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EXPANDING FRONTIERS OF FTIR AND ATR-FTIR SPECTROSCOPY FOR FOOD SAFETY: CURRENT APPLICATIONS AND EMERGING TRENDS

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Fourier transform infrared (FTIR) and attenuated total reflection fourier transform infrared (ATR-FTIR) spectroscopy are versatile, non-destructive analytical techniques that provide detailed molecular insights through infrared light absorption. This review explores their theoretical foundations, technological evolution, and diverse applications across food quality and safety assessment. Advanced modalities, including FT-NIR and FT-MIR combined with chemometrics, enable rapid, high-throughput, preparation-free detection of adulterants in milk, edible oils, and other food matrices, while facilitating protein structural analysis, nutritional evaluation, origin authentication, and spoilage monitoring. Studies demonstrate high accuracy in identifying contaminants such as pig fat, hydrogen peroxide, melamine, urea, mineral oils, and antibiotic residues, as well as monitoring molecular changes during processing and storage. The integration of vibrational spectroscopy with machine learning (ML), multivariate analysis, and complementary techniques like mass spectrometry, nuclear magnetic resonance, and hyperspectral imaging enhances predictive performance, classification robustness, and bioactive compound quantification. Furthermore, portable and real-time instruments support in situ monitoring, traceability, and regulatory compliance, advancing food safety and fraud prevention. Beyond dairy and edible oils, these techniques are increasingly applied to frozen foods, meat, plant-based alternatives, probiotics, and edible flowers, highlighting their broad versatility. Challenges such as spectral overlap, limited industrial adoption, and model standardization remain, but ongoing developments in instrumentation, chemometrics, and AI integration are expected to expand accessibility and reliability. Overall, FTIR and ATR-FTIR spectroscopy, combined with chemometric and ML approaches, provide cost-effective, rapid, and accurate solutions for authentication, quality control, and consumer safety across diverse food, nutraceutical, and biological systems.

Keywords: FTIR spectroscopy, ATR-FTIR, food authentication, adulteration detection, non-destructive analysis

1. Introduction

Fourier transform infrared (FTIR) spectroscopy has emerged as a versatile and non-destructive analytical technique that provides detailed molecular insights by measuring infrared light absorption across the mid-infrared region. This process generates unique spectral fingerprints that allow the identification of functional groups and the detection of structural changes in complex matrices. With increasing advancements in instrumentation and user-friendly software, FTIR is now accessible to both novice and expert users, enabling broad adoption across diverse scientific fields such as biochemistry, materials science, environmental studies, and food quality assessment. Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR), in particular, enhances surface-level analysis without extensive sample preparation, making it especially valuable for routine quality control and real-time monitoring in dynamic systems.

ATR-FTIR spectroscopy has become the most widely adopted mid-infrared technique due to its speed, stability, and minimal sample preparation. It allows direct contact analysis of solids, liquids, and powders, making it indispensable in fields like biology, forensics, medicine, and industrial process control. Ramer and Lendl [1] discussed both theoretical principles and practical usage, moreover highlighted emerging trends such as evanescent wave spectroscopy and miniaturized, portable ATR devices. Innovations like waveguide sensors integrated with quantum cascade lasers are paving the way for enhanced field-based applications.

Fourier transform infrared spectroscopy is a cornerstone analytical technique for exploring how infrared light interacts with matter to identify molecular components and structures. As explained by Smith [2], it operates within the mid-infrared range (4000–400 cm^{-1}), generating spectra that map light absorption versus wavenumber. FTIR spectrometers provide detailed insights into sample composition, aiding both beginners and experts in obtaining, analyzing, and interpreting

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spectra. This foundational knowledge enables users to prepare samples accurately and use FTIR software for meaningful chemical analysis, setting the stage for a wide array of scientific applications. FTIR spectroscopy is particularly powerful for studying biomolecules such as amino acids, water, and cofactors, especially when structural sensitivity is critical. Berthomieu and Hienerwadel [3] emphasized how reaction-induced FTIR difference spectroscopy allows researchers to isolate specific vibrational changes associated with active chemical groups. Advanced techniques, including isotope labeling and computational modeling, further enhance molecular resolution. These tools have illuminated dynamic biological systems, such as photosystems involved in photosynthesis, offering molecular-level insights that bridge experimental data with structural understanding. This integration underscores FTIR's capacity to decode complex biochemical mechanisms.

Within the dairy industry, FTIR, FT-NIR, and FT-MIR spectroscopy, when combined with chemometric techniques like Principal Component Analysis (PCA), Soft Independent Modeling of Class Analogy (SIMCA), and Partial Least Squares Regression (PLSR), have become powerful tools for food quality control and adulteration detection. These integrated approaches enable rapid, preparation-free analysis of milk and dairy products, allowing for the identification of adulterants such as melamine, urea, and hydrogen peroxide, as well as the assessment of protein stability and structural integrity. As food authenticity and safety gain increasing global attention, FTIR spectroscopy continues to offer efficient, high-throughput, and reliable solutions to safeguard consumer trust and uphold regulatory standards. Despite the widespread use and technological progress of FTIR and ATR-FTIR spectroscopy across various disciplines, there remains a lack of standardized methodologies and comprehensive spectral databases to ensure consistency, reproducibility, and comparability of results across laboratories. Moreover, the integration of advanced chemometric and machine learning (ML) approaches with FTIR data analysis is still underdeveloped, limiting the full exploitation of these techniques for complex, real-world applications in food, biomedical, and environmental research.

