REVIEW ARTICLE

Non-destructive analysis of Japanese table grape qualities using near-infrared spectroscopy

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Abstract

Near-infrared (NIR) spectroscopy is a useful technique for the non-destructive analysis of fruit quality. The key quality parameters of table grapes (*Vitis vinifera*) that affect consumer preference are the soluble solids content (SSC), pH, firmness, and seedlessness. This research focused on using NIR spectroscopy for assessing the quality of 'Kyoho' table grapes, as a non-destructive analysis under laboratory and field conditions. NIR spectra for each sample were acquired in the wavelength range of 400–1000 nm, using a visible/NIR spectrometer with fibre optics in the interactance mode. Partial least-square regression was used to calibrate the NIR spectral data with all the measured properties of table grapes. The best prediction model for firmness was the Savitzky–Golay first derivative (SGD1) with a coefficient of determination ($R^2_{\text{prediction}}$) of 0.7427 in the laboratory, and 0.7804 in the field. The $R^2_{\text{prediction}}$ values for pH in the laboratory and the field was 0.6276 using multiplicative scatter correction (MSC), and 0.7676 using SGD1, respectively. These values were similar to the $R^2_{\text{prediction}}$ values of SSC, which were 0.6926 using MSC, and 0.8052 using the Savitzky–Golay second derivative, respectively. In both analyses the R^2 of the calibration model was between 0.6944 and 0.8877. The partial least-square discriminant analysis was used to classify the percentage of seedlessness, which was 93.10% in the laboratory using SGD1 or MSC, and 79.31% in the field using MSC. Therefore, NIR spectroscopy is an efficient non-destructive technique for rapidly analysing Japanese table grape qualities in laboratory and field settings.

Keywords Fruit quality · Firmness · 'Kyoho' Japanese table grape · Seedlessness

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1 Introduction

The key quality parameters of table grapes are the soluble solids content (SSC), titratable acidity, and pH (Piazzolla et al. 2017). The conventional methods for the analysis of grape quality are time-consuming, expensive, involve sample destruction, and require complicated preparation procedures. Near-infrared spectroscopy (NIRS) is an alternative technique for non-destructive fruit quality assessment. It can evaluate the internal starch, SSC, oil content, water content, dry matter content, acidity, firmness, stiffness factor, and other physiological properties of fruit and vegetable products (Slaughter et al. 2003; Nicolai et al. 2007; Shao and He 2007), such as watermelon (Sun et al. 2010), passionfruit (Maniwara et al. 2014), paddy rice (Siriphollakul et al. 2015), apple (Bobelyn et al. 2010), jujube (Wang et al. 2011), and mango (Saranwong et al. 2004). It can also determine the harvest times of table grapes (Piazzolla et al. 2017), classify the phytosanitary of wine grapes (Giovenzana et al.

2017), and monitor the ripening process of wine grapes whilst they are still on the vine (González-Caballero et al. 2012).

Chemometrics allows the development of calibration and validation models from near-infrared (NIR) spectra for predicting and managing the quality of fruit products. Giovenzana et al. (2017) applied partial least-square–discriminant analysis (PLS-DA) to grape spectra in order to test the performance of visible/NIR spectroscopy in classifying healthy and infected bunches. Interestingly, the non-destructive analysis of Japanese table grapes by NIRS techniques has not yet been reported. Therefore, this study aimed to develop a non-destructive method for the rapid analysis of Japanese table grapes for quality management using the NIRS technique.

2 Materials and methods

2.1 Raw materials

Experiments were carried out at the Niigata Agricultural Research Institute, Horticultural Research Centre, Niigata, Japan. Grape inflorescences were selected in the vineyard for both seeded and seedless treatments. The seedless treatment was applied by spraying 25 ppm GA_3 twice during the flowering stages and then 14 days later, while there was no spraying for the seeded treatment. After that, three grapes berries from three positions on the fruit bunch (top, middle, and bottom) from 15 bunches of seeded and seedless treatments were collected on three harvesting dates: 28 August 2018 (79 days after flowering [DAF]), 3 September 2018 (85 DAF) and 11 September 2018 (93 DAF). Each berry was analysed by NIRS in the field (Fig. 1), and then NIRS analysis and chemometric analysis were performed in the laboratory (Fig. 2) at the Faculty of Environmental Science for Agriculture and Forestry, Niigata University (Niigata, Japan).

