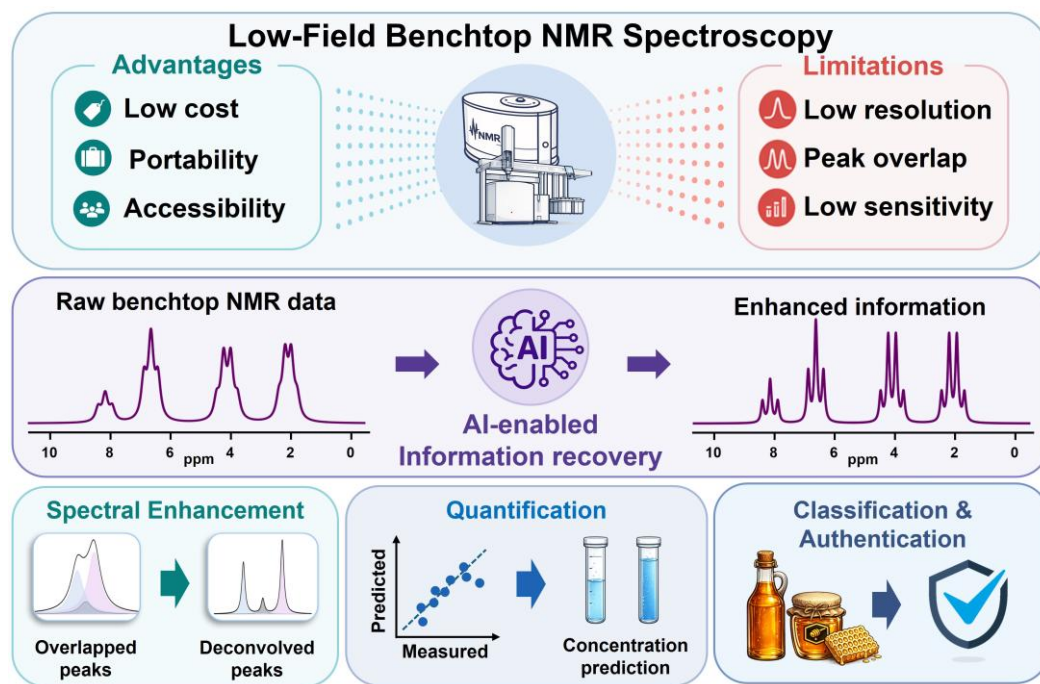


Figure 1. Schematic overview of AI-assisted low-field benchtop NMR spectroscopy and its analytical applications.

2. Low-Field Benchtop NMR and the Need for AI

Low-field benchtop NMR has significantly expanded access to NMR spectroscopy by reducing instrument size, cost, maintenance requirements, and operational complexity relative to conventional high-field systems [1,3,14,15]. These practical advantages have enabled broader deployment in routine laboratories, industrial settings, educational environments, and application-oriented analytical workflows. In this context, the value of benchtop NMR lies less in maximizing spectral performance than in providing accessible and operationally practical analytical capability.

However, these advantages are accompanied by intrinsic analytical constraints. Reduced magnetic field strength decreases chemical-shift dispersion, increases spectral overlap, and lowers sensitivity, thereby limiting the effective information content of acquired spectra [1,3,15]. In relatively simple samples, targeted analysis based on selected resonances may remain feasible. In more complex mixtures, however, analytically relevant information is often distributed across broad and overlapping spectral regions, making conventional peak-centered interpretation increasingly difficult.

This creates a distinctive analytical challenge for low-field NMR. Unlike high-field systems, where many analytical tasks can rely on well-resolved signals and direct spectral interpretation, benchtop NMR frequently requires the extraction of meaningful chemical information from compressed or partially resolved spectral patterns. As a result, the central limitation is often not data acquisition itself, but the reliable conversion of low-resolution spectral information into robust analytical outputs.

From this perspective, AI becomes particularly relevant because it enables spectra to be treated not only as collections of individually assigned resonances, but also as high-dimensional analytical fingerprints. AI-based approaches, including machine learning (ML) and deep learning (DL), can identify distributed spectral patterns, nonlinear relationships, and subtle signal variations that may not be readily accessible through conventional interpretation [6,7,15,16]. This capability is especially advantageous in low-field NMR, where analytically useful information is often encoded in overlapping composite spectral features rather than in isolated diagnostic peaks.

This rationale is further supported by the broader development of machine learning in NMR spectroscopy. Recent reviews have emphasized that AI methods are becoming increasingly important for feature extraction, spectral reconstruction, signal assignment, and automated prediction tasks across NMR application [6,7,17]. In the specific context of low-field benchtop NMR, these methodological advances are particularly meaningful because they directly address one of the principal barriers to broader analytical adoption: the difficulty of extracting reliable chemical information from spectrally constrained data.

Accordingly, AI should not be regarded simply as an optional computational add-on to benchtop NMR workflows. Rather, it represents a potentially enabling analytical strategy for extending the practical utility of low-field NMR beyond the limitations imposed by reduced spectral resolution and information density.

3. AI Methods and Preprocessing Strategies

3.1. Spectral Preprocessing for Benchtop NMR Data

The application of artificial intelligence (AI) to benchtop NMR begins not with model selection, but with the preparation of spectral data in a form suitable for robust computational analysis. Because benchtop spectra generally exhibit broader lines, reduced chemical-shift dispersion, and more extensive signal overlap than high-field NMR data, preprocessing has a particularly strong influence on downstream analytical performance [2,6,7].

Typical preprocessing steps include phase correction, baseline correction, spectral alignment, normalization, scaling, region selection, and binning. Binning refers to dividing an NMR spectrum into small contiguous chemical-shift intervals and representing each interval by an integrated or averaged signal intensity. This approach can reduce data dimensionality, average local noise, and provide some tolerance to minor peak shifts. However, it can also obscure peak shape, fine peak-position differences, and local multiplicity patterns. Inappropriate bin widths or bin boundaries may split a resonance between adjacent bins or cause the same resonance to be represented differently across samples when small chemical-shift variations occur [18]. These issues are particularly relevant in low-field NMR, where broader and more overlapped signals make the choice of bin width and alignment strategy especially important [2,6]. In low-field benchtop NMR, preprocessing is especially important because analytically relevant information is often embedded in crowded and partially overlapping spectral regions, making the definition of an appropriate feature space a critical component of analytical design.

