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Near-infrared spectrometry for rapid and real-time prediction of specific quality attributes in intact cactus pear fruits *(Opuntia ficus-indica L.)*

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Cactus pear fruits are rich sources of nutritional (essential vitamins, amino acids and minerals) and antioxidant compounds (flavonoids, carotenes, betalains, ascorbic acid and quercetin). The fruit is cultivated for fresh markets and also serves as nutraceutical and functional food, finding application in various forms such as juice, jam, wine, syrup and in dairy products. However, short postharvest life and negative perception has contributed to its underutilization in the local context. Total titratable acidity (TTA) and total soluble solids (TSS) are among the desirable attributes used to assess postharvest quality of Cactus pears. A portable near-infrared spectrometer (NIRS) can non-destructively determine the internal quality of Cactus pears' thus reducing postharvest losses. This study evaluated the potential of a handheld NIRS coupled with chemometrics of partial least square regression (PLSR) for rapid, non-destructive, and simultaneous determination of TTA and TSS in intact Cactus pear fruits. Cactus pears at different stages of maturity were sampled from Laikipia county, in Kenya, and immediately subjected to spectral data acquisition and wet-chemistry analyses. The PLSR was used to train and validate predictive models for the determination of TTA and TSS content in intact Cactus pears. The prediction model for TTA gave an R-squared (R^2) of 0.73, root mean squared error of prediction (RMSEP) of 0.28% citric acid, and residual predictive deviation (RPD) of 1.97. Additionally, the TSS model resulted in R2 of 0.75, RMSEP of 1.60° Brix, and RPD of 2.06. Overall, these findings highlight the effectiveness of NIRS in non-destructive measurement of TTA and TSS levels in whole Cactus pears. However, with further refinement and optimization of these models, the full potential of this technique for swift and precise assessment of these parameters in whole Cactus pears can be realized. This would greatly benefit farmers and processors by reducing expenses associated with quality assessment and facilitating market entry of Cactus pear derived food products.

KEYWORDS

chemometrics, total titratable acidity (TTA), total soluble solid (TSS), fruit maturity, non-destructive evaluation

1 Introduction

The cactus pear (*Opuntia ficus-indica* L.) plant, belongs to the Cactaceae family, and is known for its succulent and spiny cladodes and its adaptability to arid and semi-arid regions (Al-Naqeb et al., 2021; Ramírez-Rodríguez et al., 2020; Sipango et al., 2022). The fruit is found across several regions including Asia, Europe, Australia, Africa, the Middle East, North America, and South America (Feugang et al., 2006). In Mexico, cactus pear constitutes one of the most valuable natural resources, being a source of delicious and nutrient-rich fruits and vegetables for human consumption (Vigueras and Portillo, 2018). The berry-like fruit is characterized a fleshy pulp and a thick skin, with an average fruit weight of 100-200 g and varying considerably in terms of color (purple to orange), size, and flavor (Yahia and Sáenz, 2011). The cactus pear fruit is a source of nutritionally important vitamins (vitamin C, E, K, and beta-carotenes), carbohydrates and proteins, although it has low caloric content compared to other fruits (Ramírez-Rodríguez et al., 2020). The fruit is a also a rich source of antioxidants (carotenes, flavonoids, betalains, ascorbic acid and quercetin) essential amino acids (arginine, tyrosine, and glutamic acid) and minerals (magnesium, calcium, and potassium) and fiber in the form of pectin (Van Uytvanck et al., 2014; Cota-Sánchez, 2015; Feugang et al., 2006; El-Mostafa et al., 2014; Hailu, 2020; Guevara-Figueroa et al., 2010; Mutwa et al., 2015; Daniloski et al., 2022). The fruit pulp is also characterized by a high level of reducing sugars (12 to 17%), low level of titratable acidity (Cota-Sánchez, 2015), pigments (Felker et al., 2008; Butera et al., 2002), and mucilage (Sepúlveda et al., 2007). However, the fruit is very perishable with a life span of about two weeks depending on the ecotype (Cota-Sánchez, 2015; Amaya-Cruz et al., 2019). The Cactus pear fruit is consumed fresh and also exported to the European markets (Ramírez-Rodríguez et al., 2020). Multiple uses of Cactus pear fruits have resulted in the domestication of the plant in Mexico (Vigueras and Portillo, 2018). The Cactus pear fruit is cultivated for the fresh market but also serves as nutraceuticals and functional food, with applications in various forms such as juices, syrup, dairy products ingredients and as jam. However, short postharvest life and negative perception especially due to the presence of spines has contributed to the underutilization in the local context.

