Application of FTIR-ATR Spectroscopy for Quality Mapping and Authenticity Verification of Coffee from Traditional Markets in Padang City, Indonesia

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Abstract. Ensuring the authenticity and quality of coffee is essential, particularly in regions where traditional markets play a significant role in daily trade and consumption. This study explores the application of Fourier Transform Infrared-Attenuated Total Reflectance (FTIR-ATR) spectroscopy as a rapid, non-destructive analytical technique to assess the quality and verify the authenticity of coffee samples from traditional markets in Padang City, Indonesia. A set of reference spectra was first established using traceable, original coffee beans. These spectra were then compared to those obtained from market samples using multivariate statistical methods. The analysis revealed notable differences in spectral patterns between the original and market-sourced coffee, indicating potential adulteration or blending practices. These discrepancies suggest that some commercially sold coffee may have undergone mixing with inferior or foreign substances, compromising its quality and authenticity. While FTIR-ATR has proven to be an effective preliminary screening tool, further confirmatory analyses such as chromatographic or metabolomics-based approaches, are recommended to validate the findings. This study highlights the significance of quality assurance in traditional markets and advocates for the incorporation of spectroscopic methods into routine monitoring systems within the coffee supply chain.

1 Introduction

Coffee is one of the most widely consumed beverages globally and holds significant cultural, economic, and social value, particularly in coffee-producing countries such as Indonesia. Among various types of coffee, robusta (Coffea canephora) plays a dominant role in the domestic market due to its stronger flavor profile, higher caffeine content, and adaptability to lowland growing conditions [1]. In urban centres like Padang City, traditional markets

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remain a central hub for the distribution and daily purchase of robusta coffee, often serving as the primary point of access for consumers. However, despite their economic and social importance, traditional markets are commonly characterized by limited regulatory oversight. This creates vulnerabilities in the coffee supply chain, particularly in terms of quality assurance and authenticity. Adulteration such as the addition of filler materials or blending with lower-grade coffee can occur undetected, potentially misleading consumers and devaluing the product [2,3]. To address this issue, there is a growing interest in implementing rapid, non-destructive, and cost-effective analytical methods that can be used for on-site screening or routine quality monitoring. Fourier Transform Infrared-Attenuated Total Reflectance (FTIR-ATR) spectroscopy has emerged as a valuable tool in this regard. By capturing the molecular fingerprint of a sample, FTIR-ATR enables the detection of subtle chemical variations that may indicate adulteration, degradation, or origin differences [4-6]. This study investigates the application of FTIR-ATR spectroscopy for the quality mapping and authenticity verification of robusta coffee samples sourced from traditional markets in Padang City. By comparing spectral data from market samples with that of known, authentic robusta coffee, this research aims to evaluate the effectiveness of FTIR-ATR as a preliminary screening tool. The findings are expected to contribute to enhanced consumer protection and the development of practical quality control protocols that can be applied within informal market settings in Indonesia and beyond.

2 Materials and Method

This study involved the analysis of four robusta coffee (Coffea canephora) samples, each obtained from a different traditional market in Padang City, West Sumatra, Indonesia. The samples were coded as BT, DAS, RM, and KT, representing four distinct sources while maintaining confidentiality regarding specific market names. These codes were consistently used throughout the study to facilitate traceability and the interpretation of the results. All samples were purchased in their typical commercial form, roasted and ground, mimicking the condition in which consumers usually encounter them. To minimize external variation, the samples were collected within the same period, stored in airtight containers, and maintained at ambient room temperature (approximately 25°C), away from direct sunlight and moisture.

Spectroscopic analysis was performed using a Fourier Transform Infrared spectrometer equipped with an Attenuated Total Reflectance (FTIR-ATR) accessory. Before measurement, the instrument was calibrated and cleaned to ensure accuracy and reproducibility. Each coffee sample was analyzed with a minimum of four replicates ($n \geq 4$) to obtain statistically representative data and account for any within-sample variation. Spectral data were recorded in the mid-infrared region (4000–400 cm^{-1}) with a resolution of 4 cm^{-1} [7]. Each measurement was obtained by averaging 32 scans to enhance the signal-to-noise ratio. A fresh background scan was performed before each sample measurement to eliminate interference from environmental CO_2 and H_2O vapor.

