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Non-Destructive Characterization of *Mangifera indica* using Physicochemical Profiling and Infrared Spectroscopic Assessment

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Abstract

Mangifera indica is a nutrient-rich tropical fruit with exceptional commercial value. It can be consumed fresh or processed into pulp for use in a wide array of food and agro-based industries. As global demand for mango continues to increase, proper grading and quality assessment have become essential, particularly for export markets. The present study focuses on evaluating key nutritional and quality-related attributes of mango fruit through physical, chemical, and spectral characterization. Standard AOAC procedures were employed to determine the chemical composition, while spectral profiling was carried out using Near Infrared (NIR) spectroscopy (750–2500 nm) and Fourier Transform Infrared (FTIR) spectroscopy (4000–400 cm⁻¹). The combined physicochemical and spectral analysis provides insight into the quality indicators of indigenous mango varieties.

Keywords: FTIR, Mango, *Mangifera indica*, NIR spectroscopy, Physicochemical analysis, Tropical fruit

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Introduction

Referred to as the "king of fruits," mango is among the most widely consumed tropical fruits owing to its rich taste, high juiciness, and desirable aroma. Mangoes possess substantial nutritional value, being a good source of vitamin C, β-carotene, and essential minerals [1]. The fruit exhibits wide varietal diversity, leading to differences in colour, shape, flavour, and overall sensory attributes [2-4]. Its appealing taste, nutritional quality, and low calorific value make mangoes highly valued in international markets [5]. India contributes nearly half of the world's mango production, reporting approximately 65,000 tonnes in 2010 [6]. With rising export demands, postharvest handling and quality assessments have become indispensable. Export-quality mangoes must meet stringent physical and internal standards, including size, peel and pulp characteristics, nutrient composition, acidity, soluble sugars, and flavour-related compounds [7]. Conventionally, most of these assessments rely on destructive chemical testing, which requires trained personnel, advanced laboratory facilities, and results in the fruit being rendered unusable [1, 2].

Infrared spectroscopy—especially Near Infrared (NIR) spectroscopy—has emerged as a rapid, user-friendly, and non-destructive alternative for qualitative and quantitative food analysis [8-10]. While FTIR identifies fundamental vibrational transitions of organic molecules [11], NIR detects overtone and combination bands, enabling deeper sample penetration and faster analysis [12-13]. These methods have been successfully applied in food quality assessment, pharmaceuticals, and numerous biological samples [14-17]. This study aims to utilize non-destructive NIR and FTIR spectroscopy to assess the molecular and nutritional characteristics of mango pulp. The findings lay the foundation for developing future chemometric-based prediction models to evaluate fruit quality without the use of chemicals [8].

Previous research has extensively documented the physicochemical properties of mangoes, and several studies have utilized Fourier Transform Infrared (FTIR) or Near-Infrared (NIR) spectroscopy as independent tools for assessing biochemical composition, ripening behaviour, and quality attributes. FTIR spectroscopy provides detailed molecular-level information by identifying functional groups, monitoring structural changes, and detecting variations in sugars, organic acids, and phenolic compounds during different stages of fruit maturity. Conversely, NIR spectroscopy is widely recognized for its rapid, non-destructive ability to estimate internal quality parameters such as moisture content, total soluble solids, titratable acidity, and firmness. However, using either technique alone often results in limitations related to spectral sensitivity, penetration depth, noise interference, and restricted predictive accuracy, particularly when modelling complex biological matrices such as mango pulp and peel.

A significant research gap therefore exists in integrating FTIR and NIR to harness their complementary strengths. FTIR excels in chemical specificity, whereas NIR offers deeper penetration and faster acquisition. Their combined use can generate a more comprehensive spectral fingerprint that enhances analytical resolution. Additionally, coupling

integrated FTIR-NIR data with advanced chemometric techniques such as PCA for dimensionality reduction, PLSR for quantitative prediction, and SVM for classification—can significantly improve the robustness, accuracy, and generalizability of mango quality models. Emphasizing this gap in the introduction will establish the novelty of the present study and highlight its contribution toward developing a holistic, hybrid spectroscopic framework for high-precision mango characterization.

Materials and Methods

Sample Collection and Preparation

Mango fruits (*Mangifera indica*) were procured from a commercial orchard. Fruits were harvested at a uniform physiological maturity stage. Only fruits free from visible defects, bruises, or disease symptoms were selected for the study. Harvesting was carried out manually to minimize field heat, and the fruits were transported to the laboratory under shaded or ambient conditions. Upon arrival, fruits were immediately graded, washed, and used for subsequent physical, chemical, and spectral analyses. These controlled conditions help reduce pre-analytical variability and ensure that the observed compositional and spectral differences are primarily attributable to fruit physiology and not to handling or environmental artefacts. Whole mango fruits were initially used for physical measurements. Afterward, the peel was removed and the pulp was collected for chemical, rheological, and spectral analyses.