2.2 Analysis methods

2.2.1 NIRS analysis

Interactance spectra were recorded in the laboratory and the field using a NIRS spectrometer equipped with a PICL-NEX

Fig. 1 Near infrared spectra acquisition of table grapes performed in the laboratory
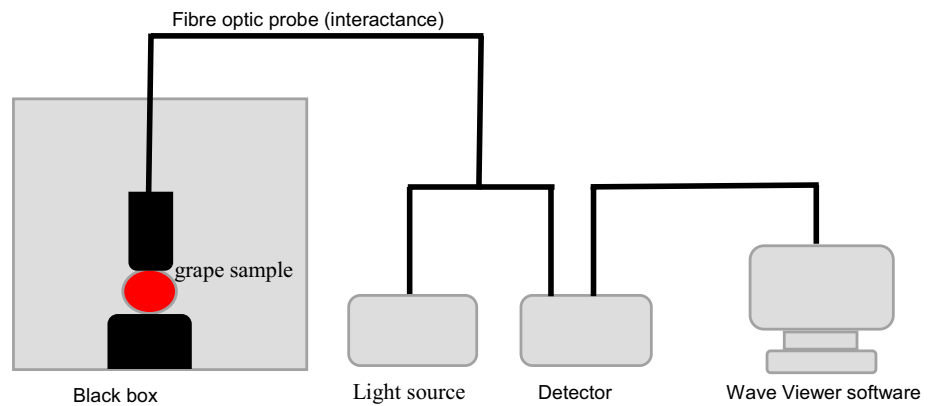

Fig. 2 Near infrared spectra acquisition of table grapes performed in the field

light source, WaveView software, a Handy Lambda II detector, and a fibre optic probe. Each spectrum was acquired in the wavelength range of 400–1000 nm, with a resolution of approximately 3 nm (total of 181 wavelengths).

2.2.2 Chemical analysis

The SSC and pH reference data for each sample were determined using a digital refractometer (PR-101α, Atago, Japan) and a pH meter (HM-30P, Japan), respectively.

2.2.3 Physical analysis

The firmness was obtained by texture analysis using a texture analyser (Shimpo, Japan), and the seedlessness was determined by cutting and counting. The percentage of seedlessness classification was calculated as follows:

$$\text{Percentage of seedlessness classification} = \frac{S_s}{S_t}100, \tag{1}$$

where S_s is the number of correctly detected or predicted as seedless berries, and S_t is the total number of berry samples.

2.2.4 Chemometric analysis

Chemometric analysis was undertaken to develop the calibration model (57 samples) and prediction model (29 samples), based on the relationship between the NIRS data and all of the measured properties (SSC, pH, firmness, and seedlessness). The pre-treatments, including the Savitzky–Golay first derivative (SGD1), Savitzky–Golay second derivative (SGD2), and multiplicative scatter correction (MSC), were studied using partial least-square regression (PLSR) and partial least-square–discriminant analysis (PLS-DA) using Unscrambler software (version 10.5; Camo, Oslo, Norway).

Moreover, in this study the model's efficiency was evaluated using the following statistical values: coefficient of determination (R^2), standard error of calibration (SEC),

and standard error of prediction (SEP), which are defined in Eqs. (2)–(4).

$$R^2 = 1 - \frac{\sum_{i=1}^{n}\left(y_i - x_i\right)^2}{\sum_{i=1}^{n}\left(y_i - \bar{y}\right)^2}, \tag{2}$$

$$SEC = \sqrt{\frac{\sum_{i=1}^{n_p}\left(x_i - y_i\right)^2}{n_p - 1}}, \tag{3}$$

$$SEP = \sqrt{\frac{\sum_{i=1}^{n_p}\left(x_i - y_i - \text{bias}\right)^2}{n_p - 1}}, \tag{4}$$

where x_i is the predicted value of firmness, SSC, or pH from each observation; y_i is the measured value; and n_p is the number of observations used in the validation set.