The objective of this review is to provide a comprehensive evaluation of FTIR and ATR-FTIR spectroscopy, including their theoretical principles, methodological advancements, and diverse applications across food safety domains. It aims to highlight their role in structural elucidation, molecular interaction analysis, and non-destructive quality assessment in food, dairy, edible oils, and plant-based products. Particular emphasis is placed on rapid, accurate, and high-throughput detection of adulterants, contaminants, and bioactive compounds, as well as monitoring protein structural changes, spoilage, and shelf-life. By critically examining recent studies, technological developments, and practical applications, this review aims to identify opportunities for scalable, cost-effective, and sustainable strategies that enhance routine quality control, regulatory compliance, consumer safety, and the overall reliability of food and dairy products in industrial and research settings.

2. Methodology

This study employs a bibliometric and narrative review approach to examine advancements in FTIR and ATR-FTIR spectroscopy within food safety applications. By applying quantitative bibliometric techniques to scholarly publications, the study provides a structured overview of research development, knowledge patterns, and emerging trends in the field. The review synthesizes recent literature to explore FTIR and ATR-FTIR Spectroscopy for Food Safety, emphasizing technological innovation and practical applications. Peer-reviewed articles published in English were systematically retrieved from major academic databases. A narrative analytical approach was applied to interpret selected studies, focusing on their relevance to technological developments, methodological advances, and practical applications in food quality and safety assessment. Literature was categorized according to technological domains, enabling a comprehensive synthesis of trends, challenges, and opportunities.

3. Applications of FTIR and ATR-FTIR spectroscopy in food safety

The broad applicability of FTIR and IR spectroscopy spans disciplines, including food safety. Ferrer [4] illustrated its use in detecting additives and examining forensic samples like paints and textiles. IR spectroscopy's non-destructive nature and molecular specificity make it invaluable for analyzing multilayered and heterogeneous materials like semiconductors, films, and geological inclusions, reinforcing its role as a universal tool for qualitative and quantitative molecular analysis. Recent research has extended FTIR spectroscopy's utility to the characterization of separation and extraction materials, especially in sample preparation processes. Gong et al. [5] highlighted its application in evaluating solid-phase sorbents along with liquid-phase extractants such as ionic liquids and deep eutectic solvents. FTIR aids in elucidating underlying extraction mechanisms, identifying key interactions like hydrogen bonding, electrostatic forces, and hydrophobic effects. These capabilities enhance the development of more effective extractants for complex targets. As a rapid and affordable tool, FTIR continues to evolve, supporting innovation in analytical and preparative sciences.

Fundamentally, ATR-FTIR works by passing infrared light through a high-refractive-index crystal, such as diamond, where it reflects internally and generates an evanescent wave that interacts with the sample. Absorption at specific wavenumbers, corresponding to molecular vibrations, provides a unique spectral fingerprint. As Metaltech Services Limited [6] explains, this method requires no elaborate sample preparation and offers rapid, non-destructive chemical

analysis, ideal for identifying functional groups and understanding molecular structures in various material states. Ensuring correct contact and critical angle alignment is essential for accurate spectral results. Continued technological integration has expanded ATR-FTIR's reach into chemical process monitoring and protein analysis. The rising global demand for food necessitates reliable, rapid quality and authenticity assessment. Vibrational spectroscopic techniques - FTIR, NIR, and Raman - offer non-destructive, efficient chemical and structural analysis, enabling species identification, adulteration detection, and compositional monitoring. Integration with chemometrics, Nuclear Magnetic Resonance (NMR), mass spectrometry, and hyperspectral imaging enhances bioactive compound profiling and traceability [7]. Overall, FTIR and ATR-FTIR spectroscopy offer rapid, non-destructive molecular analysis for food safety. They enable identification of functional groups, additives, and bioactive compounds, while supporting extraction mechanism studies and process monitoring. Integration with chemometrics, NMR, and hyperspectral imaging enhances accuracy and traceability, reinforcing FTIR's versatility and analytical value.

4. Fourier transform infrared spectroscopy in dairy quality control

Fourier transform near- and mid-infrared spectroscopy (FT-NIR, FT-MIR), when combined with chemometric tools, enables rapid, preparation-free detection of milk fat adulteration in yogurt. Temizkan et al. [8] demonstrated high classification accuracy using SIMCA and strong prediction performance through PLSR models ($R^2 > 0.98$). Both NIR and MIR effectively quantified milk fat and adulterant oil content, with NIR showing slightly better precision and predictive capability. Sen et al. [9] applied FTIR spectroscopy to detect adulteration in goat-cow and buffalo-cow milk mixtures with accuracies of 93% and 91%, respectively. Adulteration levels above 5% were reliably detected. Additionally, the method accurately predicted physicochemical properties such as fat, protein, lactose, and non-fat solids using PLSR models ($R^2 = 0.99$), demonstrating FTIR's dual capability for quality assessment and fraud detection.

