Comparison of two Vis-NIR instruments based on reflectance or interactance mode for fruit quality measurements

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Introduction

Determination of fruit quality meeting consumers' preferences is a complicated task because several parameters, such as colour, absence of surface defects, calibre, flesh firmness, soluble solids content or acidity have to be taken into account. Today, most of the quality measurements are performed using classical destructive methods, which are time consuming, costly and limited to a small number of representative fruits per batch. Non-destructive measurement using near infrared (NIR) technology, for example, provides an interesting alternative, and many studies have already illustrated the potential of such instruments for the assessment of fruit quality.[1] However, most of these studies reported results from only one type of fruit, whereas many retailers need to quickly and efficiently measure the quality of several fruit types. Finding one instrument that provides acceptable results for different fruit types is thus highly desired. Commercially available NIR instruments vary in their optical geometry, their detector type as well as their mode of measurement (reflectance, transmittance, interactance). In the present study we compared two NIR instruments using different modes, interactance or reflectance. We determined which one gives the best results for measuring total soluble solids of eight different types of fruit, varying in calibre, firmness or water content. The study reported here is a first step towards the identification of a NIR instrument useful for the measurement of many parameters regarding fruit quality.

Materials and Methods

Samples

Total soluble solids were measured in apples, pears, apricots, peaches, nectarines, melons, tomatoes and strawberries. To increase variability, fruit batches from different varieties, orchards and origins were used.

Near infrared spectroscopy

Spectra were collected using two diode-array Vis-NIR instruments working in the wavelength range of 350 to 1100 nm: NIR Case (SACMI, Italy) measuring in interactance mode and QualitySpec® Pro (Analytical Spectral Devices, Inc., USA) measuring in reflectance mode. The optical geometry of the NIR Case could be optimised for a given fruit: the device was equipped with eight halogen lights, four of them being switched off to avoid signal saturation for apricots, peaches, nectarines, tomatoes and strawberries. Integration time and sample holder were adapted according to type and size of fruit to achieve an optimal signal (Table 1). The QualitySpec® Pro instrument was equipped with a fiber optic contact probe working at 2 nm intervals. The same instrument setup was used for all the fruit types.

Each fruit batch was measured on both instruments: fruit were placed on the fruit holder with the stem-calyx axis horizontal. Spectra were collected from four positions (apples, pears, tomatoes, strawberries and melons) or from two opposite positions (apricots, peaches, nectarines) along the equator of each fruit and averaged to provide a mean spectrum for each fruit.

Table 1. Description of the NIR Case methods used for each fruit type.

	Number of halogen lamps	Size of sample holder	Number of scans	Integration time reference (ms)	Integration time sample (ms)
Apple	8	Intermediate	5	40	40
Pear	8	Intermediate	5	40	50
Peach	4	Intermediate	5	80	80
Nectarine	4	Intermediate	5	80	80
Tomato	4	Intermediate	5	80	20
Apricot	4	Intermediate	5	40	40
Melon	8	Large	5	60	120
Strawberry	4	Small	5	120	60

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Reference analysis

After NIR measurements, each fruit was crushed to extract the juice, and total soluble solids (TSS, °Brix) was determined using an electronic refractometer (Atago PR32).

Chemometrics

Calibrations were established with The Unscrambler version 9.8 (CAMO, Norway). Calibration models were developed using partial least squares regression (PLS) with full cross-validation. Several pretreatment options were investigated including spectral smoothing, standard normal variates (SNV), multiplicative scattering correction (MSC) and first derivative. For all models the wavelength range between 650 and 970 nm was used. Calibration performance was assessed in terms of R^2, root mean square error of calibration and validation (RMSECV) and ratio of standard error of prediction to standard deviation (RPD).

Results and Discussion

Typical spectra of the fruit obtained with both the NIR Case and QualitySpec® Pro instruments mainly indicated differences between spectral modes (Figure 1). NIR Case spectra of botanically related fruit, like apple and pear, or peach and nectarine, were very similar, while distinct absorption features were observed for the other fruit. The maximum peak occurred at about 700 nm for all fruit except melons (800 nm), which had an additional low-level absorbance between 500 and 680 nm. QualitySpec® Pro reflectance spectral features were particularly differentiated in the region of 450 to 700 nm. A strong absorption observed at 680 and 970 nm is attributed to chlorophyll and water, respectively.

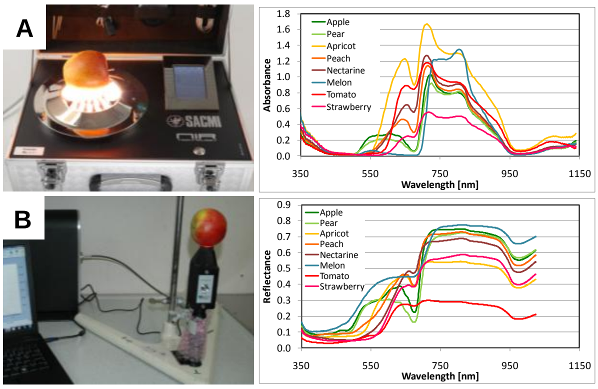

Figure 1. Examples of average spectra of the measured range of fruit (apple, pear, apricot, peach, nectarine, melon, tomato, strawberry) obtained with: **A**: NIR Case (interactance) and **B**: QualitySpec® Pro (reflectance).