In Kenya and other African countries, despite their nutritional potential, Cactus pear fruit remains underutilized (Aregahegn et al., 2013). Local communities often perceive the Cactus pear plant as a problematic weed due to its aggressive invasion of agricultural lands, posing threats to both the land, domestic animals, and native vegetation (Bakewell-stone, 2023; Van Uytvanck et al., 2014). This perception has led to efforts to eradicate the plant from farms, contributing to the fruit's underutilization. Limited knowledge of the fruit's nutritional potential, coupled with the lack of processing facilities, further diminishes the potential utilization of the Cactus pear fruits (Sipango et al., 2022; Hailu, 2020). However, efforts have been made to promote their utilization through research and publication of articles highlighting their nutritional, nutraceutical, and functional properties. Consequently, Cactus pear fruits have been partially incorporated into African cuisine and processed into various products such as juices, jams, concentrates, marmalades, oil, and cosmetic products.

The organoleptic quality of fruits is normally determined through parameters such as total titratable acidity (TTA), total soluble solids (TSS), and other attributes (Chen and Opara, 2013). The TTA is an important element of fruit quality assessment as it greatly influences the overall sensory perception of the fruits (Velardo-Micharet et al., 2021). TTA is determined by exhaustive titration of intrinsic acids with a standard base to endpoint and then expressing the acidity in terms of the predominant organic acid present in the sample such as malic, citric, and tartaric acids and is (Zhang et al., 2023). Due to its evolution during the maturation and ripening of fruits, TTA is normally used to indicate the harvesting time for fruits (Velardo-Micharet et al., 2021). The TSS content, representing the total dissolved content in fruits, is an indicator of the maturity, sweetness, and overall quality of fruits (Magwaza and Opara, 2015). It is usually determined by a refractometer and expressed as a percentage or degree brix (%/°Brix). The TTA and TSS provide valuable information about the quality of fruits and are normally used when sorting and grading Cactus pear fruits (Mutwa et al., 2015). However, the methods for determining these parameters are destructive, time-consuming, require specialized equipment and personnel, and are sometimes impractical in certain contexts (Ncama et al., 2017; Amuah et al., 2019). Therefore, it is necessary to find a non-invasive technique for determining the quality of Cactus pear fruits that are non-destructive and provide real-time and accurate information on-site.

Near-infrared spectroscopy (NIRS) is an emerging and powerful technology for probing the composition of organic matrices like biological samples (Magwaza and Opara, 2015). It has gained significant recognition as a non-invasive tool of choice in various fields (Ozaki et al., 2018). It relies on the fact that organic molecules in the sample absorb near-infrared radiation at specific wavelengths. The absorbed radiation is linked to specific chemical bonds within the sample matrix and by analyzing the absorption pattern, the chemical composition and properties of a sample can be obtained (Beć et al., 2021). The NIR spectral region typically extends from approximately 800-2500 nm and is associated with overtones and combination bands related to hydrogen-bonded molecules (O-H, C-H, and N-H) (Amuah et al., 2019; Hasanzadeh et al., 2022). The primary advantages of NIRS are; green, non-polluting, wide applicability, rapid, requires little or no sample preparation, and its ability to simultaneously determine several parameters with just a single scan (Li et al., 2019).

Recent advancements in NIR spectroscopy have led to the emergence of miniaturized NIRS systems which offer additional speed, convenience, cost-effectiveness, simplicity, and sensitivity (Beć et al., 2021). This advancement in NIR spectroscopy has seen an increasing literature on the use of smartphone or tablet-connected miniature spectroscopy for rapid assessment of quality indices of several agricultural produce (Amuah et al., 2019; Munawar et al., 2021; Shen et al., 2022; Wang et al., 2022b). Additionally, the accuracy of portable NIR spectroscopy is comparable to that of benchtop instruments (Kartakoullis et al., 2019; Savoia et al., 2021; Yegon et al., 2023). Therefore, this study aimed to evaluate the potential of portable NIRS coupled with multivariate analysis for rapid, accurate, and simultaneous determination of total titratable acidity and total soluble solids in intact Cactus pear fruits.

2 Materials and methods

2.1 Sample collection

Cactus pear fruit samples were collected from the Il Ngwesi I-Mayianat Community Ranch at Makurian in Laikipia County, Kenya. Laikipia is one of the counties in Kenya known for fast-growing and highly invasive cactus plants (Mutwa et al., 2015). To capture variation in fruit' properties, three stages of ripeness were considered for sampling; mature green, pre-ripe, and ripe fruits. Figure 1 shows different stages of Cactus pears collected for this study. Samples then were transported to Jomo Kenyatta University of Agriculture and Technology (JKUAT), postharvest laboratory, and immediately subjected to spectral data acquisition and wet-chemistry analyses.

