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# Quality evaluation of tender jackfruit using near-infrared reflectance spectroscopy

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## Abstract

Value addition of fresh tender jackfruit (*Artocarpus heterophyllus* L.) for vegetable purpose has gained much popularity due to its inherent nutritional and health benefits. For industries involved in value addition of tender jackfruit, rapid characterization of raw material is essential for screening and routine quality evaluation. But, conventional reference methods of quality evaluation are not suitable as they involve the use of chemicals, expensive, laborious and time consuming subject to the number of samples to be analyzed. As a promising alternative, the present study examined the performance of near-infrared spectroscopy (NIRS) as a novel approach to estimate pH, total soluble solid, titrable acidity, firmness and toughness of tender jackfruit. Partial least square regression (PLSR) models were used to establish linkage between reflectance spectra (1100-2450 nm) and quality attributes of fresh tender jackfruit. Based on residual prediction deviation (RPD) criteria, accuracy of PLSR model of titrable acidity was noted to be excellent (RPD=3.96) while good estimation was possible in case of firmness-tendril (RPD=2.61). Accuracy level suitable for coarse quantitative estimation (RPD=2.12) was noted in case of total soluble solids. The PLSR models of all other attributes were found to be capable of discriminating their low and high values (1.5<RPD<2.0) and hence appropriate for screening purpose. Thus, the results of the study advocate the use of NIRS approach for simultaneous estimation of multiple quality attributes of tender jackfruit in a rapid, non-destructive and non-invasive manner.

**Key words**: Tender jackfruit, near infrared reflectance spectroscopy, regression, reference method, quality, non-destructive, firmness, toughness

## Introduction

Jackfruit (*Artocarpus heterophyllus* L.) is an ancient seasonal fruit believed to be the native of the Western Ghats of India and grows abundantly in South and South East Asia. It is renowned for its richness in vitamins, minerals, calories, functional, medical and physiological properties (Swami *et al.*, 2012). Despite its usefulness, jackfruit is regarded as under exploited till recent past. However, over the last decade a variety of ready-to-eat and value added food products are being developed from jackfruit seed and mature or ripen fruit. As most of the products are either sugar or oil based, they may be of less preference for daily consumption, especially for people who are health conscious or suffering from diabetes and hypertension. In such cases, the consumption of immature or tender jackfruit as vegetable would be a better choice.

Tender jackfruit is superior to seed, matured or ripen form in terms of vitamin C (ascorbic acid); antioxidant that scavenges free radicals, strengthens the immune system, and keeps the gum healthy (Jagtap *et al.*, 2010). Moreover, it is a rich source of potassium with little sugars which may benefit people with hypertension and diabetes. These advantages added with its other nutritional values, fiber content and meat like texture made it popular as a vegetable of high market value especially in south Asian countries. In this context, development of value added products from tender jackfruit for vegetable purpose has gained much attention among business entrepreneurs. The commodity being seasonal, several preservation techniques are being employed by industries to extend shelf life and ensure its year round availability with minimum quality changes. Such industries need a rapid method for characterization of tender jackfruit for screening, routine quality analysis and quality checking protocols. However, it is difficult to achieve as the conventional methods are expensive, laborious and time consuming subject to the number of samples to be analyzed.

The aforementioned issues may be addressed using near infrared reflectance spectroscopy (NIRS) operating in visible, near-and shortwave infrared (Vis-NIR-SWIR) wavelength range of the electromagnetic spectrum (400-2500 nm). Over last few decades, the approach has been recognized as a rapid, cost effective, non-invasive, non-destructive, chemical-free approach popular for the characterization of fruits and vegetables (Schulz *et al.*, 1998; Slaughter and Abbott, 2004; Baranska *et al.*, 2006; De Oliveira *et al.*, 2014). Multiples attributes may be estimated via NIRS approach. Moreover, the approach is amenable to hyperspectral imaging system for inline/online quality estimation. The NIRS approach rely on the linkage between the attribute and spectral features defined by the overtones and combinations of fundamental vibrations of mainly C-H, N-H and O-H functional groups that occur in mid-infrared frequencies (Pasquini, 2003; Cen and He, 2007). Such linkages (also referred as calibration function) are usually developed by means of multivariate analytical methods techniques such as principal component regression, partial least squares regression (PLSR), support vector machine and artificial neural networks (Workman *et al.*, 1996; Shao *et al.*, 2011). Among them, PLSR has been widely used for its ability to address multicollinearity of spectral variables, computational efficiency and improved interpretability (De Belie *et al.*, 2003; De Oliveira *et al.*, 2014).

