

A brief review on the application of NMR relaxation methods in food metabolomics for arabica coffee

*Jauhar Dziban Assauqi*¹ and *Surjani Wonorahardjo*^{1,2*}

¹ Department of Chemistry, Faculty of Mathematics and Natural Sciences, Universitas Negeri Malang, Jl. Semarang 5, Malang 65145, Indonesia.

² Center of Advanced Materials and Renewable Energy, State University of Malang, Jl. Semarang 5, Malang 65145, Indonesia.

Abstract. Nuclear Magnetic Resonance (NMR) relaxometry has emerged as a complementary tool in food metabolomics to investigate molecular dynamics beyond conventional spectral analysis. In coffee systems, longitudinal (T_1) and transverse (T_2) relaxation times provide insights into molecular movements and interactions relevant to flavor and aroma development during brewing. T_1 relaxation is primarily associated with slower molecular motion and bulk interactions, such as water mobility and lipid matrix organization on longer timescales. In contrast, T_2 relaxation is more sensitive to faster, localized molecular dynamics, including water-solute interactions, molecular confinement, and structural heterogeneity within the coffee matrix. These short-range dynamics are directly involved in the release, diffusion, and perception of volatile and non-volatile compounds, making T_2 relaxation more closely related to aroma intensity and flavor expression during extraction. This review summarizes the principles of NMR relaxation and its applications in various food matrices, with Arabica coffee discussed as a representative complex system. Methodological challenges, inconsistencies in reporting, and limitations in interpretation are highlighted. From a sustainability perspective, NMR relaxometry aligns with the principles of green analytical chemistry by enabling rapid, non-destructive analysis with minimal solvent consumption. Future directions toward standardized and meaningful relaxation-based NMR applications in coffee research are discussed.

1. Introduction

Nuclear Magnetic Resonance (NMR) spectroscopy is a versatile and non-destructive analytical technique that provides molecular-level information on food systems without requiring extensive sample preparation or toxic solvents [1], [2]. Unlike chromatography approaches that rely on extraction, separation, and derivatization steps, NMR enables direct and simultaneous qualitative and quantitative observation of various metabolites, making it highly attractive for applications aligned with green analytical chemistry and sustainability principles [3]. In food metabolomics, this capability enables comprehensive chemical fingerprinting of complex matrices, including

*Corresponding author: surjani.wonorahardjo@um.ac.id

sugars, organic acids, lipids, amino acids, and other low molecular weight compounds that collectively determine food quality attributes [4], [5]. This positions NMR as an important analytical platform for assessing sustainable food quality.

In coffee, these chemical constituents, beyond the widely known caffeine, play a central role in shaping sensory properties such as taste and aroma [6]. Previous studies have shown that brewed coffee contains a variety of extractable components, including chlorogenic acid, carboxylic acids that contribute to acidity, tannins, terpenoids, and long-chain esters associated with aroma perception [6], [7]. Macromolecular components such as carbohydrates, proteins, and lipids further influence extraction behavior and flavor release during brewing, highlighting coffee as a chemically and structurally complex system where molecular organization is as important as chemical composition [8], [9]. Beyond conventional spectral interpretations based on chemical shifts, NMR offers access to spin relaxation parameters, namely longitudinal (T_1) and transverse (T_2) relaxation times, which provide complementary information about molecular motion, intermolecular interactions, and physicochemical environment [5], [10].

While chemical shifts primarily reflect molecular identity and composition, relaxation parameters investigate molecular dynamics across various timescales [2]. In this context, T_1 relaxation is generally associated with slower molecular motion and bulk interactions, while T_2 relaxation is more sensitive to faster and localized dynamics, molecular confinement, and heterogeneity within complex food matrices. These differences underpin the specific contributions of T_1 and T_2 data to metabolomics beyond conventional compound identification.