2.2 Spectral data acquisition

This study used a miniature NIR spectrometer model (NIR-S-G1, Tellspec, Toronto, Canada) to acquire spectral data. The instrument is incredibly small and lightweight, measuring only 77g, 75 mm in length, 58 mm in width, and 26 mm in height. It uses a digital light processing (DLP) technique to filter specific wavelengths and InGaAs detector for transforming light into signal (Crocombe, 2018). This spectrometer operates in a wavelength range of 900-1700 nm, with 256 continuous wavelengths and a resolution of 3.51 nm.

A dedicated spectral collection and management mobile application was installed on a smartphone, according to the manufacturer's instructions. The connection between the smartphone and the spectrometer was achieved through Bluetooth. The pre-installed application was used to command the sensor, manage and export acquired spectra to analytical software for multivariate analysis. Before spectral acquisition, dried sodium chloride salt (oven-dried at 105°C for 4 hours) was scanned to obtain reference value for determining the actual reflective measurement of the sample.

Before spectral data acquisition, dried sodium chloride salt was scanned to obtain reference values for determining the sample reflectance values

Spectral data were acquired by placing the Cactus pear on top of a scanning window before commanding the spectrometer to scan the sample (as shown in Figure 2). Three spectra were collected from each fruit along the equatorial line while rotating it at 120°. An average spectrum was then computed for each sample and raw intensity values were converted into absorbance values ($A = \log \frac{I_0}{I}$), where I_0 is the raw intensity of reference and I is the raw intensity of sample.

The resulting data were transferred to the Unscrambler X software (Version 10.4) and OriginPro for pre-processing and multivariate analysis.

2.3 Reference measurements

2.3.1 Total titratable acidity and total soluble solids

Reference measurements are precisely taken values for a parameter and are used together with spectral data to train predictive models. In this study, the TTA and TSS for 262 Cactus pear fruit samples were determined according to (Mutwa et al., 2015) with little modification. A Cactus pear was horizontally cut into two halves and the pulp squeezed out. Approximately 2 g of the pulp was weighed (weighing scale model no: AEG-220, Shimadzu Corporation, Japan) and diluted with 50 ml of distilled water. From the solution, 10 ml were measured into a 250 ml conical flask, and added 2-3 drops of Thymol blue indicator. The solution was then titrated against 0.1N NaOH until a permanent blue color persisted. The volume of the titer was recorded and used for calculating the amount of TTA in Cactus pears. The concentration of TTA was then expressed as a percentage of citric acid. The concentration of TTA was calculated according to Equation 1 below.

$$\%\ TTA = \frac{Titre \times Conversion\ factor \times Dilution\ factor}{Weight\ of\ the\ sample} \quad (1)$$

FIGURE 1
Cactus pears sampled at different stages of maturity.

FIGURE 2
The setup for spectral data acquisition on Cactus pear fruit samples.

The conversion factor for citric acid is 0.064.

The TSS was measured by squeezing out the juice from the other half of the Cactus pear fruit into the sample holder of a hand refractometer (ATAGO model ATC-1, Tokyo, Japan), and reading taken. The resulting measurements were expressed as °Brix. The TTA and TSS were determined in triplicate for every sample and the average values were used for calibration purposes.

2.4 PLSR model development

2.4.1 Data partitioning

As a norm in PLSR modeling, the dataset was divided into two subsets; the calibration set and the prediction set. The calibration set was used to train the models while the prediction set was used to evaluate the performance of the models. The sorting division method was used to split the dataset. This was adopted since it is simple and ensures that the range in values is well captured in both prediction and calibration sets. This was carried out as follows; the dataset was separated based on the parameter and individually sorted from the lowest to the highest, then the middle in every four samples were picked for the prediction set and the remaining three samples were assigned to the calibration set. The resulting ratio was 3:1, i.e., 196 samples picked for the calibration of models and the remaining 66 samples for evaluating the performance of constructed models.

