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Article

Discrimination of Vietnamese Coffee Products via ATR-FTIR Spectroscopy and Chemometric Techniques

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Abstract: Coffee classification involves the differentiation of coffee based on species, geographical origin, and quality attributes. In this study, ground coffee samples from seventeen commercial brands: Mai, Honey, Duong, M Ja, Con Soc, Hat A, Trung Nguyen, Huong Viet, Vina, Phuc Long, TwitterBean, Nhan, Phuong Vi, Thu Ha, Nes, and Highland were analyzed using Attenuated Total Reflectance Fourier Transform Infrared (ATR-FTIR) spectroscopy. Spectra were acquired in transmittance mode over the range 400–4000 cm⁻¹ with 128 scans per sample and a resolution of 10 cm⁻¹. Sample surfaces were smoothed consistently during measurement to minimize variability. The resulting spectral data were compressed and subjected to multivariate statistical analysis, including Principal Component Analysis (PCA) and Linear Discriminant Analysis (LDA). These techniques were applied to classify four roasted coffee types: Arabica, Robusta, Moka, and Culi. PCA revealed that the first two principal components accounted for 72.99% and 11.97% of the total variance, respectively. While PCA enabled partial brand-level discrimination, LDA provided clear separation among all four coffee types. Our findings demonstrate that ATR-FTIR spectroscopy, when coupled with chemometric modeling, offers a rapid and robust alternative to conventional methods for coffee authentication. This approach enables effective classification of Vietnamese coffee products and holds promise for future applications in fraud detection and quality control.

Keywords: coffee; ATR-FTIR; PCA; LDA; chemometric

1. Introduction

Coffee (*Coffea* spp.) has long been a widely consumed beverage in Vietnam. Globally, Vietnam ranks second only to Brazil in both coffee production and export volume, accounting for approximately 20% of the world's annual coffee output [1]. In recent years, the Vietnamese coffee industry has expanded with the aim of improving varietal quality, leading to a more diverse and dynamic market. The two primary species cultivated in Vietnam are Robusta (*Coffea canephora*) and Arabica (*Coffea arabica*). Other varieties, such as Liberica (*Coffea liberica*), Moka, and Culi, are grown in smaller quantities [2,3].

Robusta is well-suited to the basaltic soils and climate of Vietnam's Central Highlands and constitutes about 97% of the national coffee production [4–7]. Arabica, on the other hand, is mainly grown in Lam Dong province at elevations above 600 meters. Culi is a natural mutation of Arabica and Robusta, characterized by a single, rounded bean per fruit. Moka, a cultivar within the Arabica lineage introduced from France, is cultivated in Da Lat, Lam Dong [6].

The economic value associated with coffee variety has led to increasing incidences of varietal fraud and mislabeling aimed at boosting profit margins. This issue parallels similar trends reported across Vietnam's food sector, where traceability, authenticity, and origin protection have become

pressing concerns [8–10]. In addition, environmental pollution—such as pesticide residues, heavy metals, and industrial contaminants—has been shown to adversely affect the safety and quality of various agricultural products in Vietnam [11–15]. These challenges underscore the urgent need for reliable analytical approaches that not only verify product identity but also ensure food quality in the face of environmental and economic pressures. Studies have revealed widespread cases of adulteration and contamination in vegetables [11,13], rice [16–18], cashew nuts [19,20], green tea [21], and alcoholic beverages [22]. Such findings highlight the necessity of reliable analytical approaches for product verification.

Coffee is a chemically complex matrix containing more than 800 organic and inorganic compounds, each associated with different functional groups and therefore unique infrared (IR) absorption characteristics [8,23–28]. Spectroscopic fingerprinting techniques—such as Attenuated Total Reflectance-Fourier Transform Infrared (ATR-FTIR) spectroscopy—have emerged as powerful, non-destructive methods for rapid compositional analysis of coffee [25,28]. In combination with chemometric tools, including Principal Component Analysis (PCA), Linear Discriminant Analysis (LDA), and Mahalanobis distance analysis [29,30], ATR-FTIR has demonstrated high efficacy in authenticating coffee species and differentiating products by geographical origin [27,28].

Beyond coffee, these methods have been successfully applied to assess the authenticity and classify various food products in Vietnam, such as sausages [21], soybean [31], turmeric [32], mustard greens [33], ST25 rice [18], and even alcoholic beverages [22]. The use of complementary techniques like Inductively Coupled Plasma Mass Spectrometry (ICP-MS) and LC-MS/MS has further enhanced multivariate classification and traceability of food products [21,34,35].

