Non-Destructive Prediction of Quality Parameters in Alphonso Mangoes Using Near-Infrared Spectroscopy: A Comprehensive Study on Physicochemical Characteristics and Ripening Dynamics

Abstract

This study focuses on the application of Near-Infrared Spectroscopy (NIRS) to predict key quality parameters in Alphonso mangoes, namely Total Soluble Solids (TSS), Titratable Acidity (TA), pulp firmness, and carotenoid content. Alphonso mangoes, known as the "king of fruits," are a significant tropical fruit, with India being the leading global producer. Quality control is crucial for fruit export, and the mango supply chain involves various procedures. Physiological transformations occur in mangoes from production to consumption, affecting their internal quality. The challenges in assessing internal quality factors such as soluble solids, dry matter, firmness, starch, and sugar content hinder the exportation of mangoes.

The ripening process in mangoes involves metabolic changes leading to modifications in physical, mechanical, and chemical attributes. Non-destructive identification of internal defects in Alphonso mangoes is an underexplored field, with limited research on internal quality factors. The study aims to enhance understanding of light penetration into fruit tissues using numerical simulation techniques. NIR spectroscopy's significance in post-harvest technology is highlighted, and the study develops prediction models for quality parameters using Partial Least Squares (PLS) regression. The calibration models are optimized with spectral pre-processing techniques, and the Savitzky–Golay first derivative method yields favorable results. The results indicate changes in TSS, carotenoid content, firmness, and acidity during storage, providing insights into mango ripening dynamics. The Unscrambler software is employed for multivariate analysis, emphasizing the importance of the 600–1000 nm wavelength range. The study contributes to the development of portable instruments for rapid and accurate quality prediction of Alphonso mangoes in the supply chain.

1. Introduction

Mango (*Mangifera indica* L.) holds significant importance as a tropical fruit and is predominantly cultivated in nations such as India, China, Brazil, and Thailand. India stands as the leading global producer of mangoes, contributing to 50% of the total mango yield. The country annually produces 21.01 million metric tons of mangoes, covering an approximate area of 2.296 million ha (Statista, 2023).Indian mangoes, globally hailed as the "king of fruits," are immensely popular for their delicious taste, enticing aroma, exceptional flavor, low-calorie content, and high nutritional value, both domestically and internationally(Jha, 2014). Mango is enjoyed fresh or processed, with a preference for the former. Its seasonal availability restricts access to a limited time each year. Quality control plays an important role in fruit export and supply chain (Lawson et al., 2019). The mango supply chain in India involves several unit procedures, including pretreatment, cooling, packaging, and handling.

Various physiological transformations take place in mangos throughout their journey from production to consumption. These changes encompass physiological weight reduction, internal damage, and a deterioration in sensory quality (Mahto et al., 2013). Several factors, such as harvest time, seasonal variations, the impact of mulching, geographical location, elevated temperatures, reduced fruit transpiration, and biological elements, can affect the internal quality of mango fruit (Shivshankar et al., 2007). The challenges mentioned pose obstacles to the exportation of mangoes. Alphonso, a prominent mango cultivar in India, stands out as a commercially vital variety. Its delectable taste, captivating fragrance, saffron-like color, texture, and extended shelf life make it globally appealing.

Following harvest, mangoes experience a notable increase in both climacteric respiration rate and ethylene production, limiting their postharvest shelf life and diminishing eating quality. (Razzaq et al., 2013).The ripening of mango fruit entails a sequence of metabolic processes, triggering chemical alterations, heightened respiration, modification in structural polysaccharides resulting in fruit softening, breakdown of chlorophyll and carotenoid synthesis, and the hydrolysis of starch into sugars. This overall process leads to the ripening of the fruit, achieving a desirable quality with a softened texture. (Gill et al., 2017).There is a scarcity of extensive compositional data regarding the physicochemical and antioxidant characteristics of various mango cultivars.