The application of NMR relaxation techniques in food science has demonstrated its potential to distinguish food quality, composition, and authenticity across various matrices, including dairy products [11], meat [10], [12], and cereals [13]. In coffee research, Muniz et al. used ^1H LF-NMR (Low Field-Nuclear Magnetic Resonance) relaxometry to show that oil-rich Arabica varieties exhibit longer T_2 relaxation times than Robusta varieties, enabling variety discrimination through parameters such as relative hydrogen index [9]. Complementary work by Prakash and Mahar further shows that compositional differences between Arabica and Robusta can be detected using ^1H NMR spectral features [5]. These studies describe the current state of the art in applying relaxation- and NMR spectral-based approaches to coffee characterization.

Despite these advances, the current state of coffee metabolomics remains largely focused on the identification and quantification of compounds using chemical shift information, such as the use of choline and glycerophosphocholine as markers of chemical ageing in green coffee [8]. The systematic integration of T_1 and T_2 relaxation data into metabolomic interpretation, particularly to explain molecular mobility, matrix heterogeneity, and extraction-related phenomena, remains limited. This gap limits the ability to fully utilize NMR as a tool for understanding the functional and sensory properties of coffee.

From a sustainability perspective, the growing interest in LF-NMR and High Resolution Magic Angle Spinning (HRMAS) techniques reflects the demand for fast, non-destructive, and solvent-free analytical platforms consistent with the principles of Green Analytical Chemistry [1], [3], [5]. As emphasized by Khan et al. (2022), combining relaxation information with complete ^1H NMR spectra offers a more holistic framework for food quality evaluation by linking molecular identity with molecular dynamics [10]. However, a consolidated and critical synthesis of this approach within coffee systems remains lacking.

Therefore, this article is explicitly presented as a review, which aims to (i) critically summarize the current state of NMR relaxation applications in food metabolomics, (ii) discuss methodological considerations and sustainability aspects of T_1 and T_2 relaxometry, and (iii) illustrate, through literature-based discussion and conceptual examples, how relaxation parameters complement conventional metabolomic data in the characterization of Arabica coffee. By clarifying the distinct

contributions of T_1 and T_2 relaxation to metabolomic interpretation, this review highlights the novelty and importance of this conceptual framework rather than an experimental study.

2. Results and Discussion

2.1 Principles of NMR Relaxometry

NMR relaxometry describes the return of nuclear magnetization to equilibrium after radio frequency excitation and provides fundamental information about molecular dynamics and interactions within a system [5], [10]. Unlike conventional spectral analysis based on chemical shifts, which primarily reflects molecular identity and chemical composition, relaxation parameters investigate dynamic processes occurring at various time scales and length scales [2], [9]. Included in NMR relaxometry are the T_1 and T_2 relaxation.

T_1 relaxation characterizes the recovery of magnetization along the direction of a static magnetic field and is governed by energy exchange between the nuclear spin and the surrounding lattice. Therefore, T_1 relaxation is sensitive to relatively slow molecular motion, mass mobility, and long-range interactions, such as those associated with water dynamics and lipid organization in complex food matrices [10], [13]. In heterogeneous systems, variations in T_1 values can reflect differences in molecular environment and degree of molecular freedom rather than merely changes in chemical composition. In contrast, T_2 relaxation describes the loss of phase coherence of nuclear spins in a plane perpendicular to the static magnetic field and is dominated by spin-spin interactions and local magnetic field inhomogeneities [5], [10]. T_2 relaxation is highly sensitive to fast and localized molecular motion, molecular confinement, and structural heterogeneity at the micro scale. Consequently, T_2 values are strongly influenced by intermolecular interactions, pore size distribution, and the presence of macromolecular networks that restrict molecular mobility.

The complementary nature of T_1 and T_2 relaxation provides a multidimensional view of molecular dynamics in complex food systems. While T_1 reflects global and slower motion processes related to bulk physicochemical properties, T_2 captures local dynamics closely associated with diffusion, exchange processes, and short-range interactions. These differences are particularly relevant in food matrices, where the perception of taste and aroma during processing or extraction is governed not only by chemical composition but also by molecular mobility and matrix organization [6], [8].