Grewal et al. [10] explored FTIR to monitor protein structural changes due to enzymatic and thermal treatments in skim milk, aiming to predict UHT milk shelf life. Deamidation and dephosphorylation stabilized secondary structures like α-helices and β-sheets. Heating led to different changes across untreated and treated samples, and unique spectral shifts were linked to sedimentation risk, revealing FTIR's potential for evaluating protein conformational stability. Markoska et al. [11] extended this research to study protein behavior in skim milk with varying total solids (TS) content under thermal treatment. Structural transitions in β-lactoglobulin and α-lactalbumin were tracked using FTIR, revealing that high TS concentrations intensify protein denaturation. Reversible α-helical transformations and increased disorder at higher temperatures underscore FTIR's capability to study thermal responses in concentrated milk systems. Grewal et al. [12] further utilized FTIR to monitor structural changes in UHT milk during accelerated storage. Conformational rearrangements in protein–lipid interactions were observed, particularly at ≥40 °C. Sediment formation, driven by intermolecular β-sheet changes and lipid binding, was identified early using FTIR. These results establish FTIR as a sensitive method for assessing milk shelf life under varying storage conditions.

Nicolaou et al. [13] evaluated FTIR combined with Partial Least Squares (PLS) and Kernel Partial Least Squares (KPLS) regression for detecting adulteration in cow, goat, and sheep milk mixtures. Low error margins (4–8%) confirmed FTIR's ability to identify economically significant adulteration rapidly. Its non-destructive, fast analysis, completing within 30 seconds, positions it as a reliable method for high-throughput quality assurance in dairy processing. Collectively, these studies underscore FTIR spectroscopy's versatile role in dairy science, from rapid adulteration detection to tracking protein structural shifts during processing and storage. With robust chemometric integration, FTIR offers a powerful, non-destructive, and efficient approach to quality control, contributing to safer and more transparent dairy production practices.

5. ATR-FTIR spectroscopy coupled with chemometric analysis for milk quality

ATR-FTIR spectroscopy combined with chemometric techniques has emerged as a rapid, non-destructive, and sensitive method for detecting adulterants in Ultra High-Temperature (UHT) milk. Julmohammad and Tan [14] showed that hydrogen peroxide (H_2O_2), often illicitly added for preservation, can be accurately detected at concentrations as low as 0.5% v/v using multivariate models such as PCA and Multiple Linear Regression (MLR). Tan et al. [15] extended this approach to urea adulteration detection, developing an ATR-FTIR-based method capable of identifying urea concentrations down to 1% w/v. Their chemometric analysis revealed that the amide I and II regions were most significant, enabling highly accurate classification (up to 100%) and prediction of adulterant levels. The study also stressed the importance of addressing multicollinearity and recommended freeze-drying to improve spectral clarity.

In further work, Julmohammad et al. [16] explored the detection of melamine, formalin, and detergent in milk using ATR-FTIR with PCA, DA, and MLR. The method effectively identified melamine with an R^2 of 0.975 and an RMSE of 0.158%, although detergent detection posed challenges. Nonetheless, this approach remains a valuable asset for food safety assurance in increasingly complex adulteration contexts. Iñón et al. [17] demonstrated ATR-FTIR's ability to predict milk's nutritional content. By analyzing various milk types, they used PLS regression models to estimate fat, protein,

carbohydrates, and calcium content with high precision. Selectivity factors ranged from 2% to 7.6%, and relative standard deviations were below 0.07%, confirming the technique's robustness for routine nutritional quality monitoring. Dimitriou et al. [18] focused on authenticating milk origin using ATR-FTIR. They successfully differentiated cow, sheep, and goat milk through Partial Least Squares Discriminant Analysis (PLS-DA), achieving 100% classification accuracy. Freeze-drying enhanced spectral resolution, especially in the fingerprint region. This technique is crucial for detecting fraud and maintaining product integrity in culturally important dairy sectors. Hayes et al. [19] applied ATR-FTIR to study heat-induced protein denaturation and colloidal calcium phosphate (CCP) transitions in skim milk. By monitoring spectral changes, particularly in β-sheet structures and phosphate-associated regions, they linked denaturation rates to pH and temperature. These insights support process optimization in dairy manufacturing for improved shelf-life and quality.

Richardson et al. [20] demonstrated ATR-FTIR's application in monitoring milk spoilage. Analyzing dried milk films enhanced the absorbance of biochemical markers. Spoilage was indicated by shifts in lipid, protein, and sugar bands. Although early-stage spoilage prediction had limitations, the method offers a foundation for commercial spoilage detection tools to reduce food waste. Nicolaou and Goodacre [21] explored FT-IR's use in monitoring microbial spoilage. ATR and high-throughput modes, combined with PLS regression, detected bacterial loads as low as 10^3 CFU/mL. This rapid screening method outperformed traditional microbiological techniques in speed and ease, making it a strong candidate for real-time microbial quality assessment. Harshitha et al. [22] studied the interaction of aflatoxin M1 (AFM1) with milk proteins using ATR-FTIR. Spectral analysis showed conformational changes in the amide I region due to hydrophobic interactions. PCA revealed strong correlations between spectral shifts and toxin concentration, indicating the technique's sensitivity for early toxin detection. Jaiswal et al. [23] further validated ATR-FTIR for quantifying AFM1 in milk. Spectral features in the 1800–650 cm^{-1} range yielded R^2 values of 0.99 and 0.98 in calibration and validation. The method detected contamination as low as 0.02 µg/L, proving ATR-FTIR's important role in food safety surveillance and regulatory compliance. Key findings of FTIR and ATR-FTIR spectroscopy applications in milk adulteration detection, quality assessment, and safety monitoring are summarized in *Table 1*.