3 Results and discussion

3.1 Chemical and physical analyses

The firmness, pH, and SSC data of the seedless and seeded 'Kyoho' grape berries recorded at 79, 85, and 93 DAF (Table 1) were used in the calibration and prediction sets. Throughout the fruit development, the seeded grape was less firm than the seedless grape, presenting values of 9.39, 5.88, and 7.74 N versus 13.62, 9.59, and 13.38 N at 79, 85, and 93 DAF, respectively. In contrast, the SSC and pH of the seeded grapes were higher than the seedless grapes in the context of the maturity of the grape berry. The seeded grape will develop faster than the seedless grape because the exogenous GA_3 application interferes with seed development and inhibits the growth of the seeds and the berry in seeded grapes, such as 'Kyoho' and 'Red Globe' cultivars (Cheng et al. 2013). In conventional analyses of the chemical and physical qualities, berries are typically destroyed.

Table 1 Chemical and physical attributes of the 'Kyoho' table grape used in this study

		Firmness (N.)	pH	SSC (%)
Harvesting date No. 1 (79 DAF)	Seedless	13.62	3.43	16.99
	Seeded	9.39	3.62	18.72
	Average/S.D.	12.1/2.92	3.49/0.13	17.57/1.32
Harvesting date No. 2 (85 DAF)	Seedless	9.59	3.51	17.77
	Seeded	5.88	3.64	19.73
	Average/S.D.	8.36/2.17	3.55/0.09	18.42/1.25
Harvesting date No. 3 (93 DAF)	Seedless	13.38	3.61	17.96
	Seeded	7.74	3.74	20.43
	Average/S.D.	11.50/3.42	3.66/0.11	18.78/1.63

The analysis can only be carried out with random sampling. Conversely, NIRS can determine the aforementioned quality parameters and the berries can remain intact and continue to develop.