3.2. Feature Representation and Input Construction

Following preprocessing, a key methodological decision concerns how spectral information is represented for model input. One approach uses the full spectrum directly, allowing models to learn distributed spectral patterns without extensive manual feature engineering. Alternatively, spectra may be transformed into reduced representations such as binned regions, integrated windows, or selected spectral features chosen for dimensionality reduction or analytical relevance [2,6,7].

This choice involves an important trade-off between information retention, computational simplicity, and interpretability. Full-spectrum inputs preserve richer spectral detail and may be advantageous when subtle distributed patterns are analytically informative. In contrast, reduced representations can simplify model training, improve robustness in smaller datasets, and facilitate interpretation, but may also discard diagnostically relevant information. In benchtop NMR, where useful analytical variation is frequently distributed across overlapping spectral regions, this balance becomes particularly important.

Recent application studies illustrate both strategies. For example, low-field ^1H NMR studies on food analysis have employed both direct spectral inputs and reduced feature

representations for classification and regression tasks, suggesting that optimal input design depends strongly on the analytical objective and dataset characteristics [9,10].

3.3. Machine Learning and Deep Learning Models

AI-assisted benchtop NMR builds upon the broader tradition of multivariate analysis and chemometrics in spectroscopic data interpretation. Established approaches such as principal component analysis (PCA), linear discriminant analysis (LDA), partial least squares discriminant analysis (PLS-DA), and partial least squares regression (PLSR) have long served as foundational tools for extracting analytical information from spectral fingerprints [2,6]. More recently, these approaches have increasingly been complemented by machine learning (ML) and deep learning (DL) methods capable of modeling more complex and nonlinear relationships.

Among conventional ML methods, support vector machines (SVMs) are widely used because they perform well in high-dimensional spectral spaces and can remain effective even with relatively modest dataset sizes. Tree-based ensemble models such as random forests (RFs) are also attractive because of their robustness to noise, ability to model nonlinear variable interactions, and provision of feature importance measures that may support chemical interpretation.

DL approaches provide a more flexible framework for directly learning relationships from spectral inputs. Artificial neural networks (ANNs) can capture nonlinear relationships between spectral features and analytical targets, whereas convolutional neural networks (CNNs) are particularly well suited to one-dimensional spectral data because they can learn local signal motifs and neighborhood relationships directly from the spectral trace [6,7,19]. These characteristics are particularly relevant in benchtop NMR, where analytically useful information is often encoded in subtle composite spectral patterns rather than in isolated well-resolved resonances.

An important emerging direction extends AI applications beyond sample-level prediction toward computational compensation for intrinsic spectral limitations. Recent neural network-based studies have explored low-field metabolite quantification, spectral denoising, and computational transformation of low-field spectra into high-field-like representations [20,21]. As illustrated in Figure 2, these proof-of-concept studies suggest that AI may contribute not only to analytical interpretation, but also to the recovery or enhancement of chemically useful spectral information. Although such approaches are not yet integrated into routine benchtop workflows, they highlight the broader potential of AI for computational enhancement of low-field NMR data.

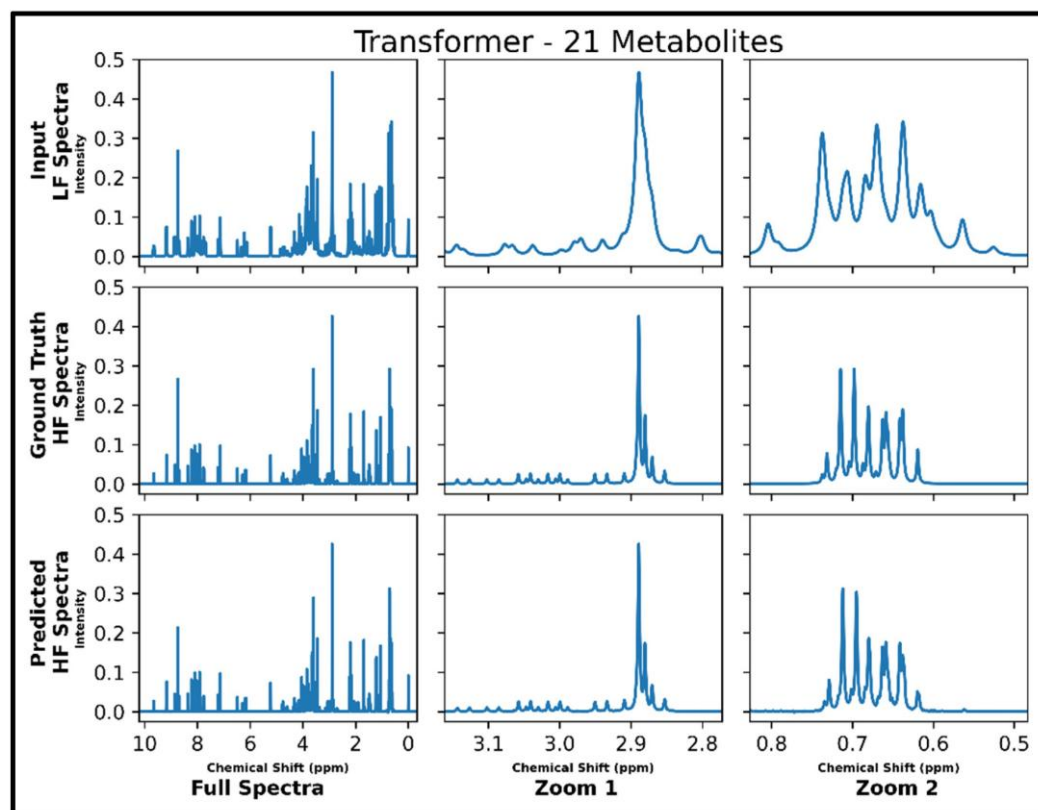


Figure 2. Transformer performance results for 100 MHz to 400 MHz conversion of one testing spectrum from the dataset of 21 metabolites. The top row shows the input LF spectrum, the middle row shows the ground-truth HF spectrum, and the bottom row shows the predicted HF spectrum. The left column shows the full spectra, and the middle and right columns show zoomed-in portions of the same spectra. Reprinted from Ref. [20], under CC BY license.