6. ATR-FTIR spectroscopy for dairy adulteration and structural analysis

Adulteration in dairy products undermines food quality and consumer trust. This review highlights that ATR-FTIR spectroscopy, combined with chemometric techniques, offers an effective, rapid, and non-destructive tool for detecting various adulterants in dairy fats and

Table 1: Key findings of FTIR and ATR-FTIR spectroscopy in milk analysis

Application Domain	Major Findings	References
Adulterant Detection (H_2O_2 in UHT Milk)	ATR-FTIR with PCA/MLR detects hydrogen peroxide adulteration in UHT milk down to 0.5% v/v accurately.	[14]
Adulterant Detection (Urea in Milk)	ATR-FTIR identifies urea ≥1% w/v; amide I/II regions critical; chemometrics enables up to 100% classification accuracy.	[15]
Multi-Adulterant Detection	ATR-FTIR with PCA/DA/MLR detects melamine (R^2 0.975); effective for multiple adulterants, though detergent detection is limited.	[16]
Nutritional Composition Analysis	ATR-FTIR with PLS accurately predicts fat, protein, carbohydrates, and calcium with low variability and high precision.	[17]
Milk Authentication (Species Origin)	ATR-FTIR with PLS-DA differentiates cow, sheep, and goat milk with 100% accuracy; freeze-drying improves spectral resolution.	[18]
Heat-Induced Protein Changes	ATR-FTIR monitors protein denaturation and CCP transitions; spectral shifts correlate with pH and temperature changes.	[19]
Milk Spoilage Detection	ATR-FTIR detects spoilage via spectral shifts in lipids, proteins, and sugars; dried films enhance detection sensitivity.	[20]
Microbial Spoilage Monitoring	FT-IR detects bacterial loads ≥10^3 cfu/mL using PLS; faster and simpler than traditional microbiological methods.	[21]
AFM1-Protein Interaction	ATR-FTIR reveals AFM1-induced conformational changes in proteins; PCA correlates spectral shifts with toxin concentration.	[22]
AFM1 Quantification	ATR-FTIR quantifies AFM1 with high accuracy (R^2 up to 0.99); detects levels as low as 0.02 µg/L.	[23]

proteins. These methods enable reliable food authentication and fraud prevention. Upadhyay et al. [24] demonstrated the capability of ATR-FTIR to detect pig body fat in ghee. Spectral data in specific wavenumber zones enabled successful differentiation between pure and adulterated samples. Principal component analysis yielded 90% classification accuracy, while PLSR predicted adulteration down to 3% levels.

In a related study, Upadhyay et al. [25] applied the same methodology to identify goat fat in ghee. The technique detected adulteration at just 1%, with 100% classification efficiency using SIMCA. PCA confirmed clear spectral distinctions, and PLS regression maintained high predictive accuracy with R^2 values above 0.99 for both calibration and validation sets. Gandhi et al. [26] addressed mineral oil adulteration in ghee. Spectral analysis in regions 1350-950 cm^{-1} and 1800–1600 cm^{-1} enabled PCA-based clustering of adulterated samples. SIMCA achieved full classification accuracy, and PLS/ Principal Component Regression (PCR) models detected adulteration as low as 2%, showcasing ATR-FTIR's reliability for routine dairy testing. Beyond fat adulteration, ATR-FTIR is also used in structural protein studies. The technique distinguishes between α-helix and β-sheet structures, making it ideal for studying protein folding, stability, and aggregation in dairy matrices. Yang et al. [27] expanded on these insights, discussing recent advancements in ATR-FTIR for protein structure analysis despite water interference. They highlighted improvements in instrumentation and sampling that enable accurate predictions. The study emphasized how ATR-FTIR rivals more complex techniques like NMR or cryo-electron microscopy in structural protein characterization.

O'Loughlin et al. [28] applied ATR-FTIR to monitor thermal denaturation in whey proteins. Protein dispersions exhibited distinct molecular changes upon heating, influenced by their manufacturing method. This study confirmed ATR-FTIR's usefulness in optimizing thermal processes for concentrated dairy products. Andrade et al. [29] assessed adulteration in whey protein concentrate using milk whey powder. Changes in amide I and II bands, and carbohydrate bands, enabled PCA and PLS modeling with R^2 values exceeding 0.99. These models provided precise quantification of adulterant proportions, confirming the method's sensitivity and accuracy. Leite et al. [30] investigated butter cheese adulteration with soybean oil. A spectral marker at 3007 cm^{-1} was key in detecting unsaturated fats. PCA and PLS effectively differentiated adulterated from pure samples, revealing that FTIR-ATR spectroscopy outperformed traditional methods in sensitivity and predictive strength. Dimitriou et al. [31] used ATR-FTIR to authenticate PDO Feta cheese. Through Principal Component Analysis-Linear Discriminant Analysis (PCA-LDA) and PLS-DA modeling of freeze-dried samples, classification accuracies reached 95.8%. Specific bands corresponding to lipids, proteins, and carbohydrates facilitated robust differentiation between Feta and imitation cheeses. Nurrulhidayah et al. [32] developed a PLS model for detecting lard in butter. The method yielded a near-perfect R^2 of 0.999 and minimal prediction errors. ATR-FTIR spectroscopy thus serves as a green, accurate, and user-friendly platform for dairy adulteration screening and quality control. Key findings of ATR-FTIR spectroscopy applications in dairy products for adulteration detection and protein characterization are summarized in *Table 2*.