2.4.2 Spectral data pre-processing

The NIR spectra can be negatively affected by several factors such as surface irregularities (scratches, bruises, or uneven textures), path length variation, and skin thickness, among others (Olmos et al., 2018). To minimize these interferences, pre-processing techniques are applied to raw spectra to remove artifacts, background noise, and interferences caused by these factors. Spectral pre-processing also improves the quality and usefulness of spectral data before modeling (Olmos et al., 2018). Here, linear baseline correction (LBC) was used to pre-process raw spectra and then mean centered (MC). The LBC was used to improve the accuracy of spectral data by removing the underlying trends or baseline drift that is not related to the chemical properties of the sample (Rinnan et al., 2009). The MC was used for offset removal and resolution enhancement (Iacobucci et al., 2016).

2.4.3 Construction and evaluation of models

The PLSR is a typical linear modeling approach for spectroscopic data. It determines components in spectral data that have the greatest correlation with reference data (Berrueta et al., 2007). To be specific, the PLSR approach models both spectral and reference data simultaneously and identifies latent variables in spectral data that best describe the latent variables in reference data. The determination of an optimum number of latent variables or factors is crucial during the training of models (Christensen and Amemiya, 2002). This ensures a balance between capturing the most relevant information contained in the dataset and avoiding overfitting or underfitting the model (Christensen and Amemiya, 2002).

In this study, leave-one-out cross-validation (LOOCV) technique was employed to determine the optimum number of factors. That is, the number of factors corresponding to the lowest prediction error. The PLSR models were constructed using the independent variables (spectral data) and the dependent variables (reference data). The spectral data from the wavelength 950-1650 nm were used for modeling as the remaining variables were considered irrelevant or noisy (Fan et al., 2018). The performances of trained models were then evaluated both internally and externally.

For internal validation, R-squared (R^2) of calibration (Equation 2) and root mean squared error of cross-validation (RMSECV) (Equation 3) were used. For external validation, external sets of data were subjected to the models, and their performance was evaluated based on R-squared (R^2) of prediction (Equation 2), root means square error of prediction (RMSEP) (Equation 4), bias

(Equation 5) and residual predictive deviation (RPD) (Equation 6) (Amuah et al., 2019; Wang et al., 2022a).

$$R^2 = 1 - \frac{\sum (y_{cal} - y_{act})^2}{\sum (y_{cal} - y_{mean})^2}, \quad (2)$$

$$RMSECV = \sqrt{\frac{\sum (y_{cal} - y_{act})^2}{n}}, \quad (3)$$

$$RMSEP = \sqrt{\frac{\sum (y_{pred} - y_{cal})^2}{n}}, \quad (4)$$

$$Bias = \frac{1}{n} \sqrt{\sum (y_{pred} - y_{act})^2}, \quad (5)$$

$$RPD = \frac{SD}{RMSEP}, \quad (6)$$

where n is the total number of samples, y_{cal} is the predicted values, y_{act} is the reference value from wet chemistry, y_{mean} is the mean of predicted values, and y_{pred} is the predicted value of the fruit parameter, SD is the standard deviation of reference data.

3 Results and discussion

3.1 Reference measurements; TTA and TSS

The TTA and TSS results are shown in Table 1. The TTA ranged from 0.21-3.70% citric acid with an average value of 1.39% citric acid. These results indicate that the pulp of a Cactus pear is moderately acidic. However, the mean of TTA expressed as % citric acid reported in this study was slightly above 0.32% citric acid reported by Mutwa et al. (2015) and outside the range of 0.72-0.83% citric acid reported by Roghelia and Panchal (2016). The possible reason for this discrepancy is that samples belonging to three different maturity stages were collected (i.e., mature green, pre-ripe, and ripe) and analyzed in this study. Varietal differences and the geographical location of Cactus pear fruit might have also contributed to the observed differences (Shewfelt, 1990).

The TSS ranged from 0.3-10.9°Brix with a mean of 5.4°Brix. However, the range of TSS reported by this study was below 11.25-13.50° Brix and 11.6-13.7°Brix reported by El-Samahy et al. (2006) and Mokoboki et al. (2009), respectively. The mean of TSS in this study was low by almost half the mean reported by Mutwa et al. (2015) (10.13° Brix) for *Opuntia monacantha* variety. The TSS results for this study slightly varied from those in the literature and the main reason for this variation was the different maturity stages samples analyzed by this study.

3.2 Cactus pear fruits' NIR spectra

Figures 3, 4 show raw spectra for Cactus pear fruits. In Figure 3, spectral variation for green, pre-ripe, and ripe samples was consistent from 950 to 1400 nm. Beyond 1450 nm, the mean

TABLE 1 Summary of reference parameters and PLSR results for prediction of TTA and TSS in Cactus pear fruits.

