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Characterization of Different Coffee (*Coffea*) Blends using Ultraviolet-Visible Spectroscopy Technique and Principal Component Analysis

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ABSTRACT

This study investigates the characterization of coffee blends using ultraviolet-visible (UV-Vis) spectroscopy combined with principal component analysis (PCA). Given the complexity of quality control in coffee production with differences in bean type, roasting degree, and processing methods, this research focuses on the comparative analysis of colour intensity, total soluble solids (°Brix), and pH of All Day (A), Mocca (M), and Espresso (E) coffee styles. The results indicate significant differences (p<0.05) across all samples, with All Day coffee having among the highest mean colour intensity (L = 26.61; a* = 7.84; b* = 10.7), Mocca coffee has the highest mean for pH level (pH = 6.08), and Espresso coffee has the highest mean for °Brix value (0.81° Bx). The UV-Vis spectral data, further analyzed using the PCA, showed distinct groupings among the coffee types, with pH and colour showing as key discriminative variables. The integration of UV-Vis spectroscopy with chemometric techniques provides a reliable, rapid analytical approach for coffee profiling. The results may promote sustainable quality assurance strategies and strengthen brand protection efforts in the coffee industry.*

Keywords: Chemometric analysis, Coffee classification, Roasting level, UV-Vis spectroscopy.

1. INTRODUCTION

Coffee is a popular beverage due to its unique taste and health benefits. The main species of coffee beans, with high economic value, are the Arabica (*Coffea arabica*) and Robusta (*Coffea canephora*) [1]. The three main regions of coffee producers are America, Africa, and Asia. Among the regions, Brazil (37%), Vietnam (17%) and Colombia (8%) are the largest coffee producers with different environmental and agronomic conditions [2]. For example, coffee produced at high altitudes was found to have less nutty and roasted notes, while sweet and caramel-like aromas are enhanced as altitude increases [3].

Coffee roasting is the process of transforming green coffee beans into roasted beans through heat, significantly affecting the quality of the beverage and making it a crucial component of product differentiation [4,5]. There are three common types of roasting: light roast, medium roast, and dark roast, with colour standards determining the degree of roasting [6]. The concentration of volatile compounds affected by roasting degree has been reported in previous research, with earthy and fruity aromas being among the most common [7-8]. Besides, bioactive compounds have been found to affect the sensory quality of coffee beans, influencing the astringency and bitterness of the coffee [5]. These characteristics contribute to the production of coffee blends to meet consumer preferences.

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Characterization of coffee, including sensory [9], aroma [10], bioactive compounds [11], and physicochemical [12] properties, is being studied because these factors are directly linked to coffee quality, market value, and consumer acceptance. Sensory evaluation by trained panels provides direct assessment of flavour, aroma, and mouthfeel, while headspace solid-phase microextraction (HS-SPME) coupled with gas chromatography–mass spectrometry (GC–MS) identifies volatile compounds with high sensitivity [13-15]. Besides, high-performance liquid chromatography (HPLC) can accurately quantify bioactives like caffeine and chlorogenic acids in coffee [16]. Analysis using spectroscopy techniques such as ultraviolet-visible (UV-Vis), near-infrared (NIR), and Fourier transform infrared (FTIR) spectroscopy provides a rapid, non-destructive means to generate spectral fingerprints that can be associated with the physicochemical properties of coffee samples [17]. As demand for coffee with different blends grows, research on the characterization of coffee blends remains limited.

The objective of this study was to characterize coffee blends using UV-Vis spectroscopy combined with principal component analysis (PCA). The findings reveal relationships between different types of coffee blends and their colour, pH, and Brix values, which may help establish unique selling points for specialty coffees, supporting branding and high consumer preference in competitive markets.

2. MATERIAL AND METHODS

2.1 Material and Sample Preparations

Three styles of Arabica coffee powder from Boncafè (M) Sdn. Bhd. were purchased from the local market. Table 1 presents the descriptions of the coffee samples' profiles for All Day Coffee, Espresso Coffee, and Mocca Coffee, based on information extracted from the packaging. The three coffee blends were selected to represent a broad spectrum of consumer preferences and market diversity. All Day reflects lighter daily-consumption brews, Mocca captures medium-roast balance and complexity, while Espresso represents a concentrated medium-dark roast beverage within the specialty segment. Together, all three coffee blends provide a representative basis for comparative analysis.

