Rapid Agro-Forensic Authentication of Food Products Using FT-IR Spectroscopy and Chemometrics

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Abstract

Economic adulteration and geographic mislabelling continue to undermine consumer trust and regulatory integrity in global food markets. As traditional laboratory-based methods remain resource-intensive and time-consuming, Fourier-transform infrared (FT-IR) spectroscopy combined with chemometric analysis has emerged as a rapid, non-destructive, and courtroom-admissible solution. This article reviews recent studies demonstrating the method's effectiveness across diverse food matrices, from honey and olive oil to dairy and coffee. It also explores the growing development of portable FT-IR systems that promise real-time surveillance at border and retail checkpoints.

Introduction

Food fraud, particularly in high-value commodities, is a growing global concern driven by economic motivations (Capuano & Ruth, 2012). It encompasses various practices such as adulteration, mislabelling, and misrepresentation of origin or production methods (Manning & Monaghan, 2019). The complexity of global supply chains has exacerbated this issue, undermining consumer trust and violating food standards (Tola, 2018).

To address such issues, the European Union has implemented quality control schemes such as the Protected Designation of Origin (PDO) and Protected Geographical Indication (PGI). These labels safeguard traditional food products by certifying their geographic origin and production techniques, contributing significantly to rural development and economic value (Sparf, 2010 and Profeta *et al.*, 2009). However, their implementation varies across EU countries, with some nations like Sweden lacking PDO products (Sparf, 2010). Consumer recognition of these labels also differs, influencing purchasing decisions. Italian consumers with excellent knowledge of EU certification labels are more likely to use PDO and PGI logos as their main purchasing motivation (Vecchio & Annunziata, 2011). The increasing global competition has led to cases of food fraud, including the misuse of geographical indications and "Italian sounding" products that mislead consumers (Carreño & Vergano, 2016). This highlights the importance of protecting authentic regional products and educating consumers about these quality labels to maintain their integrity and economic impact.

In parallel, advances in analytical technologies have enhanced the ability to detect and prevent food fraud. Vibrational spectroscopy techniques, particularly FT-IR, NIR, and Raman, have emerged as powerful tools for rapid, non-destructive food analysis (Pandiselvam *et al.*, 2024; Çebi *et al.*, 2023). These methods offer advantages over conventional techniques, including simplicity, adaptability to on-line applications, and absence of hazardous solvents (Pandiselvam *et al.*, 2024). When combined with chemometrics, they enable detailed metabolomic fingerprinting and profiling of food products, allowing for detection and quantification of key constituents (Çebi *et al.*, 2023). FT-IR spectroscopy, in particular, has been extensively used for authentication analysis of fats and oils in food products (Rohman *et al.*, 2020). While mid-infrared spectroscopy is valuable for structural characterization of food components, NIR spectroscopy has gained popularity in the food industry for routine analysis of proximate composition and detection of adulteration (Li-Chan *et al.*, 2006). These techniques offer promising alternatives to more expensive and time-consuming chromatographic and genetic approaches.

FT-IR Spectroscopy and Chemometrics: Principles and Workflow

FT-IR spectroscopy is a powerful analytical technique used to characterize molecular structures and functional groups in various compounds (Siddique, 2024). It operates by measuring the absorption of infrared radiation by molecules, which occurs when the frequency of the radiation matches the vibrational energy of molecular bonds (Álvarez-Ordoñez & Prieto, 2012). The resulting spectrum contains distinct absorption peaks corresponding to specific functional groups, serving as a molecular "fingerprint" (Bates, 1976; Tsuda & Kubouchi, 1993). FTIR spectroscopy can identify various bond types, such as O-H, C-H, and C=O, with each absorbing at characteristic frequencies (Tsuda & Kubouchi, 1993). This technique is widely applicable across scientific domains, including chemistry, biology, and material science, offering insights into molecular interactions, conformational changes, and chemical reactions (Siddique, 2024). Recent advancements, such as attenuated total reflectance (ATR) and micro spectroscopy, have further expanded its utility in both research and industrial applications (Siddique, 2024).

However, raw FT-IR spectra often contain overlapping signals, baseline drift, and scattering effects that obscure meaningful interpretation. To address this, spectral pre-processing techniques are essential. Methods such as Standard Normal Variate (SNV) correction and Savitzky–Golay (SG) derivatives are commonly used to enhance spectral resolution and minimize variability. SNV corrects for scatter-related intensity shifts, while SG derivatives sharpen peaks and highlight subtle spectral features. Optimization of SG parameters, particularly window size and polynomial order, is critical for effective resolution enhancement (Zimmermann & Kohler, 2013).

