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Original article

Non-destructive monitoring of asparagus (*Asparagus officinalis*, L) quality changes during storage using NIR spectroscopy

Zinabu Hailu Siyum,[1] Tung Thanh Pham,[1,2] Lien Le Phuong Nguyen[1,3] & László Baranyai[1]*

1 Institute of Food Science and Technology, Hungarian University of Agriculture and Life Sciences, Budapest 1118, Hungary
2 Faculty of Chemical and Food Technology, Ho Chi Minh City University of Technology and Education, Ho Chi Minh 700000, Vietnam
3 Industrial University of Ho Chi Minh City, Ho Chi Minh 700000, Vietnam

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Summary Storing asparagus under controlled conditions is crucial to preserve its freshness and quality after harvest. However, there may be changes in firmness and weight. This study aimed to evaluate surface changes of green asparagus using near-infrared (NIR) spectroscopy during storage at 2, 10 and 15 °C for 12 days. Weight loss, firmness and NIR absorbance in 900–1700 nm were measured. The results showed that the storage temperature and time had a significant influence on the weight loss and firmness values. A partial least squares discriminant analysis (PLS–DA) with first derivative spectral pre-treatment performed well and achieved an average accuracy of 86.6% in cross-validation. Furthermore, the partial least squares regression (PLSR) model accurately predicted weight loss (R_{CV}^2 = 0.97, $RMSE_{CV}$ = 1.04%) and firmness (R_{CV}^2 = 0.97, $RMSE_{CV}$ = 1.89 N). Therefore, NIR spectroscopy was efficient in monitoring asparagus quality changes during storage at different temperatures and durations.

Keywords Chemometrics, partial least squares discriminant analysis, partial least squares regression, quality assessment.

Introduction

Asparagus (*Asparagus officinalis* L.) is a healthy vegetable due to its low-calorie content, high-fibre content, and the presence of several phytochemicals (Pegiou *et al*., 2019; Sergio *et al*., 2021). However, after harvest, the quality of asparagus rapidly deteriorates due to increased respiratory and metabolic activities (Garrido *et al*., 2001; Anastasiadi *et al*., 2020). Maintaining the quality and freshness of asparagus during storage is important but challenging. Previous studies have shown that asparagus can be stored for up to 14–15 days in cold temperatures and 3–5 days in ambient conditions (Villanueva *et al*., 2005; An *et al*., 2008; Lipton, 2011). However, storage conditions affect the internal and external properties of the product, including texture, colour, moisture, and fibre content (Garrido *et al*., 2001; Villanueva *et al*., 2005; Hung *et al*., 2011). Thus, it needs to be monitored for its quality and nutritional value to satisfy customer acceptance. This leads to the demand for fast, cost-effective, and energy-efficient non-destructive measurement techniques.

Near-infrared (NIR) spectroscopy is a rapid and non-destructive analytical technique that operates based on the principle of light absorption in the wavelength range between 700 and 2500 nm (Nicolaï *et al*., 2007; Sánchez *et al*., 2009; Pham *et al*., 2023). This absorption is a result of vibrations of molecular functional groups in the sample (Büning-Pfaue, 2003; Tsenkova, 2009). The predominant spectral features in the NIR primarily originate from the vibrations of the C–H, O–H and N–H groups (Büning-Pfaue, 2003; Camps & Gilli, 2017). NIR spectroscopy has promising potential in online sorting and grading of horticultural products based on quality attributes (Nicolaï *et al*., 2007; Sánchez *et al*., 2009; De la Haba *et al*., 2014). Moreover, it is also used in post-harvest quality control and traceability (Perez *et al*., 2002; Jaren *et al*., 2006; Richter *et al*., 2019; Huang *et al*., 2020). Application of NIR helps saving energy and time while reducing waste (Sánchez *et al*., 2009; Guo *et al*., 2019). However, limited studies have established the application of NIR spectroscopy together with chemometric multivariate analysis in the quality assessment of asparagus during storage.

The aim of the present study was to evaluate the quality changes of asparagus at different storage temperatures using NIR spectroscopy. Different spectral pre-processing methods were performed to enhance the efficiency of partial least squares discriminant analysis (PLS–DA) in the classification of storage temperature groups and partial least squares regression (PLSR) in predicting weight loss and firmness of asparagus.

*Correspondent: E-mail: baranyai.laszlo@uni-mate.hu

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Materials and methods

Materials

Fresh green asparagus spears (*A. officinalis* L.) were collected directly from growers in Csengőd, Hungary, and washed with fresh water and then dried with ambient air. The asparagus spears were randomly divided into three groups, with 30 samples per group. The average length of the spears was 20.42 ± 0.58 cm, and their average diameter was 11.94 ± 3.52 mm. The samples were then packaged in low-density polyethylene plastic with ventilation holes and stored at 2, 10 and 15 °C. Ten samples were taken from each group at 4 days measurement intervals until 12 days.

Methods

Measurement of reference quality parameters

Weight loss was measured as a reduction in the weight of the stored asparagus spears and was expressed as the percentage of weight change compared with the initial value (Hung *et al.*, 2011). Weight was measured using an electronic balance (Kern PFB, Kern & Sohn GmbH, Balingen-Frommern, Germany). The firmness of asparagus was determined using a Texture Analyser (TA-XTplus, Stable Microsystems, Surrey, UK) equipped with a blade cutter (HDP/BSK). The test speed of 1 mm/s was adjusted with 0.01 s delay between consecutive data points. The maximum force required to cut the asparagus was recorded at various locations (tip, middle and base).