From a metabolomic perspective, relaxation parameters provide information beyond compound identification and quantification. By integrating T_1 and T_2 relaxation data with conventional ^1H NMR spectral information, it is possible to link molecular identity with molecular behavior, enabling a more comprehensive interpretation of food quality, structure, and functionality [2], [5]. This conceptual framework underpins the growing interest in NMR relaxometry as a complementary tool for food metabolomics and quality assessment.

2.2 Applications of NMR Relaxometry in Food Matrices

NMR relaxometry has been widely applied in food science as a rapid and non-destructive approach to investigate molecular mobility, structural organization, and compositional heterogeneity in complex matrices. By analyzing T_1 and T_2 relaxation behavior, it is possible to distinguish food systems based on their physicochemical properties without extensive sample preparation or chemical modification [1], [11]. This relaxation-based contrast reflects differences in molecular environment and interaction strength, providing information that complements conventional spectral interpretation in food metabolomics.

In aqueous and semi-aqueous food systems, relaxation parameters are strongly influenced by water dynamics and their interactions with solutes and macromolecules. T_1 relaxation is generally associated with overall water mobility and long-range molecular interactions, while T_2 relaxation is highly sensitive to water confinement, exchange processes, and interactions with proteins, polysaccharides, and other macromolecular structures [10], [12]. These characteristics have been utilized to assess hydration status, structural integrity, and textural properties in food products.

In lipid-rich matrices, NMR relaxometry provides insights into lipid mobility, phase behavior, and interactions with surrounding components. Longer T_2 relaxation times are often associated with increased lipid fluidity and reduced molecular confinement, while shorter T_2 values may indicate stronger interactions with solid or semi-solid matrices. These differences have been applied to evaluate fat content, lipid organization, and compositional differences in products such as oils, dairy systems, and processed foods [9], [14].

Protein-based food matrices, including meat and dairy products, have also been extensively studied using NMR relaxometry [10], [12]. In these systems, T_2 relaxation is highly informative for distinguishing between different water populations, such as bound, immobilized, and free water fractions. Changes in relaxation behavior have been correlated with protein denaturation, gel formation, and structural rearrangement that occur during processing and storage. Similarly, in cereal-based and carbohydrate-rich foods, relaxation parameters have been used to investigate starch gelatinization, retrogradation, and water-polymer interactions [2], [13]. Variations in T_1 and T_2 values reflect changes in molecular mobility and matrix stiffness, providing indirect indicators of texture quality and processing history.

Across these diverse food matrices, the combined interpretation of T_1 and T_2 relaxation enables the differentiation of quality attributes, detection of compositional differences, and identification of structural heterogeneity [2], [4]. Importantly, these applications highlight that relaxation-based NMR not only complements conventional compositional analysis but also offers unique insights into the molecular dynamics governing food functional properties. This capability has positioned NMR relaxometry as a valuable analytical tool in food metabolomics and quality assessment. A summary of LF-NMR applications in food matrices is provided in **Table 1**.

Table 1. Representative applications of NMR relaxometry in coffee and related food matrices.

Food Matrix	Relaxation Parameter (T_1 / T_2)	Information Obtained	Ref
Wheat seed (<i>Triticum aestivum</i> L.)	T_1 and T_2	Molecular mobility and water dynamics during rehydration; identification of bound water fractions (very tightly vs. tightly bound).	[13]
Coffee (Arabica and Robusta blends)	T_2 (LF-NMR)	Discrimination of coffee varieties in blends based on the mobility of the lipid phase and oil content.	[9]
Fresh Pork Hams	T_2 (LF-NMR)	Distribution of water populations in muscle tissue and estimation of water-holding capacity (WHC).	[12]
Milk (Adulterated)	T_2 (TD-NMR)	Rapid detection and quantification of adulterants (whey, urea, hydrogen peroxide) through water proton mobility.	[11]