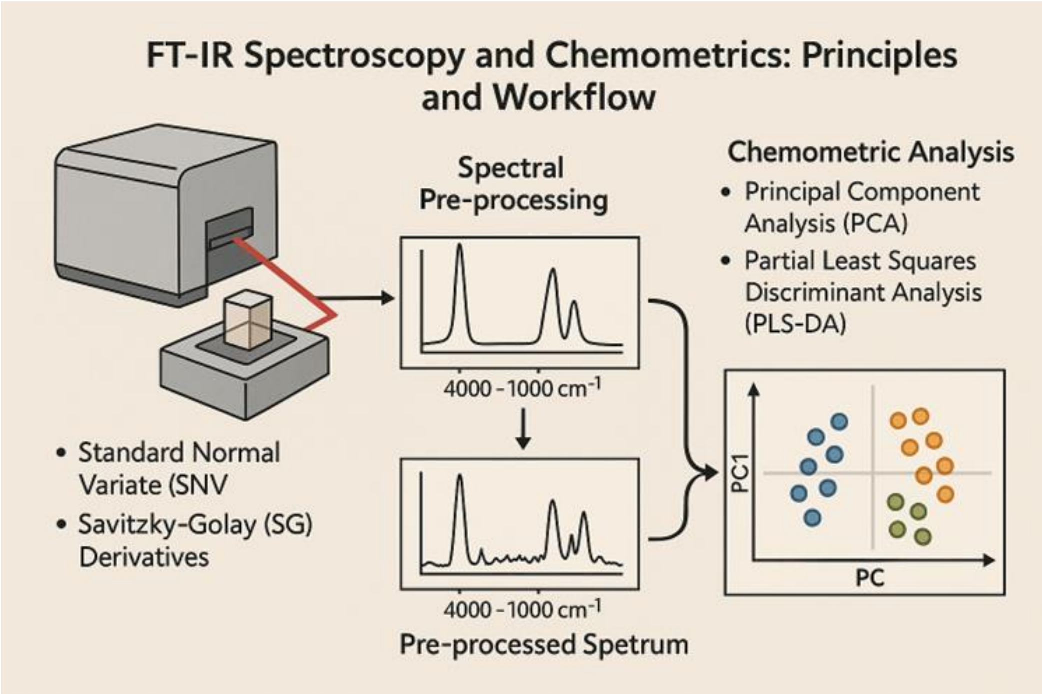

Figure 1: Principles and workflow of FT-IR spectroscopy and chemometrics

When used in combination, these techniques can significantly improve the performance of chemometric models. For instance, SG derivatives paired with Extended Multiplicative Signal Correction (EMSC) have been shown to enhance classification accuracy, although the order of application affects results (Zimmermann & Kohler, 2013). First-derivative SG transformations, for example, have improved the separation of paper types in principal component analysis (PCA) models (Lee *et al.*, 2016). Yet, caution is needed since over-processing can lead to artefacts, especially in datasets with weak signals or limited sample sizes (Delwiche & Reeves, 2010). Moreover, the interaction between SNV and derivative techniques is non-trivial, thus applying them in different sequences can yield different outcomes (Fearn, 2008).

Once spectra are pre-processed, they are typically analysed using multivariate statistical techniques. Unsupervised methods such as PCA are valuable for exploratory analysis and visualizing natural clustering without prior knowledge of sample categories (Sampaio & Calado, 2021; Muehlethaler *et al.*, 2014). In contrast, supervised techniques like Partial Least Squares Discriminant Analysis (PLS-DA) and Soft Independent Modelling of Class Analogy (SIMCA) build predictive models based on known class labels. SIMCA, in particular, has demonstrated high accuracy, sensitivity, and specificity in classifying a variety of materials, including yeast strains (Sampaio & Calado, 2021) and edible salts (Lee *et al.*, 2017), often outperforming PLS-DA. In spectral data classification, SIMCA achieved correct classification rates of approximately 95%, with notably low false-negative rates (Muehlethaler *et al*., 2014). To further address issues related to multimodality and nonlinearity in complex spectral datasets, new modeling approaches have been developed. One such method, Nearest Clusters based PLS-DA (NCPLS-DA), has shown improved classification performance compared to conventional PLS-DA, offering better handling of heterogeneous data structures (Song *et al*., 2018).

Applications Across Food Commodities

Honey:

FT-IR spectroscopy, coupled with chemometric analysis, has proven effective for authenticating honey's botanical and geographical origins. Hennessy *et al*. (2008) applied FT-IR using a germanium ATR crystal and chemometric modelling to classify 150 honey samples by both botanical and geographical origin. Their SIMCA/PLS-DA models achieved 93–100% accuracy, successfully distinguishing Irish and Argentine honeys, among others. Similarly, Ruoff *et al*. (2006) reported error rates as low as <0.1% for certain honey types using ATR-MIR spectroscopy. Additionally, Guyon *et al*. (2021) successfully classified honey varieties based on botanical origin, independent of geographical origin, using SIMCA on ATR-FTIR spectra. These studies collectively support FT-IR as a valuable tool for honey authentication and quality control.