NIR spectra acquisition

The NIR spectra were collected in reflectance mode using a handheld spectrometer NIR-S-G1 (InnoSpectra Co., Hsinchu, Taiwan). The spectrometer operated in the NIR range of 900–1700 nm with a spectral resolution of 3–4 nm (Fig. 1). Two scans were taken from the base, middle, and apex of the asparagus spears, with perpendicular rotation between their orientations.

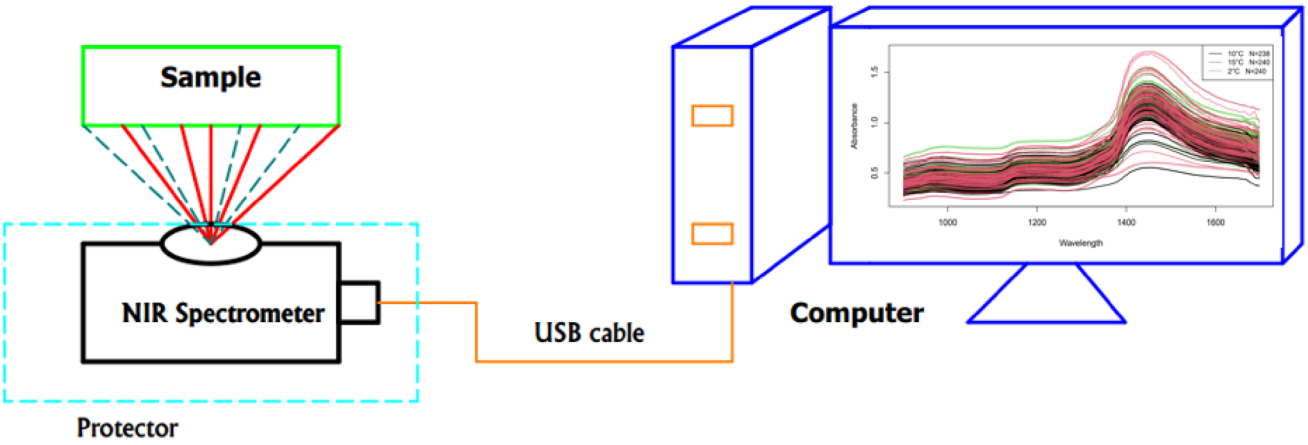


Figure 1 Schematic diagram about collecting the NIR absorption spectra in reflectance mode using a handheld spectrometer.

Table 1 PLS–DA model performance parameters

Mathematical expression	Description
$\text{Sensitivity} = \frac{TP}{TP+FN}$	Sensitivity indicates the model ability to correctly identify true positive cases.
$\text{Specificity} = \frac{TN}{TN+FP}$	Specificity is a measure of the model ability to correctly identify true negative cases.
$\text{Precision} = \frac{TP}{TP+FP}$	Precision reflects the accuracy of positive predictions among all predicted positive cases.
$\text{Accuracy} = \frac{(TP+TN)}{(TP+FN+FP+FN)}$	Accuracy assesses the overall correctness of a model by calculating the ratio of correctly predicted cases to the total number of cases.
$\text{Balanced accuracy} = \frac{\text{Specificity}+\text{Sensitivity}}{2}$	Balanced accuracy is the average of specificity and sensitivity, providing a balanced assessment of how well the model performs for both positive and negative cases.
$F-\text{score} = \frac{2\times\text{Precision}\times\text{Sensitivity}}{\text{Precision}+\text{Sensitivity}}$	*F*-score is used for evaluating the model ability to correctly classify both positive and negative cases by considering both precision and sensitivity.

Abbreviations: FN, False negative; FP, False positive; TN, True; TP, True positive.