Table 1: The profile for All Day, Espresso and Mocca coffee styles.

Profile	All Day Coffee (A)	Espresso Coffee (E)	Mocca Coffee (M)
Type of coffee bean	Arabica	Arabica	Arabica
Origin	Africa and Latin America	Africa and Central & South America	Latin America
Roast level	Medium-dark	Medium-dark	Medium
Body	Full	Full	Half
Acidity	High	Mild	Mild
Aroma and flavour	Brisk, hearty with a nutty aftertaste	Citrusy, rich and smooth	Strong and lively with a pleasant aftertaste

The coffee extracts were prepared by mixing 7 g of coffee powder with 180 mL of boiling water in a French press and stirring gently for 30 seconds. The coffee was steeped for 30 minutes and diluted to 290 mL with water. The liquid coffee was cooled to room temperature before the measurement.

2.2 Determination of Colour Parameters

A seven-gram coffee powder sample was used to measure the CIELAB colour parameters, including L* (lightness), a* (red-green axis), and b* (yellow-blue axis) using a chroma meter CR-410 (Konica Minolta, Tokyo, Japan). The sample was scanned three times, and the process was repeated for each of the triplicate samples. To measure the colour of the coffee extract, a Whatman filter paper No. 1 was dipped into the coffee extract until fully submerged and allowed to dry before colour measurement using the chroma meter. The same procedure was repeated for other samples in triplicate.

2.3 Determination of Brix Value

A digital refractometer (PAL-3, ATAGO, Japan) was used to measure dissolved sugar in three replicate samples of coffee blends at room temperature. Before the measurement, a calibration was conducted using distilled water to ensure precise measurement. Six drops of coffee extract were placed on the prism, and the triplicate measurement was recorded once the reading of the Brix value expressed in degrees Brix (°Bx) was stable. The prism was thoroughly cleaned with distilled water and dried between sample measurements.

2.4 Determination of pH Value

A pH meter (PB-10, Sartorius, Germany) was used to measure the pH of coffee extracts, which were calibrated with a pH 7 buffer solution. The meter was then soaked in the coffee sample extract, cleaned with distilled water, and stirred for ten seconds to prevent precipitation. The pH was measured in triplicate once the reading stabilized.

2.5 Determination of UV-Vis Fingerprint

The UV-Vis fingerprints of triplicate coffee extracts per sample were determined using a UV-Vis spectrometer (Lambda 365, Perkin Elmer, US) with the wavelength range from 400 to 700 nm. The spectra were recorded using a quartz cuvette at 25°C. The triplicate samples were scanned three times, resulting in 27 measurements for coffee extracts.

2.6 Analysis of Data

A statistical software add-in for Microsoft Excel (XLSTAT, Lumivero, Colorado, USA) was used for analysis of variance (ANOVA) with Tukey Honestly Significant Difference (HSD) post hoc test to assess the significant differences in terms of the mean values for colour, Brix and pH values between the three coffee blends. Additionally, PCA was conducted to analyze the relationships among coffee attributes using XLSTAT.

3. RESULTS AND DISCUSSION

3.1 Comparison of Colour, pH, and Brix Values with Different Types of Coffee Styles

Figure 1 shows the mean values of colour attributes for coffee powder and extract. The results showed that All Day coffee extract (LA) had the highest lightness (L) value and was significantly different compared to other coffees. Meanwhile, All Day coffee powder (PA), Espresso coffee extract (LE), Espresso coffee powder (PE), Mocca coffee extract (LM), and Mocca coffee powder (PM) showed no significant differences in L value. Based on the analysis, the LA coffee sample had the highest redness (a) value and the highest yellowness (b) value.