The resulting spectra were subjected to pre-processing, including baseline correction, normalization, and smoothing, to enhance data quality and facilitate robust comparisons. Multivariate statistical techniques specifically Principal Component Analysis (PCA) were employed to explore clustering patterns among the samples and detect anomalies relative to the reference robusta profile. These analyses facilitated the identification of potential adulteration or quality discrepancies in the market-sourced samples. This methodological framework provides a basis for the development of a simple yet effective strategy to monitor coffee quality in traditional market environments, where access to sophisticated laboratory facilities is often limited.

3 Results and Discussion

This study aimed to profile the metabolite composition of four traditional robusta coffee samples—coded BT, DAS, RM, and KT using Fourier Transform Infrared Spectroscopy with Attenuated Total Reflectance (FTIR-ATR). The FTIR spectral data obtained were further analyzed using Principal Component Analysis (PCA) to explore chemical variation and identify potential authenticity markers among the samples. Overview of FTIR Spectra. The FTIR spectra of the four robusta coffee samples across the range of 4000–800 cm⁻¹ are illustrated in Figure 1. Generally, the spectra exhibited characteristic absorption bands associated with the main functional groups commonly found in coffee metabolites. Key regions include: O–H stretching (~3200–3600 cm^{-1}), typically representing hydroxyl groups in phenols, alcohols, and water content;C–H stretching (~2800–3000 cm^{-1}), related to aliphatic chains in lipids and fatty acids; C=O stretching (~1700–1750 cm^{-1}), indicative of carbonyl groups in esters, acids, and caffeine-like structures; N–H bending and C=C aromatic stretching (~1500–1600 cm^{-1}), associated with proteins and aromatic compounds; C–O and C–N stretching (~1000–1300 cm^{-1}), common in carbohydrates, chlorogenic acids, and alkaloids [8-10].

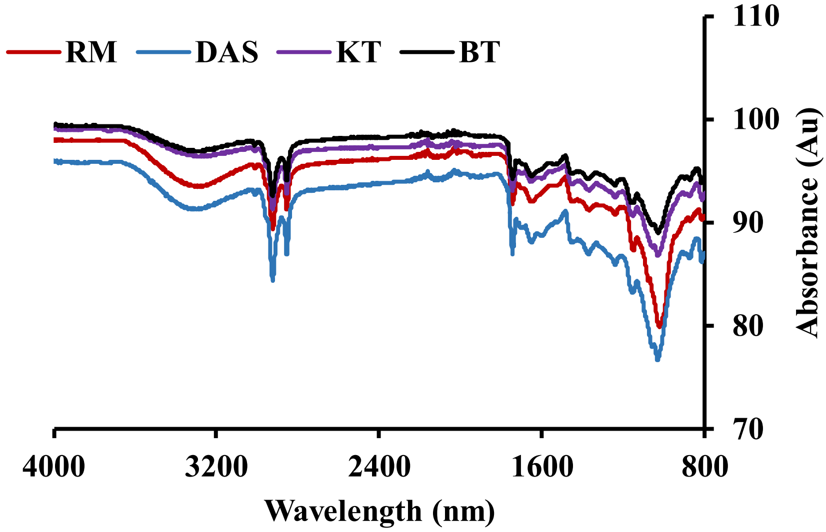

Fig. 1. FTIR spectra (4000–800 cm^{-1}) of four robusta coffee samples.

The FTIR spectra revealed characteristic peaks indicative of phenolic compounds, as shown in Figure 1. FTIR spectra (4000–800 cm^{-1}) of four robusta coffee samples. Visually, the DAS sample exhibited overall lower transmittance values in several key regions compared to the others, particularly between 1000 and 1800 cm^{-1}, which may indicate higher concentrations of certain phenolic or carbohydrate compounds. The BT sample exhibited a distinctive pattern in the fingerprint region, characterized by sharper and deeper absorption troughs, which may indicate a different origin, higher purity, or the presence of extenders/adulterants.However, visual interpretation of FTIR spectra alone is insufficient for conclusive differentiation, especially in complex matrices such as coffee. Overlapping peaks and subtle spectral variations require advanced chemometric analysis for accurate discrimination. Therefore, multivariate statistical techniques, specifically Principal Component Analysis (PCA), were applied to extract and visualize latent patterns within the spectral dataset.