The ripening process brings about changes in parameters, leading to modifications in the physical, mechanical, and chemical attributes of the fruit. Typically, fruit quality is evaluated through surface firmness, gloss, aroma, flavor, etc., which may be misleading (Jha and Matsuoka, 2004), or through destructive methods that involve intricate laboratory techniques, rendering the tested fruit inedible. The non-invasive identification of internal defects in Alphonso mangoes is a relatively unexplored field, with limited research on assessing internal quality factors like soluble solids, dry matter, firmness, starch, and sugar content. To enhance our comprehension of light penetration into fruit tissues, further research utilizing numerical simulation techniques is essential (Raghavendra et al., 2021).The growing significance of NIR spectroscopy in post-harvest technology is apparent from the recent surge in publications and the adoption of NIR systems by numerous online grading manufacturers for measuring various quality attributes (Nicolai et al., 2007).Numerous physico-chemical attributes of fruits and vegetables have been assessed non-destructively through a variety of techniques (Mahanti et al., 2022).

The primary aim of this study is to explore the feasibility of utilizing Near-Infrared Spectroscopy (NIRS) to predict Total Soluble Solids (TSS), Titratable Acidity (TA), pulp firmness, and carotenoid content in Alphonso mangoes. The ultimate goal is to contribute to the development of portable instruments or conveyor belt systems that enable rapid and accurate quality prediction of Alphonso mangoes.

2. Material and method

2.1 Sample Preparation

For experimental purposes, newly harvested samples of Alphonso mango fruits were obtained directly from farmers in Ratnagiri and Sindhudurg districts. A total of 300 mango fruits, each representing onehalf of a mango, were collected from both districts. The selection process focused on mangoes with 75 to 80% maturity, which were promptly subjected to pre-cooling after harvesting. Sorting and grading were carried out based on both weight and color criteria. Only mangoes weighing between 225 to 250 grams and exhibiting a dark green color were chosen for the subsequent experiment to ensure uniformity.

2.2 Acquisition of spectral signatures

Using the Spec3 ASD spectroradiometer, we acquired reflectance-mode spectral signatures for whole Alphonso mangoes, covering 350-2500 nm at 1nm intervals. The device underwent precise calibration with a standard white reference before scanning. Precautions were taken to prevent signal losses by ensuring no gaps between the mango and the handheld probe. Spectral signatures were collected at 0, 5, 10, 15, 20, and 25 days post-harvest, spanning the ripening period. Eight scans were conducted on each mango at different locations, and the data were averaged. For internal disorder confirmation, 10% of fruits per storage interval underwent destructive analysis by being cut open.

2.3 Determination of physico-chemical properties of mango

2.3.1 Total Soluble Solid (TSS)

The TSS levels in mango samples stored at room temperature and in cold storage were assessed using a digital handheld refractometer (ATAGO, Japan, Model: PAL Brix/RI, range: 0 to 93%, resolution: 0.2%). Calibration was conducted with distilled water (0% TSS) as the reference. To measure TSS, 10 grams of mango fruit pulp underwent crushing with a pestle and mortar, and the resulting juice was filtered through muslin cloth. For TSS determination, 1 to 2 drops of clear juice were applied to the refractometer's prism, and the corresponding TSS value was recorded. This process allowed for the accurate evaluation of soluble solids in mango samples under different storage conditions (Palafox-Carlos et al. 2012).

2.3.2 Total Carotenoid content

The carotenoid concentration in mango samples was determined using the method outlined by Ranganna (1986). In this procedure, 10 grams of mango fruit tissue were crushed with 5 ml of acetone using a mortar and pestle, repeating until the residue turned colorless. The resulting extract was then transferred to a separating funnel, where 10 ml of petroleum ether and 5 ml of 5% sodium sulfate were added. After shaking, the mixture stood undisturbed for 5 minutes to allow for phase separation. The top layer, containing the extracted carotenoids, was collected in an amber-colored bottle, and the volume was adjusted to 25 ml with petroleum ether. Optical density (OD) values were measured at 452 nm using a double-beam UV-Vis spectrophotometer (Accumax, India, Model-2201, Wavelength-195 to 1100 nm) against petroleum ether as a blank. The obtained optical density values were then utilized to determine the total carotenoid content through a standard curve, expressed in mg/10 g of fruit tissue.

