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Determination of pitaya quality using portable NIR spectroscopy and innovative low-cost electronic nose

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A R T I C L E I N F O

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A B S T R A C T

Pitaya (*Hylocereus polyrhizus*), also known as dragon fruit, is an exotic and highly valued fruit with a high amount of fiber and vitamins, and its quality is often related to attributes such as soluble solids, moisture content, and acidity. Traditional analytical techniques (e.g., gas chromatograph-mass spectrometry – GC–MS) for physicochemical quantification are costly and not environmentally friendly. This work proposes a quick and non-destructive evaluation of pitaya quality using low-cost near-infrared spectroscopy (NIRS) and electronic nose (e-nose) devices. Classification models for either NIR spectra or e-nose data as predictors presented accuracy higher than 90% when classifying samples according to their shelf-life index stage (SLI30, 50, 80, and 100). Total titratable acidity (TA) and pH could be predicted using partial least squares regression (PLSR) and NIR spectra as predictors with coefficients of determination (R^2_P) of 0.89 and 0.83, respectively, and root means square error (RMSEP) of 0.03 and 0.23, respectively. Similarly, PLSR models for the prediction of TA and pH using e-nose data achieved R^2_P of 0.85 and 0.86, and RMSEP of 0.04 and 0.22 respectively. RPD and RER values for NIRS show that all predictors can be used to at least distinguish between low and high values. The results demonstrate that inexpensive devices based on NIRS, and a novel low-cost e-nose could be used in combination for the prediction of TSS, pH, TA, moisture, and phenolics, as well as to classify pitaya according to their shelf-life stages.

Abbreviations and symbols

LV	latent variables
MC	mean centering
PCA	principal component analysis
PLS-R	Partial least squares regression
PLS-DA	Partial least square discriminant analysis
RMSEC	Root mean square error of calibration
RMSECV	Root mean square error of cross-validation
RMSEP	Root mean square error of prediction
RER	ratio error
RPD	ratio of standard deviation
R^2_C	coefficient of determination of calibration
R^2_{CV}	coefficient of determination of cross-validation
R^2_P	coefficient of determination of prediction
S-G	Savitzky–Golay
SNV	standard normal variate
SLI	Shelf-life index
(w)	window size
(o)	polynomial order

1. Introduction

Agriculture stands out in Brazil among food production since the country is one of the largest producers of agricultural products globally, highlighted by tropical fruits (FAO, 2002; Pinto and Jacomino, 2013). Delivering high-quality fruits is a common demand from consumers and has always been a concern in food safety and health (Macieira et al., 2021). Likewise, agriculture 5.0 is imminent in determining a new resolution for consumers and producers in how they perceive food since traditional farming practices have been augmented and modified by automation and implementation of modern scalable technological solutions (Ragazou et al., 2022). This scenario expedites the use of clean and smart technologies, such as smart sensors, to assure good quality

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food for the growing population (van Dijk, Morley, Rau, and Saghai, 2021).

Pitaya, also known as pitahaya or dragon fruit (*Hylocereus polyrhizus*), is a highly valued fruit, which consumption has increased in the Brazilian market, largely due to anthocyanins content, which are molecules that show nutritional properties (i.e., antioxidant), related to the maturity stage of the fruit, post-harvest conditions, ripening, and vitamin C content (Attar et al., 2022). Among the current methods to determine the phytochemicals in pitaya are the chromatographic methods (Vieira et al., 2017), such as gas chromatography-mass spectrometry (CG-MS) and high-performance liquid chromatography (HPLC) (Sanaeifar et al., 2017; Buratti et al., 2011), which are time-consuming and costly as shown in FDA guidelines for the validation of chemical methods (FDA, 2019). Therefore, developing new methods to evaluate the shelf life and target compounds present in these fruits is extremely important.

Near-Infrared Spectroscopy (NIRS) has emerged as a non-destructive analytical technique applied to agricultural products. NIRS is based on the vibration of organic chemical molecules and their interaction with the radiation of the infrared spectrum (Pasquini, 2003), and in combination with chemometrics has shown great potential for the determination of physical and chemical parameters in agricultural products, such as total soluble solids (TSS), total titratable acidity (TA), moisture (Moraes et al., 2022), and phenolic compounds (Tian et al., 2021). Recently, portable NIRS devices have been investigated as a cheaper alternative for the analysis of food and agricultural products, such as star fruit (Moraes et al., 2022), eggs (Cruz-Tirado et al., 2021) and meat (Nolasco-Perez et al., 2019) since the reduction of equipment prices is a demand for producers and traders.

Electronic nose (e-nose) is a device that uses a combination of sensors for volatile compounds to mimic the olfactive cells of mammals. Several types of e-nose equipment have been projected and investigated to identify and classify aromatic compounds related to biological and chemical alteration of food and agricultural products during processing and storage (Pearce, 2002; Sanaeifar et al., 2017). Similar to other analytical technologies processing in the food industry, the search for a low-cost device that can be used online during processing is highly required.

Both e-nose and NIRS analyses have been developed and used to replace or support consolidated techniques in the industry at a lower cost and without the use of chemicals (Moraes et al., 2022; Sanaeifar et al., 2017). NIR spectrometers and e-nose devices may be used independently or to complement each other, since NIR is a vibrational spectroscopic method that may detect major chemical compounds, but has a limit of detection of approximately 0.1% (m/m) (Pasquini, 2003), thus not being suitable for minor compounds, unless they are correlated to the major composition. E-nose, on the other hand, generates less data due to the type of sensors used, but it can detect lower concentrations of volatile compounds (e.g., ppm). These custom analytical techniques have been used to determine physicochemical properties related to several biochemical changes in agricultural products, such as the ripening of fruits (Loutfi et al., 2015). These methods produce a large amount of data that requires multivariate statistical approaches to identify the most relevant information from the large dataset and create prediction and classification models with practical applications (Li et al., 2022; Moraes et al., 2022). When applied to predict chemical information, these approaches are designed as chemometrics.

Chemometrics is used together with NIR and e-nose technology to obtain chemical information related to an enormous volume of data since both equipment do not generate direct information with a chemical value. The use of these mathematical and statistical tools allows the extraction of relevant information through each method, including principal components analysis (PCA) (exploratory analysis), linear discriminant analysis (LDA), partial least squares discriminant analysis (PLS-DA) (classification model), and partial least squares regression (PLSR) (regression model) (Moraes et al., 2022; X. Zhang et al., 2019).

