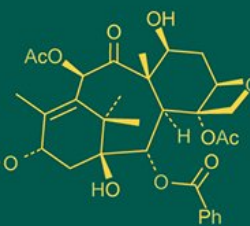
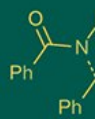


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Nuclear magnetic resonance technology in food science: Principles, instrumentation, and structural analysis of food matrices

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Abstract

Nuclear Magnetic Resonance (NMR) spectroscopy has established itself as one of the most powerful and analytically versatile technologies available in modern food science, offering a unique combination of capabilities that no single competing analytical technique can replicate. Unlike chromatographic and mass spectrometric methods that require prior separation of sample constituents, NMR generates a comprehensive molecular fingerprint of a food sample in a single measurement without requiring purification, yielding simultaneous information about the identity and abundance of hundreds of metabolites, lipids, sugars, and amino acids. This review provides a systematic and pedagogically organized account of NMR technology, beginning with the quantum mechanical foundations that underlie all NMR phenomena and progressing logically through the principal hardware components of a modern spectrometer, the diverse technical variants of NMR applied in food analysis, and the unique structural characterization capabilities that NMR offers for food matrices at both the molecular and microstructural levels. Instrumentation is described in terms of five main functional subsystems: the superconducting magnet and shim coils, the probe and radiofrequency coils, the transmitter and receiver electronics, the gradient system, and the control computer with its associated software. A systematic taxonomy of NMR types relevant to food analysis follows, spanning high-field proton and carbon NMR, benchtop NMR, time-domain NMR, low-field NMR, fast field cycling NMR, high-resolution magic angle spinning NMR, quantitative NMR, multidimensional techniques, and NMR-based metabolomics. The review then examines NMR applications in structural analysis of food matrices, covering molecular identification from chemical shift data, water state characterization by T2 relaxometry, protein structure and protein-water interaction assessment, and non-destructive lipid distribution analysis. Current limitations and future prospects conclude the review.

Keywords: Nuclear magnetic resonance, NMR principles, NMR Instrumentation, food matrix characterization, water dynamics, time-domain NMR, structural analysis, food metabolomics

1. Introduction

The safety, quality, and authenticity of food rank among the most critical concerns of modern society, and the analytical methods used to monitor these properties are accordingly of fundamental scientific and regulatory importance (Food Safety Institute, 2025) [23]. As food supply chains have become increasingly globalized, ensuring that products conform to established standards of composition, nutritional value, and geographic origin has grown considerably more complex, creating mounting pressure for analytical technologies that are simultaneously rapid, comprehensive, and adaptable to diverse food matrices (Hatzakis, 2018; Alkanan *et al.*, 2025) [3, 28]. Conventional analytical approaches including chromatography, mass spectrometry, and physicochemical testing methods have long served as the foundation of food quality control; however, these techniques frequently require extensive sample preparation, separation, or purification steps that render them time-consuming and difficult to adapt for high-throughput or real-time analysis (Alkanan *et al.*, 2025; Rashid *et al.*, 2021) [3, 59].

NMR spectroscopy has rapidly established itself as a transformative analytical tool in food science, distinguished by its capacity to analyze complex food matrices at the molecular level without requiring separation or purification steps (Hatzakis, 2018; Saifudin *et al.*, 2025) [28, 63]. In a single NMR experiment, hundreds of metabolites, lipids, sugars, amino acids, and other food constituents can be simultaneously profiled, yielding a rich molecular fingerprint that reflects

the overall chemical composition of the food sample (Alkanan *et al.*, 2025; Vignoli *et al.*, 2019) ^[3, 69]. This capability makes NMR exceptionally practical for real-time industrial quality assessments where speed, reproducibility, and minimal sample handling are of paramount importance (Saifudin *et al.*, 2025; Resende *et al.*, 2021) ^[60, 63].

NMR technology encompasses a family of related but technically distinct techniques, each optimized for different analytical objectives in food science (Hatzakis, 2018; Rashid *et al.*, 2021) ^[28, 59]. High-resolution, high-field NMR spectroscopy employing superconducting magnets provides unparalleled chemical resolution and sensitivity for detailed metabolite identification and quantification (Vignoli *et al.*, 2019) ^[69]. Low-field NMR operating at lower field strengths using compact permanent magnets offers a cost-effective alternative suitable for rapid quality assessments and on-site industrial monitoring (Alkanan *et al.*, 2025; Blümich, 2019) ^[3, 11]. Time-domain NMR, which monitors proton relaxation times rather than chemical shifts, is especially suited for non-invasive assessment of fat content, water mobility, and compositional parameters directly in intact or packaged food products without any sample preparation (Saifudin *et al.*, 2025; Kirtil *et al.*, 2017) ^[37, 63]. Specialized variants including fast field cycling NMR, high-resolution magic angle spinning NMR, and quantitative NMR each contribute distinct analytical capabilities that collectively make NMR one of the most analytically versatile platforms in food science (Ferrante and Sykora, 2005; Capitani *et al.*, 2017; Bharti and Roy, 2012) ^[10, 13, 21].

Beyond compositional characterization, NMR provides structural analysis of food at both the molecular level and the physical or microstructural level (Knicker and Nanny, 1997) ^[38]. This dual capability gives NMR a unique position among analytical techniques because it simultaneously provides information about what chemical compounds are present in a food and how those compounds are physically arranged within the food matrix, relationships that are fundamental to understanding food quality, texture, functionality, and shelf-life stability (Saifudin *et al.*, 2025; Khan *et al.*, 2016; Gilbert and Turgeon, 2025) ^[24, 35, 63]. The growing convergence of NMR technology with artificial intelligence and multi-omics approaches represents a particularly significant frontier, with AI-driven analysis supporting high-throughput screening, predictive modeling, and rapid safety diagnostics across food production systems (Alkanan *et al.*, 2025; Savorani *et al.*, 2021) ^[3, 64].

This review is organized to provide a foundational account of NMR technology for food science practitioners. The discussion begins with the fundamental physical principles governing NMR phenomena, followed by a systematic description of the principal hardware components of a modern spectrometer. Subsequent sections address the principal NMR variants employed in food analysis and examine NMR's distinctive capabilities for structural characterization of food matrices at both the molecular and microstructural levels. The review concludes with an assessment of current limitations and a forward-looking perspective on emerging technological developments.

2. Basic Principles of Nuclear Magnetic Resonance

NMR spectroscopy is founded on the quantum mechanical properties of atomic nuclei, specifically their intrinsic angular momentum called spin, which causes them to interact with external magnetic fields in ways that encode

rich information about molecular structure and dynamics (Hatzakis, 2018; Mlynárik, 2017) ^[28, 44]. When placed in a strong external magnetic field, NMR-active nuclei align with the field and precess at a characteristic Larmor frequency; the application of a radiofrequency pulse at this frequency causes resonant energy absorption, and the subsequent return to equilibrium generates the NMR signal whose frequency, phase, and decay characteristics encode the molecular environment of each nucleus (Huang, 2023; Karunakaran *et al.*, 2018; Ali, 2024) ^[2, 30, 33]. Understanding the sequential physical steps of spin alignment, resonance excitation, signal detection, and relaxation is essential to appreciating how NMR is applied across its many variants in food quality analysis (Zhonghua *et al.*, 2020; Hao *et al.*, 2014) ^[27, 78].

2.1 Nuclear Spin and the Magnetic Moment

Certain atomic nuclei possess an intrinsic quantum mechanical property called spin, which endows them with a small magnetic moment and causes them to behave like microscopic bar magnets (Zhonghua *et al.*, 2020; Karunakaran *et al.*, 2018; Hao *et al.*, 2014) ^[27, 33, 78]. The most analytically important such nuclei in food science are hydrogen-1, carbon-13, and phosphorus-31, all of which are designated as NMR-active because their non-zero spin values give them detectable magnetic moments (Adnani, 2024; Rashid *et al.*, 2021) ^[1, 59]. Nuclei with zero spin, such as carbon-12 and oxygen-16, have no magnetic moment and cannot be detected by NMR spectroscopy (Adnani, 2024; Rashid *et al.*, 2021) ^[1, 59]. Among all NMR-active nuclei, hydrogen-1 is the most widely used in food science because of its exceptionally high natural abundance of 99.98 percent and its strong magnetic sensitivity, which together yield a large and readily detectable NMR signal from the water, lipid, carbohydrate, and protein protons that are ubiquitous in all food matrices (Ritota *et al.*, 2021; Zhonghua *et al.*, 2020) ^[62, 78].