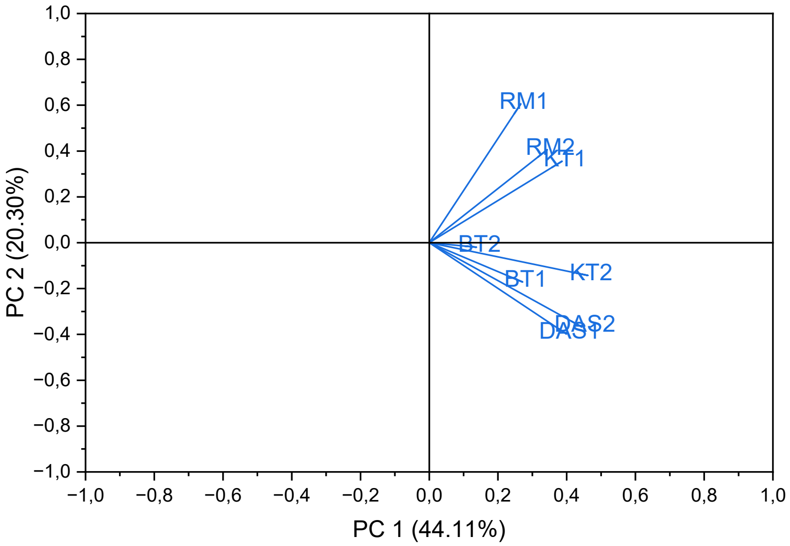

Fig. 2. PCA score plot of FTIR spectra (400–4000 cm⁻¹).

Figure 2. PCA score plot of FTIR spectra (400–4000 cm^{-1}) Figure 2 presents the PCA results for the full spectral range of 400–4000 cm^{-1}. The first two principal components (PC1 and PC2) accounted for the majority of variance among the samples, allowing a clear visual separation. Samples BT and DAS were grouped in distinct clusters apart from RM and KT, suggesting considerable differences in overall metabolite composition. This spectral range encompasses a broad set of functional groups, including O–H stretching (~3200–3600 cm^{-1}), C–H stretching (~2800–3000 cm^{-1}), C=O stretching (~1700–1750 cm^{-1}), and N–H bending (~1500–1600 cm^{-1}), reflecting the presence of diverse primary and secondary metabolites such as lipids, proteins, phenolic acids, and alkaloids. These results indicate that full-range FTIR spectra can effectively capture biochemical diversity in robusta coffee.

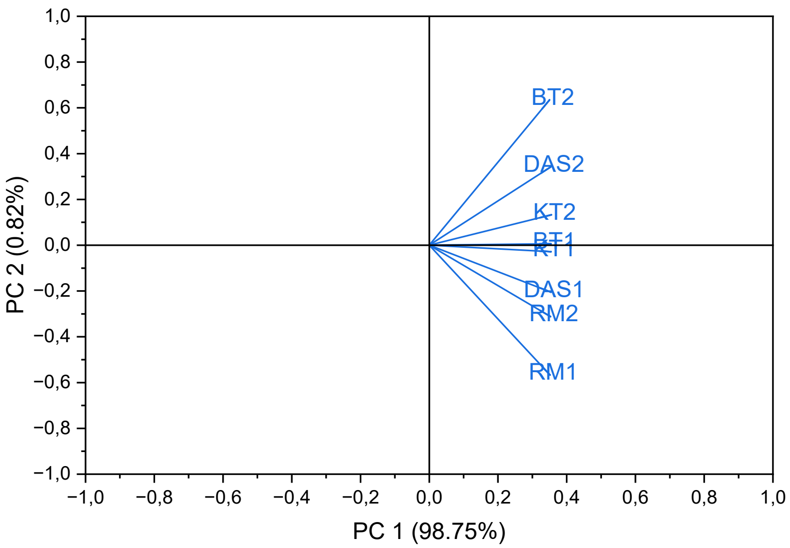

Fig. 3. PCA score plot of FTIR spectra (800–4000 cm^{-1}).