Table 2: Summary of key findings of ATR-FTIR spectroscopy for detecting dairy authentication

Application Domain	Major Findings	References
Pig Fat Adulteration in Ghee	ATR-FTIR detects pig fat in ghee; PCA/SIMCA achieve 90% classification, and PLS predicts adulteration down to 3%.	[24]
Goat Fat Adulteration in Ghee	ATR-FTIR detects goat fat at 1% level; SIMCA achieves 100% classification, and PLS shows high predictive accuracy ($R^2 > 0.99$).	[25]
Mineral Oil Adulteration in Ghee	ATR-FTIR identifies mineral oil using key spectral regions; SIMCA achieves 100% classification, and PLS/PCR detects as low as 2%.	[26]
Protein Structural Analysis	ATR-FTIR distinguishes α-helix and β-sheet structures, enabling analysis of protein folding, stability, and aggregation in dairy systems.	[27]
Thermal Denaturation of Whey Proteins	ATR-FTIR tracks structural changes in whey proteins during heating, aiding optimization of thermal processing conditions.	[28]
Whey Protein Adulteration	ATR-FTIR detects whey powder adulteration via amide and carbohydrate bands; PCA/PLS shows high accuracy ($R^2 > 0.99$).	[29]
Butter Cheese Adulteration	ATR-FTIR identifies soybean oil adulteration using 3007 cm^{-1} marker; PCA/PLS outperforms traditional methods in sensitivity.	[30]
Feta Cheese Authentication	ATR-FTIR differentiates authentic and imitation Feta; PCA-LDA/PLS-DA achieve 95.8% classification accuracy.	[31]
Lard Adulteration in Butter	ATR-FTIR detects lard with high precision; PLS model shows near-perfect accuracy ($R^2 = 0.999$).	[32]

7. Advances in FTIR spectroscopy for rapid detection of food adulteration

FTIR spectroscopy has gained significant traction in the food industry due to its rapid, simple, and non-destructive analytical capabilities. The technique enables high-throughput analysis of chemical and physical properties in food with minimal sample preparation. When integrated with multivariate data analysis, FTIR can detect trace adulterants at parts-per-billion sensitivity. Rodriguez-Saona and Allendorf [33] highlighted FTIR's established role in quality control and its growing use in detecting food adulteration. As regulatory demands for food authenticity rise, FTIR offers a powerful and efficient approach to ensure product integrity. Key findings from FTIR spectroscopy applications in food authentication and adulteration detection are summarized in *Table 3*.

High-profile fraud cases, such as the 2008 Chinese milk and 2013 horsemeat scandals, have amplified the need for reliable food authentication technologies. Valand et al. [34] emphasize FTIR's role in food fraud detection due to its analytical speed and robustness. The technique, especially when combined with multivariate analysis, can accurately detect adulterants and confirm authenticity across various food types. While FTIR is powerful on its own, its effectiveness increases when paired with complementary methods. This comprehensive approach strengthens global efforts to protect consumers and reinforce food supply chain integrity. Adulteration of high-value edible oils with cheaper substitutes is a major concern. Rohman et al. [35] reviewed how FTIR spectroscopy, especially when combined with chemometric tools like ATR and multivariate data analysis, provides a fast and cost-effective alternative to traditional techniques. This method creates distinct spectral fingerprints, allowing for reliable detection of adulterants. It also supports routine analysis with minimal technical expertise, offering an accessible solution for quality assurance labs. The authors argue for broader implementation and standardization of FTIR-based protocols in oil authentication practices.

Vlachos et al. [36] applied FTIR to detect adulteration in extra virgin olive oil and monitor oxidation in corn oil. Specific spectral bands (e.g., at 3009 cm^{-1}) reliably indicated adulteration with various vegetable oils. Oxidative changes during heating and UV exposure were also detectable. Adulteration thresholds were determined for different oils, highlighting the technique's precision. This study supports FTIR as a robust tool for real-time quality monitoring in the edible oil sector, detecting both fraudulent additions and degradation processes affecting safety and flavor. Mousa et al. [37] reviewed FTIR's advancement in oil authentication, presenting it as an efficient and eco-friendly alternative to traditional techniques. The technology rapidly evaluates multiple quality parameters from a single spectrum, significantly reducing time and cost. Integration with chemometrics enables precise detection of adulterants throughout the production cycle. This review also discusses recent innovations, practical challenges, and future directions for FTIR, positioning it as a front-line tool for preventing food fraud and ensuring consistent product quality across the edible oil industry.