3.4. Validation Strategies and Methodological Considerations

As AI-assisted benchtop NMR develops, validation strategy becomes a central methodological consideration. Many current studies rely on relatively limited datasets, meaning that apparent model performance may be strongly influenced by data partitioning, replicate handling, preprocessing design, and experimental correlation structures [6,7].

This issue is especially critical in benchtop NMR because spectra from the same sample, batch, or acquisition series may be highly correlated. If replicate scans are distributed improperly across training and test sets, model performance may be overestimated. Similarly, if preprocessing is performed before rather than within validation loops, information leakage can occur. These concerns are not unique to benchtop NMR, but their practical impact is magnified when datasets are small and spectral differences are subtle [6,7].

Accordingly, reliable evaluation of AI-assisted benchtop NMR requires validation strategies that reflect true analytical generalization rather than dataset-specific pattern recognition. Across all methodological choices, the analytical value of AI depends not simply on algorithmic sophistication, but on the coherence of the entire workflow, including preprocessing, feature construction, model selection, and validation design.

4. Applications of AI-Assisted Low-Field NMR

Recent applications of AI-assisted benchtop NMR can be broadly categorized into three areas: classification/authentication, quantification/regression, and spectral processing or automated interpretation. Among these, classification-oriented applications are

currently the most mature, because benchtop spectra often retain sufficient global compositional information for pattern recognition even when individual resonances are not fully resolved. Quantitative applications are also expanding, particularly in food and compositional analysis, whereas spectral reconstruction and automated interpretation remain comparatively exploratory but are strategically important because they more directly address the intrinsic information limitations of low-field NMR [5,6].

4.1. Classification, Discrimination, and Authentication

At present, one of the most established applications of AI- and chemometrics-assisted benchtop NMR is sample classification, discrimination, and authenticity assessment. In these applications, the analytical objective is not necessarily the complete resolution of individual resonances, but rather the discrimination of sample classes based on distributed spectral fingerprints. This characteristic makes benchtop NMR particularly suitable for applications such as food authenticity evaluation, adulteration detection, and supplement screening, where global compositional differences can remain analytically informative despite limited spectral resolution [5,22,23]. Representative studies in this category are summarized in Table 1.

Table 1. Representative studies on classification, discrimination, and authentication using AI-assisted benchtop NMR.

Target	NMR Method	AI Model	Main Content	Reference
Argan oil	60 MHz	Nearest-neighbour class model	High-throughput authenticity screening and compositional assessment of argan oil	[22]
Honey	59.7 MHz	PLS-DA	Detection and classification of adulterated honey-based supplements	[23]
Avocado oil	60 MHz	PCA, PLS-DA	Authentication and discrimination of avocado oil from other edible oils	[24]
Milk	43 MHz	ANN	Classification of milk samples by origin and production-related properties using NMR-derived features	[25]
Olive oil	60 MHz	PLS-DA	Authentication and classification of olive oil	[26]
Vegetable oils	100 MHz	PLS-DA	Classification and authentication of vegetable oils	[27]
Dietary supplements	59.7 MHz	PLS-DA	Detection and classification of adulterated slimming dietary supplements containing pharmaceutical compounds	[28]

As shown in Table 1, most classification and authentication studies have focused on food and supplement applications. A common feature across these reports is the reliance on overall spectral fingerprints rather than a small number of isolated marker peaks. For example, the argan oil study demonstrated that 60 MHz benchtop ^1H NMR spectra of neat oils contain sufficient information for both compositional assessment and authenticity screening [22]. Related chemometric approaches have also been used to classify pharmaceutical-adulterated honey-based supplements [23]. Similar approaches have been applied to avocado oil authentication [24], illustrating how fingerprint-based analysis can support practical screening tasks.

More recent studies further extend this approach. Benchtop ^1H NMR combined with multivariate or neural-network-based analysis has been used to classify milk samples according to origin and production-related properties [25], to distinguish extra virgin olive oil from other edible oils [26], and to perform preliminary screening of broader vegetable

oil categories [27]. A related strategy has also been applied to the detection of pharmaceutical adulterants in slimming dietary supplements [28]. These examples suggest that classification tasks can be effectively addressed even when spectral resolution is limited, provided that relevant information is encoded in the overall signal profile.

Taken together, these studies indicate that classification and authentication currently represent one of the most practically developed application areas for AI-assisted benchtop NMR. This may be attributed to the fact that classification models rely primarily on pattern recognition across the full spectrum, rather than on the precise resolution of individual resonances, making them inherently compatible with the spectral characteristics of low-field NMR data.

4.2. Quantification and Regression Analysis

Quantitative analysis represents a more demanding application area than classification because it requires stable and transferable relationships between spectral inputs and concentration-related variables despite peak overlap, reduced dispersion, and baseline variation. AI-assisted regression is therefore particularly informative in the benchtop NMR context, as it tests whether useful quantitative information can be extracted from partially resolved low-field spectra [6,9,10]. Representative studies are summarized in Table 2.

Table 2. Representative studies on quantification and regression using AI-assisted benchtop NMR.