Table 2. Number of samples, mean, standard deviation (S.D.) and range of values of the calibration sets.

	Number of samples	Mean	S.D.	Range
Apple	80	12.32	1.68	8.8–17.2
Pear	96	12.09	1.37	9.1–15.7
Peach	100	9.43	1.19	6.6–12.1
Nectarine	85	9.89	1.03	7.4–12.6
Tomato	94	4.62	0.82	3.1–6.6
Apricot	205	14.45	2.00	8.8–21.4
Melon	56	11.07	2.11	6.7–14.5
Strawberry	78	7.59	1.24	3.8–10.4

Table 2 shows statistics of the fruit datasets used for calibrations of TSS. The large range of TSS values for apricots (8.8–21.4 °Brix) was due to the large number of varieties used for the study (about forty). Tomatoes, on the contrary, showed a smaller TSS distribution (3.1–6.6 °Brix), despite the inclusion of different varieties and ripeness stages (green to red) in the dataset.

Based on values of R^2, RMSECV and RPD of the cross-validations, the NIR Case instrument measuring in interactance mode was more accurate at assessing TSS, across all tested fruit types, than the QualitySpec® Pro instrument operating in reflectance mode (Table 3). NIR Case R^2 values varied between 0.87–0.94 while QualitySpec® R^2 varied between 0.79 and 0.88. RMSECV values for TSS measurements obtained with NIR

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Case models were 0.1 to 0.2°Brix lower than those obtained with QualitySpec®. However, RMSECV values from both instruments were well within the range of published values.[1]

Table 3. Cross-validations of the NIR calibrations for total soluble solids (°Brix) obtained for the measured range of fruit. NC: NIR Case, QS: QualitySpec® Pro, R^2: coefficient of determination, RMSECV: root mean square error of cross-validation, RPD: residual predictive deviation.

	Pre-treatment		**R^2**		**RMSECV**		**RPD**	
	NC	QS	NC	QS	NC	QS	NC	QS
Apple	MSC	SG 5–2	0.92	0.83	0.48	0.67	3.5	2.5
Pear	MSC	SG 5–2	0.90	0.88	0.43	0.47	3.2	2.9
Peach	MSC	SG 5–2	0.87	0.82	0.44	0.51	2.7	2.3
Nectarine	SNV	SG 5–2	0.94	0.86	0.25	0.39	4.1	2.6
Tomato	SG 5-2	SNV	0.90	0.79	0.26	0.39	3.2	2.4
Apricot	MSC	SG 1–5–2	0.90	0.88	0.58	0.71	3.5	2.8
Melon	SNV	SG 5–2	0.89	0.84	0.70	0.87	3.0	2.4
Strawberry	SNV	SG 5–2	0.94	0.88	0.32	0.44	3.9	2.8

Taken together, our data showed that the NIR Case was the better instrument for measuring TSS of fruit. Our results are consistent with the studies of Schaare and Fraser[2] and of McGlone et al.,[3] who compared three different modes of measurement (reflectance, interactance and transmission) on kiwifruit and mandarins. In the first study, interactance was found to be the most accurate mode for measuring TSS of kiwifruit. In the second study, transmission was the best mode for assessing TSS of mandarins, followed by interactance, with reflectance giving the poorest results. These previous assessments were performed by changing the configuration on the same instrument. In our study, we tested commercial devices which were not only different on the mode of measurement but also on their instrumental setup. The latter could also explain the better performance of NIR Case which has been especially developed for fruit measurement. In contrast, QualitySpec® Pro has been designed for applications in different fields like pharmaceuticals, forest products, production mining or agriculture. Liu et al.[4] improved the instrumental setup of QualitySpec® Pro for fruit measurements by applying an external light source in order to get a 45° angle between light source and detector. Although this setup has been successfully implemented, adjustments such as light barrier or an external light source could improve the performance.

Few studies have compared the performance of a single NIR spectrometer for the quality assessment of different fruit types, even though this would be very helpful for fruit retailers. Walsh et al.[5] measured TSS of a range of fruit with an instrument working in transmission mode and reported RMSECV values that were lower (apples and peaches), similar (melons) or higher (tomatoes and nectarines) than the RMSECV values obtained in our study. Since Walsh et al.[5] used only fruits from a single location and harvest date, the comparability of the two studies is limited. This illustrates the challenge of calibrating a single instrument for various applications. Results from this study show that this challenge is on the way to being overcome. Further work is required to develop calibration models working efficiently with the high variability found in fruit batches of different varieties, origins and ripeness stages.

Conclusion

The present study shows that the NIR Case instrument based on interactance mode was more suitable than the QualitySpec® Pro instrument based on reflectance mode for measuring TSS of all the eight types of fruit tested. Although the current models have to be optimised by including data from additional harvesting years, and external validations of the calibrations are required, the NIR Case instrument already shows promising results for practical application.

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