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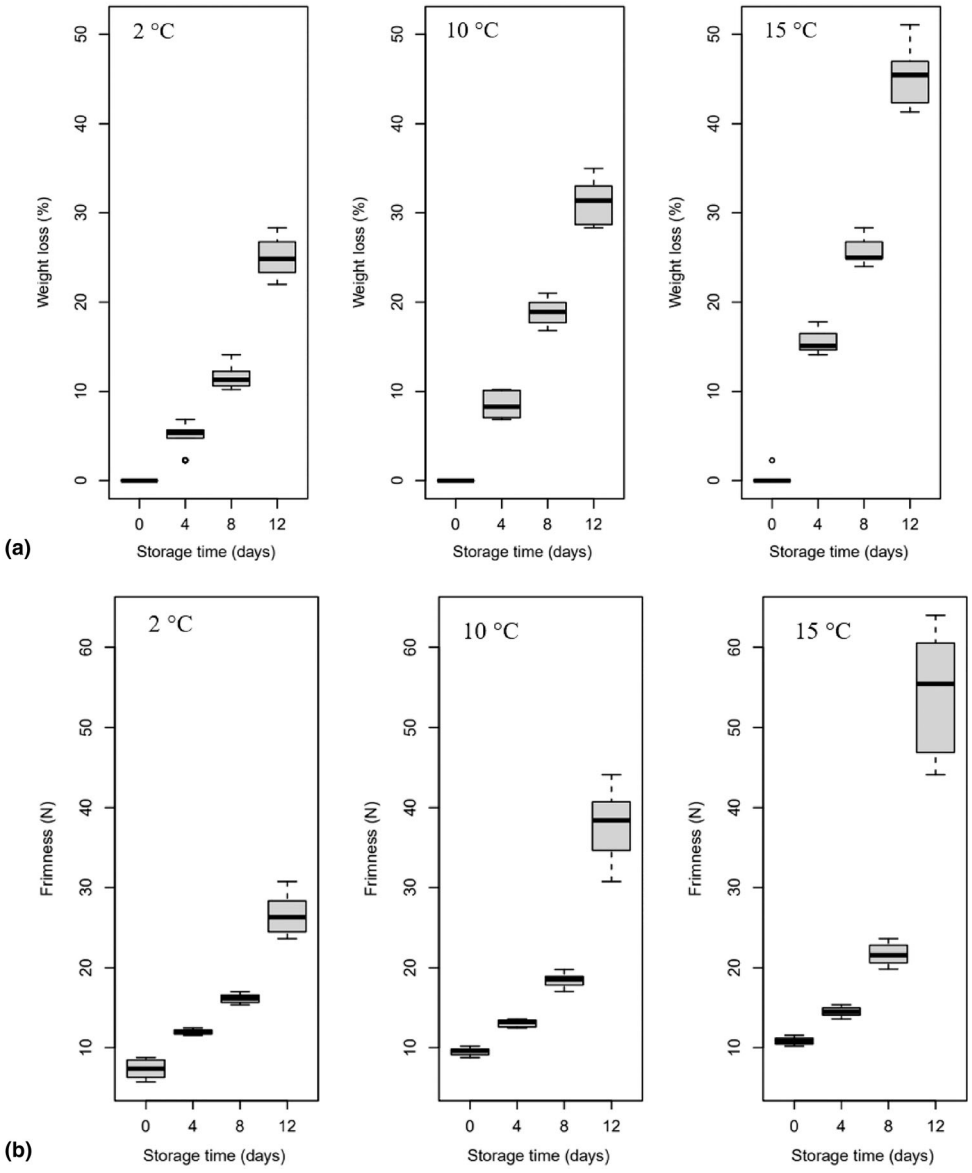


Figure 2 Changes in weight loss (a) and firmness (b) of green asparagus samples stored at different temperature and time. Ten samples were measured in each group each time.

Spectra preprocessing

The collected raw spectra were pretreated using a method that included Savitzky–Golay smoothing (with 21 data points), standard normal variate (SNV), first (D1NIR) and second (D2NIR) derivatives. These pre-processing techniques were successfully applied to remove noise and baseline interference in the signals during prediction of soluble solids (Guo *et al.*, 2019). The resulting pre-processed spectra were used to build predictive models to assess asparagus weight loss and firmness (Wang & Xie, 2014). Derivatives were also found to be successful in predicting physical properties (Garrido *et al.*, 2001; De la Haba *et al.*, 2014).

PLS–DA and PLSR models

In this study, PLS–DA model was established to classify asparagus samples that have been stored at 2, 10 and 15 °C. The dataset was randomly split into training and validation with the ratio of 75% training and 25% validation. The classification performance parameters of the model, including sensitivity, specificity, precision, accuracy, balanced accuracy and *F*-score

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Table 2 Analysis of variance (ANOVA) of asparagus quality parameters

	Factors					
	Storage time		Storage temperature		Interaction	
Parameters	*F*-Value	*P*-Value	*F*-Value	*P*-Value	*F*-Value	*P*-Value
Weight loss, %	20760.44	<2.2e-16 ***	1438.75	<2.2e-16 ***	212.41	1.434e-10 ***
Firmness, *N*	4751.08	<2.2e-16 ***	862.10	2.64e-05 ***	325.94	6.95e-10 ***

***$P < 0.001$, **$P < 0.01$, *$P < 0.05$.

Table 3 Pearson's correlation between variables from reference measurement and NIR spectroscopy

Raw NIR						
	Storage time	Weight loss	Maximum force	970 nm	1425 nm	1500 nm
Weight loss, %	0.95*					
Firmness, *N*	0.81*	0.93*				
970 nm	0.89*	0.96*	0.96*			
1425 nm	0.80*	0.85*	0.85*	0.93*		
1500 nm	0.82*	0.85*	0.82*	0.93*	0.98*	
1670 nm	0.89*	0.95*	0.95*	1.00*	0.95*	0.95*
Standard normal variate (SNV)						
Weight loss, %	0.95*					
Firmness, N	0.81*	0.93*				
970 nm	−0.90*	−0.93*	−0.88*			
1425 nm	−0.87*	−0.93*	−0.93*	0.94*		
1500 nm	0.84*	0.89*	0.88*	−0.94*	−0.98*	
1670 nm	0.90*	0.95*	0.93*	−0.98*	−0.97*	0.96*
First derivative (D1NIR)						
Weight loss, %	0.95*					
Firmness, N	0.81*	0.93*				
970 nm	−0.84*	−0.86*	−0.83*			
1425 nm	0.84*	0.89*	0.88*	−0.98*		
1500 nm	−0.81*	−0.83*	−0.81*	0.98*	−0.97*	
1670 nm	0.91*	0.95*	0.92*	−0.95*	0.97*	−0.91*
Second derivative (D2NIR)						
Weight loss, %	0.95*					
Firmness, N	0.81*	0.93*				
970 nm	0.79*	0.84*	0.86*			
1425 nm	0.80*	0.84*	0.83*	0.98*		
1500 nm	−0.83*	−0.87*	−0.86*	−0.98*	−0.99*	
1670 nm	0.82*	0.86*	0.85*	0.99*	0.99*	−0.99*

*$P < 0.05$.

were determined. Their mathematical expressions and descriptions are presented in Table 1.