Total carotenoid content (mg/10g) = (3.87×Final Volume×Optical density×100)/(Weight of sample×1000) ---- (Eq. 3.1)

2.3.3 Firmness (Peel/pulp)

Mango fruit firmness was assessed using a texture analyzer (TA-XT plus connect texture analyzer from Stable Micro Systems, Ltd., Surrey, UK) in compression mode with a 2-mm diameter cylindrical probe (SMS-P/2, Stable Micro Systems, Ltd., Surrey, UK). Operational parameters included pre-test speed (2 mm/sec), test speed (0.5 mm/sec), post-test speed (10 mm/sec), trigger force (5.0 g), and distance (15 mm). Data acquisition during the compression test had a rate of 200 points/sec, following the approach outlined by Jha et al. (2010). For pulp firmness measurement, mango fruit samples were manually peeled without disrupting the pulp texture before undergoing the compression test. Firmness was quantified as the maximum force recorded in a force–time curve during mango compression tests. Measurements were conducted in triplicates at three different locations, and average values were recorded for comparison.

2.3.4 Titratable acidity

The titratable acidity of stored mango samples, a crucial parameter indicating fruit maturity and sour taste in citrus fruits, was determined following the procedure outlined by AOAC (2000). A 1 ml portion of the fresh mango sample was placed in a 100 mL volumetric flask and made up to 100 mL with distilled water. From this, 10 ml was extracted into a conical flask and titrated against a standard 0.1N sodium hydroxide solution using phenolphthalein as an indicator. Titration continued until a faint pink color persisted for 15 seconds. The titratable acidity was then calculated and expressed as a percentage of anhydrous citric acid.

Titratable acidity= (Normality of NaOH×Titre×0.64×100)/volume of juice taken ---- (Eq. 3.2)

2.4 Development of prediction models

In the development of the NIR model for non-destructive prediction of Total Soluble Solids (TSS), acidity, carotenoid content, and firmness of Alphonso mangoes, Partial Least Squares (PLS) regression was employed to create a concise and effective model. Various pre-processing techniques, including baseline correction to address variations, second-order smoothing to reduce noise and emphasize trends, Multiplicative Scatter Correction (MSC) for handling light scattering variations, and Savitzky–Golay derivatives (first, second, and third-order) to enhance spectral features and resolution, were applied to the original spectra. Careful selection of wavelength ranges focused on relevant spectral regions associated with the target parameters. For model evaluation, full cross-validation options, likely employing techniques such as leave-one-out or k-fold cross-validation, were utilized to ensure robust performance across the dataset. Assessment criteria, such as root mean square error (RMSE) and the multiple correlation coefficient (R2) following Jha et al. (2004), were employed in model selection. Scatter plots were generated to visually assess the predictability of non-destructive NIRS measurements against measured parameters, providing an intuitive validation of accuracy and reliability. This comprehensive approach contributes to the development of robust and reliable non-destructive NIR models for predicting key quality attributes of Alphonso mangoes.

3. Results

Reflectance spectra during the ripening process of mango fruits were obtained using a Vis-NIR spectroradiometer in reflectance mode. The reflectance spectra of mango fruits are depicted in Fig. 1. To optimize predictive performance, calibration models for all quality parameters were constructed employing various spectral pre-processing methods. The most favorable outcomes were observed when employing the Savitzky–Golay first derivative. Consequently, only the outcomes obtained through the Savitzky–Golay first derivative method are presented in this study (Fig. 2).