This study aims to apply ATR-FTIR spectroscopy, in combination with multivariate statistical analysis, to differentiate commercially available Vietnamese coffee types. The findings are expected to support the development of a chemometric classification method to distinguish coffee species and brands, thereby contributing to product integrity and fraud prevention in the Vietnamese coffee market.

2. Experimental

2.1. Sample Collection and Preliminary Processing

Table 1 summarizes the information of 36 coffee samples representing four common types collected from commercial outlets in Hanoi, including 12 Arabica samples, 13 Robusta samples, 6 Moka samples, and 5 Culi samples. Each type was sampled at five different vendors to evaluate repeatability.

Table 1. Sample information, brand names, and abbreviations.

Brand	Sample information			
	Arabica	Robusta	Moka	Culi
Mai	A1	-	M1	Cu1
Honey	A2	R2	M2	Cu2
Duong	A3	R3	M3	-
Mê Trang	A4	R4	-	Cu4
M Ja	A5	R5	-	-
Con soc	A6	R6	-	-
Hat A	A7	R7	-	-
Trung Nguyen	A8	R8	-	-
Huong Viet	A9	R9	-	Cu9
Vinacafe	A10	R10	M10	-
Phuc Long	-	R11	M11	-
TwitterBean	A12	-	-	-
Nhan	A13	-	-	-

Phuong Vi	-	R14	-	-
Thu Ha	-	R15	-	-
Nescafe	-	R16	-	-
Highland	-	-	M17	Cu17

Brand names and origin information were obtained from packaging labels. Prior to analysis, all coffee samples were finely ground and homogenized.

2.2. Infrared Spectroscopy Analysis

Fourier-transform infrared (FTIR) spectra were recorded using a Nicolet™ iS50 FTIR spectrometer (Thermo Scientific, USA). Background spectra were collected and subtracted prior to each sample measurement. Samples were placed on a ZnSe crystal with a diamond element integrated into the ATR module. Spectra were acquired in the range of 400 to 4000 cm⁻¹ with 128 scans per sample and a resolution of 10 cm⁻¹. Ground coffee powders were analyzed directly on the ATR surface.

2.3. Multivariate Statistical Analysis

FTIR spectral data were exported into spreadsheet format and subjected to statistical analysis using Principal Component Analysis (PCA) with Pearson correlation (n-1) and Linear Discriminant Analysis (LDA). Data analysis was performed using XLSTAT version 2016.02.28451 integrated in Microsoft Excel and STATISTICA 12.

3. Results and Discussion

3.1. FTIR Spectral Analysis

The chemical composition of ground coffee is highly complex. In addition to well-characterized major constituents, numerous minor compounds remain unidentified but are expected to contribute significantly to the infrared spectral profile

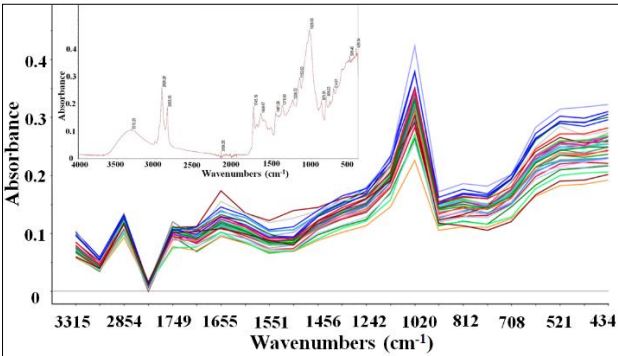


Figure 1. Summary of maximum absorbance peaks across 36 samples.

Identified functional groups included: stretching vibrations of -OH and -NH groups (3500-3050 cm⁻¹), NH⁺ (3050-3000 cm⁻¹), C-H (3000-2800 cm⁻¹), C=O (1750-1650 cm⁻¹), C=C (1650-1600 cm⁻¹), C-O (1450-1000 cm⁻¹), and deformation vibrations in the region 1000-500 cm⁻¹.