Rohman and Man [38] demonstrated FTIR's ability to detect and quantify adulteration of extra virgin olive oil (EVOO) with palm oil (PO). They applied PLS and PCR calibration models to both raw and derivative spectra, achieving high prediction accuracy (R^2 up to 0.999) and low error rates. Discriminant analysis perfectly classified pure and adulterated EVOO samples, along with other vegetable oils. The fingerprint region (1500–1000 cm^{-1}) proved critical for classification. These findings confirm FTIR's capability for precise quantification and classification in routine adulteration screening. Collectively, these studies establish FTIR spectroscopy as an essential tool for the modern food industry. Its speed, reliability, and minimal sample handling make it ideal for large-scale food authentication and fraud detection. When coupled with advanced chemometric techniques, FTIR delivers accurate, real-time results that support regulatory compliance and

Table 3: Key findings related to FTIR spectroscopy in food authentication

Application Domain	Major Findings	References
Food Fraud Detection	FTIR detects adulterants quickly and robustly; combining with multivariate methods enhances accuracy for authentication across diverse food products.	[34]
Edible Oil Adulteration Detection	FTIR with chemometrics provides rapid, cost-effective detection of oil adulteration using spectral fingerprints, supporting routine quality assurance.	[35]
Olive Oil Adulteration & Oxidation	FTIR detects olive oil adulteration and monitors oxidation via specific spectral bands, enabling real-time quality and degradation assessment.	[36]
Oil Authentication Advances	FTIR offers eco-friendly, rapid multi-parameter oil analysis; chemometrics enhances adulterant detection and supports production quality monitoring.	[37]
EVOO Adulteration with Palm Oil	FTIR with PLS/PCR accurately quantifies palm oil in EVOO (R^2 up to 0.999); fingerprint region critical for classification.	[38]

consumer safety. From detecting trace adulterants in oils to monitoring protein degradation and oxidative stability, FTIR continues to evolve into a cornerstone of quality assurance, ensuring food integrity in increasingly complex global supply chains.

8. Vibrational spectroscopy and ATR-FTIR for food quality and safety assessment

Raman spectroscopy has proven to be a powerful, non-invasive tool for analyzing frozen food quality by detecting structural changes in proteins, lipids, and water. Zhang et al. [39] discussed the capabilities of dispersive, FT-Raman, Spatially Offset Raman Spectroscopy (SORS), and micro-Raman techniques in monitoring molecular changes during freezing and storage. These methods require minimal sample preparation and offer detailed compositional insights, though challenges like signal overlap and classification inaccuracies remain. Further advancements in database standardization and cost reduction will support broader industrial adoption. In the context of meat safety, FTIR spectroscopy has gained traction for rapid, non-destructive quality control. Candoğan et al. [40] highlighted FTIR's effectiveness when combined with chemometric tools to detect spoilage, adulteration, and biochemical changes in meat products. This technique delivers sensitive physicochemical profiling, supporting both routine monitoring and regulatory compliance. As consumer demands and safety regulations grow, FTIR emerges as a reliable method to maintain integrity and trust in meat supply chains, enhancing both efficiency and traceability.

FTIR spectroscopy has also been explored as an efficient alternative to conventional methods in evaluating wheat quality. Amir et al. [41] demonstrated how FTIR identifies key components, moisture, protein, fat, and starch using characteristic vibrational peaks. Compared with traditional AACC methods, FTIR offers faster, more cost-effective, and non-destructive analysis, aiding in varietal classification and quality prediction. By mapping spectral fingerprints to functional groups, this technique supports precise, high-throughput evaluation across different wheat types, providing a practical solution for industrial and agricultural applications. To support broader applications in food and materials science, Ricci et al. [42] compiled a comprehensive FTIR spectral reference for tannins. Their work offered a valuable fingerprint database for identifying various tannin types, whether isolated in research settings or sourced commercially. Given the widespread use of tannins in pharmaceuticals, food, and agriculture, the availability of such a reference enhances quality assurance and authenticity verification. By consolidating characteristic FTIR peaks, the review contributed a foundational tool for tannin analysis, underscoring FTIR's utility in standardization.

FTIR spectroscopy, particularly when used with ATR, offers a rapid and automatable approach for food quality assessment. Its ease of use, minimal sample preparation, and broad applicability, from dairy to juices, make it a promising alternative to traditional chemical analyses. Despite clear advantages in speed and efficiency, FTIR remains underutilized in industrial settings. Van de Voort [43] emphasized the need for academic-led research to bridge this gap, especially for small food enterprises lacking R&D infrastructure. Continued methodological validation could elevate FTIR to a mainstream tool for routine quality control. Brito et al. [44] showcased ATR-FTIR's effectiveness in analyzing plant-based milk alternatives. Using PCA and HCA, the technique accurately classified soy, oat, and rice drinks based on protein bands, while also detecting inconsistencies in almond beverages. This method enables fast, non-destructive testing and could be expanded to monitor authenticity and detect adulteration, supporting wider adoption in food authentication systems.

9. Recent advances in FTIR and ATR-FTIR across food products

The application of vibrational spectroscopy, including FTIR and Raman techniques, in monitoring dairy safety and antibiotic residues is significant. These non-destructive methods enable rapid quantification of tetracyclines and β-lactams, with Raman showing higher sensitivity and FT-MIR providing better correlation accuracy. Integration with chemometrics enhances predictive reliability, supporting real-time screening, regulatory compliance, and consumer protection [45]. The detection of milk adulteration using skim milk powder in goat milk demonstrates FTIR combined with PLS-DA as a sensitive approach. Thermal treatment and freeze-drying simulated halloumi cheese production, showing that adulteration level, not geographic origin, dominates classification performance. These findings provide a robust framework for extending FTIR applications to processed dairy product authentication [46].