The Total Soluble Solids (TSS) level serves as a crucial indicator of fruit ripeness. Post-harvest, mango TSS ranged from 8.5 to 9%. During storage, a rapid increase in TSS content occurred, rising from 9.3% at 0 days to 22.1% at 20 days, followed by a decline to 18% at 25 days. Harvested at 70 to 75% maturity, all mango samples exhibited a carotenoid content of approximately 0.045 mg/10 g. Throughout storage, a rising trend in carotenoid content was observed, reaching a peak of 11.32 mg/10 g at 20 days under ambient conditions. However, thereafter, the value decreased to 8.36 mg/10 g at 25 days, indicating carotenoid degradation. Mango pulp consistently exhibited decreasing firmness during the entire storage period, with an initial recording of 6.78 N and a subsequent loss of 78% and 85% in firmness over 25 days. The acidity of mango fruits ranged from 1.89% to 1.95%, with a decline to 0.19% and 0.35% at the end of storage as ripening progressed.

The Unscrambler software (version 10x, CAMO AS, Trondheim, Norway) was used for multivariate analysis of spectral data with maturity indices. The data, spanning the wavelength range of 350–2500 nm, was visualized to examine spectral characteristics, particularly in the 600–1000 nm range, revealing peaks and depressions indicative of mango transmittance. In the wavelength range of 600–1000 nm, the multiple correlation coefficient (R^2) consistently showed stronger correlations for calibration and validation of maturity indices using PLSR models compared to other wavelength ranges. Optimal results were achieved when applying the Savitzky–Golay first derivative to the spectral data. For TSS, the PLSR model yielded a maximum R^2 value of 0.84 and an RMSE value of 1.71 in the 600–1000 nm range. Similarly, for carotenoid content, R^2 and RMSE values were 0.87 and 1.43, respectively. Titratable acidity exhibited R^2 and RMSE values of 0.85 and 0.21, while the firmness of Alphonso mango pulp reached R^2 and RMSE values of 0.95 and 0.37 (Fig. 3A to 3D).

4. Discussion

Typically, fruits and vegetables consist of approximately 80–90% water and encompass various complex molecules, including carbohydrates, organic acids, proteins, and other minor constituents. Consequently, the NIR spectra of these produce exhibit broad and intricate absorption bands due to complex hydrogen bonding interactions with different molecules. The predominant influence on NIR spectra for fruits and vegetables arises from the extensive water content, particularly with water absorption bands in the O-H bonds. These water absorption bands are generally broad and have peaks around 970, 1450, 1950, and 2250 nm (Magwaza et al., 2012). The spectral range utilized in this study allows for the observation of the characteristic water absorption bands at 970 and 1450 nm, associated with the second and first overtone of the OAH stretch, respectively (Williams & Norris, 2001).

Fruits commonly contain starch and sugars like sucrose, glucose, and fructose, which typically exhibit absorption bands near the strong water absorption regions, making their identification challenging (Delwiche et al., 2008). In the spectral range spanning 950 to 1650 nm, it is probable that the absorption bands of these carbohydrates overlap with the broader water bands around 600 to 1000 nm (Fig. 2). Notably, total soluble solids (TSS) and acidity stand out as crucial quality parameters for assessing mango quality. Ripe mangoes are characterized by high TSS content and exceptional eating quality. Total acidity (TA) and pulp firmness are anticipated to decrease during the ripening process, with the decline in TA attributed mainly to the utilization of organic acids as substrates for respiration.

NIR spectroscopy for fruit quality detection offers non-destructive analysis, rapid results, and multi-parameter assessment, reducing the need for separate analyses. It minimizes chemical usage, supports real-time monitoring, but limitations include limited penetration depth, sample homogeneity impact, high instrumentation costs, and sensitivity to environmental conditions. Careful consideration of these factors ensures accurate and reliable results.

Conclusion

This study delves into the crucial aspects of mango quality assessment, focusing on the Alphonso variety, a commercially significant cultivar in India. The research highlights the challenges faced in mango exportation, including physiological transformations, internal damage, and deterioration in sensory quality during the fruit's journey from production to consumption. The intricate processes involved in mango ripening, such as climacteric respiration, ethylene production, and various metabolic changes leading to chemical alterations, emphasize the need for accurate quality evaluation methods.The implementation of Near-Infrared Spectroscopy (NIRS) proves to be a promising approach for predicting essential quality parameters, including Total Soluble Solids (TSS), Titratable Acidity (TA), pulp firmness, and carotenoid content in Alphonso mangoes. The results obtained through the Savitzky–Golay first derivative spectral pre-processing method demonstrate the efficacy of non-destructive prediction models. The observed changes in TSS, carotenoid content, and firmness during storage offer valuable insights into the dynamics of mango ripening, contributing to the understanding of mango postharvest physiology.