PLSR model was also established to predict the weight loss and firmness of asparagus by NIR spectra. The dataset was randomly divided into 75% training to establish the model, while the remaining 25% was allocated for testing in cross-validation. The optimal number of latent variables was determined based on the root mean square error of validation ($RMSE_{CV}$). The prediction performance of the models was evaluated using coefficient of determination (R_{CV}^2), root mean square error in cross validation, ratio of deviation to prediction performance (RPD).

The cross-validation of both PLS–DA and PLSR models was repeated ten times, and the average values were used for comparison.

Statistical analysis

The PLS–DA was carried out using the 'plsdepot' package (version 0.2.0), whereas PLSR was conducted using the 'pls' package (version 2.8.2). Additionally, changes in asparagus weight loss, firmness, and NIR absorbance were depicted using box plots, and Pearson's correlation tests were performed among selected parameters (Taylor & Bates, 2013). The effects of storage time and temperature were assessed using a two-way MANOVA, followed by testing significant outcomes with a one-way ANOVA. All these statistical analyses were performed using R software (version 4.2.2, R Foundation for Statistical Computing, Vienna, Austria).

Results and discussions

Measurement of reference quality parameters

The weight loss of asparagus spears increased with storage time and temperature (Fig. 2a). This is statistically supported by the significant effects presented by the analysis of variances (Table 2). The highest variation was observed at the last stage of the storage period, mainly in samples stored at 15 °C, followed by 10 °C. Furthermore, the weight loss difference between the storage temperature groups is influenced by the humidity difference between the internal atmosphere of the products and the storage atmosphere (Villanueva *et al.*, 2005; An *et al.*, 2008; Hung *et al.*, 2011). On the other hand, weight loss in green asparagus spears had a significant positive correlation

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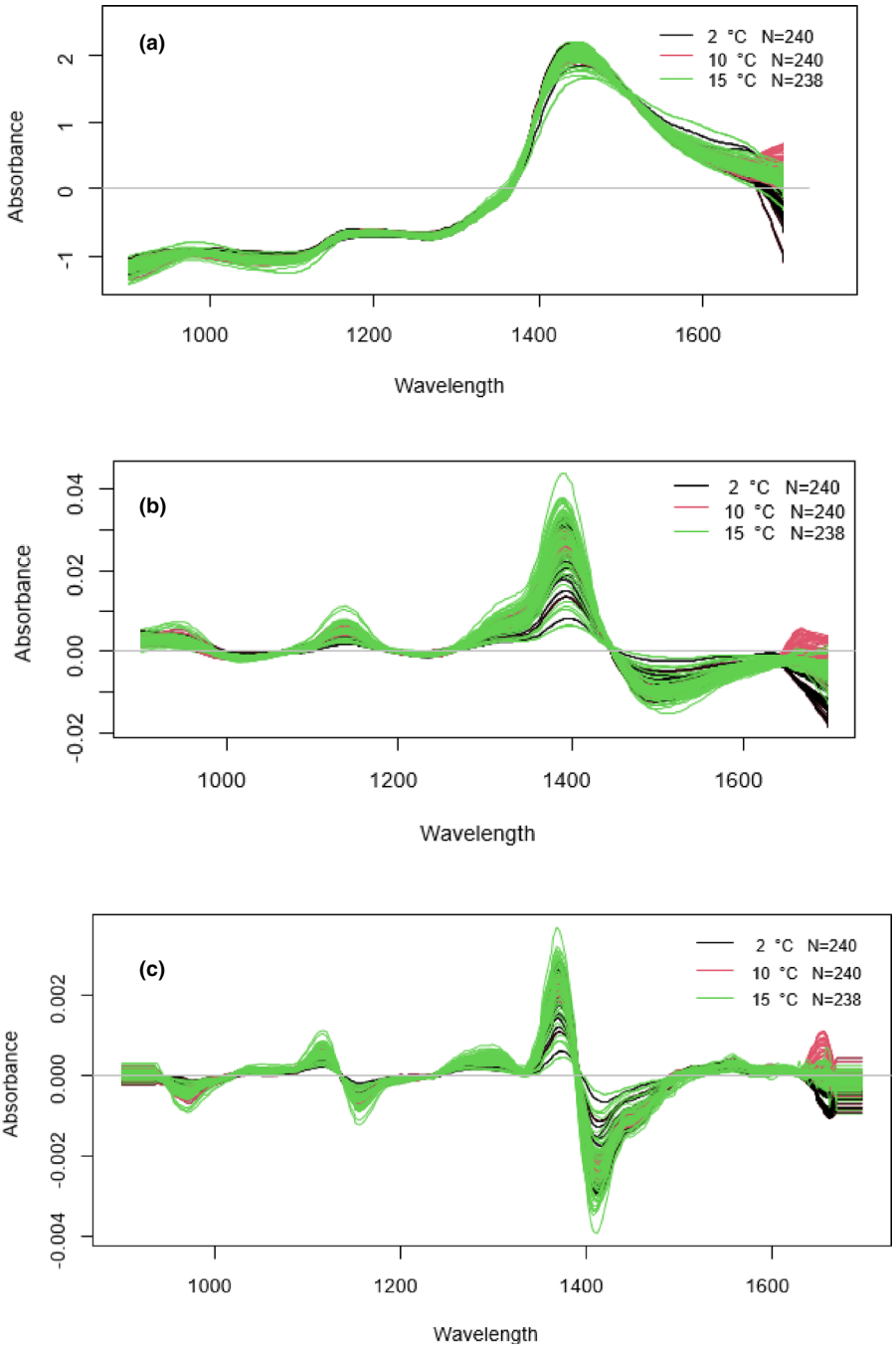