Even though a few authors (Li et al., 2022; Loutfi et al., 2015; Moraes et al., 2022) have elucidated the use of these two sensor-response equipment in single equipment assay, to the best of our knowledge, work with pitaya in combination with NIR and e-nose has not been performed in the literature. Therefore, research on the classification as well as the prediction of physicochemical properties to monitor pitaya's shelf life using NIR and e-nose combined with chemometrics is important to better assist the fruit industry.

In the current work, we propose to use an affordable NIRS and low-cost portable and novel customized e-nose devices (1) to classify pitaya according to proposed shelf-life indexes; (2) to predict properties based on physicochemical attributes, such as TSS, TA, pH, moisture and phenolics. Chemometric tools were used for classification and prediction models using the data acquired by NIRS and e-nose as predictors. Currently, there are no previous reports in the literature testing neither NIR nor e-nose to predict pitaya quality attributes or shelf-life.

2. Materials and methods

2.1. Sample acquisition and preparation

A total of 140 pitayas (red-fleshed variety) were obtained immediately after harvest from a local producer and 30 samples were analyzed for total phenolic compounds, total soluble solids (TSS), pH, titratable acidity (TA), and moisture content. Also, NIR spectra and e-nose data were acquired. The remaining samples were stored at two temperatures (15 °C and 25 °C), and the same analyses were performed after 7, 14, 21, and 25 days of storage.

2.2. Reference analysis

Total phenolics content was performed using the Folin-Ciocalteu method (Swain and Hillis, 1959) with modifications proposed by Ferreira et al. (2019) in the dilution factor of the Folin reagent (1:10). The content of total soluble solids was determined using a manual refractometer model (KASVI. K52–032, São Paulo, Brazil) following AOAC procedure, n^{o}9 32.12 (AOAC, 1980). The pH was determined using a pH meter (model MB-10; Marte, São Paulo, Brazil). Titratable acidity was measured according to Nielsen (2017) using NaOH 0.1 M. Moisture content of the samples was obtained by the gravimetric method after drying 4 g of sample in a vacuum oven at 60 °C until constant weight (AOAC, 2005). A shelf-life index (SLI) proposed by Wu (2014) was used as the ratio between TSS and TA, to identify the sample conditions regardless of the storage temperature. The fruits were then labeled as SLI 30 (day 0), 50 (day 7), 80 (day 14 and 21), and 100 (day 25), respectively.

2.3. NIR spectra acquisition

Spectral information was acquired in the NIR range (900 – 1700 nm) with a 4 nm interval applied in absorbance mode. Spectral measurement was performed directly in the fruit (peel) using a portable NIR device (DLPR NIRscanTM Nano. Texas Instruments, USA) (Fig. 1). Five measurements were taken from different parts of the fruit and averaged as representative spectra of each sample.

2.4. E-nose setup and data acquisition

A low-cost, homemade e-nose device was used in the current study. The e-nose (Fig. 1) is composed of a compartment with sensors for sample holding and a computer for data acquisition. The e-nose has a set of 8 metal oxidative semiconductor (MOS) sensors, with respective codes and sensitiveness: MQ2 (smoke and propane), MQ3 (alcohol), MQ4 (methane (CH4)), MQ6 (propane), MQ8 (inflammable gasses (hydrogen gas)), MQ9 (carbon monoxide (CO) and methane), MQ135 (ammonium (NH4+), toluene (C7H8) and hydrogen) and MQ138

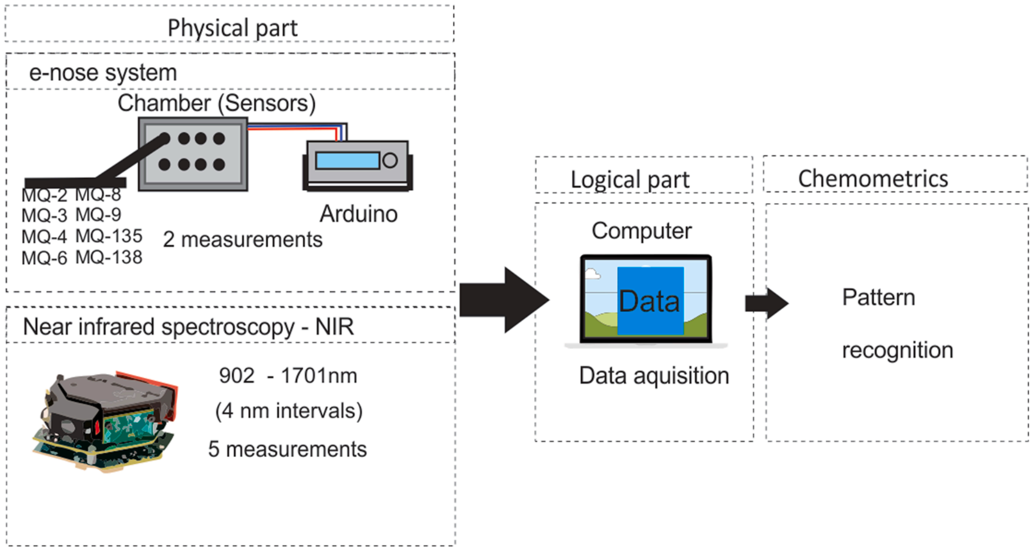

Fig. 1. Near-infrared spectroscopy system and e-nose set up.

(volatile compounds) (Zhengzhou Winsen Electronics Technology, China). The equipment also presents one sensor for temperature and another sensor for humidity measurements.

Each fruit was placed in the sample compartment for 2 min. Fresh air was used to wash the volatiles compounds out of the chamber for 2 min between each analysis so that, the ratio sample-signal/air-signal was obtained.

2.5. *Multivariate analysis*

2.5.1. *Data pre-processing*

Fruits were classified according to the shelf-life stage: SLI 30, 50, 70, and 100 (Table 1). The data used for the classification model (PLS-DA) and prediction model (PLSR) were randomly divided into a subset composed of 70% of samples for calibration and 30% for validation (external test set). NIR spectra were pre-processed using mean center (MC), smoothing Savitzky-Golay algorithm (S-G), with window size (w) of 9 to 13 by polynomial regression order (o) 0 and first (1st) and second (2nd) derivatives using S-G, with window size (w) of 9 to 11. Standard normal variate (SNV) was applied to correct the effects of light scattering (Barnes et al., 1989; Martens and Geladi, 1983). Regarding the e-nose, the voltage matrix data were pre-processed using only autoscaling (AS). For both NIR and e-nose data, Venetian blinds with 10 splits and blind thickness of 1 was used for cross-validation.