Looking ahead, the study suggests future research directions, particularly in the non-invasive identification of internal defects in Alphonso mangoes. The relatively unexplored field of assessing internal quality factors, such as soluble solids, dry matter, starch, and sugar content, presents an opportunity for further investigations. Additionally, the growing significance of NIR spectroscopy in post-harvest technology opens avenues for the development of portable instruments or conveyor belt systems that can rapidly and accurately predict the quality of Alphonso mangoes in the supply chain. This research provides a foundation for advancing mango quality assessment methods, ultimately benefiting both producers and consumers in the mango industry.

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Figure

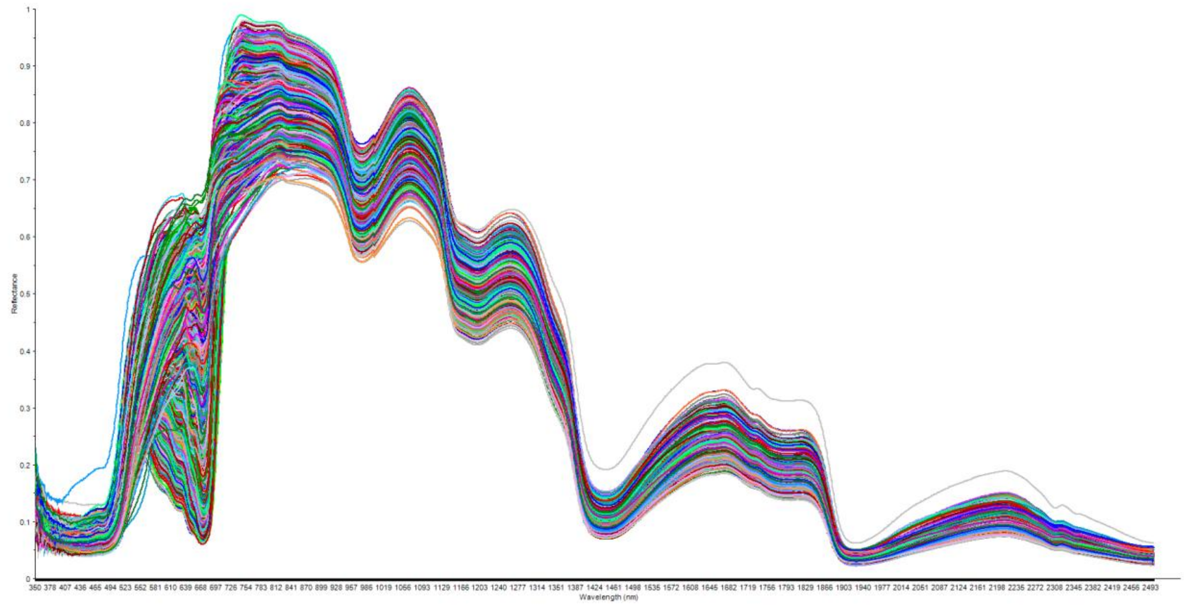


Fig. 1 Spectral Reflectance Analysis of Mango Fruits in the VNIR Region

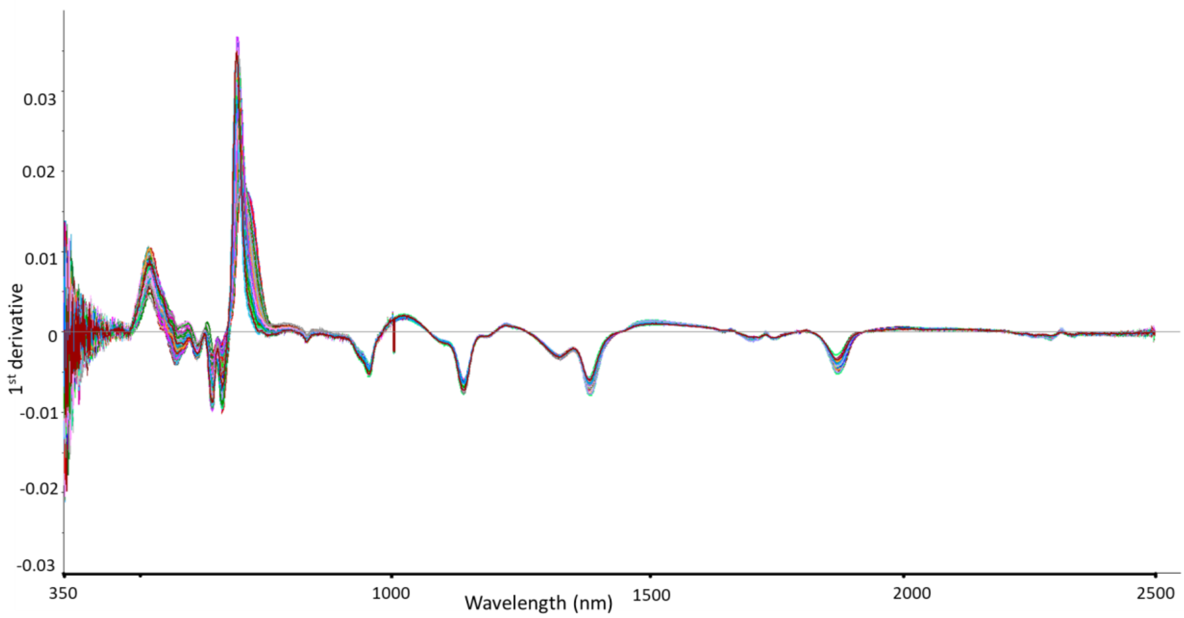
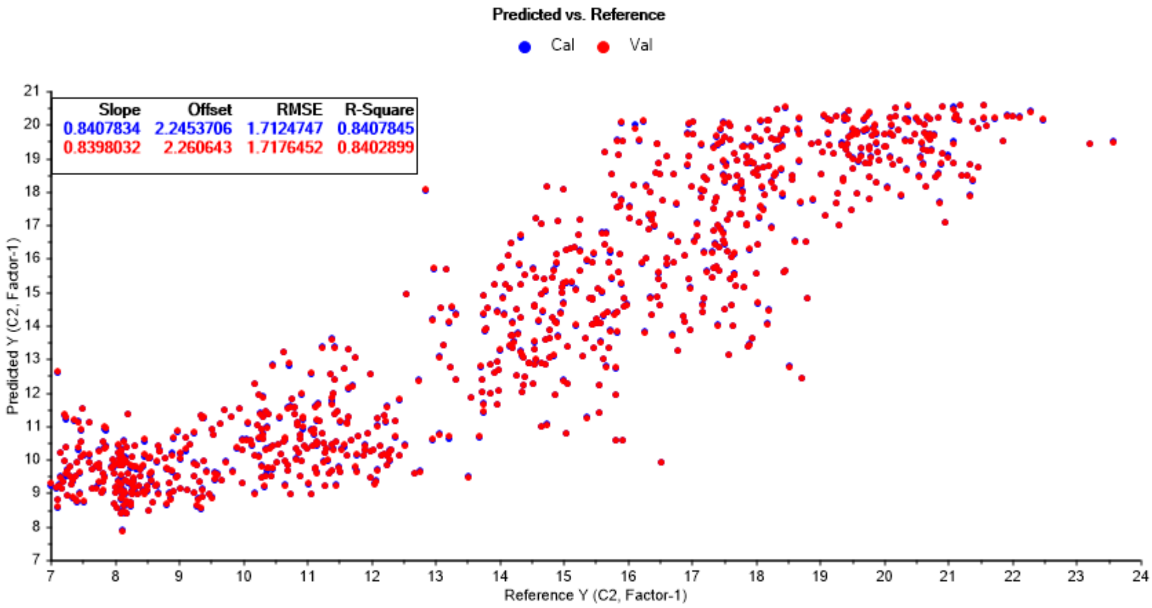
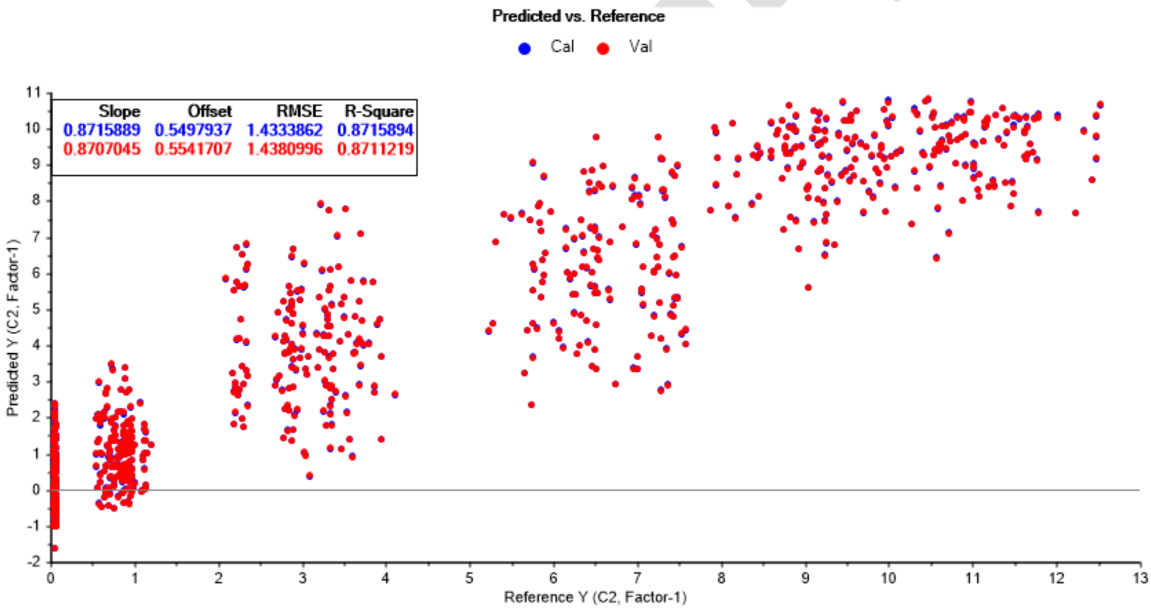