To enhance signal clarity and reduce low-frequency noise, the spectral range was narrowed to 800–4000 cm⁻¹ as shown in Figure 3. This adjustment emphasized non-metallic organic compounds relevant to coffee's biochemical profile. The resulting PCA still demonstrated distinct separation patterns, with sharper contrasts observed between BT and RM, while KT and DAS showed closer clustering, suggesting chemical similarities. Notable vibrational features in this region include aliphatic C–H stretching (~2850–2960 cm^{-1}), ester and carboxylic C=O stretching (~1700–1750 cm^{-1}), and O–H/N–H vibrations (~3200–3400 cm^{-1}), commonly associated with flavor-contributing compounds such as organic acids, lipids, and aromatic constituents. These findings reinforce the discriminative capability of the FTIR spectra within this region.

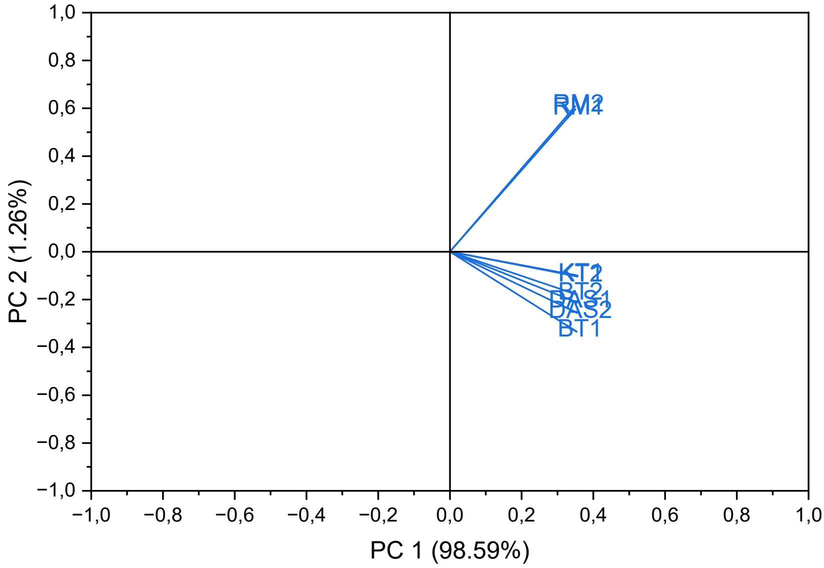

Fig. 4. PCA score plot of FTIR spectra in the fingerprint region (800–1500 cm^{-1}).

The fingerprint region (800–1500 cm^{-1}), presented in Figure 4, yielded the most distinct and informative results. This spectral window is particularly valuable for identifying specific functional groups and compound classes in complex matrices. PCA within this range revealed more apparent separation among all coffee samples, particularly between DAS and BT. This region contains vibrational modes such as C–O stretching (in carbohydrates), C–N stretching (in amino compounds), and deformation of CH_2 and CH_3 groups, which are typical of polysaccharides, phenolic acids, and alkaloids. The sharp distinctions found here affirm that fingerprint-region FTIR data are especially powerful for metabolite profiling and could be instrumental in detecting sample-specific authenticity markers.

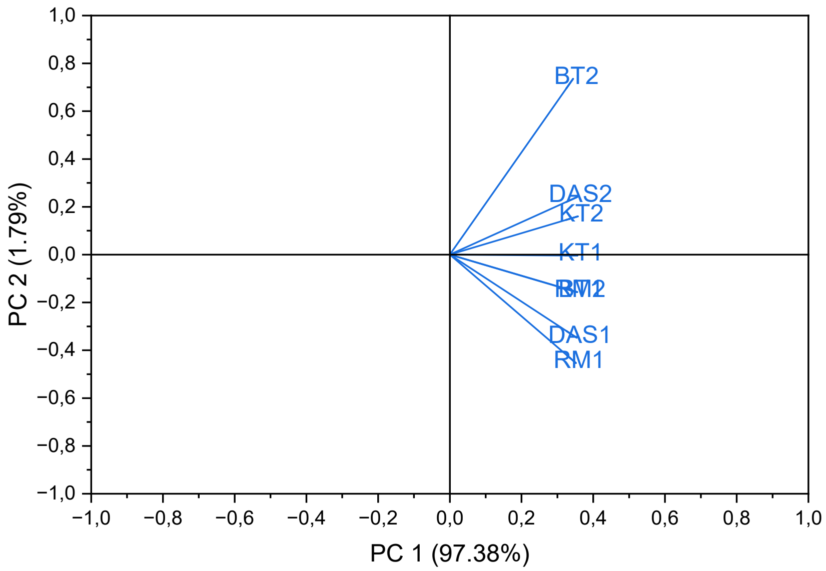

Fig. 5. PCA score plot of FTIR spectra (1500–4000 cm⁻¹).