Besides, coffee extract such as All Day coffee (LA) showed higher values across all groups compared to Espresso (LE) and Mocca (LM) coffee extracts. This could be due to roasting level, which may affect the colour intensity and hue of the brewed coffee [18]. The findings from the study showed that both roast level and brewing temperature contributed to a significant influence on the chromatic attributes of brewed coffee. Regarding roasting degree, an increase in roasting degree was associated with greater colour intensity, likely due to greater formation of melanoidins and other pigmented compounds arising from Maillard reactions. This factor highlights the critical role of thermal processing in modifying not only the visual quality of brewed coffee but also its underlying chemical composition, with broader implications for sensory perception and consumer acceptance.

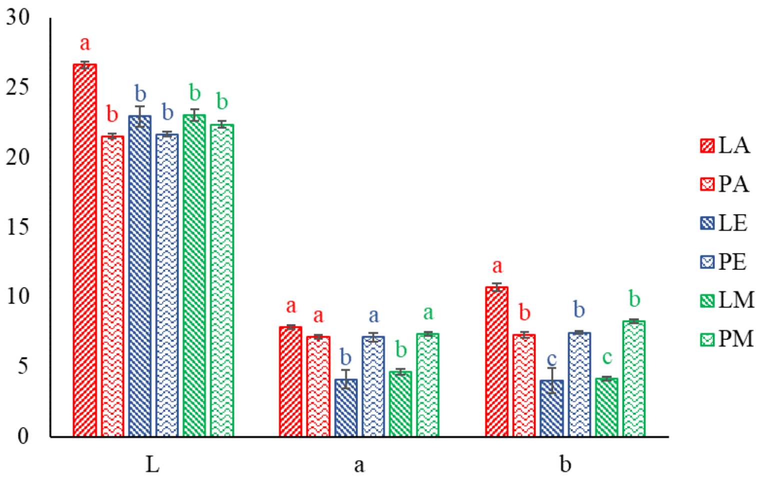

Figure 1: The mean values for colour parameters for coffee powder and extract using ANOVA and Tukey HSD post hoc test with error bars representing standard errors. Abbreviations: LA: All Day coffee extract; LE: Espresso coffee extract; LM: Mocca coffee extract; PA: All Day coffee powder; PE: Espresso coffee powder; PM: Mocca coffee powder.

Figure 2 shows the mean Brix values for the three coffee extracts and reveals that LE (0.81° Bx) has the highest Brix value, while LM (0.61° Bx) and LA (0.55° Bx) show no significant difference. All the coffee extracts, ranging from 0.81 to 0.55° Bx, showed low dissolved-solid concentrations, consistent with findings by Gloess et al. [19]. The low concentration may be associated with the extraction method using the French Press, as suggested by the authors that coffee extraction using a long extraction time, such as the French Press technique, resulted in a lower concentration of coffee components compared to the espresso extraction method, which yields a more concentrated beverage.

Figure 3 shows the mean pH values for three coffee samples, with LM (6.08) having the highest pH, while LE (6.02) and LA (5.93) were among the lowest. The ANOVA with post hoc tests showed that all coffee samples differed significantly in pH. It was observed that all pH values conform to the acidity level indicated on the packaging label, consistent with previous studies on black coffee pH [20]. In roasted coffee, the formation of formic, acetic, glycolic, and lactic acids occurs during the roasting process, contributing to a higher acidic level compared to green coffee [21].