2.3 Coffee Matrices as a Literature-Based Case Study

Coffee is a chemically and structurally complex food matrix, in which molecular composition, physical organization, and molecular mobility collectively regulate quality attributes such as aroma, taste, and extraction behavior [6], [7]. In addition to low molecular weight metabolites, including caffeine, trigonelline, and chlorogenic acid, coffee contains lipids, carbohydrates,

proteins, and cell wall components that greatly influence water accessibility and mass transfer during brewing [8]. Due to its multicomponent and heterogeneous nature, coffee is frequently used in the literature as a model system to illustrate the relevance of NMR-based approaches for food metabolomics and quality assessment.

2.3.1 Coffee Matrix Organization and the Effect of Roasting

The roasting process induces extensive physicochemical transformations in coffee beans, including polysaccharide degradation, protein denaturation, melanoidin formation, and lipid redistribution within cellular structures. These changes alter the matrix porosity, surface properties, and water-solid interactions, thereby affecting molecular mobility across multiple length scales [9]. Such structural reorganization is not fully captured by compositional analysis alone, underscoring the importance of techniques sensitive to molecular dynamics. **Fig. 1** provides a representative ^1H NMR spectral profile to conceptually illustrate the chemical complexity of Arabica coffee, rather than as a source of quantitative information.

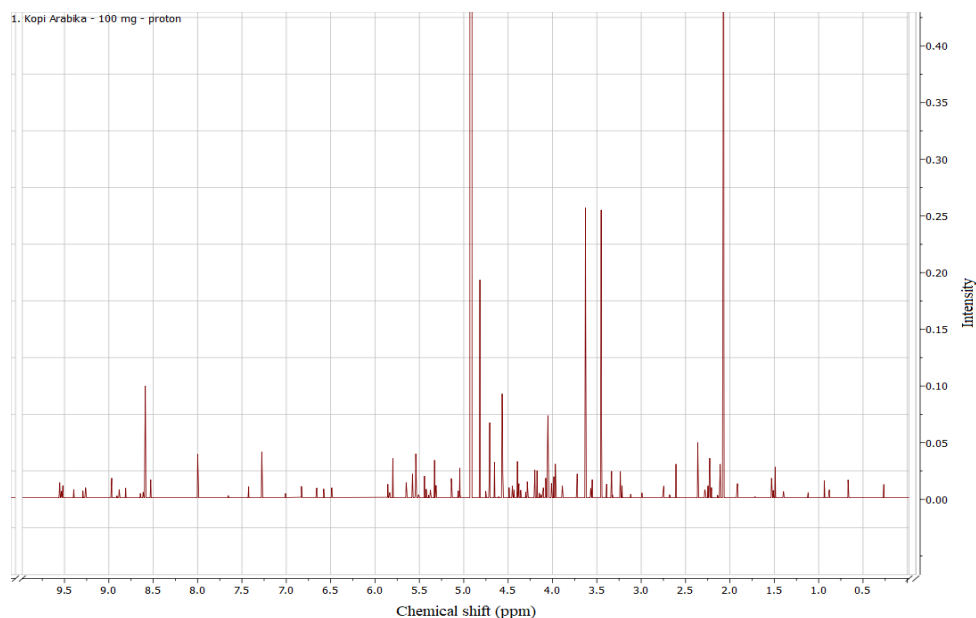


Fig. 1. Representative ^1H NMR spectral profile of Arabica coffee illustrating the chemical shift regions associated with major metabolite classes. The figure is shown for conceptual visualization of spectral complexity rather than quantitative interpretation.

2.3.2 Water–Lipid–Cell Wall Interactions and Relaxation Behavior

During the coffee brewing process, water mobility and its interaction with lipids and cell wall polymers play an important role in determining the kinetics of extraction and flavor release. From a relaxometry perspective, T_1 relaxation is generally associated with overall water mobility and long-range interactions influenced by the overall matrix organization, while T_2 relaxation is more sensitive to local molecular constraints, exchange processes, and microstructural heterogeneity [5], [10]. These differences imply that variations in T_2 relaxation are more directly related to the

diffusion and release of soluble flavor compounds during brewing, while T_1 provides complementary information about the overall hydration state of the coffee matrix.