2.5.2. *Principal component analysis (PCA)*

Principal component analysis (PCA) is an exploratory analysis that works by projecting the data points onto principal components and simultaneously keeping the most variation as possible. This method was used as an unsupervised screening method for an overview of the variation between samples, and to identify the most important wavelengths for NIR spectra and the importance of each e-nose sensor to fruit variation during shelf life. PCA plots were designed with the complete data range using the singular value decomposition algorithm (SVD) (95% confidence level) for the computation of the eigen generic sequence and a further cluster of the data. To build a PCA plot, outliers (anomalous measuring) were identified and excluded using the amount of Q residuals and Hotelling T^2 plots.

2.5.3. *Linear discriminant analysis (LDA)*

Linear Discriminant Analysis is a method derived from Fisher's linear discriminant analysis and operates by finding linear combinations from sample's features that will further characterize and classify them into different classes. LDA was applied as a supervised classification method using the most important wavelengths identified in the loadings from PCA using MINITAB® (Release 14.12.0). The performance of the classification models was evaluated by sensitivity (Eq. (1)) and specificity (Eq. (2)), accuracy (Eq. (3)), and error rate (Eq. (4)).

$$\text{Sensitivity } (\%) = \frac{TP}{(TP + FN)} \times 100 \tag{1}$$

$$\text{Specificity } (\%) = \frac{TN}{(TN + FP)} \times 100 \tag{2}$$

$$\text{Accuracy } (\%) = \frac{(TP + TN)}{TOTAL} \times 100 \tag{3}$$

Table 1
Physicochemical parameters for pitaya during different shelf-life indexes.

Analyzes	SLI30 (0)		SLI50 (7)		SLI80 (14 and 21)		SLI100 (25)	
	Min - Max	Mean ± SD	Min - Max	Mean ± SD	Min - Max	Mean ± SD	Min - Max	Mean ± SD
TSS	10.10 - 12.95	$11.74^{A} \pm 0.72$	8.95 - 13.20	$11.29^{AB} \pm 1.32$	8.45 - 14.70	$10.97^{B} \pm 1.209$	8.50 - 12.80	$10.54^{B} \pm 1.26$
pH	3.62 - 4.37	$3.96^{D} \pm 0.20$	3.88 - 4.79	$4.44^{C} \pm 0.21$	4.77 - 5.60	$5.10^{B} \pm 0.17$	5.17- 5.57	$5.35^{A} \pm 0.13$
TA	0.24 – 0.47	$0.35^{A} \pm 0.06$	0.15 – 0.32	$0.22^{B} \pm 0.04$	0.20 – 0.82	$0.15^{C} \pm 0.02$	0.09 - 0.14	$0.11^{D} \pm 0.02$
Moisture	78.61 - 89.24	$86.64^{A} \pm 1.43$	84.16 - 92.65	$87.31^{A} \pm 1.78$	78.93 - 90.01	$86.58^{A} \pm 2.23$	84.15 – 90.42	$86.81^{A} \pm 1.56$
Phenolics	0.57 - 0.87	$0.70^{B} \pm 0.08$	0.64 – 0.84	$0.73^{AB} \pm 0.05$	0.59 - 0.87	$0.75^{A} \pm 0.08$	0.49 - 0.71	$0.62^{C} \pm 0.07$
TSS/TA		$33.43^{D} \pm 2.9$		$50.25^{C} \pm 4.54$		$81.73^{B} \pm 4.74$		$104.32^{A} \pm 9.22$

*The data correspond to the mean ± SE of two repetitions. Different letters for the same parameter analyzed indicate significant differences. between the storage days. by ANOVA ($P < 0.05$). (TSS) content of total soluble solids. (TA) titratable acidity. (SLI,30,50, 80 and 100) shelf-life index for pitaya fruit for each day group 0, 7, 14 and 21, 25, respectively.

$$\text{Error rate } (\%) = \frac{(FP + FN)}{TOTAL} \times 100. \tag{4}$$

where, TP = true positive; FN = false negative; TN = true negative; and FP = false positive.

2.5.4. Partial least squares models

Partial least squares discriminant analysis (PLS-DA) is a classification method that allows dimensionality reduction as well as discriminant analysis all at once, which seems to show more flexibility over LDA. The method was used to classify the samples according to their shelf-life stage. The choice of the number of the latent variables (LVs) that should be included in the PLS-DA models was calculated based on the lowest root mean squared error for cross-validation (RMSECV) (Barbin et al., 2013). The performance of the classification models was evaluated by sensitivity (Eq. (1)) and specificity (Eq. (2)), accuracy (Eq. (3)), and error rate (Eq. (4)).

Partial Least-squares Regression (PLSR) is a method used for the quantitative relationship between predictors (X) and response (Y) measured values (i.e., reference analysis). Both NIR spectra (900 – 1700 nm) and e-nose datasets were used as predictors for each characteristic analyzed. The performance of the regression models was assessed by the coefficient of determination (R^2), the number of latent variables (LV), and root mean squared error (RMSE) for calibration (RMSEC), cross-validation (RMSECV), and prediction (RMSEP) (Skibsted et al., 2004), residual predictive deviation (RPD) and the range error ratio (RER) (Barbin et al., 2015), where RPD indicates the model as unusable (RPD < 1.5), able to distinguish between high and low values (1.5 < RPD < 2.0), quantitative prediction (2.0 < RPD < 2.5), an indication of a good prediction (2.5 < RPD <3.0) and excellent prediction (RPD > 3) (Saeys et al., 2005). While RER ≥ 4 means that the model is qualified for screening calibration, RER ≥ 10 the model is acceptable for quality control, and RER ≥ 15 the model is very good for quantification (Rambo et al., 2013).

$$RMSEP = \sqrt{\frac{\sum_{p=1}^{P} \left(y_p - \hat{y}_p\right)^2}{P}} \tag{5}$$

$$RMSECV = \sqrt{\frac{\sum_{i=1}^{I} \left(y_i - \hat{y}_i\right)^2}{I}} \tag{6}$$

$$RPD = \frac{SD}{RMSEP \ ou \ RMSECV} \tag{7}$$

$$RER = \frac{Range}{RMSEP \ ou \ RMSECV} \tag{8}$$

3. Results and discussion

3.1. Reference analysis

Results for physical and chemical analysis of pitaya (Table 1), and Pearson correlation (Table 2) among features, demonstrated that changes in TSS, pH, TA, and phenolic compounds occurred during storage. Moisture did not have significant variation within the tested days ($p < 0.05$). A recent study suggested that TSS content does not change significantly within the maturity stages. On the other hand, TA decreased during maturation (shelf-life) (Freitas and Mitcham 2013). However, it was observed that TSS decreased continuously until the latest stage SLI100 10.54 ± 1.26.