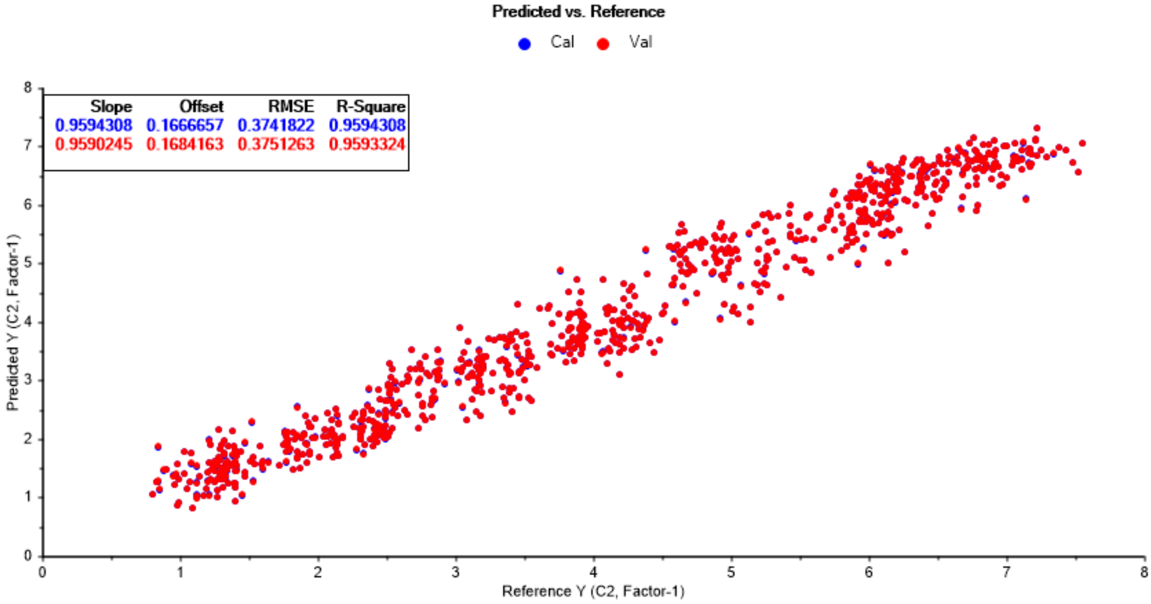
Fig. 2 First derivative of mango spectral signatures