3.2 Raw spectrum

The raw spectra (400–1000 nm) of the 'Kyoho' grape were pre-processed in the laboratory and the field, as shown in Fig. 3. In both locations, the spectra showed the same peak at around
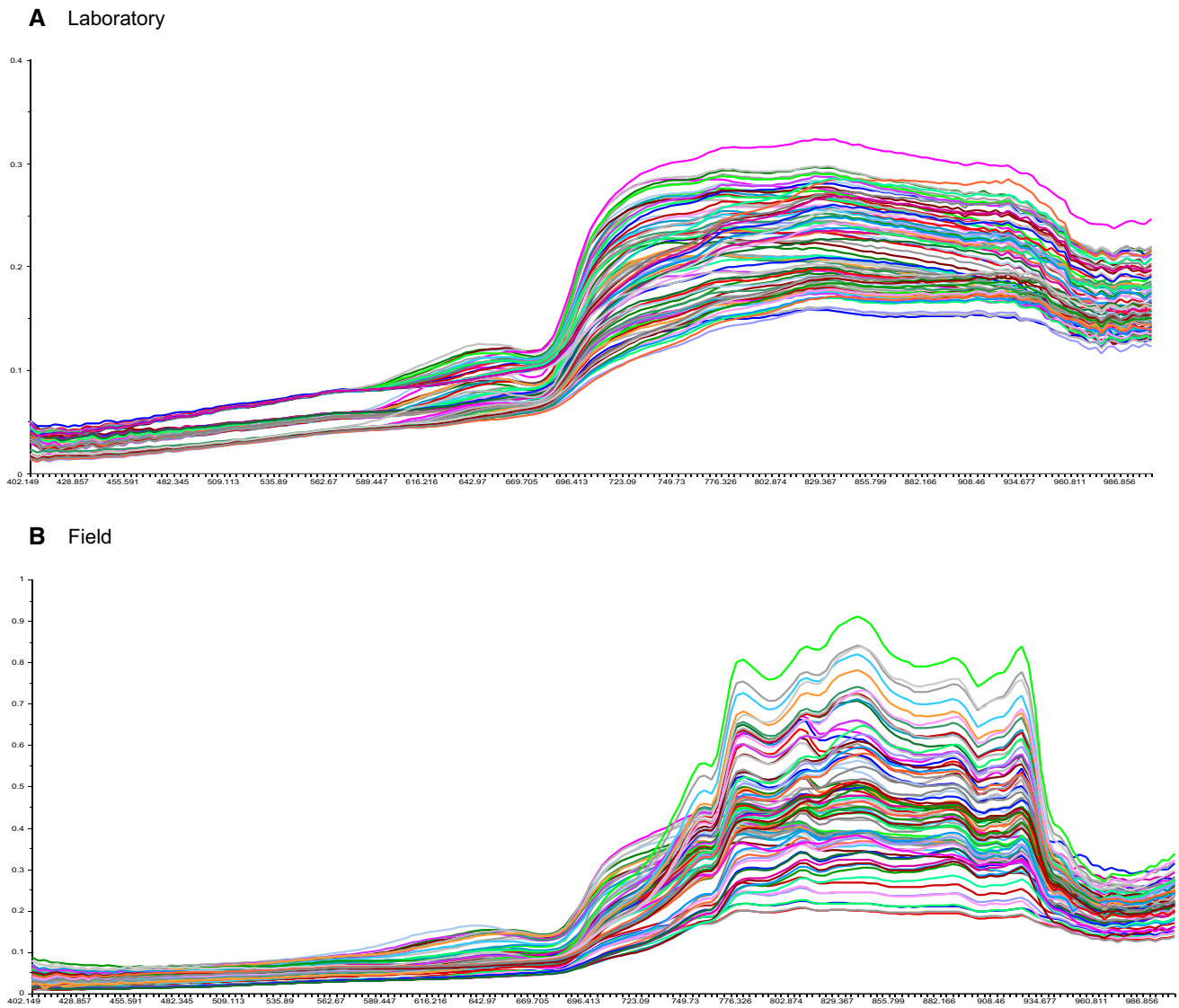
A Laboratory

B Field

Fig. 3 Raw spectrum of the 'Kyoho' table grape over the wavelength range 400–1000 nm, in the laboratory (**a**) and in the field (**b**)

Table 2 Calibration and prediction models with the best pre-treatment techniques in the laboratory and the field

Parameter	Location	Pre-treatment	PLS Factors	Calibration (57 samples)		Prediction (29 samples)	
				SEC	R^2	SEP	R^2
Firmness	Laboratory	SGD1	3	1.3902	0.8249	1.6101	0.7427
	Field	SGD1	7	1.1135	0.8877	1.4870	0.7804
pH	Laboratory	MSC	1	0.0637	0.7198	0.0699	0.6276
	Field	SGD1	6	0.0525	0.8099	0.0552	0.7676
SSC	Laboratory	MSC	2	0.7938	0.6944	0.8129	0.6926
	Field	SGD2	3	0.7016	0.7613	0.6452	0.8052

720–950 nm, but the original spectrum acquired in the field was noticeably higher compared with that recorded in the laboratory. There were several environmental factors affecting the in-field spectral wavebands. Variations in the air humidity and berry temperature, as well as instrumental noise significantly affected the spectral information, especially for the near infrared region. Such variations were addressed with suitable data preprocessing techniques thereafter (Ji et al. 2015).