Target	NMR Method	AI Model	Main Content	Reference
Milk	100 MHz	ANN, PLS-R	Quantitative determination of milk fat and lactose-related classification	[9]
Pork	80 MHz	KNN, RF, GBRT, GLM, SVM, SVM-RBF	Simultaneous classification and fatty-acid-related quantification from one spectral dataset	[10]
Simulated metabolomics	100 MHz	MLP, Transformer	Spectral conversion to improve downstream low-field quantification	[20]
Avocado oil	60 MHz	PLS-R	Authentication with compositional information relevant to quantitative assessment	[24]
Vegetable oils	100 MHz	PLS-R	Quantitative analysis of oil composition and adulteration	[27]
Crude oil	60 MHz	PLS-R	Rapid quantitative characterization of crude oil properties from benchtop ^1H NMR spectra	[29]
Reactants	43 MHz	ANN	ANN-based quantification for online reaction monitoring	[30]

As summarized in Table 2, current studies can be broadly grouped into two approaches. One approach relies on experimental benchtop spectra for direct regression analysis, as illustrated by studies on pork lipid composition, milk and avocado oil analyses [9,10]. In these cases, a single low-field ^1H NMR dataset has been used to support both classification and quantitative prediction, suggesting that compositional information can be encoded in the overall spectral profile even when individual peaks are not fully resolved. A related observation has been reported in vegetable oil studies, where benchtop NMR enabled the prediction of selected major compositional parameters, particularly those associated with fatty-acid content, although with somewhat lower accuracy than high-field measurements [27]. As shown in Figure 3, Kern et al. demonstrated the use of 43 MHz low-field ^1H NMR combined with ANN-based regression for quantitative online reaction monitoring. The predicted component areas of four reactants were compared

with 500 MHz NMR reference data, illustrating the potential of AI-assisted low-field NMR for process-oriented quantitative applications [30].

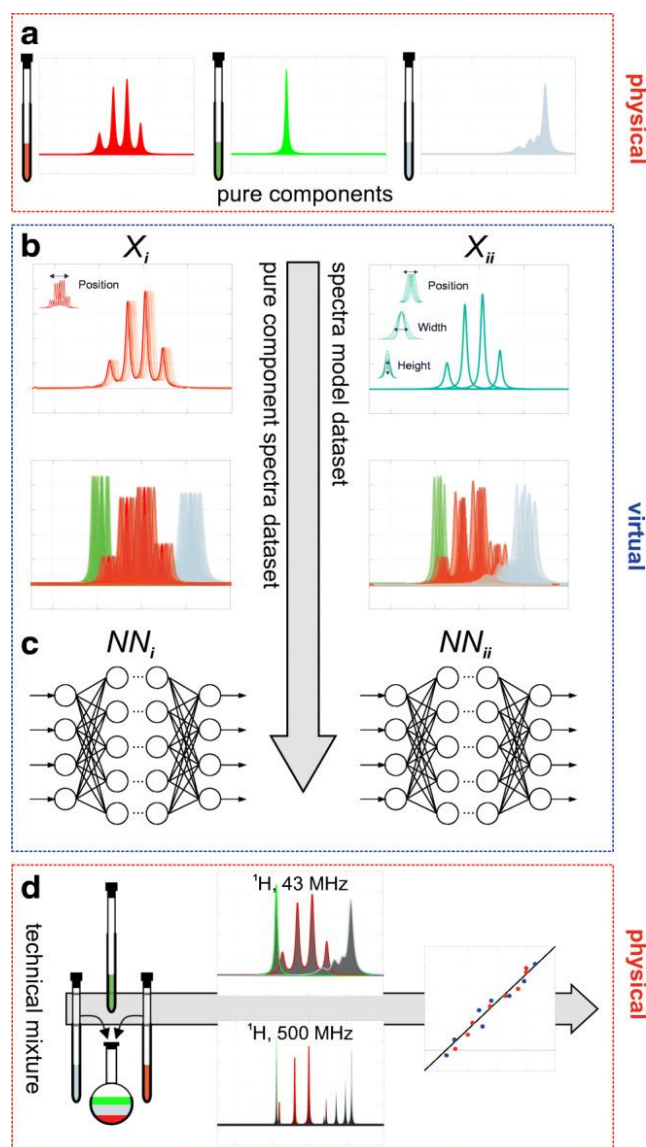


Figure 3. Workflow of ANN-assisted quantitative analysis using low-field NMR for online reaction monitoring. (a) Acquisition of pure-component ^1H NMR spectra for individual chemical species. (b) Generation of synthetic training datasets from experimentally measured pure-component spectra (X_i) and spectral models based on peak-function representations (X_{ii}). (c) Development and training of two independent artificial neural network (ANN) models using the synthetic spectral datasets. (d) Application of the trained ANN models to quantitative analysis of reaction mixtures using 43 MHz low-field ^1H NMR spectra, followed by comparison with indirect hard modeling (IHM) and 500 MHz high-field ^1H NMR reference data. The results demonstrate the potential of AI-assisted low-field NMR for process-oriented quantitative applications. Reproduced from Ref. [30], licensed under CC BY 4.0.

A second approach involves computational or simulation-based strategies aimed at improving the quantitative usability of low-field spectra. For example, recent studies have explored AI-assisted analysis across different magnetic field strengths using both simulated and experimental datasets. Johnson et al. demonstrated that metabolite quantification can be reliably performed directly from simulated low-field (100 MHz) spectra using neural networks, while other studies using experimental 60 MHz data showed that

machine-learning performance can approach high-field levels when appropriate spectral preprocessing is applied. Taken together, these findings suggest that although low-field NMR suffers from intrinsic spectral limitations, AI-based approaches can effectively mitigate these constraints and enable reliable chemical analysis [20,21]. While these studies are not directly equivalent to routine analytical workflows, they provide insight into how AI-based methods may extend the effective information content of low-field data.

Additional applications further illustrate the potential of regression-based analysis. In crude oil characterization, 60 MHz benchtop ^1H NMR combined with partial least squares regression has been used to predict refinery-relevant properties such as API gravity, sulfur content, total acid number (TAN), and distillation yields [29]. These results suggest that even highly overlapped low-field spectra may contain sufficient multivariate information to support practical quantitative predictions in complex industrial systems.

Taken together, these studies indicate that quantitative analysis using benchtop NMR is feasible under certain conditions, particularly when the target variables are strongly correlated with global spectral features. However, compared to classification tasks, quantitative applications appear to be more sensitive to spectral quality, preprocessing design, and model selection, reflecting the additional requirement for stable and transferable relationships between spectral data and concentration-related variables.

4.3. Spectral Processing, Reconstruction, and Automated Interpretation

A third application direction involves the use of AI not only for classification or quantitative prediction, but also for computationally addressing the intrinsic spectral limitations of benchtop NMR. This includes spectral processing, resolution enhancement, and automated interpretation workflows. Compared with classification and regression, this area remains less mature, but is strategically important because it directly addresses the limited spectral resolution and information density of low-field NMR data [6,20,21]. Representative studies are summarized in Table 3.