2.2 Alignment in a Magnetic Field: The Zeeman Effect

Under ordinary conditions, the magnetic moments of nuclei in a sample point in random directions and their collective effects cancel one another (Zhonghua *et al.*, 2020; Hao *et al.*, 2014) ^[27, 78]. When a food sample is placed inside the strong external magnetic field B_0 of an NMR instrument, however, the nuclear spins adopt one of two quantized orientations relative to the field: a lower-energy parallel alignment and a higher-energy antiparallel alignment (Hao *et al.*, 2014; Karunakaran *et al.*, 2018) ^[27, 33]. This splitting of nuclear energy levels in the presence of an external magnetic field is known as the Zeeman effect, named after the physicist who first described the field-induced splitting of spectral lines (Zhonghua *et al.*, 2020; Karunakaran *et al.*, 2018) ^[33, 78]. Because the Boltzmann distribution at thermal equilibrium dictates that slightly more nuclei occupy the lower-energy parallel state, a small but measurable net magnetization develops along the direction of B_0 , and this net magnetization constitutes the physical basis of the detectable NMR signal (Hao *et al.*, 2014; Karunakaran *et al.*, 2018) ^[27, 33]. The magnitude of the energy difference between the two spin states increases proportionally with field strength, which explains why higher-field NMR instruments produce greater signal sensitivity: a larger population difference between spin states generates proportionally larger net magnetization and a stronger

detectable signal (Huang, 2023; Zhonghua *et al.*, 2020) [30, 78].

2.3 Resonance and the Larmor Frequency

Each NMR-active nucleus resonates at a specific frequency known as the Larmor frequency ν_0 , which is determined by both the identity of the nucleus type and the strength of the external field B_0 , according to the relationship ν_0 equals the magnetogyric ratio γ divided by 2π , multiplied by B_0 (Huang, 2023; Hao *et al.*, 2014; Karunakaran *et al.*, 2018) [27, 30, 33]. The magnetogyric ratio is a fundamental physical constant unique to each nuclear species and determines the intrinsic NMR sensitivity of that nucleus (Karunakaran *et al.*, 2018) [33]. When a brief radiofrequency pulse at exactly ν_0 is applied perpendicular to B_0 , the nuclei absorb energy resonantly and are tipped away from their equilibrium alignment into the higher-energy spin state (Huang, 2023; Ali, 2024) [2, 30]. The exact resonance frequency of each nucleus in a molecule is not solely determined by B_0 but is also shifted slightly by the surrounding electron cloud through a phenomenon known as the chemical shift δ , which is measured in parts per million relative to an established reference standard (Adnani, 2024; Rashid *et al.*, 2021; Nishiyama *et al.*, 2022) [1, 59]. Because different functional groups and molecular environments produce characteristic and highly reproducible chemical shifts, the NMR spectrum serves as a detailed molecular fingerprint of the sample that enables identification and quantification of individual compounds within complex mixtures without prior separation (Adnani, 2024; Rashid *et al.*, 2021; Alkanan *et al.*, 2025) [1, 3, 59].

2.4 Signal Detection: The Free Induction Decay

When the radiofrequency pulse is switched off, the excited nuclei begin returning to their equilibrium alignment through relaxation processes that collectively determine the information content of the measured NMR signal (Balci, 2025; Karunakaran *et al.*, 2018; Ali, 2024) [2, 33]. As the precessing nuclear magnetization relaxes back toward B_0 , it induces a small but measurable oscillating electrical voltage in a receiver coil surrounding the sample (Karunakaran *et al.*, 2018; Ali, 2024) [2, 33]. This time-domain signal, which decays progressively as nuclear spins lose their phase coherence and return to thermal equilibrium, is called the Free Induction Decay or FID (Balci, 2025; Karunakaran *et al.*, 2018; Paniagua and Pons, 1963) [33, 52]. The FID contains all the frequency information, relaxation time information, and molecular environment information of the sample and serves as the raw data from which the NMR spectrum or image is subsequently produced through mathematical processing (Paniagua and Pons, 1963; Ali, 2024; Huang, 2023) [2, 30, 52]. The rate and character of the FID decay are directly and sensitively influenced by the molecular environment of each contributing nucleus, making this signal informationally rich before any formal spectral processing is applied (Huang, 2023; Mlynárik, 2017) [30, 44].

2.5 Relaxation Processes: T1 and T2

After the radiofrequency pulse, nuclear spins return to equilibrium through two independent relaxation mechanisms that each carry distinct and complementary information about the physical and chemical environment of food components (Huang, 2023; Graaf, 2019; Mlynárik, 2017; Ali, 2024) [2, 26, 30, 44]. Both relaxation times are

fundamental to understanding the water-state and microstructure analysis applications of NMR in food science.

2.5.1 T1: Longitudinal or Spin-Lattice Relaxation

T1, also called longitudinal or spin-lattice relaxation time, describes how quickly the component of magnetization aligned along the B_0 direction recovers to its equilibrium value by transferring energy from excited nuclear spins to the surrounding molecular environment, referred to as the lattice (Huang, 2023; Paniagua and Pons, 1963; Graaf, 2019) [26, 30, 52]. This energy transfer process is strongly influenced by molecular mobility, because the efficiency of energy transfer depends on how closely the tumbling frequency of surrounding molecules matches the Larmor frequency (Mlynárik, 2017) [44]. In food matrices, tightly bound water molecules or crystallized fat exhibit markedly shorter T1 values than free water or liquid oil, because bound molecules tumble at frequencies closer to the Larmor frequency and transfer energy more efficiently to the lattice (Mlynárik, 2017; Ali, 2024) [2, 44]. In food science applications, T1 measurements therefore serve as informative indicators of the physical state and degree of molecular organization of food components, with direct relevance to texture assessment, crystallization monitoring, and processing history verification (Kirtil *et al.*, 2017) [37].

2.5.2 T2: Transverse or Spin-Spin Relaxation

T2, also called transverse or spin-spin relaxation time, describes how quickly the component of magnetization perpendicular to B_0 decays due to the progressive loss of phase coherence among the precessing nuclear spins, without requiring any net energy transfer out of the spin system itself (Huang, 2023; Graaf, 2019; Mlynárik, 2017) [26, 30, 44]. T2 is always equal to or shorter than T1 because all mechanisms contributing to T1 also contribute to T2, while T2 has additional dephasing pathways through spin-spin coupling and local field fluctuations (Mlynárik, 2017; Graaf, 2019) [26, 44]. In food science applications, T2 measurements are particularly valuable for characterizing the distribution and mobility of water populations within food structures, for assessing fat content and physical state, and for monitoring structural changes during processing and storage (Ali, 2024; Gilbert and Turgeon, 2025; Kirtil *et al.*, 2017) [24, 37]. Together, T1 and T2 determine signal intensity and image contrast in NMR and MRI experiments, and their systematic measurement across multiple exponential components underpins the time-domain NMR applications described in subsequent sections of this review (Ali, 2024; Kirtil *et al.*, 2017; Cheng *et al.*, 2022) [2, 14, 37].

2.6 Fourier Transformation: From Time-Domain Signal to Frequency-Domain Spectrum

The time-domain FID is converted into a frequency-domain NMR spectrum through the mathematical operation of Fourier transformation, which decomposes the complex oscillating and decaying FID signal into its constituent frequency components (Huang, 2023; Paniagua and Pons, 1963; Graaf, 2019) [26, 30, 52]. The resulting spectrum displays signal intensity as a function of chemical shift, with each peak corresponding to a chemically distinct group of nuclei and its integrated area proportional to the number of those nuclei present in the sample, which underpins the quantitative accuracy of NMR spectroscopy (Huang, 2023;

Karunakaran *et al.*, 2018; Ali, 2024) [2, 30, 33]. For MRI applications, additional magnetic field gradients are applied to encode the spatial position of nuclear spins into the frequency and phase of the detected signal; Fourier transformation of this spatially encoded multi-dimensional dataset then produces cross-sectional images of the food sample interior in which contrast reflects differences in proton density, T1, or T2, thereby enabling non-destructive visualization of internal food architecture without any

physical cutting or sample destruction (Huang, 2023; Gladden, 1994; Alkanan *et al.*, 2025) [3, 25, 30]. The ability to extract both comprehensive chemical spectral information and spatial structural imaging information from the same fundamental NMR phenomenon through different data acquisition and processing strategies underlies the remarkable analytical versatility of NMR technology across its diverse applications in food science.