Acidity decreased during storage, and pH values increased, which may explain the spoilage in some fruits after two weeks. This degradation might be linked to the oxidation process that consumes some of the organic acids present in the fruit. As a result, an increase in SLI (TSS/TA) occurred during the period. Previous work reported an abrupt increase in pH after three weeks of storage, although in a different variety of pitaya (Franco et al., 2022). In this work, it was also observed a decrease in total phenolics in the late shelf-life stages, which is following previous studies (Angonese et al., 2021; Franco et al., 2022).

Table 2
Pearson correlation for physicochemical parameters of pitaya.

	TSS	pH	Moisture	Phenolics	TA
TSS	1.00				
pH	−0.39	1.00			
Moisture	−0.46	0.35	1.00		
Phenolics	−0.24	0.49*	0.28	1.00	
TA	0.31	−0.90**	−0.28	−0.38	1.00

* Values in modulus are equal to 0.5,.
** values in modulus are > 0.5.

3.2. Principal components analysis (PCA)

PCA was performed using data from the whole data set for all 8 sensors used in the e-nose. Fig. 2 shows the PCA scores (PC1vs PC2) for NIR spectra and the data obtained by e-nose device.

PC1 and PC2 explain more than 80% of the total variance (Fig. 2a). It is also possible to observe a trend to split samples stored for long periods (SLI 100) on the negative side of PC1, to fresher samples (SLI 50, 70) on the positive side of PC1. The loadings (Fig. 2b) show that the wavelengths 905, 1010, 1130, 1320, 1400, 1480, and 1660 are responsible for the variation in the PC1. The wavelengths at 905, 1010, and 1130 nm are related to hydrogen and oxygen (H—O) (Osborne, 1986), and carbon and hydrogen interaction, second and first vibration of O—H related to aromatic compounds (Magwaza et al., 2012); 1320 and 1400 nm might be related to organic acids (Weyer and Lo, 2006). From those, 1010 and 1400 nm overlap with water which is correlated to the moisture present in the fruit. The peaks at 1480 and 1660 nm are associated with glucose (Osborne, 1986), and some authors have reported this wavelength to be related to lignin, starch, and cellulose (Ertlen et al., 2010). The variations observed during the storage period of the fruit as well as the response for phenolic compounds may be attributed to acid compound degradation, such as ascorbic acid, gallic acid, and malic acid (Cheah et al., 2016). The region responsible for the picks in the spectra at 1000 and 1440 nm could be related to organic acids, which for pitaya is represented by malic acid ($C_4H_6O_5$) since it is the major component in the fruit (Angonese et al., 2021).

For the e-nose system, it is possible to observe that samples from SLI 30 were on the positive side for PC1 scores (Fig. 2c) while SLI 50, 70, and 100 were on the negative side. PC1, PC2, and PC3 together, explained 66.64% of the total variation. It can be seen in Fig. 2c that the e-nose system can differentiate the storage days of pitaya in the aforementioned groups. The loadings for the PCA with e-nose data (Fig. 2d) show the contribution of each sensor to the separation of the fruits. All sensors identified some type of compounds; however, the biggest peaks were presented by sensors MQ138 and MQ3, which are responsible for the volatile compounds present in fruit and alcohols derived molecules, respectively. Some of the compounds previously reported in pitayas include alcohols, 1-hexadecanol, and 2-ethyl-hexanol, aldehydes - octenal and octanal, and ketones – diphenyl-1- (2-furanyl)-ethanone (Attar et al., 2022), related to most of the volatile compounds. While, MQ3 sensitivity to alcohol may explain the sensor's selectivity towards the molecule of malic acid and other organic acids due to its OH group, others, such as MQ8 did not respond considerably well to pitaya, yet it still might be relevant to PCA separation. A reason for that may be linked to hydrogen sulfide (H_2S) in the fruit respiration process in the post-harvest (Hu et al., 2012). Previous work has demonstrated a correlation between the presence of this gas and the delay in senescence of the fruit, which helps to prolong the fruit's shelf-life (Hu et al., 2012). Likewise, carbon monoxide (CO) plays a role in fruit respiration (Young et al., 1962) and are related to food quality (Krupa and Tomala, 2021), therefore MQ9 was an important sensor to monitor this gas level that