Table 3. Representative studies on spectral processing, reconstruction, and automated interpretation using AI-assisted benchtop NMR.

Target	NMR Method	AI Model	Main Content	Reference
Simulated metabolomics	100 MHz	Transformer	Spectral conversion to improve downstream low-field quantification	[20]
Simulated metabolomics	Simulated ^1H NMR (400 MHz, validated at 100 & 800 MHz)	MLP, CNN, Transformer	Optimization of direct metabolite quantification from simulated NMR spectra	[21]
New psychoactive substances	80 MHz	CNN	Nontargeted screening of new psychoactive substances in low-S/N benchtop data	[31]
Structural group elucidation of unknown mixtures	60 MHz	DSM	Automated NMR fingerprinting for structural group assignment in mixtures with data augmentation for improved low-field interpretation.	[32]
Organic mixtures	80 MHz	SVC	Automated structural group assignment for complex mixtures	[33]

As shown in Table 3, studies in this area remain methodologically diverse. Simulation- and computation-based investigations provide initial proof-of-concept evidence that AI may support not only interpretation of low-field spectra, but also computational recovery or enhancement of analytically useful spectral information [20,21]. Although these approaches are not yet equivalent to routine benchtop analytical workflows, they

illustrate a potentially important direction for overcoming information loss associated with reduced magnetic field strength.

More direct analytical applications have also been reported. Deep learning-based methods have been applied to the screening of complex mixtures such as new psychoactive substances, where low signal-to-noise ratios and extensive spectral overlap create substantial analytical challenges [31]. In such contexts, AI appears capable of extracting diagnostically relevant patterns even when conventional interpretation is difficult.

Beyond mixture fingerprinting and automated screening, AI-assisted spectral processing methods such as denoising, reconstruction, and baseline correction are emerging in broader NMR and magnetic resonance research [34,35]. However, their direct validation in low-field benchtop FT-NMR workflows remains limited, and their practical analytical utility for compact benchtop systems requires further investigation.

More exploratory studies have also examined AI-assisted structural interpretation workflows. One study employed a 60 MHz benchtop NMR instrument combined with a deep set model (DSM) to assign structural group information from ^1H , ^{13}C , ^{13}C DEPT, and HSQC spectra [32]. As shown in Figure 4, another study employed a support vector classifier (SVC) for automated NMR fingerprinting and structural group assignment using ^1H , ^{13}C , and ^{13}C DEPT spectra, and validated the approach using mixture spectra acquired at 80 MHz on a benchtop NMR spectrometer [33]. In both cases, predicted structural-group profiles showed reasonable agreement with the composition of test mixtures, suggesting that partial automation of spectral interpretation may be feasible under controlled conditions.

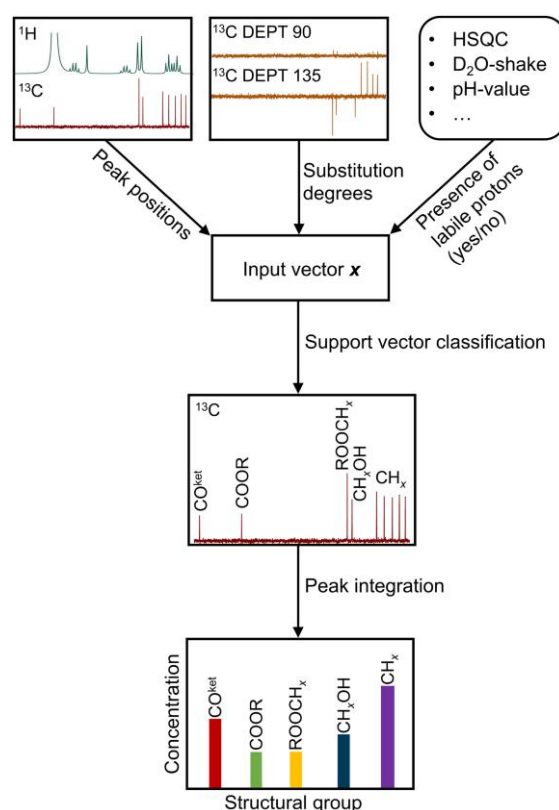


Figure 4. Workflow of the developed NMR fingerprinting method using an SVC for predicting structural groups based on spectral information from ^1H , ^{13}C , and ^{13}C DEPT NMR spectra as well as using binary information about the presence or absence of labile protons in the sample Reprinted from Ref. [33], under CC BY license.

At present, most AI-assisted benchtop NMR applications remain focused on proton spectroscopy. Although benchtop instruments are capable of heteronuclear measurements and more advanced experiments, AI-assisted applications in these areas remain limited. Accordingly, such directions are better regarded as emerging opportunities rather than established analytical practice.

Taken together, the studies reviewed in this section suggest that AI-assisted benchtop NMR is evolving from largely application-specific proof-of-concept studies toward more structured analytical use. Although many current implementations remain dependent on specific datasets and experimental conditions, they collectively demonstrate that meaningful chemical information can be extracted from spectrally constrained low-field data through appropriate computational strategies [30,32,36]

5. Challenges and Limitations of AI-Assisted Low-Field NMR

Despite the growing promise of AI-assisted benchtop NMR, several important challenges continue to constrain its broader analytical adoption. These limitations arise not only from the intrinsic spectral characteristics of benchtop instruments, but also from dataset design, validation strategy, model interpretability, transferability, and the lack of standardized workflows. Accordingly, the central challenge is no longer simply whether benchtop NMR can generate analytically useful data, but whether AI-based analysis can be implemented in a robust, transferable, and chemically meaningful manner [2,6]. The following subsections therefore consider these issues not as isolated technical limitations, but as interrelated factors that determine whether reported model performance can be translated into reliable analytical use.

5.1. Limited Dataset Size and Restricted Representativeness

One of the most persistent challenges in AI-assisted benchtop NMR is the limited size and diversity of many published datasets. In contrast to large-scale machine learning applications, benchtop NMR studies often rely on relatively narrow experimental datasets involving limited sample numbers, classes, or concentration ranges. Under such conditions, apparently strong classification or regression performance may reflect dataset-specific characteristics rather than broad analytical generalizability [6,37].