Usually, calibration functions are developed using large spectral libraries with appropriate variability in spectra and attribute values. To the best of our knowledge, no such spectral library exists for fresh tender jackfruit. Also, no studies have examined the potential of NIRS to characterize fresh tender jackfruit. Thus, the present study was undertaken as a preliminary step towards the development of a comprehensive spectral library with a view to enable rapid and non-destructive characterization of tender jackfruit via NIRS. The present study is the first attempt for NIRS based quality evaluation of tender jackfruit.

## Materials and methods

**Tender jackfruit sample collection and reference analysis**: The present study was conducted using tender jackfruit samples ($n$=58) collected from Alappuzha ($n$=19), Kollam ($n$=7), Malappuram ($n$=27) and Pathanamthitta ($n$=5) districts of Kerala state in India. All the samples were manually picked from jackfruit trees and subjected to analysis the very next day. Initially, each sample was cut axially in two similar parts; one part was used for reference analysis of attributes while the other was used for spectra acquisition. Then the part kept for reference analysis was peeled and sliced. A few slices were subjected to measurements of texture attributes (firmness and toughness) using a Texture Analyser (Stable Micro Systems, UK) equipped with a cylindrical probe of 5 mm diameter. The force-deformation curve was observed and the firmness (peak force) and toughness (area under the curve) were measured separately for core, tendril and skin (between tendril and peel) of the peeled tender jackfruit. The pH and TSS of the crushed sample juice were determined using a digital pH meter and refractometer, respectively. The titrable acidity of homogenized pulp of tender jackfruit was determined by titrimetric analysis against sodium hydroxide solution using phenolphthalein indicator (Ranganna, 1986).

**Spectral data collection**: The sample portion kept for spectral measurements was initially peeled. Then, grating was performed for more uniform presentation of core, tendril and skin portions of the sample for spectral measurements. The grated sample was taken in a circular sample container (10 cm diameter and 2 cm thickness) and the surface was levelled using the lower part of a glass Petri dish. It was ensured that there was no light penetration through the sample after preparation. Bi-directional spectral measurements of the grated sample were measured using a portable spectroradiometer Fieldspec 4 (Analytical System Devices, USA) in 350-2500 nm wavelength range. The sensing end of the fiber optic cable (25$^o$ conical angle) was located at a height of about 11 cm above the center of sample container. Thus, the field of view of the sensor has approximately 5 cm diameter at the sample surface. The sample was illuminated using a 200 W quartz-halogen lamp (45$^o$ illumination angle) and spectral measurements were performed. Prior to spectral measurement of each sample, a white reference spectrum was acquired using a Spectralon panel of size 5”×5” (Labsphere, USA). Four reflectance spectra of the sample were acquired by rotating the container at an angle of 90$^o$ after each spectrum measurement. Then, they were subjected to Savitsky-Golay smoothing of third-order and span of 9 nm (Sahadevan *et al.*, 2013). A characteristic spectrum of the sample was generated by averaging the smoothed spectra.

**Data pre-processing and regression modeling**: All the data pre-processing and modelling were performed using MATLAB software (R2017a, Mathworks). Pre-processing mainly intent to remove scattering and other undesired variations in the reflectance spectra and thus play a vital role in the development of reliable NIRS multivariate models. The reflectance spectra of samples were subjected to different pre-processing techniques categorized as scatter correction and derivatives (Rinnan *et al.*, 2009). Multiplicative scatter correction (*MSC*), de-trend (*DT*) and standard normal variate (*SNV*) constitute the former category while the latter consisted of first (*FD*) and second derivatives (*SD*). The reflectance without any pre-processing (*Raw*) was also included in the analysis. Apart from the use of individual spectral pre-processing techniques, a pairwise combination of all scatter correction and derivative techniques were also examined in the study. As *DT* and its combination with *SD* (*DT*+*SD*) yielded same results, the latter pre-processing was excluded from the analyses. Thus, an overall of 11 pre-processing techniques (6 individual + 5 combinations) were examined in this study.