Table 1: Sequential Steps in NMR Signal Generation: Physical Basis and Analytical Outcome

Step	Physical Basis	Analytical Outcome	Key References
Placement in B0 field	Zeeman splitting; spins align parallel or antiparallel to B0; net magnetization forms along field direction	NMR-active nuclei prepared in state of measurable net magnetization; signal generation becomes possible	Zhonghua <i>et al.</i> (2020) [78]; Hao <i>et al.</i> (2014) [78]; Karunakaran <i>et al.</i> (2018) [33]
Radiofrequency pulse at ν_0	Resonant energy absorption at Larmor frequency tips magnetization perpendicular to B0; chemical shift differentiates nuclei by environment	Nuclear spins enter excited state; Free Induction Decay (FID) begins when pulse is withdrawn	Huang (2023) [30]; Hao <i>et al.</i> (2014) [78]; Adnani (2024) [1]; Ali (2024) [2]
T1 and T2 relaxation	Longitudinal recovery along B0 via energy transfer to lattice (T1); loss of transverse phase coherence (T2) without energy leaving spin system	Time-domain FID decay encodes molecular environment, water state, mobility, and physical food structure	Huang (2023) [30]; Mlynárik (2017) [44]; Graaf (2019) [26]; Ali (2024) [2]
Fourier Transformation	Mathematical decomposition of time-domain FID into constituent frequency components	NMR spectrum revealing chemical shifts and peak areas proportional to nuclear number, or spatial MRI image of internal food structure	Huang (2023) [30]; Paniagua and Pons (1963) [52]; Gladden (1994) [25]; Karunakaran <i>et al.</i> (2018) [33]

3. Principal Components of a Modern NMR Spectrometer

A standard NMR spectrometer is assembled from several core hardware subsystems that work in close coordination to generate the required magnetic fields, excite nuclear spins with radiofrequency pulses, detect the resulting signals, and process the raw data into interpretable spectra or images (Neiss, 2006; Bai, 2008; Kroeker, 2015; Webb, 2016) [4, 39, 48, 72]. Each subsystem plays a specific and functionally irreplaceable role in the overall analytical performance of the instrument, and familiarity with these functions is important for understanding both the capabilities and the practical constraints of different NMR configurations used across food science applications.

3.1 The Magnet and Shim Coil System

The magnet is the most fundamental and physically dominant component of any NMR instrument, responsible for generating the strong, stable, and highly homogeneous static magnetic field B0 required to align nuclear spins and establish the conditions for resonance detection (Neiss, 2006; Bai, 2008; Kroeker, 2015; Webb, 2016) [4, 39, 48, 72]. In modern high-resolution NMR spectrometers used for food metabolomics and structural analysis, the main magnet is a superconducting solenoid consisting of niobium-titanium alloy wire wound inside a cryostat vessel maintained at approximately 4 Kelvin using liquid helium, which allows the coil to carry large persistent electrical currents without resistance and thereby sustain field strengths from 9.4 to 28.2 Tesla corresponding to proton Larmor frequencies from 400 to 1200 MHz (Neiss, 2006; Bai, 2008) [4, 48]. The stability and strength of B0 directly determine the sensitivity and spectral resolution of the NMR measurement, making field consistency absolutely critical for reliable quantitative food analysis (Kroeker, 2015; Webb, 2016) [39, 72]. Installed within the magnet bore is a complementary set of auxiliary electromagnetic coils known as shim coils, which

generate small spatially varying corrective magnetic fields to fine-tune the homogeneity of B0 across the sample volume (Neiss, 2006; Bai, 2008; Kroeker, 2015) [4, 39, 48]. Even minor residual inhomogeneities in B0 cause NMR peaks to broaden and degrade spectral resolution, so systematic shimming of the magnet before each experiment is a standard and indispensable operational procedure in all food NMR applications (Neiss, 2006; Webb, 2016) [48, 72]. In benchtop NMR instruments used for industrial food quality monitoring, the magnet is a permanent assembly of rare-earth alloy magnets that require no cryogenic maintenance but produce lower and less homogeneous fields; in low-field NMR instruments used for time-domain food analysis, compact electromagnet or permanent magnet assemblies operate at fields corresponding to proton frequencies from 10 to 80 MHz (Blümich, 2019; Pullen and Booth, 2021) [11, 58].

3.2 The Probe and Radiofrequency Coils

The probe is the mechanical and electrical assembly that positions the sample tube precisely within the most homogeneous region of B0 and contains the radiofrequency coil or coil assembly that both delivers the excitation pulse to the sample and detects the resulting NMR signal (Neiss, 2006; Bai, 2008; Kroeker, 2015; Kelz *et al.*, 2021) [4, 34, 39, 48]. The RF coil generates the oscillating magnetic field B1 perpendicular to B0 during the excitation pulse and then immediately functions as a highly sensitive receiver to capture the weak FID signal that the relaxing spins emit after the pulse is withdrawn (Neiss, 2006; Kelz *et al.*, 2021) [34, 48]. The design and sensitivity of the probe coil strongly influence the signal-to-noise ratio of the measurement, which is the single most important determinant of the minimum detectable concentration and the data acquisition time required for acceptable quality in food NMR analysis (Kelz *et al.*, 2021; Webb, 2016) [34, 72]. In MRI configurations used for non-destructive food structural

imaging, the RF coil design is more varied, with large body coils used for signal transmission and local receive arrays placed close to the food sample to improve detection sensitivity and spatial resolution beyond what a single large coil can achieve (Serai *et al.*, 2021) ^[65].

3.3 The RF Transmitter and Receiver Console

The NMR console houses the electronic systems responsible for generating the precisely timed and calibrated radiofrequency pulses needed to excite nuclear spins and for detecting, amplifying, and digitizing the resulting FID signals from the probe (Neiss, 2006; Fan *et al.*, 2022; Webb, 2016) ^[20, 48, 72]. The transmitter chain within the console includes an RF synthesizer producing the precise Larmor frequency, a pulse programmer controlling the timing, duration, and shape of each pulse, amplitude and phase modulators adjusting the RF waveform, and a power amplifier boosting the signal to levels sufficient to efficiently excite nuclear spins throughout the entire sample volume (Neiss, 2006; Fan *et al.*, 2022; Webb, 2016) ^[20, 48, 72]. The receiver chain performs the complementary function of capturing and processing the weak FID from the probe coil: a low-noise preamplifier immediately amplifies the microvolt-level FID signal, filters remove out-of-band noise, a demodulator converts the signal to a lower intermediate frequency, and a high-resolution analog-to-digital converter transforms the continuous time-domain signal into digital data for computer processing (Neiss, 2006; Fan *et al.*, 2022; Yang, 2022; Webb, 2016) ^[20, 48, 72, 74]. High-resolution spectrometers additionally include a lock channel that continuously monitors the deuterium resonance of the NMR solvent and feeds field-stabilization corrections back to the magnet power supply, compensating for slow B₀ drifts during long food metabolomics acquisition sessions (Neiss, 2006; Bai, 2008) ^[4, 48].

3.4 The Gradient System

The gradient system, found primarily in MRI scanners and high-performance NMR spectrometers used for diffusion measurements and spatially resolved analysis, consists of three orthogonal sets of gradient coils oriented along the X, Y, and Z axes driven by dedicated high-current power amplifiers (Serai *et al.*, 2021; Webb, 2016) ^[65, 72]. By superimposing spatially varying magnetic fields onto B₀, these gradient coils cause the Larmor frequency of nuclear

spins to vary linearly with position along each axis in the sample (Serai *et al.*, 2021) ^[65]. Through controlled sequences of gradient switching, the system encodes the spatial origin of each NMR signal into its frequency and phase, information that is then decoded by multi-dimensional Fourier transformation to produce two-dimensional or three-dimensional images of the food sample interior (Serai *et al.*, 2021; Webb, 2016) ^[65, 72]. In food science applications, gradient-enabled MRI provides non-destructive visualization of internal food architecture including fat distribution, moisture gradients during drying, ice crystal formation during freezing, and microstructural changes during processing, all without any physical sectioning of the sample (Alkanan *et al.*, 2025; Kamal *et al.*, 2019; Wang *et al.*, 2021) ^[3, 32, 71].

3.5 The Control Computer and Data Processing Software

The control computer serves as the central coordinating unit for the entire NMR instrument, communicating with the console to define and execute pulse sequences, controlling the precise timing of RF pulses, gradient switching, and data acquisition windows, and collecting the digitized FID data from the receiver (Neiss, 2006; Bai, 2008; Kroeker, 2015; Yang, 2022) ^[4, 39, 48, 74]. Following acquisition, the control software applies a series of processing steps including Fourier transformation, phase correction, baseline correction, and peak integration to convert the raw FID into a readable NMR spectrum with chemical shift assignments and quantitative peak areas (Neiss, 2006; Yang, 2022; Kroeker, 2015) ^[39, 48, 74]. Modern NMR processing software also incorporates automated shimming routines, solvent suppression algorithms, spectral referencing tools, and database-matching functions that substantially reduce the specialist expertise required for routine food quality NMR analysis (Savorani *et al.*, 2021; Hatzakis, 2018) ^[28, 64]. For time-domain and low-field NMR applications in food science, specialized software performs multi-exponential curve fitting of T₂ relaxation decay data using algorithms such as CONTIN or non-negative least squares, decomposing the complex overall relaxation curve into component populations that correspond to distinct water states or structural environments within the food matrix (Cheng *et al.*, 2022; Gilbert and Turgeon, 2025) ^[14, 24].