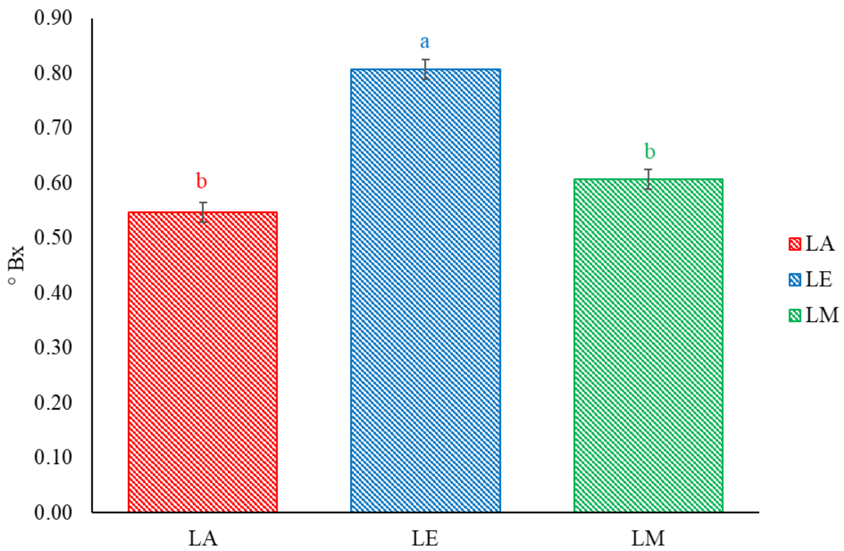

Figure 2: The difference in coffee extract for Brix value using ANOVA and Tukey HSD post hoc test with error bars representing standard errors. Abbreviations: LA: All Day coffee extract; LE: Espresso coffee extract; LM: Mocca coffee extract.

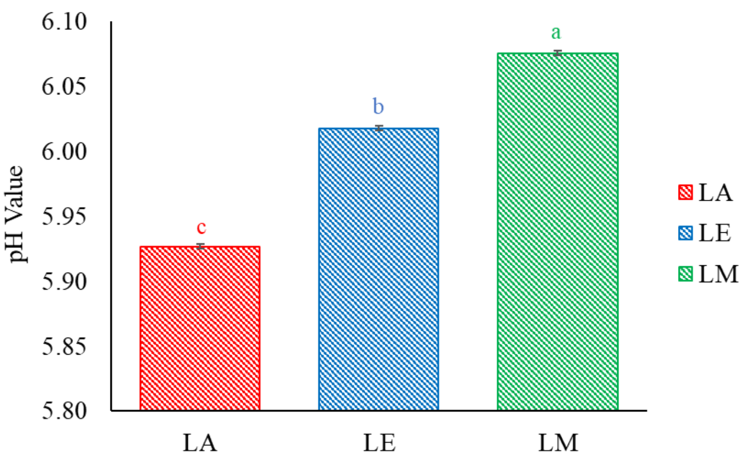

Figure 3: The mean pH level of coffee extracts using ANOVA with Tukey HSD post hoc test with error bars representing standard errors. Abbreviations: LA: All Day coffee extract; LE: Espresso coffee extract; LM: Mocca coffee extract.

3.2 UV-Vis Fingerprinting of Different Types of Coffee Styles

Figure 4 shows the raw spectral UV-Vis fingerprints of three coffee extracts, with a decreasing trend over the UV-Vis wavelengths (400-700 nm). Based on the mean values of the UV-Vis absorbance, All Day coffee extract (LA) has the highest absorbance across the entire wavelength range, followed by Espresso coffee extract (LE) and Mocca coffee extract (LE). This elevated absorbance, particularly in the blue region at 400–425 nm, suggests the presence of brown colouration in roasted coffee, resulting from thermal Maillard reaction products (MRPs) attributed to melanoidins during the coffee roasting process [22].