Parameter	No. of samples	Range Ref	Av. Ref	STD Ref	% CV Ref	R^2C	LV	RMSEC	Range Pred	Av. Pred	STD Pred	R^2P	RMSEP	RPD	%CV Pred	Bias
TTA	262	0.21- 3.70	1.39	0.57	41.01	0.65	7	0.31	0.17-2.08	1.32	0.55	0.73	0.29	1.97	41.67	-0.01
TSS	262	0.3-10.9	5.4	3.30	61.11	0.72	5	1.64	0.10-11.08	5.73	2.74	0.75	1.60	2.06	47.82	-0.09

TTA, Total Titratable Acidity (% citric acid); TSS, (: °Brix) Total Soluble Solids; Av, Average; Ref, Reference values; STD, Standard Deviation; R^2C, R-squared for model calibration; R^2P, R-squared for model prediction; LV, Latent Variables; RMSEC, Root Means Square Error of Calibration; RMSEP, Root Means Square Error of Prediction; RPD, Residual Prediction Deviation.

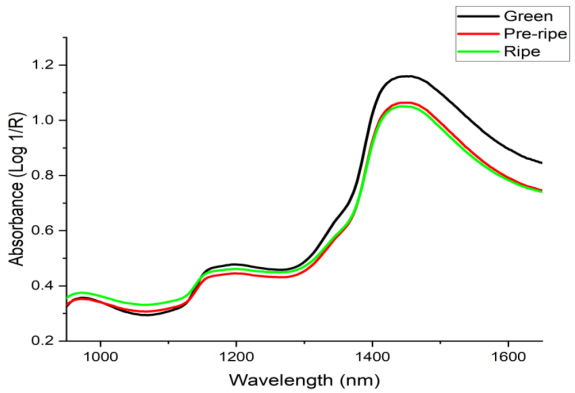

FIGURE 3
Raw spectra for green, pre-ripe, and ripe Cactus pears fruits.

spectrum for green Cactus pears significantly deviated from the other samples. Even though there were differences in the intensities of absorbances, all spectra portrayed similar trends and shapes throughout the entire wavelength. Also, there were three common absorption peaks, one prominent at around 1450 nm and two minor peaks at around 1180 nm and 960 nm. The major band at around 1450 nm is associated with the first overtone O-H stretch in water molecules (Liang et al., 2018; Li et al., 2019). The absorption signal at 1180 nm is likely due to a blend of two stretching vibrations; one is associated with C-H stretching of CH_3 and the other one is the first overtone O-H stretching (Shen et al., 2022). The peak at around 960 nm is associated with the second overtone O-H and C-H (Workman and Weyer, 2007).

Considering the penetration depth of NIR radiation which is up to 3 mm (Huang et al., 2016), the spectral signals acquired were a combination of the contributions from both the skin and the pulp of the fruit. The hydroxyl (O-H) groups represented by the absorption signals at 1445 nm, 1000 nm, and 800 nm for the first, second, and third overtone O-H stretch (Workman and Weyer, 2007) are associated with sugars, organic acids (Amuah et al., 2019), vitamins (Borba et al., 2021), water (Guan et al., 2019) and the cell wall components (cellulose, hemicellulose and pectin) (Fang, 2015). Citric acid belongs to the carboxylic acid functional group. It is characterized by the presence of a carboxyl group which consists of a carbonyl group (C=O) and a hydroxyl (OH) group (Wilhelm and Gardette, 1994). Citric acid is a predominant organic acid in Cactus pear (Mutwa et al., 2015). Water, glucose, sucrose, and cellulose of Cactus pears contain O-H and C-H chemical bonds in their chemical structures. The TSS and TTA are organic molecules that typically contain C-H, O-H, C-O, and C-C bonds in their structure (Amuah et al., 2019) and NIR spectroscopy could be a suitable tool for rapid screening of these parameters in Cactus pears non-invasively.

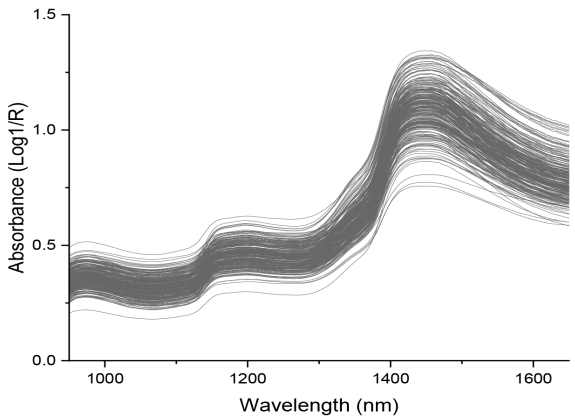

FIGURE 4
Stacked spectra for all sampled Cactus pears in all different stages of maturity.