Table 2: Principal Hardware Subsystems of a Modern NMR Spectrometer and Their Roles in Food Analysis

Subsystem	Core Function	Relevance to Food NMR Analysis	Key References
Magnet and shim coils	Generates stable, homogeneous B ₀ field; shims correct residual field inhomogeneity	Field strength determines chemical resolution and metabolite detection sensitivity; shimming quality controls spectral peak width in metabolomics	Neiss (2006) ^[48] ; Bai (2008) ^[4] ; Kroeker (2015) ^[39] ; Webb (2016) ^[72]
Probe and RF coils	Delivers excitation pulse to sample; detects weak FID signal with high sensitivity	Probe sensitivity determines minimum detectable concentration of food metabolites; coil design affects SNR in tissue and product imaging	Neiss (2006) ^[48] ; Kelz <i>et al.</i> (2021) ^[34] ; Serai <i>et al.</i> (2021) ^[65] ; Webb (2016) ^[72]
RF transmitter and receiver console	Generates calibrated RF pulses; amplifies, filters, and digitizes the FID	Pulse accuracy controls quantitative fidelity; receiver noise floor sets detection limits for minor food components and adulterants	Neiss (2006) ^[48] ; Fan <i>et al.</i> (2022) ^[20] ; Yang (2022) ^[74] ; Webb (2016) ^[72]
Gradient system (MRI)	Superimposes spatially varying fields to encode the spatial position of each NMR signal	Enables non-destructive 3D imaging of internal food structure, fat distribution, moisture gradients, and ice crystal patterns during processing	Serai <i>et al.</i> (2021) ^[65] ; Webb (2016) ^[72] ; Alkanan <i>et al.</i> (2025) ^[3]
Control computer and software	Coordinates all subsystems; processes FID into spectra or images; performs multi-exponential T ₂ fitting	Automation and spectral processing software reduces analyst workload and enables routine food quality control at scale	Neiss (2006) ^[48] ; Yang (2022) ^[74] ; Kroeker (2015) ^[39] ; Savorani <i>et al.</i> (2021) ^[64]

4. Types of NMR Spectroscopy Used in Food Analysis

NMR spectroscopy for food analysis encompasses a family of technically distinct approaches that differ in magnetic field strength, the physical domain in which signals are detected (frequency versus time domain), the pulse sequences employed, and the types of nuclei observed (Hatzakis, 2018; Rashid *et al.*, 2021) ^[28, 59]. Each variant has been developed and optimized for specific analytical objectives and food matrix types, and understanding their respective strengths and limitations is essential for selecting the most appropriate method for a given food quality challenge (Hatzakis, 2018) ^[28]. The following sections provide a systematic review of each major NMR type organized from high-field spectroscopic methods through to specialized variants.

4.1 High-Field NMR Spectroscopy

High-field NMR spectroscopy employs large superconducting magnets operating at proton resonance frequencies between 400 MHz and 1.2 GHz to achieve the strong and stable magnetic fields that maximize both spectral resolution and detection sensitivity (Vignoli *et al.*, 2019; Adnani, 2024) ^[1, 69]. The exceptional spectral resolution of these instruments enables precise identification and quantification of individual compounds even within the highly complex metabolite mixtures found in food samples, because closely spaced resonances of chemically similar nuclei can be clearly separated and independently integrated (Vignoli *et al.*, 2019; Rashid *et al.*, 2021) ^[59, 69]. Recent advances in superconducting magnet technology have extended the frontier of commercial high-field NMR to proton frequencies of 900 MHz and above, including a 1.1 GHz spectrometer installed at St. Jude Children Research Hospital in Memphis and a 1.2 GHz instrument at the University of Florence (Patching, 2025) ^[53]. High-field NMR is the method of choice for comprehensive metabolite profiling and unambiguous structural identification in food research, although its high acquisition and operating costs limit its deployment primarily to specialized research and reference testing laboratories (Hatzakis, 2018; Pullen and Booth, 2021) ^[28, 58].

4.1.1 Proton NMR Spectroscopy

Proton or ¹H NMR spectroscopy is the most widely applied high-field NMR technique in food science, exploiting the high natural abundance of ¹H nuclei at 99.98 percent and their strong magnetic sensitivity to simultaneously profile diverse food components including oils, proteins, carbohydrates, and organic acids (Ritota *et al.*, 2021; Rashid *et al.*, 2021) ^[59, 62]. A single ¹H NMR measurement provides a comprehensive molecular fingerprint from which hundreds of metabolites can be identified and quantified without any prior separation of the food sample, making it exceptionally efficient for compositional screening (Vignoli *et al.*, 2019; Savorani *et al.*, 2021) ^[64, 69]. In extra virgin olive oil quality analysis, for example, ¹H NMR spectroscopy has delivered improved quantification of fatty acid ester composition even in the presence of signal overlap from high-concentration constituents, providing a critical determinant of oil quality grade and geographic origin authentication (Savorani *et al.*, 2021) ^[64]. Proton NMR metabolomics has become a cornerstone approach for food authentication, adulteration detection, and geographical origin verification across dairy

products, wines, honeys, and plant-derived foods (Hatzakis, 2018; Savorani *et al.*, 2021) ^[28, 64].

4.1.2 Carbon-13 NMR Spectroscopy

Carbon-13 or ¹³C NMR spectroscopy measures the resonance of the ¹³C nucleus and provides structural information that is complementary to and in important respects not obtainable from proton NMR alone (Bertelli *et al.*, 2020) ^[8]. While ¹H NMR excels at identifying functional groups and quantifying metabolite concentrations, ¹³C NMR reveals carbon skeleton architecture, molecular connectivity through carbon-carbon bonds, and most importantly site-specific isotopic composition at individual molecular positions (Bertelli *et al.*, 2020; Tenaillon *et al.*, 2004) ^[8, 66]. Quantitative ¹³C NMR has been particularly valuable for determining natural abundance stable carbon isotope ratios in high-value food compounds such as vanillin, enabling differentiation of natural from synthetic sources based on the distinctive isotopic fractionation patterns associated with different biosynthetic versus chemical synthetic pathways (Bertelli *et al.*, 2020; Tenaillon *et al.*, 2004; Pironi *et al.*, 2021) ^[8, 55, 56, 66]. This isotopic authentication capability is directly applicable to verifying the botanical and production origin of flavouring compounds, essential oils, and other high-value food ingredients whose premium market value rests on confirmed natural origin (Tenaillon *et al.*, 2004) ^[66].

4.1.3 Advanced Pulse Techniques for Food-Matrix Proton NMR

Several specialized pulse sequences have been developed specifically to address the analytical challenges posed by complex food matrices in high-field ¹H NMR spectroscopy (Savorani *et al.*, 2021) ^[64]. The Double Pulsed-Field-Gradient Echo technique selectively excites specific spectral regions, such as the aromatic region between 5 and 10 ppm in wine analysis, with substantially enhanced sensitivity relative to conventional broadband excitation, revealing broad resonances from macromolecular assemblies and trace aromatic metabolites that are not visible in standard one-dimensional spectra (Savorani *et al.*, 2021; Herbert-Pucheta *et al.*, 2021) ^[29, 64]. The DISPEL technique, standing for Destruction of Interfering Satellites by Perfect Echo Low-pass filtration, suppresses the ¹³C satellite peaks that arise from the small natural abundance of ¹³C and that otherwise obscure minor metabolite signals adjacent to major resonances, significantly improving quantitative accuracy in matrices such as olive oil and fruit juices without requiring complicated experimental optimization (Savorani *et al.*, 2021) ^[64]. Automated solvent suppression methods remove the dominant water resonance that would otherwise prevent detection of low-concentration food metabolites across the full chemical shift range, which is a practically important consideration given the high water content of most food samples encountered in quality control settings (Savorani *et al.*, 2021; Hatzakis, 2018) ^[28, 64].