Figure 3 NIR spectra pre-processing techniques: SNV (a), 1st derivative (b) and 2nd derivative (c) by storage temperture.

with storage time ($r = 0.95$) and firmness ($r = 0.93$) (Table 3). This result indicates that asparagus lost moisture continuously and, as a result, became harder during storage.

The firmness (maximum cutting force) of the asparagus samples also increased with storage temperature and time (Fig. 2b). This is supported by the statistical analysis (Table 2), which showed significant effect (F-value = 4751.08, $P < 0.001$) and had significant positive correlation ($r = 0.81$) with storage time (Table 3). The degradation of organic compounds and the presence of heterogeneous fibre content across asparagus

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Table 4 Confusion matrix table of PLS–DA model based on validation data set

	Training				Validation		
	2 °C	10 °C	15 °C		2 °C	10 °C	15 °C
Raw NIR, LV = 14, average recognition of 95.0% and accuracy of 84.4%							
2 °C	45	0	0	2 °C	15	0	0
10 °C	0	43	4	10 °C	0	12	4
15 °C	0	2	41	15 °C	0	3	11
SNV, LV = 14, average recognition of 97.7% and accuracy of 86.6%							
2 °C	45	0	0	2 °C	15	0	0
10 °C	0	42	1	10 °C	0	12	3
15 °C	0	3	44	15 °C	0	3	12
D1NIR, LV = 12, average recognition of 99.2% and accuracy of 86.6%							
2 °C	45	0	0	2 °C	15	0	0
10 °C	0	44	0	10 °C	0	14	2
15 °C	0	1	45	15 °C	0	1	13
D2NIR, LV = 12, average recognition of 99.0% and accuracy of 84.0%							
2 °C	45	0	0	2 °C	14	0	0
10 °C	0	44	0	10 °C	0	13	4
15 °C	0	1	45	15 °C	1	2	11

Table 5 Performance parameters of PLS–DA model for classification of storage temperature groups

	Training (n = 135)			Validation (N = 45)		
Parameters	2 °C	10 °C	15 °C	2 °C	10 °C	15 °C
Raw NIR						
Accuracy	1	0.96	0.96	1	0.84	0.84
Precision	1	0.96	0.91	1	0.8	0.73
Sensitivity	1	0.91	0.95	1	0.75	0.79
Specificity	1	0.98	0.96	1	0.9	0.87
Balanced accuracy	1	0.91	0.95	1	0.75	0.79
F score	1	0.93	0.93	1	0.77	0.76
SNV						
Accuracy	1	0.97	0.97	1	0.87	0.87
Precision	1	0.93	0.98	1	0.8	0.8
Sensitivity	1	0.98	0.94	1	0.8	0.8
Specificity	1	0.97	0.99	1	0.9	0.9
Balanced accuracy	1	0.98	0.94	1	0.8	0.8
F score	1	0.95	0.96	1	0.8	0.8
D1NIR						
Accuracy	1	0.99	0.99	1	0.87	0.87
Precision	1	0.98	1	1	0.87	0.93
Sensitivity	1	1	0.98	1	0.91	0.74
Specificity	1	0.99	1	1	0.85	0.96
Balanced accuracy	1	1	0.98	1	0.91	0.74
F score	1	0.99	0.99	1	0.77	0.82
D2NIR						
Accuracy	1	0.99	0.99	0.98	0.87	0.84
Precision	1	0.98	1	0.93	0.87	0.73
Sensitivity	1	1	0.98	1	0.76	0.79
Specificity	1	0.99	1	0.97	0.93	0.87
Balanced accuracy	1	1	0.98	1	0.76	0.79
F score	1	0.99	0.99	0.96	0.81	0.76

spear sections (base, middle and tip) negatively affect the firmness (Garrido *et al*., 2001; Villanueva *et al*., 2005; Anastasiadi *et al*., 2020). The most significant variability was observed in samples stored at 15 °C on the final storage day, followed by 10 and 2 °C. This variation would arise due to the development of lignin and an increase in crude fibre, attributed to the enzymatic activity of phenylalanine–ammonia lyase (An *et al*., 2008; Lipton, 2011; Anastasiadi *et al*., 2020).