The PLSR (Wold *et al.*, 2001) models were established between pre-processed spectra and different quality attributes of tender jackfruit. To avoid either over-fitting or under-fitting tendencies of PLSR, optimum number of latent variables (*LV*) was selected on the basis of minimum mean squared error of leave-one-out cross-validation (Viscarra Rossel, 2007). The cross-validation performance of PLSR models was evaluated in terms of coefficient of determination ($R^2$) (Equation 1), root mean squared error (RMSE) (Equation 2), residual prediction deviation (RPD) (Equation 3) and Akaike Information Criterion (AIC) (Equation 4). The RPD criteria suggested by Nicolaï *et al.* (2007) was used to classify models as excellent (RPD>3.0), good (2.5<RPD<3.0), suitable for coarse quantitative estimation (2.0<RPD<2.5), capable of discriminating their low and high values (1.5<RPD<2.0) and poor (RPD<1.5). The minimum AIC criteria (Akaike, 1973) was used to identify the best model from those developed using different pre-processing techniques. Several preliminary analyses noted better performance of PLSR models when wavelengths in 1100-2450 nm range were used (Schulz *et al.*, 1998) instead of entire spectral range of the instrument. Thus, the data modelling involved in this study was performed using spectral reflectance in 1100-2450 nm wavelength range.

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2}{\sum_{i=1}^{n}(Y_i - \bar{Y})^2} \quad (1)$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2} \quad (2)$$

$$RPD = \frac{\sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(Y_i - \bar{Y})^2}}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2}} \quad (3)$$

$$AIC = n \times \ln(RMSE) + 2 \times LV \quad (4)$$

Where, $Y$, $\hat{Y}$ and $\bar{Y}$ represents observed, predicted and average value of quality attribute, respectively and $n$ indicates the sample size.

## Results and discussion

**Descriptive statistics of quality attributes of tender jackfruit**: To ensure high variability in the database, tender jackfruit samples (about 50-70 days of maturity) were collected from different geographical locations irrespective of their variety (soft or hard) and other physical attributes. The length, diameter, geometric mean diameter, and sphericity of samples vary in the range 11.40-27.60 cm, 4.93-11.87 cm, 8.36-15.32 cm, 0.33-0.80 (unit less), respectively. The descriptive statistics of chemical and textural attributes of tender jackfruit examined in the study are given in Table 1. The pH value represents low acidic nature of tender jackfruit while titrable acidity represent an estimate of its citric acid content. The total soluble solid content being a proxy of sugar content, its low values noted for tender jackfruit samples in this study against that of mature jackfruit (19.03-32.53 °Brix) reported by Shamsudin *et al.* (2009) may be ascribed to non-conversion of starch to sugars. Both firmness and toughness appeared to be higher in the skin portion followed by core and tendril. Among these attributes, pH and titrable acidity has low (3.79 %) and high (42.55 %) values of coefficient of variability. The variability of attribute values observed in this study was similar to that reported for NIRS analysis of fruits and vegetables (De Oliveira *et al.*, 2014; Maniwara *et al.*, 2014).

Table 1. Descriptive statistics of quality attributes of tender jackfruit samples

| Attribute | Range | Mean | CV[†] |
|---|---|---|---|
| pH | 5.13 - 6.37 | 5.79 | 3.79 |
| Total soluble solids, °Brix | 3.70 - 8.00 | 5.06 | 16.84 |
| Titrable acidity, % | 0.13 - 0.51 | 0.22 | 42.55 |
| Firmness (core), N | 5.52 - 12.41 | 8.25 | 18.86 |
| Firmness (tendril), N | 1.69 - 8.33 | 4.30 | 35.72 |
| Firmness (skin), N | 8.35 - 15.15 | 10.75 | 13.73 |
| Toughness (core), N.s | 16.67 - 36.25 | 25.51 | 19.66 |
| Toughness (tendril), N.s | 3.87 - 20.69 | 10.42 | 42.24 |
| Toughness (skin), N.s | 22.17 - 42.06 | 31.36 | 12.72 |

[†]Coefficient of variation in percentage

**Spectral characteristics of tender jackfruit**: Fig. 1 depicts the mean spectrum of fresh tender jackfruit samples examined in this study. Typically, a spectrum in Vis-NIR-SWIR is broad due to overlapping of complex absorption patterns allied with the overtones and combinations of spectrally active functional groups. This is evident in case of Vis-NIR-SWIR spectrum of fresh tender jackfruit. It consists of broad and distinct characteristic absorptions around 970, 1200, 1450 and 1930 nm. The absorption around 970 nm may be associated with second overtone of water while that around 1200 nm may cause due to C-H stretching vibration (Fu and Ying, 2016) related to cellulose. The spectral characteristics around 1400-1450 nm band may be linked with the first overtone of water and may also be related to sucrose (Cen and He, 2007). The broad absorption around 1930 may be indicative of combination mode related to water (Fu and Ying, 2016). Apart from these features, a small absorption around 1790 nm was also noted which may be attributed to fructose content of tender jackfruit.