Beyond the nominal dataset size, the effective number of independent observations may be smaller when replicate measurements, spectra from the same batch or product, or systematically prepared mixture series are included [5]. If such spectra are randomly partitioned at the spectral level, closely related observations may appear in both training and test sets, potentially leading to optimistic performance estimates. Validation at an independent sample, product, batch, or source level is therefore important for assessing generalizability.

This issue is particularly important because many benchtop NMR applications target real-world materials such as foods, supplements, oils, or biofluids, whose compositions may vary substantially across origin, batch, season, processing history, or storage conditions. Models trained on restricted datasets may therefore capture local compositional regularities rather than robust analytical relationships. In practical terms, many current studies remain more convincing as proof-of-concept demonstrations than as evidence of broadly deployable analytical performance [5,38].

5.2. Instrument Effects, Preprocessing Dependency, and Poor Transferability

A second major challenge is the sensitivity of benchtop NMR workflows to instrument effects and preprocessing choices. Because benchtop spectra exhibit broader lines, lower dispersion, and greater signal overlap than high-field spectra, relatively small differences in phase correction, baseline treatment, normalization, or feature representation

can substantially influence model behavior. As a result, preprocessing dependency can become a major source of variability and reduced reproducibility across studies [2,6].

These issues become even more pronounced when models are transferred across instruments or laboratories. Gunning et al. demonstrated that inter-instrument differences in 60 MHz ^1H NMR spectra of edible oils were sufficient to compromise direct transfer of classification models trained on raw data, requiring mitigation through preprocessing strategies such as piecewise direct standardization, standard normal variates, or rank transformation [39]. These findings indicate that transferability cannot be assumed even between nominally similar benchtop platforms, representing a major barrier to practical deployment.

5.3. Validation Strategy and Analytical Robustness

The increasing use of AI also raises important concerns regarding validation and analytical robustness. In relatively small benchtop NMR datasets, model performance may be strongly influenced by data partitioning strategy, sample correlation, and insufficient independent validation [6].

Such concerns are especially relevant in datasets built from replicate spectra or systematically prepared mixture series, where spectral-level random partitioning may place closely related observations in both training and test sets [5,40]. Accordingly, validation should, where possible, be organized at the independent product, source, or sample level and supported by provenance-diverse or blind test samples, as illustrated in studies that explicitly considered source variation or applied blind workflow validation [22,37].

From an analytical perspective, strong statistical performance under constrained validation conditions does not necessarily translate into reliable real-world analytical performance. Practical applications require robustness against matrix variation, batch effects, instrumental drift, and other experimental sources of variability. This is particularly important for applications such as routine identification, process monitoring, or decentralized analysis.

Napolitano et al. noted that broader adoption of benchtop NMR for rapid automated identification remains limited not only by instrumental constraints such as reduced sensitivity and spectral dispersion, but also by challenges in workflow automation and robustness [37]. Accordingly, validation in AI-assisted benchtop NMR should be understood not only as a computational requirement but also as an analytical one. External validation and robustness testing under realistic analytical conditions are therefore essential, rather than relying solely on internal performance metrics.

5.4. Limited Interpretability and Uncertain Chemical Meaning

Another major challenge concerns model interpretability. Although machine learning and deep learning approaches may improve predictive performance, it is not always clear which spectral features drive model decisions or whether these relationships reflect chemically meaningful variation rather than dataset-specific artifacts. This issue is particularly relevant in benchtop NMR, where extensive spectral overlap complicates direct chemical interpretation [6,41].

More broadly, explainability is increasingly recognized as an important requirement across spectroscopic AI applications. Recent reviews of explainable artificial intelligence (XAI) in spectroscopy have noted that such methods remain relatively underutilized and are often adapted from approaches originally developed for image-based applications [41]. In benchtop NMR, limited spectral resolution further complicates interpretation of attribution maps or feature importance analyses. This raises an important methodological question as to whether model predictions reflect chemically meaningful variation or merely statistical correlations within the available dataset. Predictive performance alone

is insufficient to establish that an AI model has captured chemically meaningful variation. Model outputs should be considered analytically credible only when important spectral regions are consistent with known resonances or plausible compositional differences, reproducible across independent samples or experimental conditions, and stable against reasonable changes in preprocessing or validation strategy. Conversely, high accuracy based on unstable or chemically ambiguous features may reflect dataset-specific optimization rather than robust analytical interpretation. Therefore, performance metrics should be interpreted together with chemically informed attribution, external validation, and robustness testing.

Recent benchtop NMR studies illustrate both progress and remaining gaps in model interpretability. Some classification and screening studies have primarily emphasized predictive performance or chemometric class separation, with limited formal feature-attribution or XAI analysis to clarify which spectral variables drive model decisions [23,25,28]. In contrast, other studies have begun to relate discriminating spectral regions to chemically plausible signals, such as fatty-acid-associated regions in edible-oil classification, and recent deep learning-based screening of new psychoactive substances indicates a move toward chemically informed interpretation [26,31]. These examples suggest that high predictive accuracy or class separation should not be treated as self-evident chemical explanation. Addressing this challenge will require stronger links between AI outputs, spectral assignment, and analytically defensible decision frameworks [6,41].

5.5. Standardization, Reporting Quality, and Translation to Real-World Practice

A further challenge lies in the lack of standardized protocols for sample handling, acquisition, preprocessing, and reporting. This issue is well recognized in NMR metabolomics and becomes even more critical when benchtop NMR is combined with AI, because model outputs may be highly sensitive to upstream variation introduced during sample preparation or acquisition [42,43].

These considerations are directly relevant to benchtop NMR. Reviews of biomedical benchtop NMR have noted that, although compact systems show promising diagnostic performance in several contexts, broader translation depends on continued hardware development, improved pulse sequences, and more robust integration of computational methods [38]. In this sense, successful implementation requires not only improved algorithms, but also standardization of the full analytical workflow. Without such standardization, the reproducibility and transferability of AI-assisted benchtop NMR remain inherently limited [38,42,43].