3.3 Characterization of cactus pear fruits

Principal component analysis (PCA) was used to reduce the complexity of the dataset while retaining as much as possible the variation within the datasets. Figure 5 shows a PCA score plot with clusters of Cactus pears based on the different ripening stages. Three distinct groups corresponding to green, pre-ripe, and ripe stages of Cactus pears are observed. Along the PC1 axis, the green and pre-ripe groups overlap slightly while pre-ripe and ripe clearly separate. The amount of total explained variations were 81% and 15% for PC1 and PC2, respectively. The PC1 explained a substantial amount of variation which relates to the progression of ripening of Cactus pears.

3.4 Quantification models

The performance of the PLSR models trained for predicting TTA and TSS in intact Cactus pear samples are shown in Figure 6. Measured and predicted values are displayed by the x-axis and y-axis, respectively. The blue points represent the training set while the red points correspond to the independent set of data used for the internal validation. Apart from internal validation using LOOCV, model's performance was also assessed using an independent set of samples (prediction set) that was not part of the training set. The prediction set was meant to test the model's performance on new set of samples and evaluate its predictive power. Table 1 provides the statistical results of the models.

The TTA model showed reasonably fair performance as it presented an R^2 of 0.65 and an RMSEC of 0.31% citric acid. This meant that the model was able to explain about 65% of the total variation in TTA content in cactus pears. However, considering a range of 0.21-3.70% citric acid within the samples, an error of ±0.31% citric acid suggests that the model may not be reliable in predicting TTA in Cactus pears. Despite that, the model resulted in improved statistics upon validation with an external set of samples. The model resulted in an R^2 and RMSEP of 0.73 and 0.29% citric acid, respectively.

The TSS model resulted in an R^2 and RMSEC of 0.72 and 1.64° Brix, respectively for the calibration set. Additionally, it also returned an R^2 and RMSEP of 0.75 and 1.60°Brix, respectively for the prediction set. The TTA and TSS models presented better results when subjected to an external set of samples. This proved the models' potential of providing estimates of TTA and TSS content on new cactus pear samples.

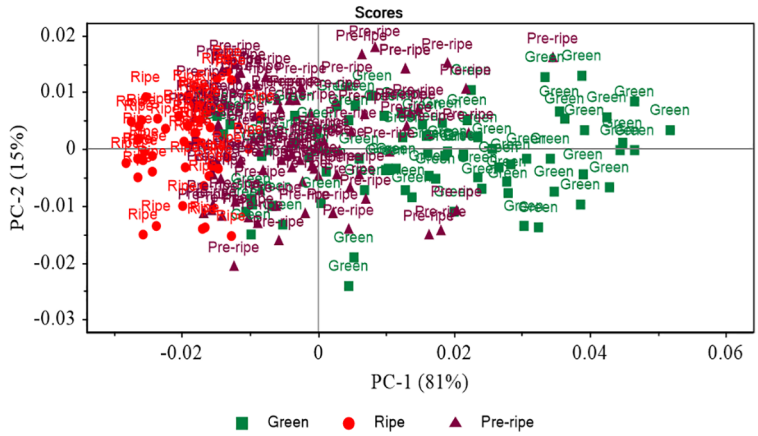

FIGURE 5
A PCA score plot for three ripening stages of Cactus pears.