3.3 Calibration and prediction analyses

The raw spectra of the 'Kyoho' grape both in the laboratory and the field, along with the physical parameters (firmness, pH, and SSC) were analysed and modified by PLSR using three different pre-treatments: SGD1, SGD2, and MSC. A total of 57 samples was used for developing the calibration model, and 29 samples were used for developing the prediction model. The results are displayed in Table 2 and Fig. 4.
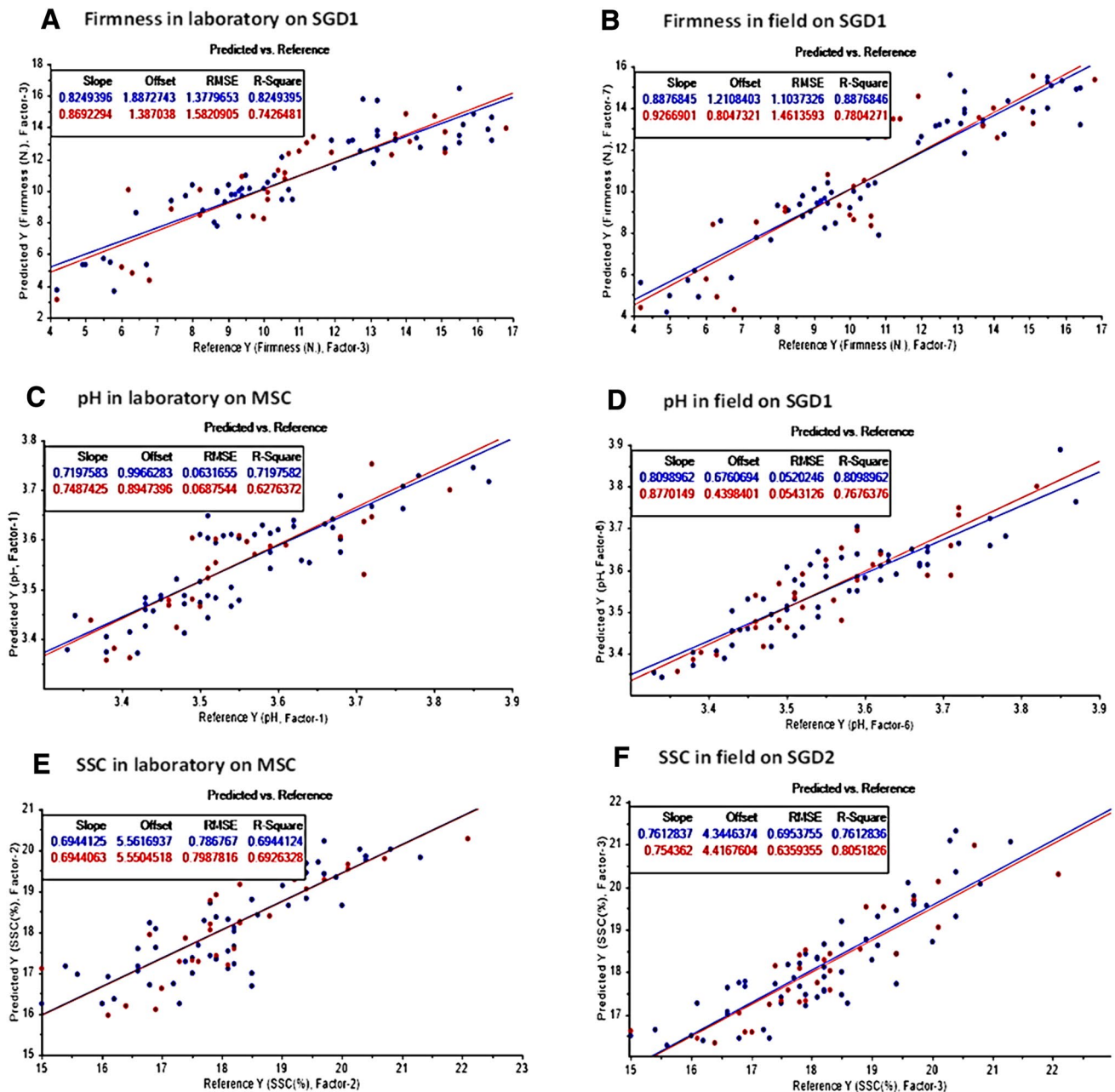