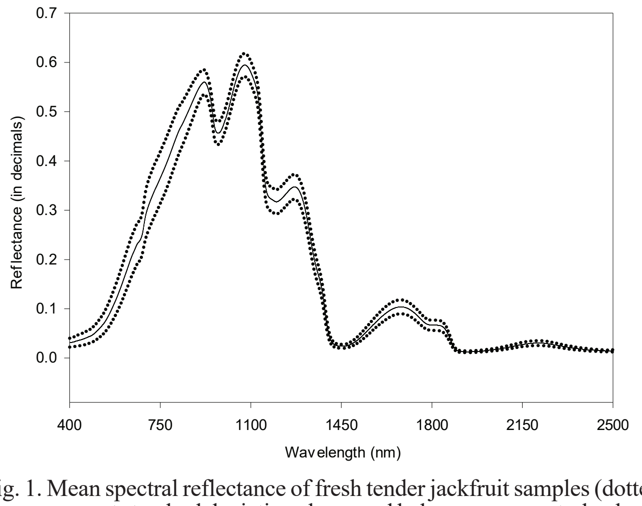


Fig. 1. Mean spectral reflectance of fresh tender jackfruit samples (dotted lines represent standard deviation above and below mean spectral values)

**Data modeling**: Initially, PLSR models linking quality attribute and spectra subjected to different spectral preprocessing were developed. The $R^2$ and RPD of cross-validation of quality attributes varied in the range 0.07-0.67 and 1.05-1.75 (pH), 0.39-0.77 and 1.29-2.12 (total soluble solids), 0.53-0.93 and 1.47-3.78 (titrable acidity), 0.01-0.64 and 1.02-1.68 (firmness-core), 0.25-0.85 and 1.16-2.61 Firmness (tendril), 0.17-0.69 and 1.10-1.82 (firmness-skin), 0.07-0.63 and 1.05-1.65 (toughness-core), 0.28-0.74 and 1.19-1.99 (toughness-tendril), 0.11-0.71 and 1.07-1.88 (toughness-skin) across different spectral preprocessing methods. Among them, the selection of best spectral treatment and the associated PLSR model was based on AIC criteria. The main reason for its use for model selection rely on its ability to account for the information loss of a statistical model by considering its accuracy and complexity together. A statistical model may be treated as good if it has minimum information loss and hence low AIC value. On the contrary, high AIC values represents poor statistical models. Hence, we implemented minimum AIC criterion to identify the best PLSR model for each quality attribute of tender jackfruit. Fig. 2 depicts the AIC values in the cross-validation of PLSR models based on different spectral preprocessing noted in case of toughness (tendril) shown as an illustrative example. Based on minimum AIC criterion, PLSR model based on *SD* of reflectance was found to be the best among

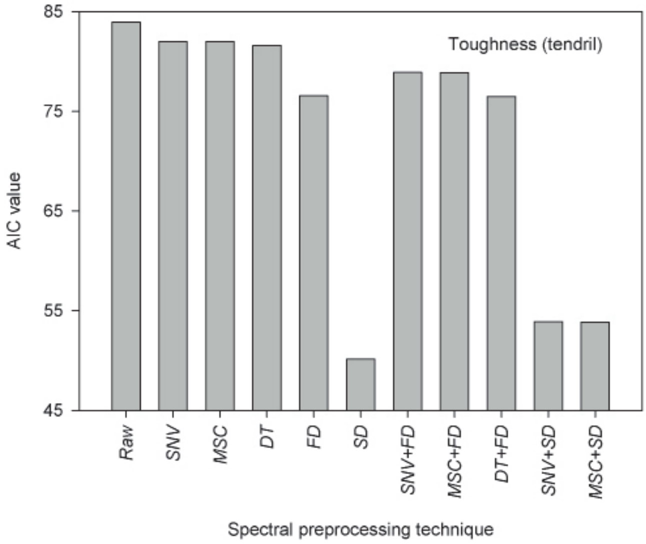


Fig. 2. Akaike Information Criteria (AIC) of cross validation of toughness (tendril) *Raw*: reflectance, *SNV*: standard normal variate, *MSC*: multiplicative scatter correction, *DT*: detrending, *FD*: first derivative, *SD*: second derivative.