To reduce data redundancy, only the spectral maxima were extracted for all samples. *Figure 2* displays 23 selected peak intensities from the 36 coffee spectra. Visual inspection of the spectral profiles revealed insufficient resolution to discriminate coffee types by eye. Repeated measurements (n = 5) demonstrated a relative standard deviation (RSD) of 0.7%, with mean peak deviation within ±3%. Replicate samples, used to assess production-related variation, yielded an RSD of 1.0% and average deviation of ±5%.

3.2. Application of Principal Component Analysis (PCA)

Principal Component Analysis (PCA) was applied to evaluate both the origin effect and classification potential across the 36 samples. In the original dataset, many variables are expected to be correlated. PCA eliminates this redundancy via linear transformation, producing uncorrelated variables called principal components (PCs). These PCs reorder the data such that the first components retain the majority of the original information. The number of meaningful PCs is always less than the number of original variables, enabling further multivariate analysis [27]. Figure 3 shows a scree plot indicating eigenvalue and eigenvector contributions. The first two PCs accounted for 72.99% and 11.97% of total variance, respectively, together explaining over 80% of the dataset variability.

Although PCA was applicable to this dataset, it did not successfully classify coffee samples by species (see Figure 2). However, brand-based clustering within each coffee type was relatively effective. Moka and Culi samples were more clearly differentiated (Figures 3c, 3d, 4d). The loading scatterplot (Figure 4c) indicated that wavelengths at 1947 cm⁻¹ (combination bands and overtones) and 2854 cm⁻¹ (intramolecular hydrogen-bonded -OH stretch) contributed most strongly to PC1, while other wavelengths contributed to the separation along PC2.

For Arabica coffee, the PCA model could clearly distinguish the Mai and M Ja brands (Figure 3a). The corresponding loading plot (Figure 4a) showed strong PC1 contributions from 766 and 870 cm⁻¹ (deformation modes), and PC2 contributions from 1703 cm⁻¹ (C=O stretch) and 1975 cm⁻¹ (fingerprint region).

In the case of Robusta, the PCA model revealed some similarity between samples from Phuc Long, Duong, Vina, Me Trang, and Honey, as well as between Thu Ha and Phuong Vi. In contrast, M Ja, Trung Nguyen, and Hat A samples were distinctly separated (Figure 3b). The loading plot (Figure 4b) indicated that the 1975 cm⁻¹ peak (fingerprint region) was the primary contributor to PC2 separation.

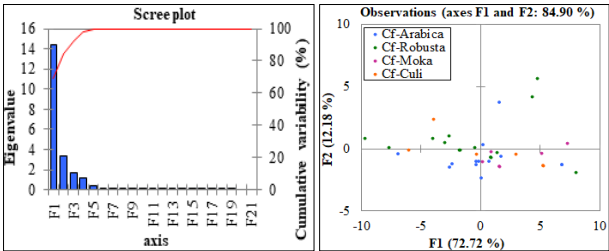


Figure 2. Classification results using PCA.

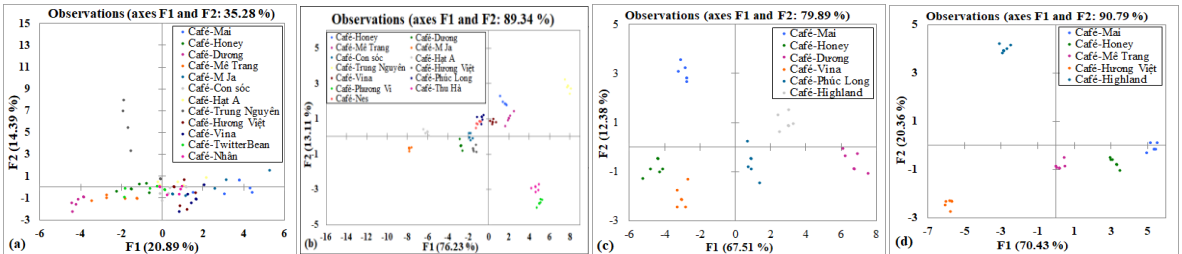
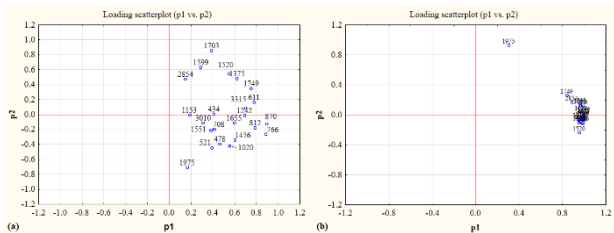


Figure 3. PCA brand discrimination within Arabica (a), Robusta (b), Moka (c), and Culi (d) samples.