Fig. 4 Calibration (blue) and prediction (red) models of firmness, pH and SSC, showing important statistical values (Slope, Offset, RMSE, and R^2) for the best pre-treatments (SGD1, SGD2, and MSC) in the laboratory and the field conditions

Table 3 Peak wavelengths of firmness, pH, and SSC in the laboratory and the field

Parameter	Location	Pre-treatment	Peak wavelength (nm.)
Firmness	Laboratory	SGD1	**693.1, 769.7**, 944.5
	Field	SGD1	**693.1, 773.0**, 918.3, 924.9
pH	Laboratory	MSC	719.8, 928.1, **934.7**, 944.5, 980.4
	Field	SGD1	766.4, **931.4**
SSC	Laboratory	MSC	719.8, **928.1, 934.7**, 944.5
	Field	SGD2	**924.9, 934.7**

Bold figures are the similar peak wavelengths in the laboratory and the field of each parameter

From the analysis, the R^2 of prediction and SEP of firmness were 0.7427 and 1.6101 N in the laboratory, and 0.7804 and 1.4870 N in the field, respectively, when pre-treated by SGD1. For the calibration model, the R^2 and SEC of firmness were 0.8249 and 1.3902 N in the laboratory, and 0.8877 and 1.1135 N in the field, respectively. There were no notable differences between the values recorded in the laboratory and in the field, thus suggesting that NIRS can be applied in the field as a decision-making tool for determining harvesting date and quality management. These R^2 values were greater than 0.64, which indicates that the models were suitable for screening the physical attributes (SSC, pH, and firmness) of the grapes ($R^2 = 0.64$–0.81) and produced reliable predictions ($R^2 = 0.81$–0.90) (Williams 2007). Fu et al. (2008) verified the usefulness of NIRS in predicting the firmness of white peach using the PLSR method. In that work, 120 peaches were used for calibration, and 60 for prediction. For each sample, reflectance spectra were acquired in the range of 800–2500 nm. The best results were obtained with MSC spectra pre-treatment ($R^2_{calibration} = 0.948$ and $R^2_{validation} = 0.864$) (Fu et al. 2008).

The $R^2_{prediction}$ of pH in the laboratory and the field were 0.6276 and 0.7676 while the SEP were 0.0699 and 0.0552, respectively. The $R^2_{calibration}$ of pH in the laboratory and the field were 0.7198 and 0.8099 when pre-treated using MSC and SGD1, respectively. Thus, this PLSR model was acceptable. A similar result was found when analysing the NIR reflectance spectra (350–2500 nm) of Satsuma mandarin (*Citrus reticulata*) (Gómez et al. 2006). For pH, the $R^2_{calibration}$ was 0.865, and the SEC was 0.106 (Gómez et al. 2006). When the calibration model was used to predict the data for 30 unanalysed mandarins, the prediction result was reasonable ($r = 0.81$), and the SEP was 0.18 with a bias of –0.028 (Gómez et al. 2006). The PLS approach appeared to be acceptable since seven factors were used in the calibration model (Gómez et al. 2006).

For SSC in the laboratory and the field, the $R^2_{prediction}$ were 0.6926 and 0.8052, the SEP were 0.8129% and 0.6452%, and

the $R^2_{calibration}$ were 0.6944 and 0.7613 by MSC and SGD2, respectively. The performance of these models was somewhat comparable to that developed for the SSC of the 'Nebbiolo' wine grape, which showed an $R^2_{prediction}$ of 0.82, SEP of 7.31%, $R^2_{calibration}$ of 0.72, and SEC of 5.89% (Guidetti et al. 2010). These values were based on data obtained using NIRS (380–1650 nm) on 25 wine grapes (red and white) whilst they were ripening on the vine. Cross-validation results indicated that the NIRS technique provided excellent precision for SSC ($R^2 = 0.94$). This confirms that the NIRS technique is well-suited for evaluating the internal quality characteristics related to firmness, pH, and SSC. Moreover, according to González-Caballero et al. (2011), this approach enables the non-destructive quantification of chemical changes that take place during on-vine ripening and helps with the decision regarding the optimal timing for harvesting.