FTIR and Raman spectroscopies have emerged as essential tools for probiotic and bacterial analysis, allowing high-throughput, non-invasive characterization of cell composition, structure, and encapsulation. Integration with chemometrics enables strain identification, process monitoring, and stability evaluation. Technological advances and AI-driven analysis further overcome challenges such as water interference and fluorescence, enhancing quality control in food and biotechnology [47]. Synchrotron-based FTIR microspectroscopy, combined with chemometrics, effectively differentiates plant proteins from casein in hybrid cheeses. Protein-protein and protein-lipid interactions vary with plant protein type, while lipid mapping shows preferential association with casein. These findings highlight the power of high-resolution vibrational spectroscopy for characterizing complex dairy-plant systems, offering insights for product formulation and structural optimization [48].

ATR-FTIR spectroscopy enables rapid, on-site quantification of ethanol and acetic acid in fermentation products. The method requires minimal preparation, delivers accurate results, and supports small-scale producers in real-time monitoring. Its simplicity and robustness provide cost-effective solutions for optimizing fermentation, improving product quality, and enhancing economic outcomes in agricultural industries [49]. Spectroscopic fingerprinting combined with chemometric modeling allows precise classification and authentication of sunflower oils. ATR-FTIR achieves high predictive accuracy for oleic acid content, while portable Fibre Optic Reflectance Spectroscopy (FORS) enables rapid on-site screening. Integration of these approaches provides a complementary, scalable solution for food quality assurance, supporting nutritional verification and market compliance [50]. Overall, vibrational spectroscopy, including FTIR, ATR-FTIR, and Raman, offers rapid, non-destructive analysis across dairy, fermentation, and edible oils. Combined with chemometrics and portable devices, these methods enhance contaminant detection, product authentication, and quality monitoring, supporting regulatory compliance, consumer safety, and sustainable production practices across the food industry.

10. FTIR and ATR-FTIR spectroscopy coupled with machine learning for rapid food quality and safety assessment

Integrating FTIR and ATR-FTIR techniques with machine learning (ML) enhances predictive accuracy and enables rapid, non-destructive analysis across diverse food matrices. Together, these approaches exemplify how emerging trends in spectroscopy and data-driven modeling are transforming routine food quality monitoring and regulatory compliance.

FTIR spectroscopy has been applied to differentiate sweet and bitter almonds using shell material, offers a non-destructive alternative to kernel analysis. Spectral preprocessing, including normality testing and Box-Cox transformation, improved data distribution. Supervised models, particularly a hybrid Random Forest-Support Vector Machine (SVM), achieved nearly 99% classification accuracy. The approach reduces labor, time, and environmental impact, providing scalable quality control solutions in industrial almond processing [51]. Mid-infrared FTIR spectroscopy combined with ML enables rapid characterization of fig seed oil's bioactive compounds, including phenolics, flavonoids, and antioxidant activity. Spectral preprocessing methods, such as Savitzky-Golay smoothing and multiplicative scatter correction, enhanced predictive accuracy, with R^2 values exceeding 0.82 for most analytes. The technique allows fast, environmentally sustainable, and high-throughput quality assessment, promoting the valorization of underutilized plant-derived oils [52].

FTIR spectroscopy integrated with artificial intelligence demonstrates effective detection of buffalo milk adulteration, with sensitivity to cow milk levels as low as 1%. Multiple ML algorithms, including ensemble bagged trees, optimized through particle swarm feature selection, achieved over 90% accuracy. This rapid, non-destructive methodology minimizes reliance on conventional laboratory analysis, supporting routine authentication and dairy industry safety compliance [53]. ATR-FTIR spectroscopy coupled with advanced ML allows rapid detection of deoxynivalenol (DON) in wheat. Recursive feature elimination identified critical spectral wavenumbers, while TabPFN and CatBoost models provided high quantitative accuracy ($R^2 = 0.86$) and classification reliability. The approach reduces matrix interference, enabling efficient, reproducible, and scalable food safety monitoring, offering an alternative to traditional LC-MS/MS and ELISA techniques [54]. Overall, FTIR and ATR-FTIR spectroscopy, integrated with chemometrics and ML, provide rapid, non-destructive, and accurate assessment for food safety and quality.

11. Implications of FTIR and ATR-FTIR for innovation

The integration of FTIR, ATR-FTIR, and Raman spectroscopy with chemometric modeling has significant implications for advancing analytical precision, efficiency, and scalability across food products. These complementary techniques enable accurate quantification and sensitive detection of contaminants. Their non-destructive nature supports rapid, real-time monitoring while preserving sample integrity, making them highly suitable for routine industrial applications. In dairy systems, these approaches enhance adulteration detection, protein stability assessment, and spoilage monitoring, thereby strengthening regulatory compliance, consumer protection, and supply chain transparency. Similarly, in edible flowers and other plant-based products, spectroscopic integration facilitates authentication, compositional analysis, and bioactive compound profiling, contributing to improved traceability and product standardization across nutraceutical and medicinal sectors.