Overall, the current literature suggests that the principal limitations of AI-assisted benchtop NMR extend beyond instrumental constraints such as reduced sensitivity and spectral resolution. Rather, they reflect a broader methodological challenge: translating information-limited low-field spectral data into reliable, interpretable, and transferable analytical outcomes. Addressing these limitations will require coordinated advances in dataset design, validation practice, preprocessing robustness, model interpretability, and reporting standardization [2,6,37–39,41–43].

6. Future Perspectives

The future development of AI-assisted benchtop NMR will depend largely on whether current methodological limitations can be translated into practical opportunities for analytical improvement. As summarized in Figure 5, future progress is unlikely to depend solely on increasingly complex algorithms, but rather on the integration of computational methods with robust analytical workflows, improved data practices, and application-oriented validation strategies [4,6,44].

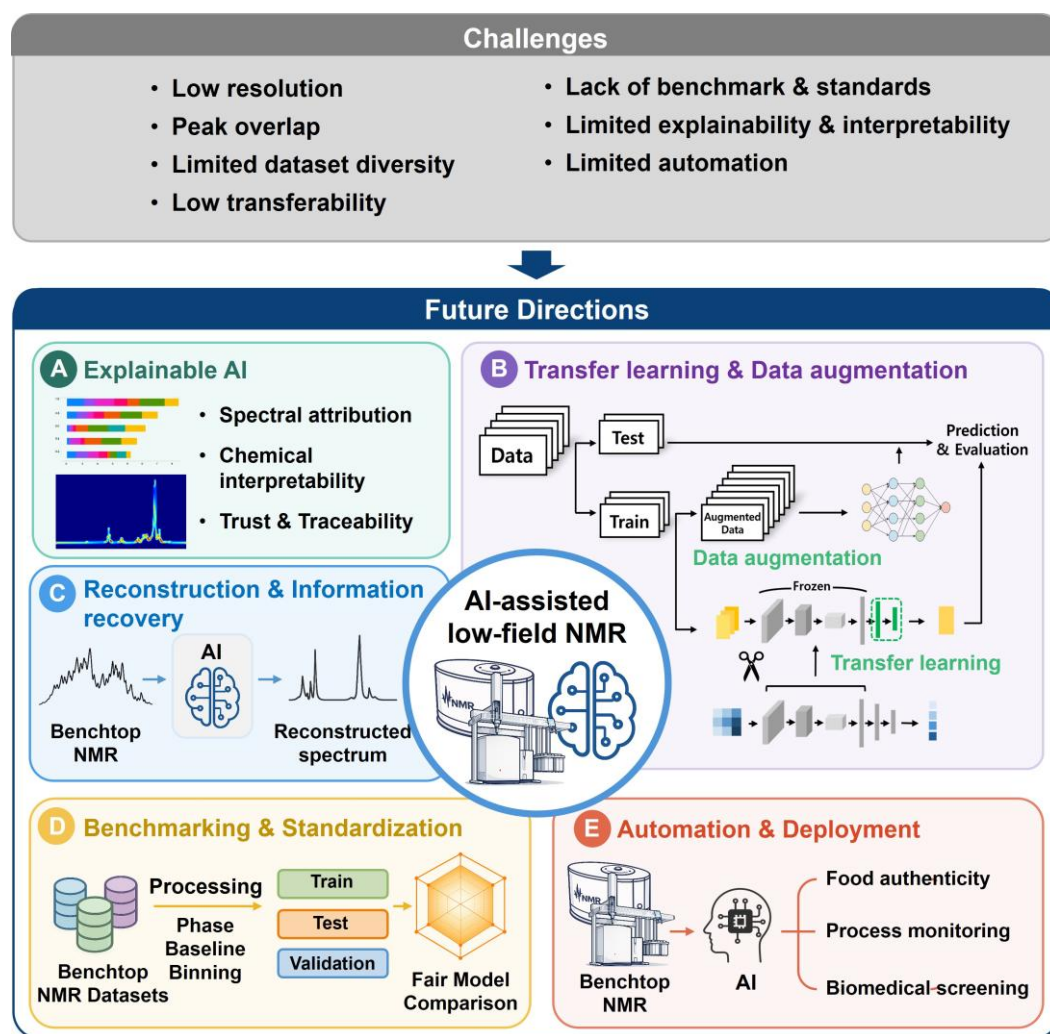


Figure 5. Challenges and future directions of AI-assisted low-field benchtop NMR.

One important direction involves improving model interpretability. As discussed in Section 5, limited explainability remains a barrier, particularly in applications requiring traceability, analytical confidence, or regulatory acceptance [41]. Future progress will likely require stronger connections between AI outputs and chemically meaningful spectral features, especially in low-field benchtop NMR, where spectral overlap complicates direct interpretation. Emerging XAI approaches, including SHAP-based feature attribution, integrated gradients, and attention-based interpretation, may help relate model decisions to relevant spectral regions [26,31,45,46]. In parallel, uncertainty quantification may provide an additional reliability layer by flagging low-confidence or potentially over-confident predictions and supporting more risk-aware interpretation of AI-assisted NMR outputs [11,47]. Because uncertainty-aware modeling has not yet been established in low-field benchtop NMR, future studies should validate uncertainty estimates under practical analytical conditions, including independent samples, matrix variation, instrumental variability, and preprocessing-dependent effects.

A closely related priority is improving model transferability and data efficiency. Many current benchtop NMR studies rely on relatively small, application-specific datasets, and model performance may depend strongly on instrument-specific or experimental conditions [36,39]. In this context, transfer learning, data augmentation, synthetic dataset generation, and simulation-to-experiment strategies may provide practical routes toward more robust and transferable analytical models [48,49]. In low-field benchtop NMR, synthetic spectra generated from pure-component spectra and physically

motivated spectral models have been used to train neural networks for quantitative online reaction monitoring [30]. Simulated low-field spectra have also recently been used for neural-network-based low-to-high-field spectral transformation and metabolite quantification, illustrating their potential value under data-limited conditions [20,21]. In high-field NMR contexts, synthetic NMR signals have been used to train deep neural networks for accelerated reconstruction of non-uniformly sampled multidimensional spectra [50]. Broader NMR studies, including FID-Net-based spectral reconstruction/virtual decoupling and machine-learning-assisted structure elucidation using simulated or predicted spectra, provide further methodological precedents [51]. However, simulated spectra may not fully reproduce experimental noise structures, matrix effects, instrumental variability, baseline distortions, or preprocessing-dependent artifacts. Therefore, synthetic-data strategies should be regarded as complementary tools for pretraining, augmentation, and robustness testing rather than substitutes for validation with independent experimental low-field benchtop NMR data.