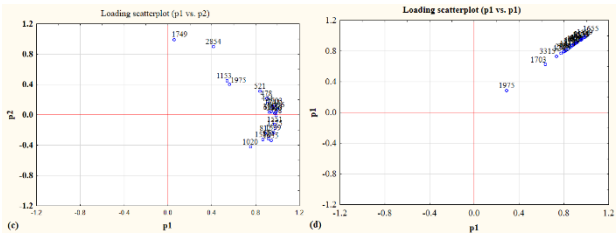


Figure 4. PCA loading scatterplots for Arabica (a), Robusta (b), Moka (c), and Culi (d) samples.

3.3. Application of Linear Discriminant Analysis (LDA)

Linear Discriminant Analysis (LDA) is a classification tool that constructs linear combinations (discriminant functions) of the original variables to maximize intergroup variance while minimizing intragroup variance [37,38]. When applied to the 36 sample dataset, LDA produced satisfactory discrimination. The analysis successfully separated the four coffee types: Robusta, Arabica, Moka, and Culi (Figure 5). Furthermore, brand-specific discrimination was also achieved for each type (Figure 6).

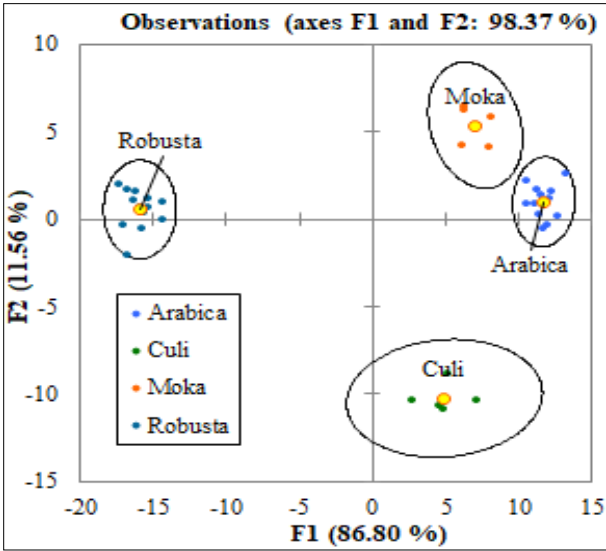


Figure 5. Discriminant analysis results for coffee type classification.

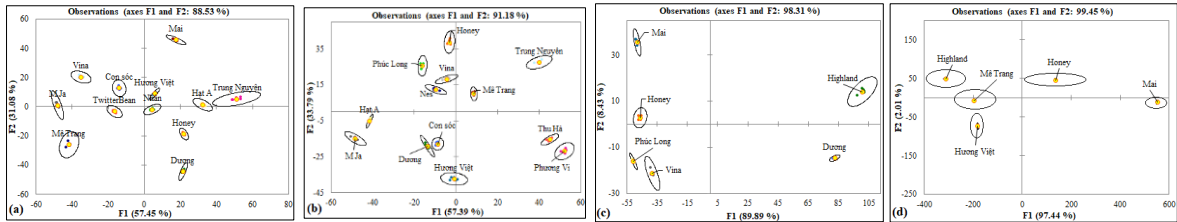


Figure 6. Brand discrimination using LDA for Arabica (a), Robusta (b), Moka (c), and Culi (d).

Compared to PCA, LDA demonstrated superior performance in both species-level and brand-level classification. The four coffee types were distinctly separated (Figure 5), and samples within each type were grouped according to supplier (Figure 6). In practice, differences in post-harvest processing or roasting methods between suppliers may introduce composition variability even within the same coffee type.

4. Conclusions

This study demonstrates that FTIR spectroscopy, when combined with Principal Component Analysis (PCA) and Linear Discriminant Analysis (LDA), is effective for the classification of roasted Arabica, Robusta, Moka, and Culi coffee from 17 commercial brands available in the Vietnamese market. The analytical workflow, which employs PCA followed by LDA using PC scores as input, provided clear discrimination among the coffee types.

These results represent an initial step toward developing a reliable analytical method for the classification of pure coffee products by type. Future investigations will address whether this approach can also detect blends of Arabica and Robusta. If successful, such capability would offer a rapid tool for detecting adulteration and verifying product authenticity.

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