Figure 5 shows the PCA results for the higher frequency region (1500–4000 cm^{-1}), which includes many key functional groups relevant to coffee biochemistry. The second principal component (PC2) contributed strongly to sample separation, with BT emerging as the most distinct sample in terms of metabolite profile. Functional groups driving the separation include O–H and N–H stretching (3200–3500 cm^{-1}), and C–H stretching (2800–3000 cm^{-1}), which are associated with phenolic compounds, organic acids, and lipid constituents. Notably, DAS and KT displayed closer metabolic profiles, potentially reflecting similar processing or sourcing practices.

The results of this study confirm that FTIR-ATR spectroscopy, when coupled with multivariate statistical analysis such as PCA, is capable of revealing distinct chemical profiles among robusta coffee samples obtained from traditional markets [11-12]. The separation observed in PCA plots, particularly in the fingerprint region, highlights how small variations in metabolite content can be detected and associated with sample-specific characteristics. The clustering of samples BT and DAS apart from RM and KT, for instance, may reflect different origins, handling practices, or degrees of adulteration. BT, which consistently appeared as the most chemically distinct in multiple spectral ranges, could potentially represent either a purer coffee source or, conversely, one that is more heavily adulterated, depending on the spectral features. Further targeted analyses would be required to determine whether these differences stem from the presence of non-coffee substances (e.g., corn, rice, or other extenders) or natural variation due to terroir and processing. In the fingerprint region (800–1500 cm^{-1}), the presence of clear vibrational signals corresponding to C–O, C–N, and CH_2/CH_3 groups suggests the influence of complex biomolecules such as polysaccharides, chlorogenic acids, and alkaloid compounds known to contribute to the flavor and functional quality of coffee [13,14]. The separation among samples in this region confirms that FTIR-ATR is not only sensitive to gross adulteration but can also differentiate nuanced compositional differences resulting from natural biochemical variability. Moreover, the clustering pattern between DAS and KT in the higher spectral ranges (1500–4000 cm^{-1}) suggests a degree of chemical similarity, possibly due to similar post-harvest practices or shared geographic supply chains. This supports previous findings in the literature, where FTIR spectroscopy has been effectively used to trace the geographical origin and post-harvest treatment effects in coffee and other plant-based commodities. While FTIR-ATR spectroscopy has proven effective in this study as a rapid screening method, its semi-quantitative nature suggests that it should be complemented with confirmatory methods, such as GC-MS or LC-MS-based metabolomics, for precise identification and quantification of metabolites [15]. Nonetheless, its ease of use, speed, and non-destructive nature make it highly suitable for routine quality monitoring and early-stage authenticity checks in the coffee supply chain, especially in low-resource settings such as traditional markets. Ultimately, these findings underscore the potential for implementing portable FTIR-ATR systems in local regulatory or producer cooperatives to ensure product integrity, protect consumers from adulterated goods, and strengthen the value of Indonesian robusta coffee in both domestic and international markets.

4 Conclusion

This study demonstrated the potential of FTIR-ATR spectroscopy combined with multivariate analysis (PCA) to differentiate metabolite profiles among four traditional robusta coffee samples. The full-spectrum FTIR data (4000–800 cm^{-1}) revealed variations in functional groups associated with lipids, organic acids, phenolic compounds, and polysaccharides. PCA applied to various spectral ranges, especially the fingerprint region (800–1500 cm^{-1}), provided clear clustering and separation of samples, indicating its suitability for rapid authentication and quality assessment. These findings support the application of FTIR spectroscopy as a powerful, non-destructive tool for profiling coffee biochemical diversity and could be developed further for traceability and origin identification.

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