Another important opportunity lies in computational compensation for intrinsic spectral limitations. While most current applications focus on classification or regression using acquired spectra, relatively few directly attempt spectral enhancement, signal separation, or information recovery [20]. Future advances in spectral reconstruction, denoising, baseline correction, signal separation, and related computational enhancement strategies may therefore expand the analytical capabilities of low-field benchtop NMR. Recent AI and deep-learning approaches have shown promising results for denoising, reconstruction, and information recovery across broader NMR applications [11,35,51,52]. In addition, decomposition-based approaches may help resolve overlapping signals and improve spectral interpretability [53]. AI-enabled pure-shift NMR also represents a promising example of computational spectral enhancement. Recent deep-learning studies have demonstrated accelerated pure-shift reconstruction and improved apparent spectral resolution by suppressing homonuclear J-coupling patterns and reducing multiplet complexity [54,55]. In parallel, recent benchtop NMR studies indicate that pure-shift methods may be useful for simplifying crowded spectra in compact low-field systems. However, the practical utility of these approaches for low-field benchtop FT-NMR remains largely unexplored and will require validation under realistic analytical conditions. Advanced computational deconvolution and signal-separation approaches may also complement future AI-assisted low-field benchtop NMR workflows. Recent Bayesian model-based and decomposition-based methods have shown potential for quantitative analysis, spectral deconvolution, signal separation, and noise reduction in overlapped NMR spectra [56,57]. Although not all of these approaches are deep-learning models, they may help extract analytically useful information from low-resolution spectra and should be evaluated in future low-field benchtop NMR studies.

AI-enabled interpretation may also extend toward inverse spectral problems, including molecular structure prediction from low-field benchtop NMR spectra. Recent machine-learning studies using conventional NMR data have shown promising progress in automated structure elucidation [58]. However, reduced spectral dispersion, extensive signal overlap, and limited low-field training datasets currently constrain *de novo* structure prediction in low-field benchtop NMR. At present, AI is more realistically positioned for structural-group assignment, library-assisted identification, automated fingerprinting, and decision-support tasks. Future progress will require improved spectral quality, curated spectral databases, additional spectral information, computational enhancement strategies, and uncertainty-aware validation [11,58].

In addition to these developments, multimodal integration may further enhance the analytical potential of benchtop NMR. Although benchtop systems are unlikely to replace other analytical techniques across all applications, their value may increase when

combined with complementary information sources. Broader spectroscopy studies have emphasized the integration of AI with multiple sensing modalities as a route toward more robust analytical systems [2]. In future work, this may include the fusion of benchtop NMR data with FT-IR, Raman, mass spectrometry, or targeted chemical metadata, particularly in applications such as food authentication, process monitoring, and biomedical screening.

Benchmarking and standardization will also be essential for future progress. Variability in preprocessing, dataset construction, and validation strategy currently complicates comparison across studies and limits reproducibility [38,39]. The development of shared benchmark datasets, transparent evaluation protocols, and standardized reporting practices would provide a stronger foundation for rigorous comparison and methodological progress. Similar trends are observed in broader machine learning and spectroscopy research, where benchmark-driven development is increasingly used to support reproducible and comparable model evaluation [59].

Another emerging opportunity lies in extending AI-assisted benchtop NMR beyond the current emphasis on proton spectroscopy. While most existing studies focus on ^1H NMR, benchtop platforms are also capable of heteronuclear measurements. Recent work has demonstrated that benchtop ^{19}F NMR can support sensitive quantification and reaction screening in fluorinated systems [60–63]. However, direct AI-assisted applications in heteronuclear benchtop NMR remain limited, suggesting that this area may represent an underexplored direction for future research.

Finally, the broader impact of AI-assisted benchtop NMR will depend on its integration into automated and application-oriented analytical workflows. Current studies already suggest its potential in areas such as food authenticity assessment, process monitoring, and biomedical analysis [5]. However, wider adoption will likely require improvements in workflow automation, user-independent operation, and system-level integration of instrumentation and data analysis. In this sense, the long-term role of benchtop NMR may not be to replicate high-field systems, but to evolve as a distinct analytical platform that combines accessibility, automation, and AI-enabled interpretation.

7. Conclusions

AI-assisted benchtop NMR spectroscopy has emerged as a promising strategy for extending the analytical utility of low-field NMR beyond the limitations imposed by reduced spectral resolution and extensive signal overlap. The studies reviewed here indicate that the current strongest evidence lies in classification and authentication applications, where distributed spectral fingerprints can be effectively translated into reliable analytical decisions. Quantitative applications are also progressing, although their broader applicability remains dependent on rigorous validation, dataset diversity, and robustness across experimental conditions. In contrast, spectral reconstruction and automated interpretation remain comparatively early-stage, but represent strategically important directions because they directly address the intrinsic information limitations of low-field NMR data.

The future development of this field is unlikely to depend solely on increasingly complex AI models. Rather, meaningful progress will require robust analytical workflows, improved dataset quality, rigorous validation strategies, greater model interpretability, and stronger standardization across experimental and computational practices. Without such developments, AI-assisted benchtop NMR may remain limited to promising application-specific demonstrations rather than evolving into a broadly transferable analytical framework.

More broadly, benchtop NMR should not be regarded simply as a lower-performance alternative to high-field instrumentation. Its distinctive value lies in accessibility, portability, and suitability for rapid, routine, and decentralized analysis. Within this context, AI is likely

to play an increasingly important role in transforming benchtop NMR from a compact measurement platform into a more intelligent and integrated analytical system.

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