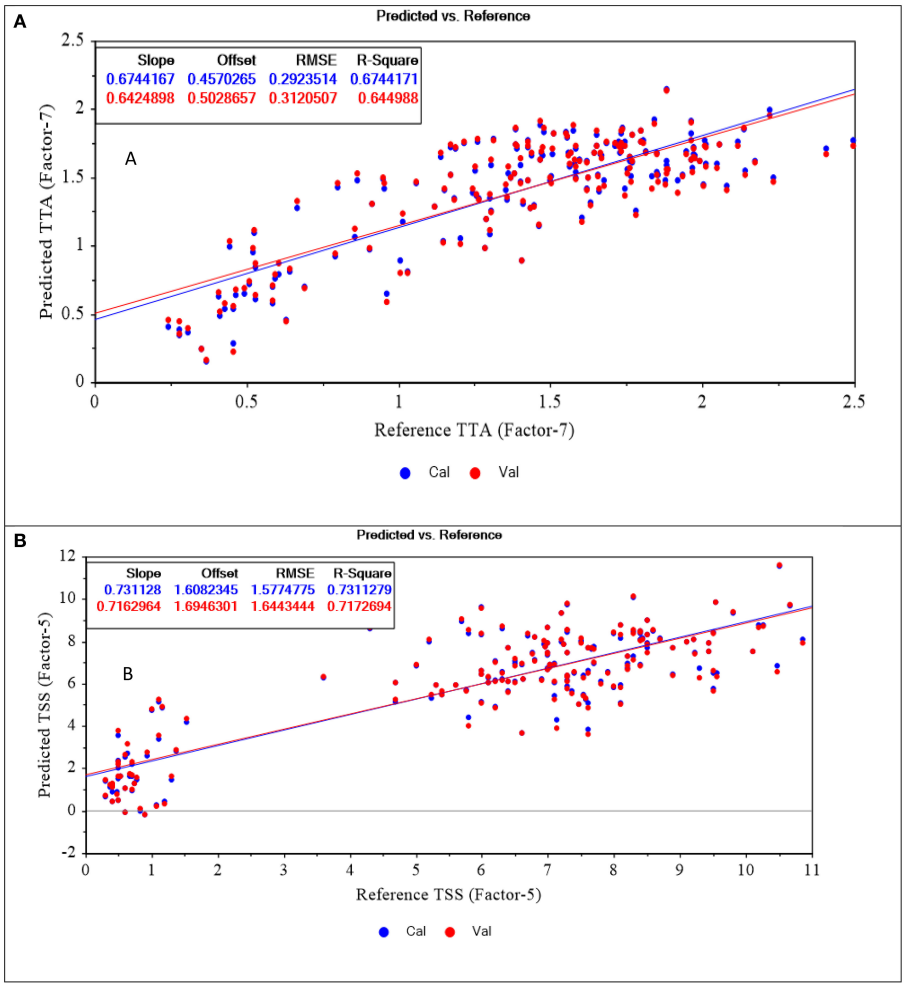

FIGURE 6
PLSR scatter plots for; **(A)** TTA model and **(B)** TSS model.

The mean of predicted TTA (1.32% citric acid) and TSS (5.73° Brix) (Table 1) were so close to the mean of conventionally measured TTA (1.39% citric acid) and TSS (5.4° Brix) (Table 1). This suggested that both PLSR models performed well in explaining the overall patterns of TTA and TSS in Cactus pears and provided an estimate that aligned well with the average values of measured parameters. The standard deviation for predicted TTA and TSS were slightly lower than that of the actual values. This meant that the predicted values were closer to the mean when compared with the reference data. It was a good trend because predicted samples deviated normally from the mean. It also indicated that there were very low chances of predicting samples as outliers since their actual values were close to the mean.

The predicted % CV was smaller than the actual %CV except for TTA. This confirmed that the TSS model was able to accurately predict TSS values in new samples with reduced variability compared to the original data. Since all predicted values were lower than the actual measurements, it resulted in a bias of -0.01 and -0.09 for the TTA and TSS models, respectively. This was a confirmation of the underestimation of predictions made by the models. Another parameter that was used to validate the models was RPD. It is a metric for evaluating the practical usefulness of a PLSR model in a real-world scenario (Bellon-Maurel et al., 2010). This parameter affirmed that the TSS model was more precise in predicting the TSS content in Cactus pears as it presented an RPD of 2.06. According to (Bellon-Maurel et al., 2010), a model with an RPD of above 2.00 is considered excellent and reliable.

In addition to statistical metrics of PLSR models, scatter plots are necessary for the visualization of the relationships between the predictor variable (spectral data) and the response variable (reference data). Scatter plots indicate patterns, clusters, similarities, and differences among the samples. Figure 6 shows the scatter plots for TTA and TSS calibration models. The data points for both predicted and conventionally measured values were distributed along the regression line. This suggested that predicted and actual values were so close and NIR spectroscopy could be used for non-invasive determination of TTA and TSS in intact Cactus pears.