Previous studies have reported that oil-rich Arabica coffee varieties tend to exhibit longer T_2 relaxation times compared to Robusta varieties, reflecting increased molecular mobility in lipid-related domains [9]. This observation suggests that relaxation behavior can provide insights into how matrix organization affects aroma retention and release, complementing information obtained from conventional spectral analysis. An illustrative example of T_1 and T_2 relaxation behavior plotted against representative chemical shift regions is shown in **Fig. 2** to support the conceptual discussion of relaxation mechanisms reported in the literature.

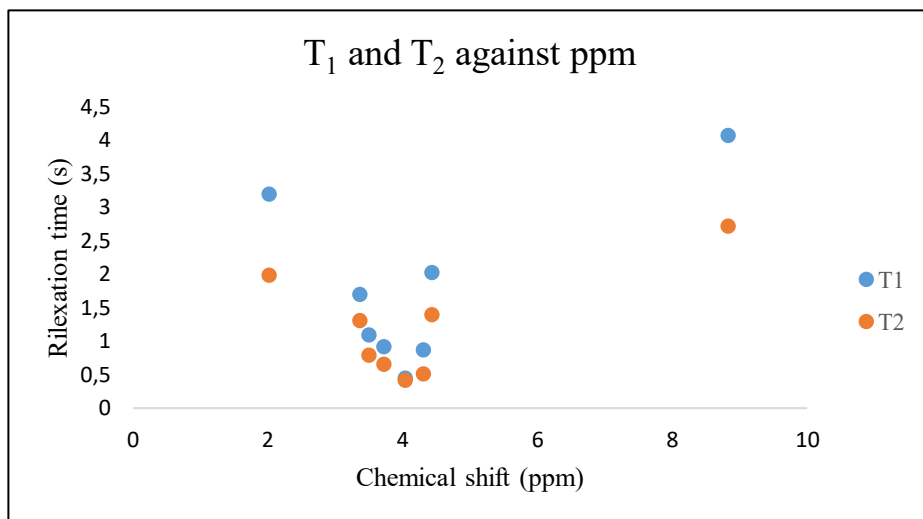


Fig. 2. Illustrative representation of T_1 and T_2 relaxation behavior plotted against chemical shift regions, based on representative relaxation trends reported for coffee systems. The figure is intended to support conceptual discussion of relaxation mechanisms rather than to present experimental results.

2.3.3 Integration of Relaxation Parameters in Coffee Metabolomics

Although most coffee metabolomics studies rely primarily on chemical shift information for compound identification and quantification, relaxation parameters provide complementary insights into collective molecular behavior within the matrix [4], [9]. Unlike spectral markers, T_1 and T_2 relaxation times do not correspond to individual metabolites but reflect ensemble dynamics influenced by interactions between water, lipids, and solid components. This distinction is particularly relevant for coffee systems, where samples with similar chemical compositions may exhibit different sensory characteristics due to differences in molecular mobility and microstructure. In this context, relaxation parameters serve as descriptors of matrix organization and dynamic behavior, helping to rationalize variations in extraction efficiency, aroma release, and taste perception that are not easily explained by composition data alone [4], [5].

In the context of coffee analysis, authentication refers to the verification that a coffee product corresponds to its botanical origin or declared composition, specifically the confirmation of Arabica–Robusta purity and the detection of undeclared blending or adulteration. LF NMR relaxation parameters contribute to authentication not by identifying specific molecular markers, but by exploiting systematic differences in matrix dynamics associated with variety composition.