3.4 Loading weight analysis

The $R^2_{prediction}$ of the best pre-treatment of each parameter was analysed by the loading weight. The results are shown in Table 3 and Fig. 5 The SGD1 was the best pre-treatment for firmness in both the laboratory and the field, which both showed the peak at 693.1 nm was similar to that at 769.7–773.0 nm. The best pre-treatment for pH was MSC in the laboratory and SGD1 in the field. The peak wavelength was 931.4–934.7 nm. The best pre-treatment for SSC was MSC in the laboratory and SGD2 in the field, the peak wavelengths were 928.1–924.9 and 934.7 nm, respectively. From the R^2 and peak wavelength data, the parameters (firmness, pH, and SSC) were quite similar between the laboratory and the field. This suggests that in-field NIRS analysis will provide results that are comparable to those obtained from analysis in the laboratory. When evaluating the loading weight vectors from the PLS-DA of wine grape NIR spectra (1600–2400 nm) between ripening stages, the sugar peaks were around 1750 and 2067 nm, and the water peaks were around 1900 and 1970 nm (González-Caballero et al. 2012).

3.5 Percentage of seedlessness classification

The seedlessness of the 'Kyoho' table grape, which was exposed to GA₃ applications during cultivation, is very important for obtaining a premium price in Japan. It is difficult to detect the presence or absence of seeds without destroying the sample. In this context, NIRS analysis is an interesting approach. The NIR spectrum of the 'Kyoho' grape and the seedlessness data in the laboratory and the field were analysed using the PLS-DA prediction model. A total of 57 grape samples on the last harvesting date (93 DAF) were analysed by Unscrambler software for
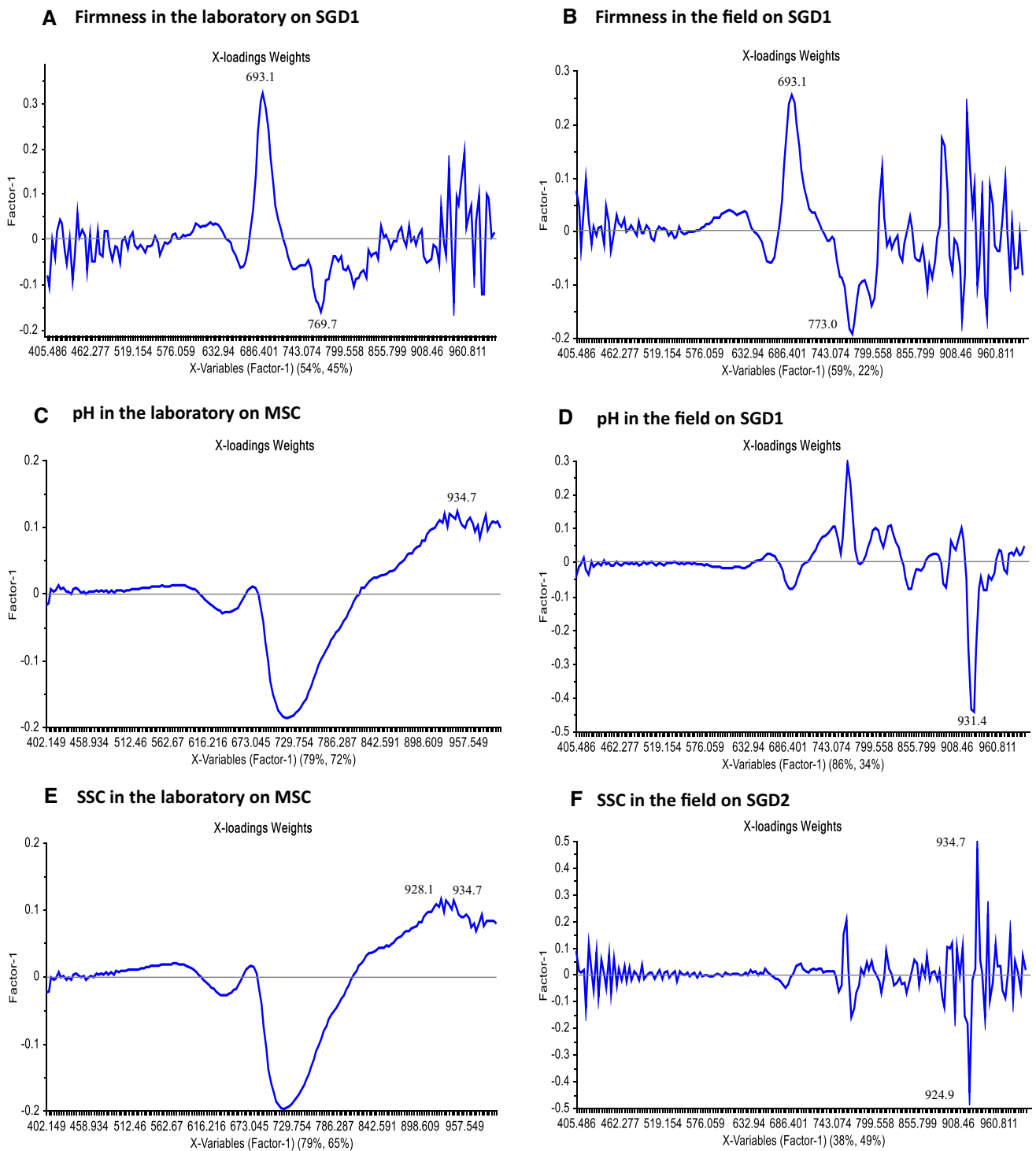
Fig. 5 Loading weight analysis of firmness, pH, and SSC for the best pre-treatment (SGD1, SGD2, and MSC) in the laboratory and the field