others for estimating toughness (tendril) of tender jackfruit. Similarly, the best PLSR models of other quality attributes were also identified. The *SNV+SD* of reflectance appeared to be the best preprocessing technique for pH and toughness (skin), while *SNV+SD* yielded better result in case of titrable acidity. For all the remaining attributes examined, preprocessing of spectral reflectance by *SD* yielded best performing PLSR models. The

Table 2. Regression statistics of cross-validation of quality attributes of tender jackfruit samples using best spectral pre-processing technique

| Attribute | Preprocess | *LV* | $R^2$ | RMSE | RPD |
|---|---|---|---|---|---|
| pH | SNV+SD | 2 | 0.67 | 0.13 | 1.75 |
| Total soluble solids | SD | 2 | 0.77 | 0.40 | 2.12 |
| Titrable acidity | SNV+FD | 5 | 0.94 | 0.02 | 3.96 |
| Firmness (core) | SD | 2 | 0.64 | 0.93 | 1.68 |
| Firmness (tendril) | SD | 3 | 0.85 | 0.59 | 2.61 |
| Firmness (skin) | SD | 2 | 0.69 | 0.81 | 1.82 |
| Toughness (core) | SD | 2 | 0.63 | 3.04 | 1.65 |
| Toughness (tendril) | SD | 2 | 0.74 | 2.22 | 1.99 |
| Toughness (skin) | SNV+SD | 2 | 0.71 | 2.13 | 1.88 |

*LV*: number of latent variables, $R^2$: coefficient of determination, RMSE: root mean squared error, RPD: residual prediction deviation, SNV: standard normal variate, MSC: multiplicative scatter correction, FD: first derivative, SD: second derivative, the sign '+' indicates pairwise combination of preprocessing techniques

regression statistics of cross-validation of best performing PLSR models of different quality attributes of tender jackfruit are given in Table 2.

Based on the accuracy criteria recommended by Nicolaï *et al.* (2007), excellent (RPD>3.0) performance was noted for best PLSR model of titrable acidity. The performance of best PLSR model of firmness-tendril was found to be good (2.5<RPD<3.0), while an accuracy suitable for coarse quantitative estimation (2.0<RPD<2.5) was noted in case of total soluble solids. The best PLSR models of all other attributes were found to be capable of discriminating their low and high values (1.5<RPD<2.0) and hence appropriate for screening purpose. As limited literature is available on NIRS analysis of tender jackfruit, the performance of PLSR models obtained in this study were compared with that of other fruits and vegetables subject to the variability in spectral measurements (instrument, wavelength range), sample type and its representation (intact, chopped, homogenized). The regression statistics noted for best PLSR models of this study were similar or even better than that reported in the literature for pH (Shao *et al.*, 2011), total soluble solids (Xu *et al.*, 2012), titrable acidity (De Oliveira *et al.*, 2014; Maniwara *et al.*, 2014) and texture (Kjølstad *et al.*, 1990; Lu, 2001).

Fig. 3 depicts the regression coefficient (grey colored bars) values of quality attributes of tender jackfruit. The spectral features roughly in 2200-2450 nm range appeared to be more significant (based on absolute magnitude of regression coefficient) in the estimation of all quality attributes of tender jackfruit examined in this study. The spectral features in this region may be linked to characteristic absorptions due to $CH_3$ combination, C-H stretching & C-H bending modes (around 2260 nm), second overtone of O-H bending mode (around 2364 nm) and combination of C-H stretching & C-C stretching vibrations (around 2430 nm) associated with cellulose (Cen and He, 2007; Xu *et al.*, 2013; Guimarães *et al.*, 2014). The other significant wavelength band which was almost consistent across different attributes occur roughly around 1800 nm which may be related to the first overtone of C-H stretching (Fu and Ying, 2016) of cellulose. The spectral