As demonstrated by Muniz et al. (2023), Arabica and Robusta coffee exhibit markedly different lipid contents, which translate into distinct contributions from mobile proton populations characterized by longer T_2 relaxation components [9]. By isolating this moving phase and measuring its signal amplitude using parameters such as the relative hydrogen index (RHI), T_2 -based relaxometry enables strong discrimination between pure varieties and their blends, with a strong linear relationship between relaxation-derived metrics and Arabica content. Within this framework, relaxation parameters act as indirect yet quantitative indicators of authenticity, sensitive to variety-dependent matrix organization rather than individual metabolites, thus providing a complementary and practical pathway for coffee authentication beyond conventional compositional profiles.

Overall, the literature indicates that coffee serves as a valuable model system for describing how NMR relaxometry bridges molecular composition and molecular dynamics [2]. By integrating relaxation behavior with conventional ^1H NMR spectral information, it is possible to interpret coffee quality attributes in a more mechanistic way, emphasizing matrix effects and molecular mobility rather than just compositional changes [4], [5]. Such an approach enables interpretation of sensory and extraction-related phenomena that are not fully captured by compositional analysis. Thus, coffee provides a representative platform to demonstrate the conceptual value of relaxation-based NMR in food metabolomics.

2.4 Strengths, Limitations, and Practical Challenges

NMR relaxometry offers several advantages as an analytical approach for food metabolomics and quality assessment, particularly in the context of complex matrices such as coffee [4], [5]. One of its main strengths lies in its non-destructive nature and minimal sample preparation requirements, enabling rapid analysis while preserving the original structure and molecular organization of the sample. This feature is particularly valuable for studying molecular dynamics and matrix effects that are often altered by extraction- or separation-based techniques.

Another key advantage of NMR relaxometry is its ability to investigate molecular mobility and intermolecular interactions, in addition to chemical composition. By providing complementary information through T_1 and T_2 relaxation parameters, relaxometry enables insights into bulk and local dynamics that influence functional properties such as extraction behavior, texture, and sensory perception [2], [8]. This dynamic perspective is difficult to obtain using conventional metabolomics techniques, which primarily focus on compound identification and quantification.

Despite these advantages, several limitations must be considered when applying NMR relaxometry to food systems. The main challenge is the indirect nature of relaxation parameters, which reflect collective molecular behavior rather than specific metabolites [2]. As a result, interpreting T_1 and T_2 values often requires careful consideration of matrix composition, microstructure, and physicochemical context, and may not be straightforward without complementary analytical information. Overlap of relaxation components, especially in heterogeneous systems, is another practical limitation. In complex food matrices, multiple molecular populations may exhibit similar relaxation times, leading to broad or overlapping T_2 distributions that complicate data interpretation and model fitting [9], [12]. This issue is particularly relevant in coffee, where water, lipids, and solid components coexist at various spatial scales.

Instrumental and methodological factors also influence the practical application of NMR relaxometry. High-field NMR instruments provide better spectral resolution but are associated with high acquisition and maintenance costs, which can limit accessibility [1]. Although LF-NMR relaxometry offers a more cost-effective and portable alternative, reduced sensitivity and resolution may limit its application to certain analytical questions [14]. Furthermore, variations in pulse

sequences, acquisition parameters, and data processing approaches across studies hinder direct comparison and reproducibility.

From a practical standpoint, the lack of standard protocols and reporting guidelines is a significant barrier to the wider adoption of relaxation-based NMR in food metabolomics. Inconsistent reporting of experimental conditions, relaxation models, and adjustment procedures complicates comparisons between studies and limits the development of robust databases or predictive models [2]. Overcoming these challenges will require coordinated efforts toward methodological harmonization and transparent reporting. Overall, while NMR relaxometry provides unique and valuable insights into molecular dynamics and matrix organization, its effective application in food systems depends on careful experimental design, complementary analytical approaches, and critical interpretation of results [5]. Recognizing the strengths and limitations of this technique is essential for its meaningful integration into metabolomics and food quality research.