4.2 Benchtop NMR Spectroscopy

Benchtop NMR spectroscopy employs small permanent magnets operating at proton frequencies between 40 and 80 MHz in place of the large superconducting magnets required by high-field instruments (Bernstein *et al.*, 2019; Blümich and Singh, 2018) ^[7, 12]. Although the spectral resolution of benchtop instruments is considerably lower than that of

high-field systems due to the smaller chemical shift dispersion at lower field strengths, these instruments offer compelling practical advantages for industrial food quality applications (Bernstein *et al.*, 2019; Pullen and Booth, 2021) [7, 58]. Benchtop NMR systems are compact enough to be placed on a laboratory workbench or within a food processing environment, require no cryogenic cooling or associated infrastructure, and can be operated for real-time monitoring directly within food production facilities (Bernstein *et al.*, 2019; Blümich, 2019) [7, 11]. These characteristics make benchtop NMR an increasingly cost-effective and accessible option for routine quality control where high throughput and operational simplicity are prioritized (Pullen and Booth, 2021; Yu *et al.*, 2021) [58, 76]. The ongoing improvement of permanent magnet homogeneity and digital signal processing is steadily expanding the analytical range of benchtop systems, and their adoption in industrial food quality laboratories is growing rapidly (Blümich, 2019; Pullen and Booth, 2021) [11, 58].

4.3 Time-Domain NMR

Time-domain NMR measures the rate at which nuclear magnetization decays in the time domain following radiofrequency excitation, characterizing the transverse relaxation time T2 and often also T1, rather than acquiring a conventional frequency-domain chemical shift spectrum (Saifudin *et al.*, 2025; Kirtil *et al.*, 2017) [37, 63]. In TD-NMR, the decay rate of nuclear magnetization after excitation pulses reflects the molecular mobility of nuclei within the food matrix and is sensitive to the physical state and spatial distribution of water and fat within food structures without requiring any sample preparation (Saifudin *et al.*, 2025; Kirtil *et al.*, 2017) [37, 63]. Different molecular environments produce characteristically distinct T2 values: water bound tightly to macromolecular surfaces exhibits very short T2 values typically between 0.01 and 1 milliseconds; water immobilized or entrapped within cellular structures shows intermediate T2 values from 1 to 100 milliseconds; and free bulk water exhibits long T2 values from 100 to 1000 milliseconds (Saifudin *et al.*, 2025; Gilbert and Turgeon, 2025) [24, 63]. TD-NMR relaxation curves from food samples are analyzed by multi-exponential curve fitting, decomposing the complex overall decay into multiple exponential components each representing a distinct water population or structural compartment within the food matrix (Cheng *et al.*, 2022; Gilbert and Turgeon, 2025) [14, 24]. The sensitivity of TD-NMR to the physical state and distribution of water makes this technique exceptionally powerful for non-invasive characterization of moisture and fat states in intact food products throughout processing and storage (Kirtil *et al.*, 2017; Kamal *et al.*, 2019) [32, 37].

4.4 Low-Field NMR

Low-field NMR refers broadly to instruments operating at magnetic field strengths below 100 MHz proton frequency, a range that overlaps substantially with TD-NMR in both instrumentation and application domains (Alkanan *et al.*, 2025; Wang *et al.*, 2021) [3, 71]. The LF-NMR designation emphasizes the low field strength of the instrument rather than a specific detection methodology, and most LF-NMR applications in food science use time-domain relaxometry as their primary analytical approach (Alkanan *et al.*, 2025) [3]. LF-NMR has been extensively applied to characterize water

dynamics, moisture migration, and quality changes in diverse food products because of its sensitivity to water physical states, high analysis speed, non-destructive nature, and relatively low instrument cost compared to high-field systems (Alkanan *et al.*, 2025; Wang *et al.*, 2021) [3, 71]. Combined with magnetic resonance imaging, LF-NMR has become particularly valuable in the aquatic food industry for simultaneously measuring water content, fat composition, and protein levels, as well as for monitoring quality changes during storage, processing, and cold chain distribution (Wang *et al.*, 2021; Alkanan *et al.*, 2025) [3, 71]. In drying applications, LF-NMR enables real-time monitoring of internal moisture release patterns with quantitative correlations to final product quality parameters, supporting data-driven process optimization in food manufacturing (Cheng *et al.*, 2022; Zhu *et al.*, 2021; Kamal *et al.*, 2019) [14, 32, 80].

4.5 Fast Field Cycling NMR

Fast Field Cycling NMR measures nuclear relaxation properties across a wide and continuously variable range of magnetic field strengths, typically spanning from 10 kilohertz to 10 megahertz equivalent proton frequency, rather than at the single fixed field strength used by all other NMR instruments (Ferrante and Sykora, 2005) [21]. By measuring relaxation at many different field strengths and generating a complete nuclear magnetic relaxation dispersion profile, FFC-NMR provides uniquely comprehensive information about molecular dynamics occurring across a broad range of timescales within the food matrix (Ferrante and Sykora, 2005) [21]. Fast molecular motions contribute most strongly to relaxation at high measurement fields, while progressively slower motions become apparent at lower measurement fields, so the relaxation dispersion profile simultaneously encodes information about rotational dynamics, translational diffusion through food structures, and frequency-dependent intermolecular interactions (Ferrante and Sykora, 2005) [21]. In food science, FFC-NMR has been applied to characterize the complex molecular dynamics of water, sugar, and protein assemblies in gel-based confectionery products such as Turkish delights, revealing distinct rotational and translational dynamic populations that reflect the organizational structure of the gel matrix at the molecular level (Öztürk *et al.*, 2020; Pocan *et al.*, 2021) [51, 57]. Benchtop FFC-NMR relaxometry has also been used to differentiate cheeses produced from raw milk versus pasteurized or heat-treated milk, a distinction of direct relevance to Protected Denomination of Origin product certification, by identifying characteristic differences in relaxation dispersion profiles that reflect distinct protein and water matrix structures produced by different milk thermal treatments (Nagmutdinova *et al.*, 2025; Conte *et al.*, 2020) [17, 47].

4.6 High-Resolution Magic Angle Spinning NMR

High-Resolution Magic Angle Spinning NMR enables direct analysis of intact or minimally processed solid and semi-solid food tissue samples with chemical resolution approaching that of conventional solution-state NMR, without requiring the extraction and dissolution that liquid-state analysis demands (Capitani *et al.*, 2017; Ritota *et al.*, 2021) [13, 62]. The technique achieves this capability by rapidly rotating the sample at the magic angle of 54.74

degrees relative to the B0 field direction, a rotation that averages out the anisotropic magnetic interactions including dipolar couplings and chemical shift anisotropy that otherwise produce broad featureless peaks in solid samples and converts them into sharp, resolved resonances (Capitani *et al.*, 2017) [13]. This makes HRMAS-NMR particularly valuable for food quality and authenticity research where the native tissue structure contains essential compositional information that would be altered or destroyed by extraction (Ritota *et al.*, 2021; Pironti *et al.*, 2021) [55, 56, 62]. In meat authentication research, HRMAS-NMR applied directly to intact muscle tissue from Protected Geographical Indication Chianina beef revealed comprehensive metabolic profiles encompassing amino acids as indicators of protein quality, carnosine as a marker of post-mortem aging, nucleosides reflecting ATP degradation, and fatty acid profiles influenced by feeding systems, enabling classification by geographical origin and discrimination between PGI-certified and non-PGI samples through combined multivariate analysis (Capitani *et al.*, 2017; Pironti *et al.*, 2021; Ritota *et al.*, 2024) [55, 56, 61, 13].

4.7 Quantitative NMR

Quantitative NMR applies carefully optimized experimental conditions to convert NMR spectral intensities into accurate absolute concentration measurements without requiring compound-specific external calibration curves, exploiting the fundamental quantitative proportionality between NMR peak area and the number of nuclei contributing to that peak (Bharti and Roy, 2012) [10]. Reliable qNMR requires that the relaxation delay between successive scans be long enough to allow complete T1 recovery of all resonances; that pulse flip angles be accurately calibrated; that an appropriate concentration reference be included; and that baseline correction be applied carefully before peak integration (Bharti and Roy, 2012) [10]. When these conditions are rigorously met, qNMR delivers highly accurate and reproducible absolute concentration measurements across a wide range of food components simultaneously in a single experiment (Bharti and Roy, 2012; Vignoli *et al.*, 2019) [10, 69]. Quantitative NMR combined with global spectral deconvolution enabled simultaneous structural identification and absolute quantification of 26 distinct aqueous components in *Cordyceps sinensis*, including amino acids, sugars, and nucleotides, from a single measurement, while the compositional profiles simultaneously differentiated natural from cultivated samples and identified counterfeit products (Yang *et al.*, 2021; Liu *et al.*, 2023) [41, 75].