Figures 7, 8 shows factor 1 spectral loading weights for models predicting TTA and TSS in cactus fruits, respectively. Spectral loading weights for a model predicting TTA explained 76% and 22% of variance in spectra data and measured TTA, respectively, while the model predicting TSS was responsible for 55% and 24% variance in spectral data and measured TSS, respectively. These spectral loading weights demonstrates how well the wavelengths were considered by

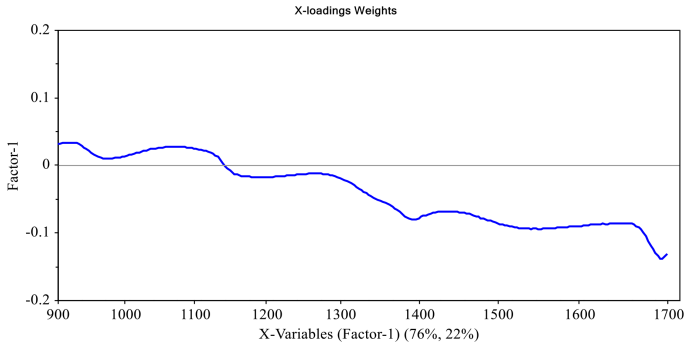

FIGURE 7
Factor 1 X-loadings plot for PLSR model predicting TTA in cactus fruits, showing contribution of wavelengths (900-1700 nm), which explains 76% of variance.

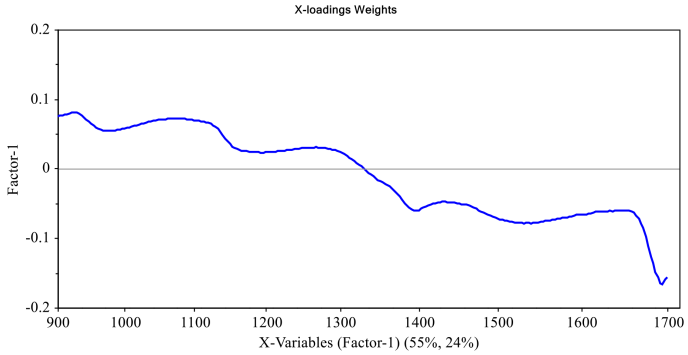

FIGURE 8
Factor 1 X-loadings plot for PLSR model predicting TSS in cactus fruits, showing contribution of wavelengths (900-1700 nm), which explains 55% of variance.

the models. Figures 7, 8 shows several peaks at different wavelengths that were responsible for prediction of TTA and TSS in cactus fruits. Particularly, peaks at around 1050-1110, 1240, 1400, 1450, 1600-1650 nm and 1040-1100, 1270, 1400, 1450, 1550, and 1650 nm were responsible for prediction of TTA and TSS in cactus fruits. These wavelengths contributed significantly to the formation of latent variables responsible for predicting TTA and TSS in cactus fruits, with those from 1400 nm onwards being the most influential. In addition, these wavelengths correspond to the vibrational modes belonging to C-H, O-H, and N-H chemical bonds (Workman and Weyer, 2007; Liu et al., 2015; Amuah et al., 2019) which are normally found in carbohydrates, organic acids and proteins, and contributes to TTA and TSS in cactus fruits (Cota-Sánchez, 2015; Hernández García et al., 2020).

4 Conclusion

This study assessed the feasibility of a portable NIR spectrometer (wl 900 – 1700 nm) for rapid and non-destructive determination of total titratable acidity (TTA) and total soluble solids (TSS) content in cactus fruits. Partial least squares regression (PLSR) algorithm was adopted for training and validating predictive models. While the TTA model achieved an R^2 of 0.73, RMSEP of 0.29% citric acid, and RPD of 1.97, its accuracy in terms of prediction error, was low considering a small range of TTA reported in this study. Conversely, the TSS model performed better with an R^2 of 0.75, RMSEP of 1.60° Brix, and RPD of 2.06. Nonetheless, these results demonstrated the potential of a portable NIR spectrometer for non-invasive and rapid quantification of TTA and TSS content in cactus fruits. Implementation of this technique by farmers or processors would greatly improve quality assessment of cactus fruits, specifically in terms of TTA and TSS. It would also help in reducing expenses associated with quality assessment and promote utilization of cactus fruits by facilitating market entry of cactus derived food products.

Data availability statement

The raw data supporting the conclusions of this article will be made available by the authors, without undue reservation.

Author contributions

WO: Conceptualization, Funding acquisition, Investigation, Project administration, Resources, Supervision, Visualization, Writing – original draft, Writing – review & editing. DL: Conceptualization, Data curation, Formal analysis, Investigation, Writing – original draft. SI: Conceptualization, Methodology, Resources, Supervision, Validation, Writing – original draft. PK: Conceptualization, Investigation, Methodology, Resources, Supervision, Writing – review & editing. WN: Investigation, Methodology, Writing – review & editing. DY: Data curation, Investigation, Methodology, Software, Visualization, Writing – original draft, Writing – review & editing.

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Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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