2.5 Future Perspectives and Sustainability Considerations

Future research of NMR relaxometry in food metabolomics is closely linked to advances in data analysis, instrumentation, and sustainability-oriented analytical design. Although current studies have demonstrated the ability of T_1 and T_2 relaxation parameters to capture molecular mobility and matrix organization, their full potential has not yet been realized through systematic integration with multivariate analysis and environmentally friendly analytical strategies [4]. One promising direction is the integration of NMR relaxation data with chemometric and machine learning approaches. Multivariate techniques such as principal component analysis (PCA), partial least squares regression (PLSR), and supervised classification models can improve the interpretation of complex relaxation datasets by linking relaxation behavior to compositional, structural, or quality-related attributes [11].

In the context of coffee, combining T_1 and T_2 relaxation parameters with complete ^1H NMR spectral features can enable improved discrimination of roast level, botanical origin, and matrix composition, while reducing dependence on extensive chromatographic profiles. Such data-driven frameworks are invaluable for translating relaxation parameters, often considered abstract, into practically meaningful quality indicators. Another key perspective relates to the increasing accessibility of low-field and portable NMR technology. Recent developments in LF-NMR relaxometry have enabled compact, cost-effective instruments capable of rapid on-site analysis [9].

Although this system offers lower spectral resolution than high-field NMR, its sensitivity to molecular mobility and relaxation behavior remains adequate for many food quality applications. The application of portable NMR devices throughout the food production and supply chain opens up new possibilities for decentralized quality monitoring, authenticity assessment, and process control, including coffee roasting and brewing operations [2], [5]. In this context, relaxation-based parameters provide robust, field-tolerant descriptors that are well suited for implementation on low-field, portable NMR platforms.

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From a sustainability perspective, NMR relaxometry is highly aligned with the principles of Green Chemistry and Green Analytical Chemistry [3]. This technique is essentially non-

destructive, requires minimal or no sample pretreatment, and avoids the use of hazardous organic solvents commonly associated with chromatography methods [1]. These characteristics position NMR relaxometry as a sustainable alternative for routine food analysis, particularly in large-scale or repetitive quality assessments.

Looking ahead, the development of standard protocols for relaxation measurement, data processing, and reporting will be crucial for improving reproducibility and comparability between studies [2], [5]. Establishing reference relaxation ranges for major food matrices, including Arabica coffee, could facilitate the wider adoption of relaxometry as a complementary tool in metabolomics and quality assessment. When combined with chemometric modelling and sustainable analytical practices, NMR relaxometry has the potential to evolve from a specialised research technique into a practical, environmentally friendly, and scalable platform for food analysis.

3. Conclusion

This review highlights the role of NMR relaxometry as a complementary approach in food metabolomics, offering insights into molecular dynamics and matrix interactions that go beyond conventional spectral analysis. By focusing on T_1 and T_2 relaxation parameters, NMR relaxometry enables the characterization of overall and localized molecular motion relevant to extraction behavior and sensory-related properties in complex matrices such as Arabica coffee. Future development of NMR relaxation-based metabolomics should prioritize standardized acquisition protocols, including clear specifications of pulse sequences, relaxation delays, echo times, and temperatures, as these parameters directly control the measured T_1 and T_2 values and determine reproducibility across studies. Integration of T_1 and T_2 relaxation data with full ^1H NMR spectra and chemometric analysis is recommended to translate molecular mobility into chemically and functionally meaningful quality indicators. Importantly, NMR relaxation measurements can be applied at various magnetic field strengths, including high-field, medium-field, and low-field NMR instruments, provided that acquisition parameters are appropriately optimized for each system. Although absolute relaxation times may vary with magnetic field strength, relative relaxation trends related to molecular dynamics remain comparable, enabling cross-platform interpretation and broader application. Overall, the alignment of NMR relaxometry with green analytical chemistry principles, combined with methodological standardization and instrument flexibility, positions this technique as a sustainable and scalable platform for future food metabolomics studies and quality assessment.

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