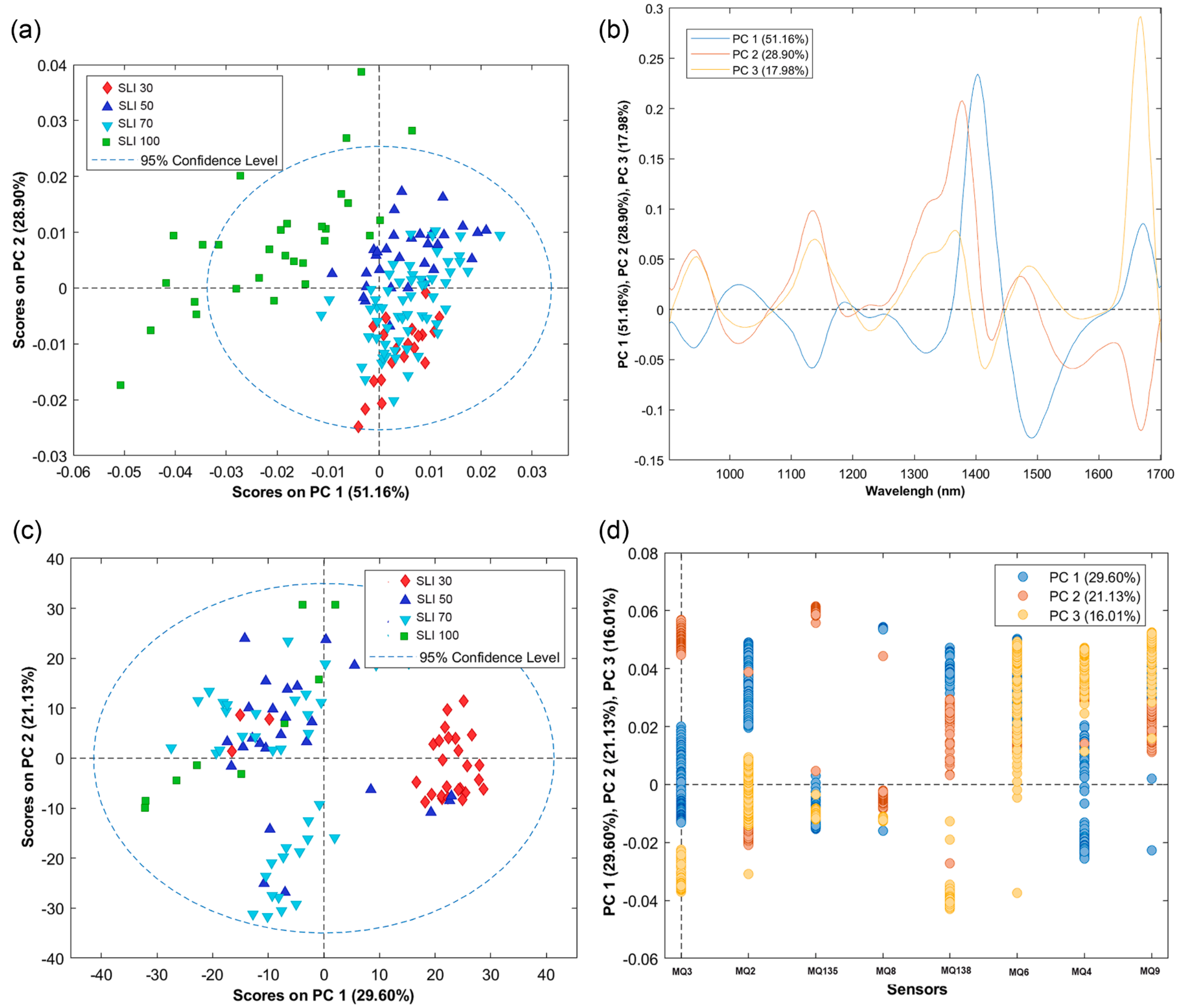

Fig. 2. PCA (a) scores and (b) loadings for NIR spectra absorbance mode; PCA (c) scores and (d) loadings for e-nose data.

increases over time during storage. MQ4 and MQ6 responses for methane and propane might be related to the release of these gasses during storage since they are related to the rotten process in fruit waste (Gunaseelan, 2004). Even though pitaya is classified as non-climacteric fruit, the mechanisms involving ethylene production in fruits are still unknown (Aizat et al., 2013), and perhaps small variations in this hormone levels may be enough to obtain a response in MQ138 and MQ4 sensors.

3.3. Classification model using LDA

LDA classification of pitaya according to SLI using NIR spectra provided good results, using a few selected wavelengths. The wavelengths of 930, 950, 1010, 1020, 1140, 1190, 1320, 1400, 1480, 1660, 1670 nm

Table 3
Confusion matrix for LDA and PLS-DA classification of pitaya using NIR spectra and e-nose data.

Classification method	Equipment		SLI30	SLI50		SLI80	SLI100
LDA	NIR spectrometer	SLI30	25	2		0	0
		SLI50	2	21		3	0
		SLI70	0	1		58	0
		SLI100	0	0		1	27
	e-nose	SLI30	26	3		0	0
		SLI50	2	18		0	0
		SLI70	0	4		37	1
		SLI100	0	0		1	10
PLS-DA	NIR spectrometer	SLI30	10	2	0		0
		SLI50	0	8	5		0
		SLI70	0	1	9		1
		SLI100	0	0	0		7
	e-nose	SLI30	11	0	0		0
		SLI50	0	6	0		0
		SLI70	0	1	8		0
		SLI100	0	0	3		4

were used in the models. Mainly, misclassification of samples observed for neighboring classes (Table 3). FT-NIR in combination with LDA has been successfully used to detect variation in morphological and chemical properties of lemon (Ruggiero et al., 2022), where the major component was attributed to polysaccharide content. This finding could be related to sugar and phenolic compounds since Jamila et al. (2020) also obtained a perfect classification rate using NIR spectroscopy and chemometrics for garcinia fruit.

The LDA results for e-nose showed lower overall accuracy (95%) when compared to portable NIR spectrometer (97%). These results could be related to the transformations of volatile compounds compared to other chemical changes related to water and solid contents since NIR spectra are influenced by vibrational bonds in molecules related to major components such as water content, which may lead to a better classification, whereas the generated volatiles might not be sufficiently sensitive to MOS sensors in e-nose. From that, all classes had misclassified samples, where SLI100 presented the highest accuracy (99%). The SLI50 accuracy (91%) for e-nose was the lowest among classes, similar to the result obtained using NIR spectra (94%). All parameters sensitivity, selectivity, accuracy, and error rate are presented in Table 4.

LDA has been used together with a low-cost electronic nose to classify oranges in different ripening stages, shelf life, and storage time as well as, early stages of contamination (Srivastava and Sadisatp, 2016). Other authors tested multiple e-nose systems for recognition of different odors (i.e., C_7H_8 C_6H_6 NH_3 CO, NO_2 and CH_2O) with LDA and obtained an average accuracy of 70.06% (Zhang et al., 2017). Some of these components are equal to the ones attested in the equipment presented in this work, explaining the high classification rate found for pitaya. This gain in performance may be associated with the equipment robustness, sensor choice, and meticulous data treatment, despite the fact that the device used in this work is a low-cost one.

3.4. Classification model using PLS-DA

The confusion matrix of PLS-DA models for pitaya using NIR spectra is shown in Table 3, while sensitivity, selectivity, accuracy, and error rate are presented in Table 4. The four classes (SLI30, 50, 70, and 100) represent the storage indexes and the numbers on the diagonal of the matrix represent the samples correctly classified according to their respective classes, on the other hand, values that do not fall in that position are misplaced values. The transformations performed in the data were mean center, smoothing S-G order (o) 0, (w) 11 in combination with 1st S-G derivative (o 2, w 9), since they showed the best results. Regarding the best model for PLS-DA using NIR spectra, it showed 95%, 81%, 84%, and 98% for SLI30, 50, 70, and 100, respectively, where the overall accuracy for the prediction model was 90%.

NIR has been used to discriminate nectarine's shelf-life over 21 days using different irrigation strategies. They build models varying from 57 to 84% of accuracy (Pérez-Marín et al., 2011), it should be pointed out that the spectra acquisition was performed using different equipment. A similar approach was performed for kiwi, this time using NIR-HSI used PLS-DA for the classification of ripeness evaluation reached good accuracy, classifying the fruit during ripening with a sensitivity of over 73.3% (Benelli et al., 2021). Therefore, the results found in this work are promising compared to the ones found in the literature, considering the low-cost device that was used.

E-nose results (Table 3) showed better classification performance when compared to NIR. The overall accuracy was > 94% whereas the accuracy for SLI30 and SLI50 were 100 and 97%, respectively. Sensitivity, selectivity, accuracy, and error rate are presented in Table 4. The accuracy of the calibration model for each equipment was similar to those of the prediction model, which attests to the absence of over and underfitting. The data suggest e-nose equipment is suitable for the classification of pitaya in the presented shelf-life indexes with excellent accuracy (>93%), higher than (91.7%) found by Zhang et al. (2019) when discriminating the content of aspergillus carbonarius in grapes based on their volatile compounds. Both NIR and e-nose presented accuracy over (91%). The results found in this research are promising for the classification of fruits according to the shelf-life stages.