constructing the calibration model, and 29 samples were used for the prediction model.

Table 4 shows the percentage of seedlessness classification using PLS-DA, the best result was obtained from the laboratory with 93.1% accuracy using the SGD1 spectral pre-processing technique. In contrast, a percentage of seedlessness classification of 79.3% was obtained in the field test upon MSC pre-treatment. This is the first study to report a seedlessness analysis for Japanese table grapes using NIRS. In the PLS-DA models developed by Guidetti et al. (2010),

Table 4 Percentage of seedlessness classification in the laboratory and the field

Location	Pre-treatment	No. of samples for model	No. of samples for prediction			Grand total	% Seedlessness
			Correct	Mistake	Total		Classification
Laboratory	SGD1	57	27	2	29	86	**93.10**
	SGD2	57	23	6	29	86	79.31
	MSC	57	27	2	29	86	**93.10**
Field	SGD1	57	21	8	29	86	72.41
	SGD2	57	13	16	29	86	44.83
	MSC	57	23	6	29	86	**79.31**

Bold figures are the highest percentage seedlessness classification of pre-treatment under laboratory and field

for 77.1% of both ripe and unripe wine grapes their SSC was correctly classified by the calibration model and 68.8% was correctly classified by the validation model.

4 Conclusion

The results from this study confirmed that the quality of Japanese table grapes can be efficiently predicted both in the laboratory and in the field. Interactance measurements of wavebands from 400 to 1100 nm with spectral acquisition of PLSR are considered promising techniques for predicting berry firmness, juice pH levels, and SSC, as well as the percentage of seedlessness classification. Some modifications of the optical apparatus for NIR measurements are still needed in order to increase prediction accuracy and reproducibility.

Compliance with ethical standards

Conflict of interest The authors declare that they have no conflict of interest.

Ethical standards All the procedures performed in studies that involved human participants were in accordance with the ethical standards of the institutional and/or national research committee and with the 1964 Helsinki declaration and its later amendments or comparable ethical standards. All applicable international, national, and/or institutional guidelines for the care and use of animals were followed.

Human and animal participants This article does not contain any studies with human participants or animals performed by any of the authors.

Informed consent Informed consent was obtained from all individual participants included in the study.

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