Spectra preprocessing

The NIR absorption peaks appeared according to the expected vibrations of molecular functional groups in the sample (Büning-Pfaue, 2003; Tsenkova, 2009; Camps & Gilli, 2017). These spectral features are caused by overtones and combinations of fundamental molecular vibrations occurring at infrared wavelengths (Tsenkova, 2009; Camps & Gilli, 2017). The NIR absorption spectra of asparagus, pre-processed by standard normal variate (SNV), first and second derivatives are presented in Fig. 3. The spectral peaks near 970, 1190, 1450, 1500 and 1670 nm are related to the vibrations of the C–H, O–H and N–H groups (Sinelli *et al*., 2008; Tsenkova, 2009). According to these observed specific changes in the spectra, both moisture content and fibre density are likely to affect spectral readings.

PLS–DA and PLSR models

The classification with PLS–DA shows whether sample groups of different storage temperature could be distinguished. The accuracy of the PLS–DA model using the first derivatives was notably higher (86.6% in cross-validation) for classification compared to the second derivatives, SNV, and raw NIR data, as it is presented in Tables 4 and 5, respectively. The samples stored at 2 °C achieved the highest classification performance indicating their difference from the others. This observation with the smaller changes of asparagus kept at 2 °C suggests better storability than those stored at temperatures of 10 and 15 °C. Similar studies have demonstrated that asparagus can be stored for up to 16 days on 2 °C (Villanueva *et al*., 2005) and 21 days on 1 °C (Anastasiadi *et al*., 2020). Lower temperature effectively slows down enzymatic and microbial activity, therefore maintains freshness and texture (An *et al*., 2008; Anastasiadi *et al*., 2020). In contrast, higher storage temperature accelerates chemical reactions, microbial growth and moisture loss, resulting in rapid deterioration and diminished appearance (Villanueva *et al*., 2005; An *et al*., 2008; Hung *et al*., 2011). The PLS–DA method based on NIR spectra reached high accuracy, above 81%, in recognition of asparagus storage time (Sánchez *et al*., 2009). The identification

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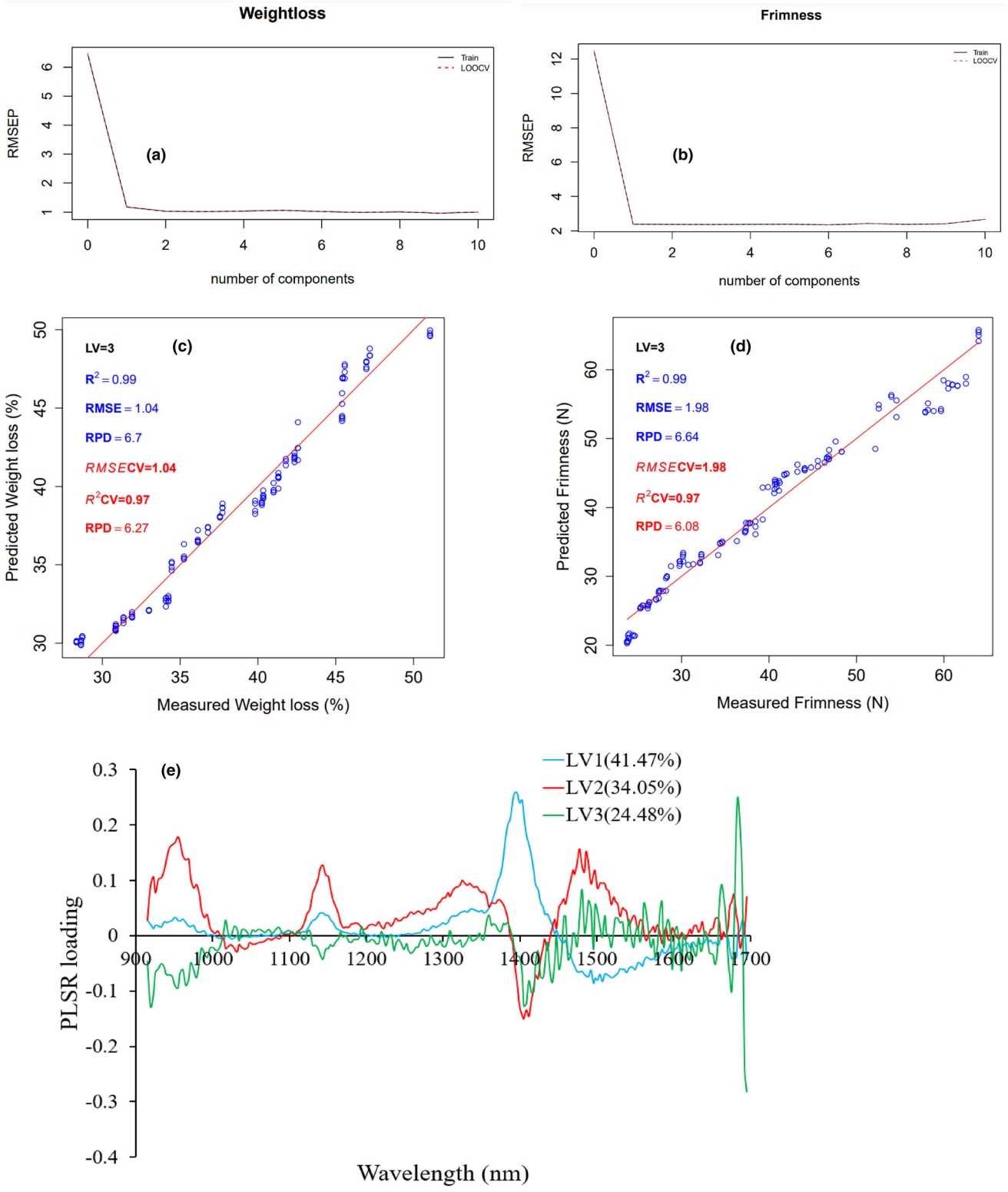