3.5. PLSR prediction of physicochemical features

Partial Least Squares Regression (PLSR) was used to model the relationship for each of the analyses (NIR and E-nose) with the physicochemical features TSS, pH, TA, moisture, and total phenolics of pitaya. RMSEC and RMSEP as well as the coefficient of determination (R^2) for both techniques are presented in Fig. 3 and Fig. 4. The spectral region from 900 to 1700 nm was used for the NIR spectra acquisition and various pre-treatments were tested, where mean center, smoothing (o) 0 (w) 9, and SNV presented the best results, while, for e-nose, autoscaling was used for all models.

Regarding the PLSR models using NIR spectra (Table 5), pH and TA presented higher values of R^2 for calibration and prediction models compared to moisture and phenolics. Xu et al. (2019) found good models for TSS in oranges. They used NIR and e-nose in a fusion system to improve the prediction of the total sugar content. In the postharvest of fruits using NIR the prediction of direct correlation (e.g., TSS and water absorption) and secondary ones (e.g., TA and pH), where the latter are predicted indirectly from maturity stages or a compound such as chlorophyll, can be made to the stages of the fruit, as long as, the relationship is robust based on the variation that they may have (e.g., environmental and seasonal). The drawback is to assure the robustness of the correlation between these measured variables and the compound of interest in the fruit or vegetable (i.e., TA with chlorophyll content) to make such

Table 4
Sensitivity, specificity, accuracy, and error rate values for classification of pitaya according to shelf-life index by using NIR spectra and e-nose.

Statistical method	Equipment	Shelf-life index	Sensitivity	Specificity	Accuracy	Error rate
LDA	NIR spectrometer	SLI30	0.93	0.98	0.97	0.02
		SLI50	0.88	0.96	0.94	0.06
		SLI70	0.94	0.99	0.96	0.04
		SLI100	1	0.99	0.99	0.01
	e-nose	SLI30	0.93	0.96	0.95	0.05
		SLI50	0.72	0.97	0.91	0.09
		SLI70	0.97	0.92	0.94	0.06
		SLI100	0.91	0.99	0.98	0.02
PLS-DA	NIR spectrometer	SLI30	1.00	0.94	0.95	0.05
		SLI50	0.73	0.84	0.81	0.19
		SLI70	0.64	0.93	0.84	0.16
		SLI100	0.88	1.00	0.98	0.02
	e-nose	SLI30	1.00	1.00	1.00	0.00
		SLI50	0.86	1.00	0.97	0.03
		SLI70	0.73	0.95	0.88	0.12
		SLI100	1.00	0.90	0.91	0.09

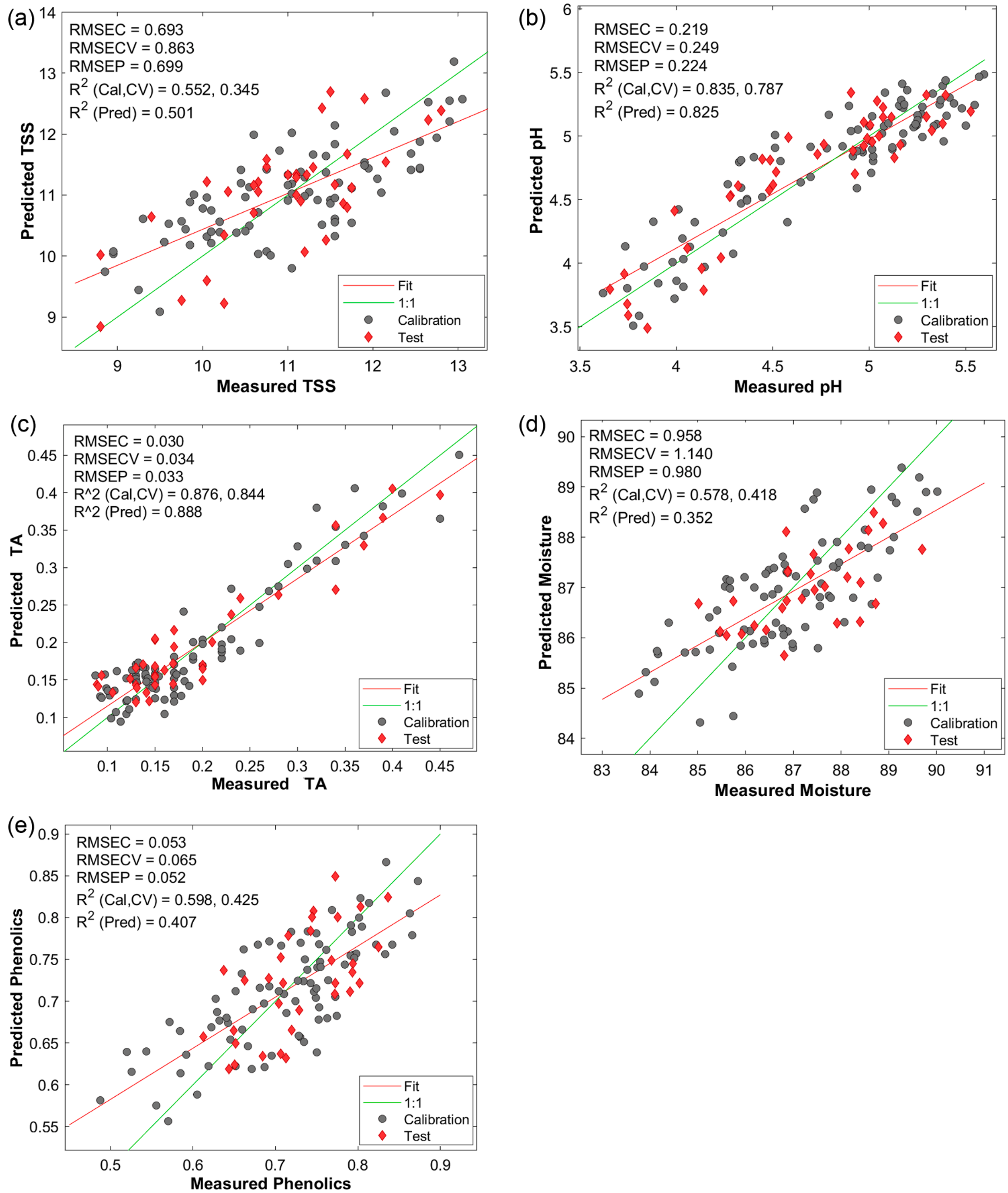

Fig. 3. PLSR models with the best performance for (a) total soluble solids (TSS), (b) pH, (c) titratable acidity (TA), (d) moisture, and (e) total phenolics, using NIR spectra.

assumptions (Walsh et al., 2020). This challenge reinforces the difficulty in obtaining a good correlation between the analyzed features (i.e., TSS, TA, pH, moisture, and phenolics) for pitaya as observed in the Pearson correlation table (Table 2). The good responses for pH and TA rely on the fact that pitaya presents many organic acids, whereas malic acid (451 mg/100 g) is the main one in the red-fleshed variety (Angonese et al., 2021), therefore O—H bonds that are absorbed on the overtone by NIR in some wavelengths (i.e., 970 and 990 nm) is present in the structure of this molecule.