4.8 Two-Dimensional and Multidimensional NMR

Two-dimensional and multidimensional NMR techniques create spectra with two or more frequency axes that provide connectivity information between nuclei and enable resolution of overlapping signals that cannot be separated in the one-dimensional spectrum (Vignoli *et al.*, 2019; Hatzakis, 2018) [28, 69]. The most widely used two-dimensional NMR techniques in food science include Correlation Spectroscopy, which reveals pairs of protons coupled through chemical bonds and thereby maps molecular connectivity; Heteronuclear Single Quantum Coherence spectroscopy, which correlates each proton resonance to the chemical shift of its directly bonded carbon; and Heteronuclear Multiple Bond Correlation spectroscopy, which reveals through-bond connectivity

between protons and carbons separated by two or three bonds (Vignoli *et al.*, 2019) [69]. These two-dimensional techniques enable unambiguous structural identification of metabolites in food extracts even when one-dimensional spectra show extensive peak overlap, making them particularly valuable for structural confirmation of novel or unexpected compounds in complex food matrices such as wine, honey, and plant-derived extracts (Hatzakis, 2018; Vignoli *et al.*, 2019) [28, 69].

4.9 NMR-Based Metabolomics

NMR-based metabolomics exploits the comprehensive, simultaneous, and highly reproducible molecular fingerprinting capability of NMR spectroscopy to analyze the complete low-molecular-weight metabolite complement of a food sample in a single experiment (Savorani *et al.*, 2021; Vignoli *et al.*, 2019) [64, 69]. The approach can be conducted in two complementary modes: in targeted metabolomics, specific known compounds of established quality or authenticity relevance are identified and precisely quantified; in untargeted metabolomics, the complete spectral fingerprint is captured and statistical methods detect all deviations from authentic reference patterns, including those arising from unanticipated adulterants or novel quality-affecting processes (Savorani *et al.*, 2021) [64]. The untargeted approach is particularly powerful for food authentication because it can detect any compositional anomaly rather than only those specifically anticipated by the analyst in advance (Savorani *et al.*, 2021; Hatzakis, 2018) [28, 64]. The combination of NMR metabolomics with multivariate statistical analysis methods including Principal Component Analysis for unsupervised pattern recognition, Partial Least Squares Discriminant Analysis and Orthogonal PLS-DA for supervised classification, and Partial Least Squares Regression for quantitative prediction of continuous quality parameters is central to extracting actionable authentication and quality information from high-dimensional NMR spectral datasets in food analysis (Savorani *et al.*, 2021; Vignoli *et al.*, 2019) [64, 69].

4.10 Specialized NMR Techniques

4.10.1 Continuous Wave Free Precession NMR

Continuous Wave Free Precession NMR was developed specifically for rapid, high-throughput fat and oil analysis in food and agricultural products (Colnago *et al.*, 2011) [15]. CWFP applies continuous radiofrequency pulses under conditions that maintain nuclear magnetization in a steady state, producing substantially higher sensitivity per unit acquisition time compared with traditional pulsed spin-echo detection schemes (Colnago *et al.*, 2011) [15]. This sensitivity advantage translates into faster analysis times well suited for high-throughput quality control of intact oilseeds, fats, and oil-containing food products directly in commodity processing operations (Colnago *et al.*, 2011; Moraes *et al.*, 2024) [15, 45].

4.10.2 Self-Diffusion Coefficient NMR

Self-diffusion coefficient measurements using pulsed-gradient TD-NMR assess the translational mobility of molecules within food matrices, providing information about chemical and structural changes that is complementary to relaxation time measurements (Vackier *et al.*, 2019; Osheter *et al.*, 2022) [50, 68]. Strong linear correlations have been established between the self-

diffusion coefficients of protons in edible oils measured by NMR and conventional chemical indicators of oxidative deterioration including peroxide value, conjugated diene concentration, and aldehyde content, enabling rapid non-destructive assessment of oil oxidation status without chemical reagents or sample destruction (Vackier *et al.*,

2019^[68]; Osheter *et al.*, 2022^[50]; Wiesman *et al.*, 2022)^[73]. This approach is particularly attractive for industrial oil quality monitoring because it provides results within minutes from intact oil samples and is therefore compatible with real-time process monitoring on production lines (Wiesman *et al.*, 2022)^[73].

Table 3: NMR Variants Used in Food Analysis: Characteristics and Representative Applications

NMR Type	Field Strength	Principal Analytical Strength	Representative Application	Key References
High-field 1H NMR	400 to 1200 MHz	Comprehensive metabolite profiling with maximum chemical resolution	Food authentication; metabolomics; adulteration detection	Hatzakis (2018) ^[28] ; Vignoli <i>et al.</i> (2019) ^[69] ; Savorani <i>et al.</i> (2021) ^[64]
High-field 13C NMR	400 to 1200 MHz	Carbon skeleton architecture and site-specific isotopic analysis	Authentication of natural flavorings; vanillin origin verification	Bertelli <i>et al.</i> (2020) ^[8] ; Tenailleau <i>et al.</i> (2004) ^[66] ; Pironti <i>et al.</i> (2021) ^[55, 56]
Benchtop NMR	40 to 80 MHz	Compact, cryogen-free, on-site deployment	Routine quality control; process monitoring in food factories	Bernstein <i>et al.</i> (2019) ^[7] ; Blümich (2019) ^[11] ; Pullen and Booth (2021) ^[58]
Time-Domain NMR	Low field below 50 MHz	Non-destructive characterization of water and fat physical states	Water state analysis; solid fat content; moisture in intact products	Saifudin <i>et al.</i> (2025) ^[63] ; Kirtil <i>et al.</i> (2017) ^[37] ; Cheng <i>et al.</i> (2022) ^[14]
Low-Field NMR	10 to 80 MHz	Fast, low-cost, sensitive to water mobility and distribution	Aquatic product freshness; drying monitoring; cold chain quality	Wang <i>et al.</i> (2021) ^[71] ; Alkanan <i>et al.</i> (2025) ^[3] ; Kamal <i>et al.</i> (2019) ^[32]
Fast Field Cycling NMR	10 kHz to 10 MHz variable	Complete molecular dynamics dispersion profile across timescales	Gel structure in confectionery; PDO cheese authentication	Ferrante and Sykora (2005) ^[21] ; Öztürk <i>et al.</i> (2020) ^[51] ; Nagmutdinova <i>et al.</i> (2025) ^[47]
HRMAS-NMR	400 to 700 MHz	Intact tissue analysis with high resolution without extraction	Meat geographical origin authentication; cheese metabolomics	Capitani <i>et al.</i> (2017) ^[13] ; Ritota <i>et al.</i> (2024) ^[61] ; Pironti <i>et al.</i> (2021) ^[55, 56]
Quantitative NMR	Any field strength	Absolute quantification without compound-specific calibration curves	Multi-component food analysis; adulteration quantification	Bharti and Roy (2012) ^[10] ; Yang <i>et al.</i> (2021) ^[75] ; Liu <i>et al.</i> (2023) ^[41]
2D Multidimensional NMR	400 to 1200 MHz	Resolves spectral overlap; provides molecular bond connectivity	Novel biomarker elucidation; complex food matrix structural analysis	Vignoli <i>et al.</i> (2019) ^[69] ; Hatzakis (2018) ^[28]

5. NMR for Structural Analysis of Food Matrices

Structural analysis using NMR operates at two complementary and mutually reinforcing levels of food organization (Knicker and Nanny, 1997; Saifudin *et al.*, 2025)^[38, 63]. At the molecular level, NMR identifies and characterizes individual chemical compounds from their characteristic spectral signatures, providing information about molecular structure, functional group composition, and isotopic identity (Saifudin *et al.*, 2025; Eisenreich and Bacher, 2007)^[19, 63]. At the physical or microstructural level, NMR relaxometry and imaging reveal how water, proteins, fats, and other components are organized, distributed, and dynamically interacting within the three-dimensional architecture of the food matrix (Knicker and Nanny, 1997; Khan *et al.*, 2016; Bertram *et al.*, 2002)^[9, 35, 38]. This dual capability is analytically distinctive because NMR simultaneously provides answers to both what compounds are present in a food and how those compounds are physically arranged within it, a combination of information that is directly relevant to food quality, texture, processing behavior, shelf life, and authenticity (Saifudin *et al.*, 2025; Gilbert and Turgeon, 2025; Kirtil *et al.*, 2017)^[24, 37, 63].