Beyond food applications, the interdisciplinary potential of vibrational spectroscopy extends to broad scientific relevance. The combination of spectroscopy with ML, hyperspectral imaging, and advanced analytical platforms enables high-throughput screening, predictive modeling, and automated decision-making. These advancements reduce operational costs, minimize sample waste, and enhance analytical reliability for both small-scale producers and large industries. However, maximizing these benefits requires standardized protocols, robust calibration models, and effective data preprocessing strategies to address spectral variability and interference. Overall, the continued development and adoption of spectroscopic and chemometric approaches will drive innovation in quality assurance, support sustainable production practices, and reinforce consumer confidence in global food and agricultural systems.

12. Technical and practical barriers to the optimization of FTIR applications

Despite the versatility of FTIR and ATR-FTIR, several challenges limit their widespread application in food products. Spectral overlap and interference, particularly in complex matrices such as milk, processed dairy products, or edible flowers, reduce resolution and complicate accurate identification of target analytes. Water absorption and fluorescence can further obscure signals, affecting sensitivity and detection limits for low-concentration contaminants or bioactive compounds. Sample heterogeneity, matrix variability, and inadequate penetration depth introduce additional complexity, requiring careful optimization of sample preparation techniques such as freeze-drying or homogenization. Calibration and spectral interpretation are often challenging, necessitating advanced chemometric methods like PCA, PLS-DA, and ensemble ML to achieve reliable classification and quantification.

Industrial adoption and field-deployable applications face further obstacles. Standardized protocols, robust calibration models, and comprehensive spectral libraries are often insufficient, hindering reproducibility and scalability across diverse product types and production conditions. Operator expertise, equipment costs, and limited access to portable or IoT-enabled systems restrict real-time, on-site monitoring. Integration with AI-driven predictive models and multimodal analytical platforms remains underexplored, limiting automation and rapid decision-making. Overcoming these limitations requires coordinated efforts in method standardization, development of universal reference databases, optimization of preprocessing strategies, and enhanced chemometric and ML integration. Addressing these challenges is essential to fully harness the potential of vibrational spectroscopy for reliable, high-throughput, and field-deployable quality assurance, adulteration detection, and product authentication across food, dairy, and plant-based matrices.

13. Prospective developments in FTIR and ATR-FTIR spectroscopy

Emerging advancements in FTIR and ATR-FTIR technologies offer significant potential to transform analytical practices across food, dairy, and plant-based industries. Miniaturized, portable devices equipped with waveguide sensors and quantum cascade lasers will enable rapid, on-site analysis, reducing dependence on centralized laboratories. Integration with advanced chemometric and ML algorithms promises automated spectral interpretation, improving classification accuracy, sensitivity, and predictive capability. These innovations will facilitate continuous quality monitoring, real-time adulteration detection, and rapid assessment of protein structures, bioactive compounds, and molecular interactions. Expanding spectral libraries and standardized preprocessing protocols will further enhance reproducibility, robustness, and cross-product comparability, fostering broader industrial adoption.

Future developments are expected to integrate ATR-FTIR with complementary techniques such as Raman spectroscopy, hyperspectral imaging, nuclear magnetic resonance, and mass spectrometry, creating hybrid analytical platforms capable of high-resolution molecular profiling. Cloud-based data systems, IoT-enabled devices, and AI-assisted predictive models will allow real-time monitoring, automated decision-making, and traceability throughout supply chains. Applications may extend to novel dairy products, probiotics, hybrid plant-dairy systems, and edible flowers, supporting regulatory compliance, fraud prevention, and sustainable production practices. Overall, these technological advancements will provide scalable, cost-effective, and environmentally sustainable solutions for ensuring product authenticity, safety, and consumer confidence, positioning ATR-FTIR as a frontline analytical tool in global food quality assurance and industrial monitoring.

14. Conclusion

This review highlights the critical role of FTIR and ATR-FTIR spectroscopy as versatile, non-destructive, and rapid analytical tools across chemical, biological, and environmental research. Emphasis is placed on their integration with advanced chemometric and ML techniques, enabling highly accurate detection of dairy adulterants, monitoring of protein structural changes, and prediction of physicochemical properties. Their rapid analysis, minimal sample preparation, and high-throughput capabilities make them indispensable for food quality control, shelf-life assessment, and regulatory compliance. Collectively, these technologies support safer, more authentic dairy production, enhance consumer confidence, and foster transparency across global food supply chains. Moreover, FTIR and ATR-FTIR applications extend to broader sectors, including edible flower authentication, bioactive compound profiling, and environmental monitoring, demonstrating their interdisciplinary impact.

This review also underscores the future potential of FTIR and ATR-FTIR spectroscopy through technological innovations such as portable and miniaturized devices, quantum cascade lasers, enhanced spectral databases, and AI-driven chemometric modeling. Integration with complementary techniques like Raman spectroscopy, hyperspectral imaging, and mass spectrometry promises real-time monitoring, automated decision-making, and comprehensive molecular characterization. These advancements will further improve sensitivity, reproducibility, and scalability for industrial and field applications. By addressing current limitations, such as spectral interference, calibration variability, and matrix complexity, these technologies are poised to become frontline tools for rapid, reliable, and sustainable quality assurance. Overall, continued innovation and

interdisciplinary integration will ensure FTIR and ATR-FTIR spectroscopy remain pivotal for enhancing food safety, authenticity, and consumer trust across dairy systems and beyond.

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