For the PLSR models using the full spectra, NIR models for TSS and moisture showed RPD values of 1.73 and 1.98, which fell into the 1.5 < RPD < 2 range suggesting that TSS and moisture models can distinguish between high and low values (Saeys et al., 2005). pH and TA showed RPD 2.40, 2.78, falling into 2.0 < RPD < 2.5 and 2.5 < RPD <3.0, respectively, which suggests a model for quantitative predictions (Saeys et al., 2005). On the other hand, phenolics presented 1.55 for RPD which is the threshold for the group that includes TSS and moisture. Even though it shows a moderate correlation with pH (Table 2), it did not present good prediction values, at least using the total phenolics method, as proposed in this work. A study on phenolics in red wine grapes found models with an RPD of 1.2 (Rouxinol et al., 2022), which may indicate the difficulty of working with these compounds. A reason for that lies on the complexity of the molecules that also have a hydroxyl functional group (-OH) since they are a group of aromatic carbon

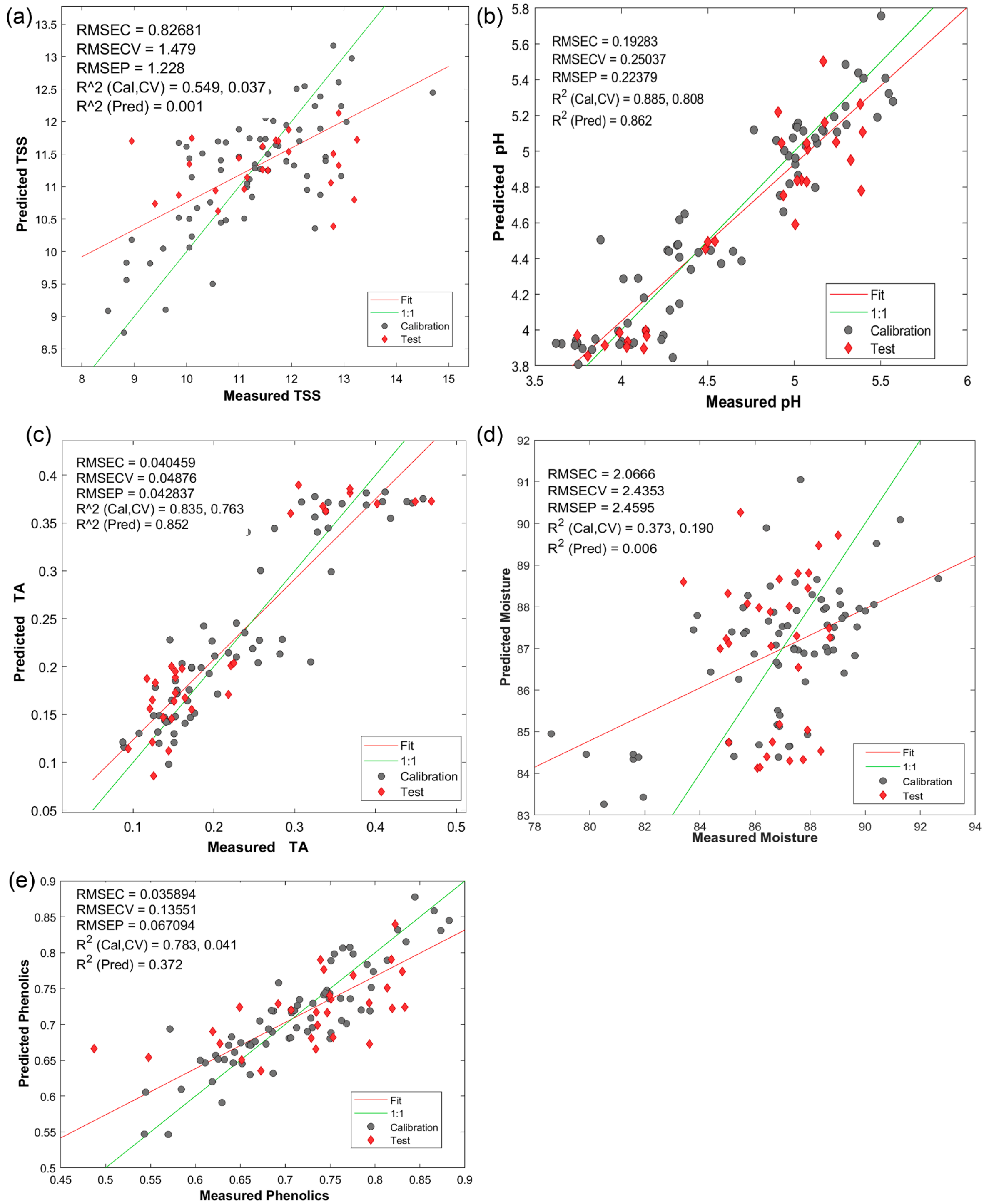

Fig. 4. PLSR models with the best performance for (a) total soluble solids (TSS), (b) pH, (c) titratable acidity (TA), (d) moisture, and (e) total phenolics, using e-nose data.

compounds derived from alcohols. As per RER for NIR equipment, TSS, pH, and moisture presented values 8.94, 8.81, and 8.82 making them fall into the RER $\geq$ 8 thresholds, which means they are qualified for screening calibration. While TA RER was 11.57, which attests that the model is acceptable for quality control.

As per e-nose, PLSR models for e-nose (Table 5) presented similar results. However, models for pH and TA generated high R^2 for calibration and prediction models. A possible reason for that may be linked to the presence of organic acids (Angonese et al., 2021; Balois-Morales et al., 2013) and its degradation during the evaluated time confirmed by the increase in pH. TSS and moisture presented low R^2 values since it was not possible to build good models for those parameters, as these parameters are not related to any feature that would be captured by MOS sensors; therefore, it is not a surprise these two models did not present a good fit. Although the models for phenolics presented an R^2 of 0.78 for calibration, the prediction models were not so good, thus not suitable for prediction in the current work. The poor correlation may rely on the fact that the measurements were performed in the non-violated fruit; therefore, the volatile compounds that were being released from the peel might not be enough to be captured by the

Table 5
Parameters for the calibration and prediction sets for reference analysis in pitaya using portable NIR and e-nose with PLSR.