Physical, Chemical, and Rheological Analysis

Vernier calipers were used to measure the major, minor, and intermediate diameters. These parameters were employed to calculate size, sphericity, and surface area. The weights of intact fruit, pulp, peel, and seed were also recorded. Chemical composition was evaluated using AOAC standard protocols [18], including: Oven drying for moisture, Muffle furnace for ash content, Soxhlet extraction for fat, Kjeldahl method for protein, Acid-alkali digestion for crude fibre [19, 20].

Carbohydrate content was calculated using:

Carbohydrate (%) =
$$100 - [Protein (\%) + Fibre (\%) + Fat (\%) + Moisture (\%) + Ash (\%)]$$
 (1)

Energy value (kcal/100 g) was calculated using Osborn and Voogt's formula:

Energy =
$$9 \times \text{Fat } (\%) + 4 \times \text{Carbohydrate } (\%) + 4 \times \text{Protein } (\%)$$
 (2)

Viscosity of mango pulp was determined using a viscometer.

Spectral Data Collection

NIR spectra (700–2500 nm) were recorded using a NIR DOSS2500 spectrometer. FTIR spectra (4000–700 cm⁻¹) were obtained using a PerkinElmer FTIR instrument with KBr pellets.

Results and Discussion

The physicochemical characteristics of mango pulp are summarised in **Table 1**, with size, sphericity, and surface area calculated using the following equations:

Size (Dg) =
$$(a \times b \times c)^{1/3}$$
 (3)

Where a, b, and c represent the major (10.77 cm), minor (7.97 cm), and intermediate (9.06 cm) axes.

Surface Area (Sa) =
$$\pi \times (Dg)^2$$
 (4)

Sphericity
$$(\Phi) = (Dg/a) \times 100 \%$$
 (5)

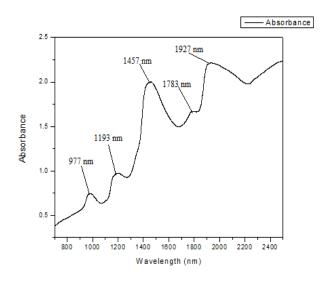
The data show that pulp constitutes the majority of the fruit mass, indicating a fleshy and juicy variety. A high moisture percentage supports this observation. The pulp also exhibits considerable protein and carbohydrate content, making mango a moderate-energy fruit. The pH value (4.215) confirms its acidic nature, which is expected for ripe mangoes.

Physical & Rheological Parameter	Value
Intact fruit weight (g)	507.000
Pulp weight (g)	385.000
Peel weight (g)	68.000
Kernel weight (g)	54.000
Size (cm)	9.1960
Surface area (cm²)	265.625
Sphericity	0.8538
Viscosity (mPa·s)	30.651
Biochemical Parameter	Value (g/100g)
Moisture	86.851
Ash	0.405
Crude fat	0.455
Crude protein	5.15
Crude fibre	0.695
Energy (Kcal)	50.475
Carbohydrate	6.445
Total Soluble Solids (°Brix)	15.000
pH	4.215

Table 1 Physical and Biochemical Attributes of Mango Pulp

Spectral Interpretation

Both NIR and FTIR techniques provided molecular fingerprints of mango pulp without requiring elaborate sample preparation. FTIR, due to its shallow penetration depth, primarily revealed fundamental vibrational bands. Major peaks include: 3394 cm⁻¹: Broad O–H stretching (indicative of high moisture), 2916 cm⁻¹: asymmetric C–H stretchingof methylene (–CH₂) and methyl (–CH₃) groups, which are abundant in carbohydrates and minor lipid components of mango pulp, 2137 cm⁻¹: a weak band associated with a combination/overtone transition or a minor background/instrumental artefact, rather than a distinct functional group., 1637 cm⁻¹: Amide (N–H) bending and C=C stretching. NIR spectra showed overtone and combination bands with broader, less intense peaks due to higher harmonic frequencies: 977 nm: Second overtone of O–H (water), 1193 nm: Second overtone of C–H (lipids), 1457 nm: N–H first overtone (proteins), 1780 nm & 1927 nm: C–H and O–H combination bands (cellulose, starch) [19]. Thus, NIR provides deeper structural insights than FTIR and is more suitable for non-destructive fruit analysis [21].



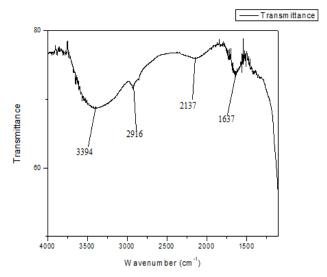


Figure 1 Near infrared fingerprint of the mango pulp

Figure 2 Fourier Transform infrared fingerprint of mango pulp

Conclusion

This study offers a fundamental assessment of mango quality using both destructive and non-destructive analytical approaches. Chemical analysis confirmed mango pulp to be rich in moisture, carbohydrates, and protein, with a moderate energy value. Physical characterization showed a high pulp-to-peel ratio, making the fruit suitable for processing industries.

The use of IR-based non-destructive tools—NIR and FTIR—proved effective in identifying key organic components. While FTIR detects fundamental vibrations, NIR provides overtone and combination bands, offering deeper penetration and broader analytical scope. Future studies combining chemometrics with large datasets can enable predictive modelling for rapid, chemical-free quality assessment of mangoes.

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