Carob Beans:

Recent studies have explored the use of spectroscopic and chemometric techniques for classifying carob pods and products based on geographical origin and quality parameters. Christou *et al*. (2017) used FT-IR spectroscopy and orthogonal PLS (OPLS) to classify carob pods from seven Mediterranean countries. Spectra focused on the 1200–900 cm^{-1} region, rich in carbohydrate signals, allowed 100% correct classification by origin, showing promise for PGI applications in carob-derived foods. Kokkinofta *et al*. (2020) further investigated nutritional composition as a marker for provenance, achieving 79% overall classification success using chemometric techniques. Ioannou *et al*. (2023) demonstrated that phenolic profile and antioxidant activity could serve as chemical markers for classifying carob products, with geographical origin significantly affecting these parameters. These studies collectively highlight the potential of spectroscopic and chemometric methods for authenticating carob origin and assessing quality attributes in carob-derived products.

Olive Oil:

Bendini *et al*. (2007) analyzed mono-varietal Italian olive oils using ATR-FT-IR and PCA, achieving clear regional separation based on subtle compositional differences. Similarly, Laouni *et al*. (2022) demonstrated accurate classification of Moroccan olive oils into coastal, continental, and Saharan groups. Similarly, Laouni *et al*. (2022) achieved 84-100% correct classification rates for Moroccan olive oils using FTIR and PCA-LDA/PLS-DA. These studies highlight the potential of spectroscopic methods coupled with chemometrics as rapid, cost-effective tools for verifying olive oil geographical origin and supporting authenticity claims.

Coffee and Dairy:

Wang *et al*. (2011) differentiated Arabica coffees by origin and roast level using FT-IR and SIMCA. The method also detected Robusta adulteration. Moreover, Tarapoulouzi *et al*. (2020) applied FTIR and PCA-OPLS to distinguish cow, goat, and sheep milk cheeses, focusing on bands in the amide I and II regions. Tarapoulouzi & Theocharis (2023) extended this approach to classify traditional Cypriot Halloumi and Anari cheeses by milk species origin. Duliński et al. (2025) utilized FTIR spectroscopy with machine learning techniques to authenticate sheep's milk, identifying characteristic spectral signatures, particularly in the amide I and II bands. These studies highlight the potential of FTIR spectroscopy as a rapid and reliable tool for food authentication, with applications in detecting adulterations and ensuring product quality across various food industries

Handheld FT-IR Instruments: Field Applications

Recent studies demonstrate the effectiveness of portable FT-IR devices for on-site food quality control and adulteration detection. Cebi *et al*. (2023) demonstrated that modern portable FT-IR devices equipped with diamond ATR optics and MEMS interferometers offer spectral performance comparable to laboratory instruments. These devices require minimal sample preparation, operate on batteries, and transmit results via wireless connections. Such instruments are capable of detecting adulterants at concentrations as low as 0.4% and achieve R^2 values over 0.98 with root mean square error (RMSE) below 2%.

The versatility of portable spectrometers has been demonstrated across a wide range of food matrices, including milk powder, spices, marine oils, olive oils, honeys, and coffees (Moskowitz & Yakes, 2023). A global study on oregano adulteration found that 33 out of 34 portable near-infrared devices correctly classified 5 out of 6 samples, demonstrating the potential for real-time remote testing throughout supply chains (McGrath *et al.*, 2020). These portable spectroscopic techniques, combined with chemometrics, offer rapid, accurate, and non-destructive analysis for maintaining food integrity from farm to fork (Çebi *et al.*, 2023).

Limitations and Future Directions

Despite its advantages, FT-IR spectroscopy has some limitations. Variability due to seasonality, climate, or cultivar can affect spectral interpretation. Standardized spectral databases are still under development, and inter-instrument variability can complicate cross-border enforcement.

Moreover, chemometric models require careful calibration and external validation to ensure reproducibility and legal admissibility. Future work should focus on building harmonized spectral libraries and incorporating AI-assisted modelling for improved accuracy and adaptability.

Conclusion

FT-IR spectroscopy combined with chemometrics represents a fast, non-destructive, and scalable approach to agro-forensic analysis. Its successful application across various food commodities highlights its potential as a frontline tool in detecting fraud and verifying origin. With further validation and wider adoption of portable systems, FT-IR could become central to modern food authentication and regulatory enforcement.

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