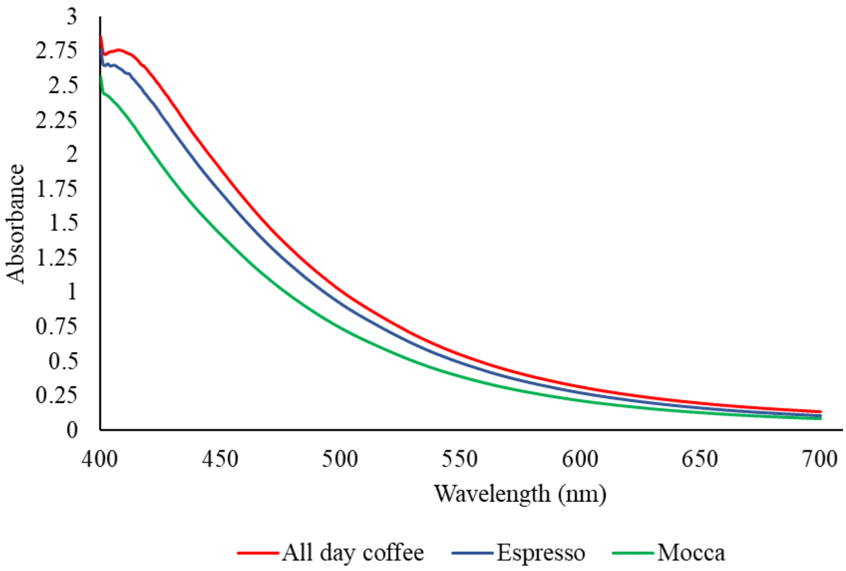

Figure 4: The UV-Vis fingerprints (400 – 700nm) for different types of coffee extracts.

3.3 Relationship Between Different Types of Coffee and Quality Characteristics

The PCA biplot in Figure 5 shows the relationship between coffee extract, LA, LE, and LM with the coffee characteristics, which include colour parameters, Brix values, and pH levels. The F1 variable captures 86.6% of the variance, indicating that pH levels and °Brix play a major role in the variations observed among different coffee extracts. The All Day coffee extract (LA) is positively correlated with colour parameters. In contrast, the LE and LM showed a negative correlation with colour parameters on the negative side of F1. It was observed that all three coffee extracts are clearly distinguished by colour, °Brix, and pH. Overall, the LA is associated with high colour parameters, LE with high °Brix (sweetness), and LM with low acidity (high pH).

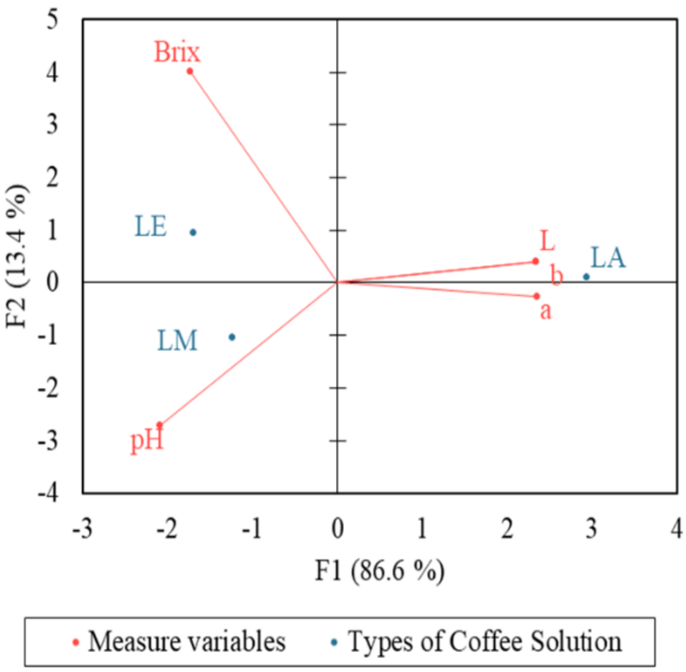

Figure 5: The biplot of principal component analysis for different coffee styles and the measured variables, which include colour, Brix value, and pH level. Abbreviations: LA: All Day coffee extract; LE: Espresso coffee extract; LM: Mocca coffee extract.

4. CONCLUSION

The study used UV-Vis Spectroscopy, ANOVA, and PCA to characterize different types of coffee blends. The results showed that the All Day coffee (A) style had the highest colour parameter values, Mocca coffee (M) had the highest pH, and Espresso coffee (E) was the sweetest among all. The UV-Vis analysis shows that the All Day coffee extract (LA) exhibits the highest absorbance across the UV-Vis spectrum, indicating a greater presence of colour-related compounds compared to Espresso and Mocca. The PCA results showed that pH and colour parameters were the major factors to differentiating among coffee samples. The findings presented in this study offer valuable insights for adoption by the coffee industry to enhance quality control measures by integrating UV-Vis and PCA as a rapid screening technique. Besides, the findings may be valuable for guiding product development by ensuring the preservation of the unique coffee characteristics revealed by the PCA. Future research should expand the scope to include a broader range of coffee types with varying characteristics to achieve a more comprehensive characterization of coffee properties.

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