Predicted vs. Reference
Cal
Val
Slope Offset RMSE R-Square
0.8407834 2.2453706 1.7124747 0.8407845
0.8398032 2.260643 1.7176452 0.8402899
Predicted Y (C2, Factor-1)
Reference Y (C2, Factor-1)

(A)


Predicted vs. Reference
Cal
Val
Slope Offset RMSE R-Square
0.8715889 0.5497937 1.4333862 0.8715894
0.8707045 0.5541707 1.4380996 0.8711219
Predicted Y (C2, Factor-1)
Reference Y (C2, Factor-1)

(B)



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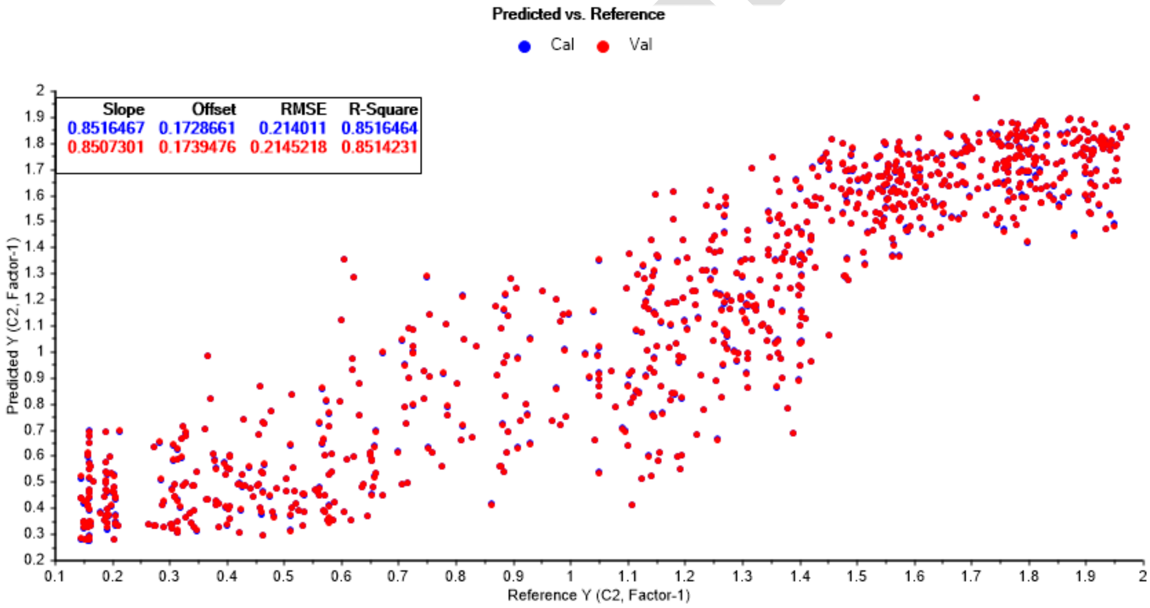

(D)

Fig. 3 Observed and predicted physico-chemical parameters of Alphonso mango A) TSS, B) Carotenoid content, C) Firmness, D) Titratable acidity in PLSR model