Reference Analyses	Equipment	Pre- Processing	LV	R^2C	RMSEC	R^2Cv	RMSECV	R^2P	RMSEP	RPD	RER
TSS	NIR spectrometer	MC. SM S-G (o) 0 (w) 11. 1st S-G (o)2. (w) 9. SNV	9	0.55	0.69	0.35	0.86	0.50	0.70	1.73	8.94
	e-nose	autoscaling	4	0.55	0.83	0.04	1.48	0.00	1.23	0.98	5.04
pH	NIR spectrometer	MC. SM S-G (o) 0 (w) 11. 1st S-G (o)2. (w) 9 2nd (o) 2 (w) 9.SNV	6	0.83	0.22	0.79	0.25	0.83	0.23	2.40	8.81
	e-nose	autoscaling. smoothing S-G o (0) (w) 9	7	0.89	0.19	0.81	0.25	0.86	0.22	2.50	8.71
TA	NIR spectrometer	MC. SM S-G (o) 0 (w) 11. 1st S-G (o)2. (w) 9 2nd (o)2. (w) 9.SNV	5	0.88	0.04	0.84	0.03	0.89	0.03	2.78	11.57
	e-nose	AS. SM S-G (o) 0 (w) 9	7	0.84	0.04	0.76	0.04	0.85	0.04	2.6	9.54
Moisture	NIR	MC. SM S-G (o) 0 (w) 11. 1st S-G (o)2. (w) 9 2nd (o)2. (w) 9.SNV	8	0.58	0.96	0.49	1.14	0.35	0.98	1.98	8.82
	e-nose	autoscaling	5	0.37	2.06	0.19	2.46	0.00	2.46	0.96	5.86
Phenolics	NIR	MC. SM S-G (o) 0 (w) 11. 1st S-G (o)2. (w) 9 2nd (o)2. (w) 9.SNV	9	0.60	0.05	0.43	0.07	0.41	0.05	1.55	7.41
	e-nose	autoscaling smoothing S-G (o) 0 (w) 9	20	0.78	0.04	0.04	0.14	0.37	0.07	1.02	5.86

*All models were built using full spectra and maximum variable number NIR (228) and e-nose (928).

sensors. The evaluation of odor in fruit peel using e-nose is usually performed by grinding the peel and resuspending in solvent (Li et al., 2022), which was not the scope of this paper.

E-nose RPD values for TSS, moisture, and phenolics were below 1.5 which indicates an unusable model; however, pH fell into $2.5 < \text{RPD} < 3.0$, which indicates a good prediction model, and TA RPD > 2 indicates a model for quantitative predictions. Regarding RER for e-nose models, only TA and pH fell into the RER ≥ 8 thresholds, which means they are qualified for screening calibration. Some of the unsatisfactory prediction models obtained could be because measurements were performed again with intact fruits. Pitaya has a thick peel that obstructs the penetration of the light from NIRS sensors, thus affecting the model for attributes such as TSS and moisture content, for example.

There are only a few studies on pitaya regarding fruit quality, yet volatile compounds and primary metabolites (e.g., sugar) appears as urgent indicators of fruit quality and flavor that will ensure the acceptability by consumers (García-Cruz et al., 2017; Walsh et al., 2020). However, variability within them can affect prediction models regarding their robustness when using NIR sensors (Walsh et al., 2020). Likewise, moisture and TSS, for example, affect fruits (e.g., strawberries) abruptly, in which small variation in intracellular structure may lead to an interference in model performance when using NIR spectroscopy (Xie et al., 2021). Similarly, even though e-nose MOS sensors are well-established in determining and identifying a vast number of gasses, such as ethanol, toluene, and benzene, allowing them to be used with LDA and PLS models, a drawback in this technology is the difficulty of the sensor to detect small concentrations (i.e., ppb) (Spinelle et al., 2017). The fact that the release of phenolic compounds from the peel might be low combined with the high detection limit (100–1000 ppm) by the sensors may explain the poor response for e-nose TPC PLS model.

4. Conclusions

The use of tools to assist food production is required to assure good quality food for the growing population (Ragazou et al., 2022). Thus, the use of smart technologies (NIRS and e-nose) that contribute to this movement will be demanded in the years to come. These technologies have shown promising capability in delivering solutions for fruit quality control (Mishra et al., 2021; Xu et al., 2019). When evaluating NIR spectroscopy and e-nose as possible equipment to evaluate pitaya shelf-life, LDA showed excellent classification with data from both techniques, even though NIR spectra presented higher overall accuracy ($>$ 97%) compared to e-nose ($>$ 95%). PLS-DA showed excellent accuracy in classifying fruits in the 4 shelf-life indexes for both equipment, which suggests that both techniques could be used to discriminate the shelf-life of pitaya in the 4 proposed stages (SLI, 30, 50, 70, and 100) even when fruits are kept in different temperatures. In addition, it was possible to predict TA and pH for both e-nose and NIR spectra and distinguish between high and low values for TSS, moisture, and phenolics for NIR spectra. The major chemical constituent for classification and prediction may be the volatile compounds associated with malic acid. Albeit the effort in elucidating the chemicals involved in the senescence of pitaya, the biggest challenge and novelty of this work was to offer a 200 dollars portable device to evaluate pitaya shelf life without compromising the equipment's performance. The price to evaluate each sample using NIR and e-nose together would be less than $ 0.10. This cost was calculated based on the 3 - 5% of the retail price of each equipment charged upon one day of analysis. Thus, low-cost NIR spectroscopy and novel low-cost customized e-nose devices combined with chemometrics can be used in the industry to distinguish the different shelf-life stages of pitaya, which would facilitate the selection of these fruits for fresh consumption or specific applications as processed products, such as juices and ice cream.

CRediT authorship contribution statement

Marcus Vinicius da Silva Ferreira: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Writing – original draft. **Ingrid Alves de Moraes:** Methodology, Software, Investigation, Data curation, Writing – review & editing. **Rafael Valsani Leme Passos:** Methodology, Software, Investigation, Data curation, Writing – review & editing. **Douglas Fernandes Barbin:** Conceptualization, Methodology, Software, Data curation, Writing – review & editing, Supervision, Project administration, Funding acquisition. **Jose Lucena Barbosa:** Conceptualization, Writing – review & editing, Supervision.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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