5.1 Molecular Structure Identification and Characterization

NMR spectroscopy detects the response of atomic nuclei, particularly 1H and 13C, to applied magnetic fields with

exquisite sensitivity to the local chemical environment of each nucleus (Knicker and Nanny, 1997; Saifudin *et al.*, 2025)^[38, 63]. The chemical shift is highly specific to each functional group and molecular context, making it a powerful and reliable identifier of molecular structure without requiring physical separation of compounds from the food matrix (Saifudin *et al.*, 2025; Adnani, 2024)^[1, 63]. Systematic analysis of the proton and carbon chemical shifts observed in an NMR spectrum against standardized reference charts and spectral databases allows food scientists to identify whether detected resonances originate from amino acids, carbohydrates, fatty acids, organic acids, phenolic compounds, or other metabolite classes (Saifudin *et al.*, 2025; Eisenreich and Bacher, 2007)^[19, 63]. The combination of one-dimensional and two-dimensional NMR experiments provides a framework for complete de novo structural elucidation of unknown food components, a capability not available from chromatographic retention data alone (Vignoli *et al.*, 2019; Hatzakis, 2018)^[28, 69]. The structural identification power of NMR has been demonstrated across numerous food science examples of direct commercial and regulatory relevance. The isotopic composition of individual carbon atoms in vanillin has been determined by quantitative 13C NMR at natural isotopic abundance, enabling differentiation of natural from synthetic vanillin through site-specific isotopic analysis of specific carbon positions in the molecule whose isotopic signature arises from differential fractionation through

different biosynthetic versus synthetic production routes (Tenailleau *et al.*, 2004) ^[66]. Piperine from black pepper has been structurally confirmed by combined ¹H and ¹³C NMR analysis, with both spectra providing independently consistent molecular structural evidence while supporting chromatographic purity determination (Pawar *et al.*, 2025) ^[54]. Quantitative NMR combined with global spectral deconvolution has enabled simultaneous structural identification and absolute quantification of 26 distinct aqueous components in *Cordyceps sinensis*, including amino acids, sugars, and nucleotides, from a single measurement, while simultaneously differentiating natural from cultivated samples and identifying counterfeit products based on their compositional profiles (Yang *et al.*, 2021; Liu *et al.*, 2023) ^[41, 75].

5.2 Water State Characterization in Food Matrices

One of the most distinctive and practically valuable structural analysis capabilities of NMR in food science is its ability to characterize the different physical states, populations, and dynamic properties of water within food matrices without any sample preparation or destructive measurement (Khan *et al.*, 2024; Gilbert and Turgeon, 2025) ^[24, 36]. Water in foods exists in multiple distinct forms with widely different mobility characteristics that reflect the structural environment constraining each water population, and NMR relaxometry based on multi-exponential T2 analysis can quantify the proportion and relaxation dynamics of each water type simultaneously from the measured relaxation decay curve (Khan *et al.*, 2024; Kirtil *et al.*, 2017) ^[36, 37]. This non-destructive and simultaneous characterization of multiple water populations is of immense practical value because the distribution and state of water within a food matrix directly determines its quality, texture, shelf life, microbial safety, and processing behavior (Kirtil *et al.*, 2017; Kamal *et al.*, 2019; Cheng *et al.*, 2022) ^[14, 32, 37].

5.2.1 Classification of Water Populations in Food Systems

Multiple research groups have established a consistent framework for classifying and quantifying the distinct water populations present in diverse food systems using T2 relaxometry (Gilbert and Turgeon, 2025) ^[24]. Khan *et al.* (2016) ^[35] applied ¹H NMR T2 relaxometry to plant-based foods and identified three water populations: strongly bound water comprising 1 to 6 percent of total water content, loosely bound water comprising 80 to 92 percent, and free or bulk water comprising 6 to 16 percent. In meat systems, Bertram *et al.* (2002) ^[9] identified three distinct water compartments designated T2b, T21, and T22 corresponding to water associated with the myofibrillar protein lattice, water within the myofibrils, and extramyofibrillar water respectively, and demonstrated that T21 correlated strongly with myofibrillar ultrastructure with a correlation coefficient of 0.84, establishing a direct quantitative link between NMR-measured water dynamics and protein organizational state. In cheese matrices, Kruk *et al.* (2021) demonstrated through nuclear magnetic relaxation dispersion that confined water populations in the protein-fat gel matrix exhibit dynamics up to four orders of magnitude slower than bulk water, quantifying the profound influence of the protein network architecture on water molecular mobility. Across a broad survey of food systems, Gilbert and Turgeon (2025) ^[24] confirmed that between one and four distinct water populations are routinely resolvable by LF-NMR T2 relaxometry and that water mobility consistently correlates

with the underlying microstructural organization of the food matrix, establishing water state as a universal NMR-accessible indicator of food microstructure.

5.2.2 Water dynamics during food processing and storage

The distribution and state of water in food products evolves dynamically during processing and storage in ways that directly and sensitively reflect structural changes in the food matrix, and NMR water state analysis provides a non-destructive window into this microstructural evolution with strong predictive value for product quality outcomes (Kirtil *et al.*, 2017; Kamal *et al.*, 2019) ^[32, 37]. During hot-air oven drying of Fuji apple slices at temperatures from 50 to 80 degrees Celsius, Kamal *et al.* (2019) ^[32] identified four distinct water relaxation peaks by LF-NMR corresponding to strongly bound water, lightly bound water, water entrapped within cellular structures, and free water with T2 values spanning from 0.01 milliseconds to 1000 milliseconds across the four populations. Free water content and relaxation times decreased systematically and progressively with drying duration, and strong positive correlations were established between specific NMR parameters and sensory quality metrics including color, hardness, chewiness, and shear force, demonstrating that NMR water state data can serve as a reliable and non-destructive predictor of final product sensory quality (Kamal *et al.*, 2019) ^[32]. In dough systems, Lu and Seetharaman (2013) detected three water populations with T2 values ranging from 2 to 5 milliseconds for water tightly bound to the starch-gluten matrix, 10 to 40 milliseconds for water at gluten-starch interfaces, and 100 to 200 milliseconds for weakly associated bulk water, providing molecular-level insight into the hydration microstructure that determines dough rheological behavior.

During cold chain storage of bigeye tuna with temperature fluctuations, LF-NMR tracked quality deterioration through T2 relaxation measurements that detected the progressive redistribution of water from immobilized to free populations as muscle protein denaturation advanced, and the resulting NMR parameters correlated with multiple physicochemical quality indicators including texture, oxidation status, and total viable bacterial count (Zhang *et al.*, 2023) ^[77]. For quality assessment of dried icefish processed by different drying methods, LF-NMR revealed that cold air drying at 8 to 12 degrees Celsius better preserved muscle fiber structure and water absorption capacity relative to hot air drying at 40 to 60 degrees Celsius, with these structural differences manifested as distinct water population distributions upon rehydration that correlated directly with sensory quality and textural properties of the rehydrated product (Zhu *et al.*, 2024) ^[79].

5.3 Protein Structure and Dynamics in Food Matrices

5.3.1 Myofibrillar Protein Organization in Meat Systems

Proteins in food undergo significant structural changes during processing, cooking, storage, and aging, and these changes have direct and profound consequences for food quality, texture, nutritional value, and authenticity (Tilgner *et al.*, 2019; Fontes *et al.*, 2018). NMR is uniquely suited to characterize these protein structural changes in intact or minimally processed food samples, avoiding the artefacts and structural disruptions that extraction and purification procedures inevitably introduce (Capitani *et al.*, 2017; Ritota *et al.*, 2021) ^[13, 62]. HRMAS-NMR analysis applied directly to intact beef muscle tissue has identified

characteristic profiles of amino acids and protein-derived metabolites that serve as quantitative indicators of post-mortem proteolysis and aging progress, providing verifiable molecular evidence of maturation history relevant to premium aged meat products (Tilgner *et al.*, 2019; Pironti *et al.*, 2021) [55, 56]. By detecting specific amino acids, dipeptides, and structural breakdown products including carnosine, NMR reveals the progressive structural degradation and reorganization of myofibrillar proteins during aging in a manner not accessible to chromatographic or physicochemical methods applied to tissue extracts (Fontes *et al.*, 2018; Ritota *et al.*, 2024) [61]. Magnetic resonance imaging combined with NMR relaxometry has further demonstrated how physical processing treatments including ultrasound combined with magnetic nanoparticles during thawing of Antarctic krill affect protein network organization and oxidation state in ways quantifiable by NMR-detectable microstructural parameters (Ding *et al.*, 2025).