Figure 4 Selection of latent variables for weight loss (a) and maximum force (b) prediction, the PLSR model based on the first derivatives to predict weight loss (c) and maximum force (d) of asparagus, and the PLSR loading plot (e).

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Table 6 Performance parameters for PLSR models with different spectral preprocessing methods

			Training (n = 135)			Validation (n = 45)		
Quality parameters	**Treatment**	**LV**	R^2	**RMSE**	**RPD**	R^2_{cv}	$RMSE_{CV}$	**RPD**
Weight loss, %	Raw NIR	5	0.9898	1.001	6.46	0.9755	1.001	5.88
	SNV	5	0.9997	1.014	6.53	0.9772	1.014	5.99
	1st derivative	3	0.9999	1.041	6.70	0.9720	1.041	6.27
	2nd derivative	5	0.9990	1.073	6.18	0.9733	1.073	6.18
Firmness, *N*	Raw NIR	6	0.9957	1.839	6.60	0.9835	1.838	6.35
	SNV	5	0.9992	2.019	6.26	0.9763	2.018	6.09
	1st derivative	3	0.9989	1.986	6.64	0.9754	1.985	6.08
	2nd derivative	4	0.9984	2.175	6.60	0.9764	2.172	5.17

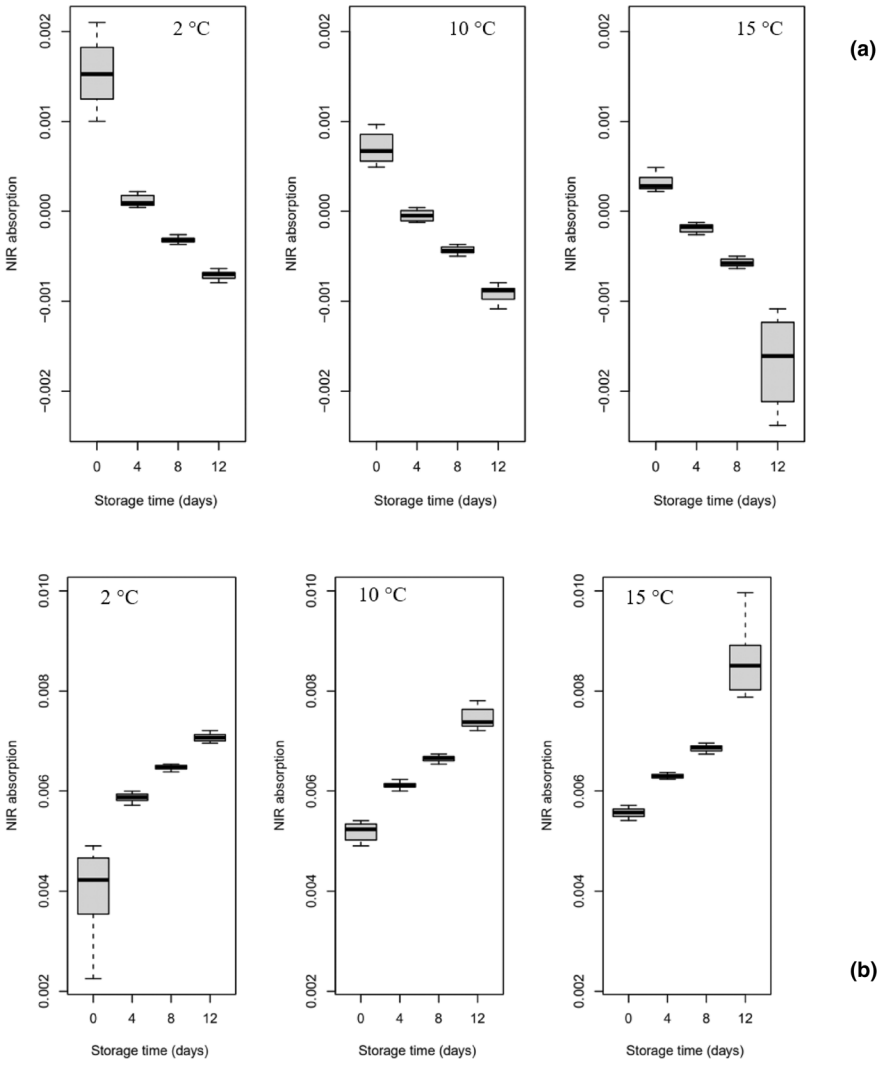


Figure 5 Changes in the first derivatives of the NIR absorbance (two replicates/sample position) at 970 nm (a) and 1425 nm (b) of green asparagus samples stored at different temperature and time. Ten samples were measured in each group each time.