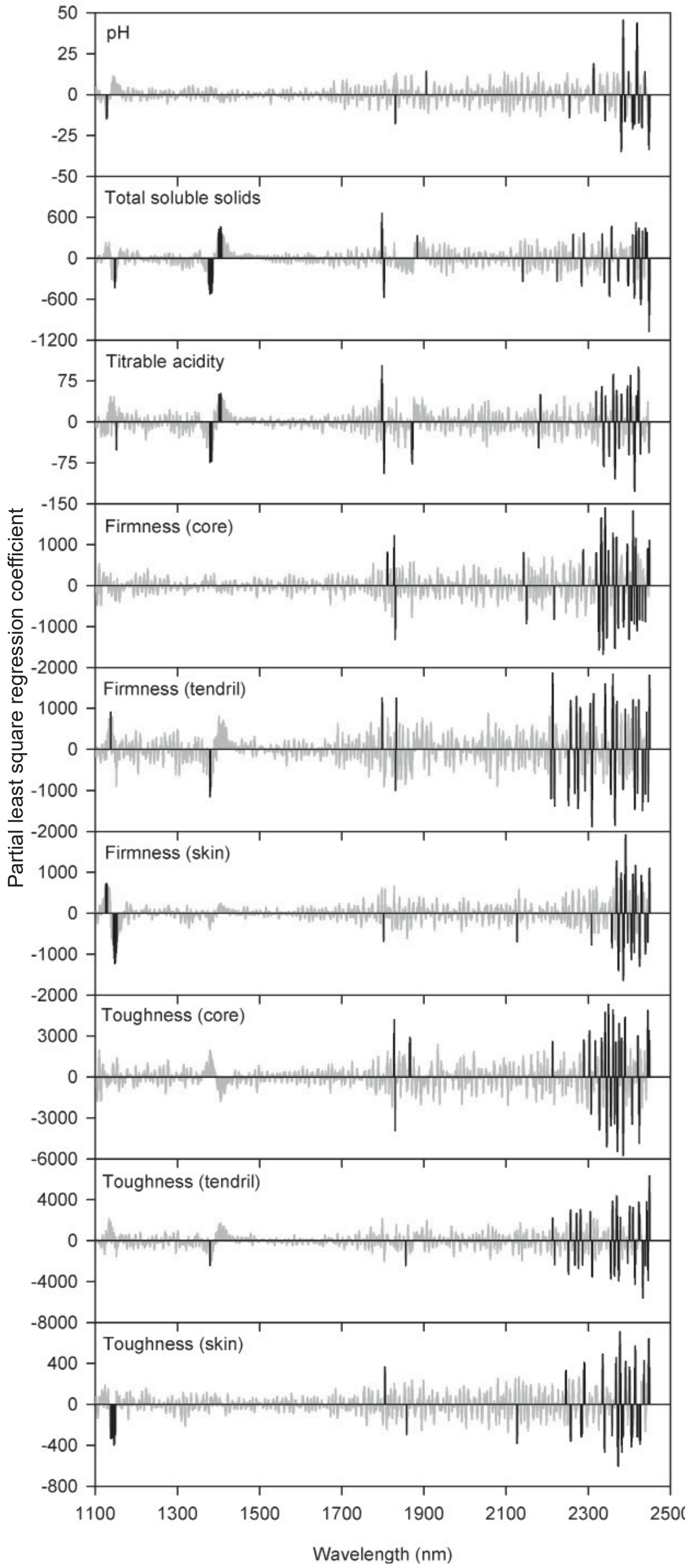


Fig. 3. Partial least square regression coefficient values of quality attributes of tender jackfruit. Most prominent wavelengths are represented as black colored bars.

features due to first overtone of O-H stretching (Guimarães *et al.*, 2014) around 1400 nm appeared to have significant contribution in the estimation of total soluble solids, firmness and toughness of tendril. The significant wavelengths around 1150 nm noted in case of all chemical attributes and texture attributes of tendril may be linked to the second overtone of C-H stretching (Fu and Ying, 2016).

The present study is the first attempt to use NIRS in conjunction with PLSR for quality evaluation of tender jackfruit. Among different attributes examined, best performance was noted for tritrable acidity followed by firmness (tendril). The performance of PLSR models was found to be primarily influenced by the overtones and combinations of C-H functional group which may be related to cellulose composition. The overall result of the study endorses NIRS as a rapid, non-destructive, non-invasive and reliable approach to estimate multiple quality attributes of tender jackfruit.

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