5.3.2 Protein-Water Interactions and Their Structural Implications

The structural organization of proteins in food matrices directly and profoundly determines how water molecules are distributed, how tightly they are bound, and how rapidly they exchange between different spatial environments, all of which are reflected in NMR-measurable relaxation parameters (Bertram *et al.*, 2002; Mulas *et al.*, 2013; Nagmutdinova *et al.*, 2025) [9, 46, 47]. In aged cheeses such as Parmigiano Reggiano and Fiore Sardo, NMR relaxometry characterizes the complex and evolving structural matrix of proteins, fat, mineral crystals, and water that develops progressively during months-long aging, with changes in relaxation parameters providing quantitative markers of aging progress and final product quality development (Nagmutdinova *et al.*, 2025; Consonni and Cagliani, 2008). Mulas *et al.* (2013) [46, 47] applied MRI relaxometry to 36 Sardinian Pecorino cheese samples divided equally between cheeses from heat-treated milk and cheeses from raw milk, finding that heat-treated milk cheeses consistently exhibited significantly higher proportions of fast-relaxing water protons comprising 70 to 80 percent of total water, while raw milk cheeses showed proportionally greater long-relaxation-time water populations. This differentiation reflects fundamental differences in protein network structure and water binding at the microscale that arise from the different thermal histories of the milk, allowing NMR to reliably distinguish production methods from one another without any chemical extraction or separation procedure (Mulas *et al.*, 2013) [46]. In rehydration studies of cold air dried versus hot air dried icefish, NMR analysis revealed that cold air dried products maintained 92 percent immobilized water and only 2 to 3 percent free water upon rehydration, reflecting well-preserved protein network integrity, while hot air dried products showed measurably higher free water fractions indicating greater protein network disruption during the more aggressive drying treatment (Zhu *et al.*, 2024) [79].

5.4 Lipid Structure and Fat Distribution

NMR provides distinctive capabilities for the non-destructive characterization of lipid molecular structure and the spatial distribution of fat within intact food matrices, complementing the chemical composition information available from chromatographic lipid analysis (Hwang and Bakota, 2016; Wiesman *et al.*, 2022) [31, 73]. Time-domain

NMR sensors measuring two-dimensional T1-T2 relaxation parameter maps and self-diffusion coefficients can simultaneously quantify total fat content and distinguish solid fat fractions from liquid oil fractions within a single measurement on an intact food sample, which is directly relevant to characterizing texture, mouthfeel, thermal behavior, and stability of fat-containing foods (Hwang and Bakota, 2016; Kirtil *et al.*, 2017) [31, 37]. Self-diffusion coefficient measurements using pulsed-gradient TD-NMR are particularly informative for assessing the degree of lipid oxidative deterioration in edible oils, because strong linear correlations have been established between diffusion coefficients and conventional chemical oxidation markers including peroxide values and conjugated diene concentrations, enabling rapid non-destructive quality assessment without requiring chemical reagents (Vackier *et al.*, 2019; Osheter *et al.*, 2022; Wiesman *et al.*, 2022) [50, 68, 73]. During deep frying operations, LF-NMR can simultaneously identify and quantify three distinct proton populations corresponding to residual moisture, surface-absorbed fat, and internally incorporated fat in fried food products, enabling concurrent and non-destructive monitoring of frying oil quality degradation and product fat uptake throughout the frying cycle (Wang *et al.*, 2019; Wiesman *et al.*, 2022) [70, 73].

6. Limitations and Challenges of NMR in Food Science

Despite its powerful and wide-ranging analytical capabilities, NMR spectroscopy faces significant limitations that constrain its broader adoption in food science and industry, and an honest assessment of these barriers is necessary for realistic deployment planning (Hatzakis, 2018; Pullen and Booth, 2021) [28, 58].

The most fundamental analytical limitation is NMR's inherently low sensitivity relative to mass spectrometry and chromatographic detection systems (Hatzakis, 2018) [28]. The minute energy difference between nuclear spin states produces only a very small equilibrium population difference, resulting in a weak signal that requires relatively high analyte concentrations and extended data acquisition times to achieve acceptable signal-to-noise ratios (Hatzakis, 2018) [28]. This intrinsic sensitivity limitation means NMR is generally unsuitable for detecting trace-level food contaminants such as pesticide residues, mycotoxins, and veterinary drug residues at regulatory limit concentrations, where mass spectrometry-based techniques such as LC-MS/MS and GC-MS offer orders-of-magnitude superior sensitivity (Hatzakis, 2018; Rashid *et al.*, 2021) [28, 59].

High-field NMR spectrometers, which provide the best combination of sensitivity and spectral resolution, depend on cryogenically cooled superconducting magnets that are very expensive to acquire, requiring capital investments from several hundred thousand to over one million euros per instrument, and incur substantial ongoing costs for liquid helium replenishment, maintenance contracts, and expert technical personnel (Pullen and Booth, 2021; Hatzakis, 2018) [28, 58]. These cost barriers effectively restrict routine high-field NMR to large food companies and specialized reference laboratories, limiting access for small and medium food enterprises (Hatzakis, 2018) [28]. Benchtop NMR instruments address the cost and portability limitations but sacrifice spectral resolution and sensitivity, restricting application to major food constituents at millimolar concentrations and precluding detection of minor trace

components (Pullen and Booth, 2021; Blümich, 2019) ^[11, 58]. The complexity of NMR data and the requirement for specialized chemometric expertise present additional practical barriers, because developing, validating, and maintaining statistical classification models requires statistical training not universally available in food production or regulatory environments (Hatzakis, 2018; Savorani *et al.*, 2021) ^[28, 64]. Inter-laboratory transferability of NMR-based chemometric models remains a significant unresolved challenge, because models optimized for one instrument may not perform reliably on different instruments due to subtle differences in field homogeneity, shimming, and probe characteristics (Savorani *et al.*, 2021) ^[64].

7. Future prospects

The future trajectory of NMR technology in food science is shaped by converging advances in instrumentation miniaturization, signal enhancement, digital data processing, and regulatory framework development (Pullen and Booth, 2021; Beek, 2021; Alkanan *et al.*, 2025) ^[3, 6, 58]. The continued development of benchtop NMR instruments operating at 40 to 100 MHz with permanent magnets is progressively making NMR analytical capabilities accessible in industrial production environments without the infrastructure requirements of high-field superconducting magnet systems (Beek, 2021; Blümich, 2019) ^[6, 11]. As permanent magnet homogeneity and digital signal processing continue to improve, the spectral resolution and sensitivity achievable by benchtop systems is narrowing the performance gap with low-end high-field instruments for standard food composition analysis tasks, and future developments may enable handheld or truly portable NMR devices suitable for use at farm gates and retail inspection points (Beek, 2021; Pullen and Booth, 2021) ^[6, 58].

Hyperpolarization techniques represent a scientifically promising frontier for overcoming NMR's inherent sensitivity limitations, with approaches such as Signal Amplification By Reversible Exchange capable of transiently enhancing NMR signal intensity by several orders of magnitude at relatively modest additional cost (Pullen and Booth, 2021) ^[58]. If successfully adapted for routine food analysis protocols, hyperpolarization could extend NMR detection capabilities toward trace-level analytes currently accessible only by mass spectrometry, potentially broadening NMR's regulatory relevance to contaminant monitoring applications (Pullen and Booth, 2021) ^[58]. The integration of NMR with artificial intelligence and machine learning approaches is expected to substantially expand NMR's practical accessibility in food science, as AI algorithms can identify complex non-linear patterns in large spectral datasets with greater speed and accuracy than traditional chemometric methods, supporting high-throughput food authentication decisions, predictive quality modeling, and real-time process anomaly detection (Alkanan *et al.*, 2025; Savorani *et al.*, 2021) ^[3, 64]. The convergence of NMR with blockchain-based traceability systems and digital supply chain platforms represents a further transformative opportunity, where NMR-generated metabolic fingerprints could serve as cryptographically secure chemical identifiers recorded on immutable digital ledgers to provide verifiable proof of food origin and authenticity throughout the supply chain (Lukacs *et al.*, 2025) ^[43].

8. Conclusion

This review has traced the technology from its quantum mechanical foundations through instrumentation design and across the diverse technical variants applied in food analysis, demonstrating how each variant's distinctive analytical strengths serve specific food science objectives. High-field NMR provides unmatched chemical resolution for comprehensive metabolite profiling and structural identification; benchtop NMR delivers accessible process-side quality monitoring without cryogenic infrastructure; time-domain and low-field NMR enable rapid non-destructive characterization of water and fat states in intact food products; HRMAS-NMR enables metabolomic analysis of intact tissue without extraction; fast field cycling NMR reveals molecular dynamics information inaccessible to fixed-field instruments; and quantitative and multidimensional NMR extend the range of structural and compositional information extractable from complex food matrices. The structural analysis capabilities reviewed in this paper, encompassing molecular identification from chemical shift data, water population characterization by T2 relaxometry, protein-water interaction assessment by combined relaxometry and spectroscopy, and non-destructive fat distribution analysis, collectively provide an information-rich window into the molecular and physical architecture of food with direct relevance to quality, texture, processing optimization, shelf life, and authenticity verification. While important challenges related to instrument cost, limited sensitivity at trace analyte levels, and the requirement for chemometric expertise remain, ongoing advances in benchtop instrumentation, hyperpolarization signal enhancement, and AI-driven spectral analysis are progressively addressing these limitations and expanding NMR's practical accessibility.

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