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Table 7 Analysis of variance of NIR spectra frist derivatives at selected wavelengths

	Factors					
	Storage time		Storage temperature		Interaction	
Wavelength	*F*-Value	*P*-Value	*F*-Value	*P*-Value	*F*-Value	*P*-Value
970 nm	3885.79	<2.2e-16***	902.16	<2.2e-16***	138.50	<2.2e-16***
1425 nm	2492.45	<2.2e-16***	576.53	<2.2e-16***	84.59	<2.2e-16***
1500 nm	1723.01	<2.2e-16***	452.89	<2.2e-16***	83.32	<2.2e-16***
1670 nm	3995.96	<2.2e-16***	560.37	<2.2e-16***	83.57	<2.2e-16***

***$P < 0.001$.

of geographical origin of white asparagus was successful with SVM and reached 89% accuracy (Richter *et al.*, 2019). Presented result of 86.6% in cross-validation is in agreement with literature.

On the other hand, Fig. 4 shows the optimal number of latent variables and PLSR model to predict weight loss (Fig. 4a,c) and firmness (Fig. 4b,d) and the PLSR loading plot (Fig. 4e). The Model performance parameters with different spectral preprocessing methods are presented in Table 6. The PLSR model with the first derivatives and 3 latent variables demonstrated relatively good performance for weight loss ($R^2 = 0.972$, $RMSE_{CV} = 1.04\%$, $RPD = 6.27$) and firmness ($R^2 = 0.975$, $RMSE_{CV} = 1.98$ N, $RPD = 6.08$) in the validation datasets. Flores-Rojas *et al.* (2009) and De La Haba *et al.* (2014) estimated the shear force using PLSR on NIR data but obtained lower performance ($R^2 < 0.67$) compared to present study. Perez *et al.* (2002) achieved similar performance to this study in estimation of cutting force, in terms of $R^2 = 0.84$ and $SE_{CV} = 5.73$ N.

According to the PLSR model loadings based on the first derivatives, variations in NIR absorbance were observed at wavelengths of 970, 1425, 1500 and 1670 nm. The changes corresponding to temperature and time are visually depicted through box plots, as presented in Fig. 5. Observed differences are supported by significant *F*-values of ANOVA test at $p < 0.05$ (Table 7). Besides the expected significant effects of storage time and temperature, the significant interactions suggest different behaviour of sample groups in time. In addition, Pearson's correlation for raw spectra, SNV, D1NIR and D2NIR pre-processing methods are presented in Table 3. The NIR absorbance refined using the first derivatives at wavelengths of 1425 and 1670 nm achieved the highest significant positive correlations with weight loss and firmness. Conversely, NIR absorbance at 970 and 1500 nm were negatively correlated with those reference values (Table 3). According to the performance of classification and regression models, as well as the correlation among reference parameters with the NIR spectra, the NIR spectroscopy was successful in quality assessment of asparagus during storage. According to the results, the NIR based measurement technique is suitable for quality assessment of asparagus from farm to retail stores. The presented results were acquired with a handheld device, supporting the application of portable instruments. Such smart tools enable on site measurements and provide information to decision making, without long chemical analysis and need for a laboratory. The NIR spectroscopy with portable instruments offers improved farming and integration into digitalized technology.

Conclusions

In this study, NIR spectroscopy was used to assess the quality of stored asparagus. Storage time and temperature influenced its weight loss, firmness and NIR absorbance. The computation of first derivatives was the optimal preprocessing method for enhancing NIR spectral analysis compared to SNV, second derivatives and raw spectra. PLS–DA and PLSR models, based on the first derivatives, efficiently classified storage temperature groups with classification accuracy of 86.6% in cross-validation and predicted weight loss ($R_{cv}^2 = 0.97$, $RMSE_{CV} = 1.04\%$) and firmness ($R_{cv}^2 = 0.97$, $RMSE_{CV} = 1.89$ N). Therefore, NIR spectroscopy is a promising non-destructive method to monitor quality changes of asparagus during storage. Due to the application of portable instrument in the study, results also enable on site quality control from farms to retail.

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Author contributions

Zinabu Hailu Siyum: Conceptualization (equal); formal analysis (equal); investigation (equal); methodology

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(equal); writing – original draft (lead). **Tung Thanh Pham:** Formal analysis (equal); investigation (equal); methodology (equal). **Lien Le Phuong Nguyen:** Methodology (equal); supervision (equal); validation (equal); writing – review and editing (equal). **László Baranyai:** Conceptualization (equal); supervision (equal); validation (equal); writing – review and editing (equal).

Conflict of interest

Authors declare no conflict of interest.

Peer review

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Data availability statement

Data is available upon request from the corresponding author.

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The calibration and validation method used in modified partial least square regression model is similar the current work, and its results are used to compare the predicted firmness parameter of asparagus.

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The results of physical changes were important input to the current work. MAP was evaluated by means of weight loss and firmness of the asparagus during storage at 2 and 10 °C for up to 12 days.

Wang, A. & Xie, L. (2014). Technology using near infrared spectroscopic and multivariate analysis to determine the soluble solids content of citrus fruit. *Journal of Food Engineering*, **143**, 17–24.

The authors used NIR and multivariate analysis to determine the total soluble solid content of citrus fruits. In the current work, a similar approach using the Partial Least Squares Regression (PLSR) model was used to estimate asparagus weight loss and firmness.

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