Use of near infrared spectroscopy for the determination of internal quality of entire apples

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Introduction

This work is performed in the framework of the HiDRAS program (High - Quality Disease Resistant Apples for a Sustainable agriculture). The aim is to build up a specific apple data base which should allow the breeders to make a much better use of the tremendous diversity available in many European Genetic Resources collections.

The present work investigated the use of NIRS to assess the internal quality of apples by determining Vitamin C, total polyphenol and sugar contents (brix).

Material and methods

Samples

In this study, a large amount of apple samples ($n = 2500$) were collected to cover a broad variability including several varieties and cultivars harvested between 2004 and 2007.

Wet chemistry

Concerning the reference values, the vitamin C content was determined by HPLC, the total polyphenol content was obtained by the Folin–Ciocalteu method and the sugar content was obtained on the basis of a polarimetric Brix determination.

Table 1. Characteristics of the apple data base and performances of the LS-SVM models.

Criteria	Units	Min-Max	Mean	*SD*	Calibration			Validation		
					n	*SEC*	*SD/ SEC*	*n*	*SEP*	*SD/ SEP*
Vitamin C	Mg/100 DM	0.27–75.0	13.5	12.4	800	3.4	3.7	295	4.9	2.0
Polyphenol	µg g^{-1}	276–7300	1186	720	2000	178	4.1	627	140	5.1
Brix	°brix	7.2–20.9	12.3	1.6	1000	0.45	3.6	853	0.37	4.3

Data acquisition

The spectra were acquired by a FOSS NIRSystems 6500 scanning monochromator (400–2500, 2 nm) with the DCA module (Direct Contact Analysis). The instrument is placed upside down in
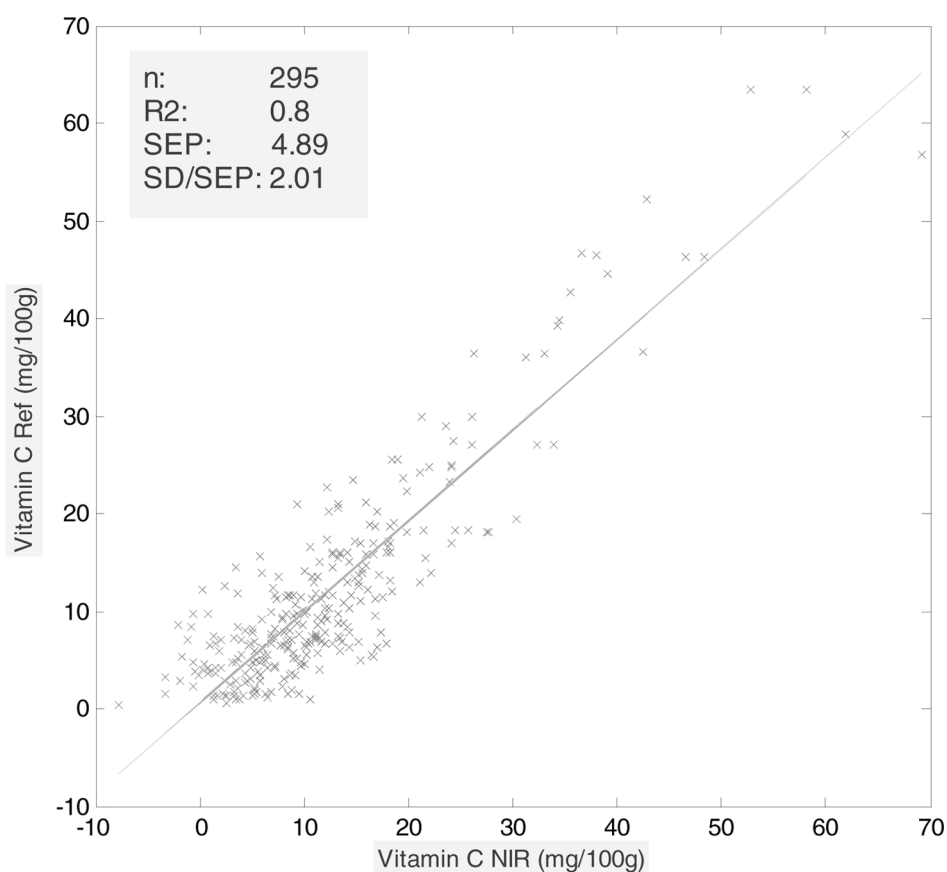
Figure 1. Scatter plot obtained for Vitamin C.
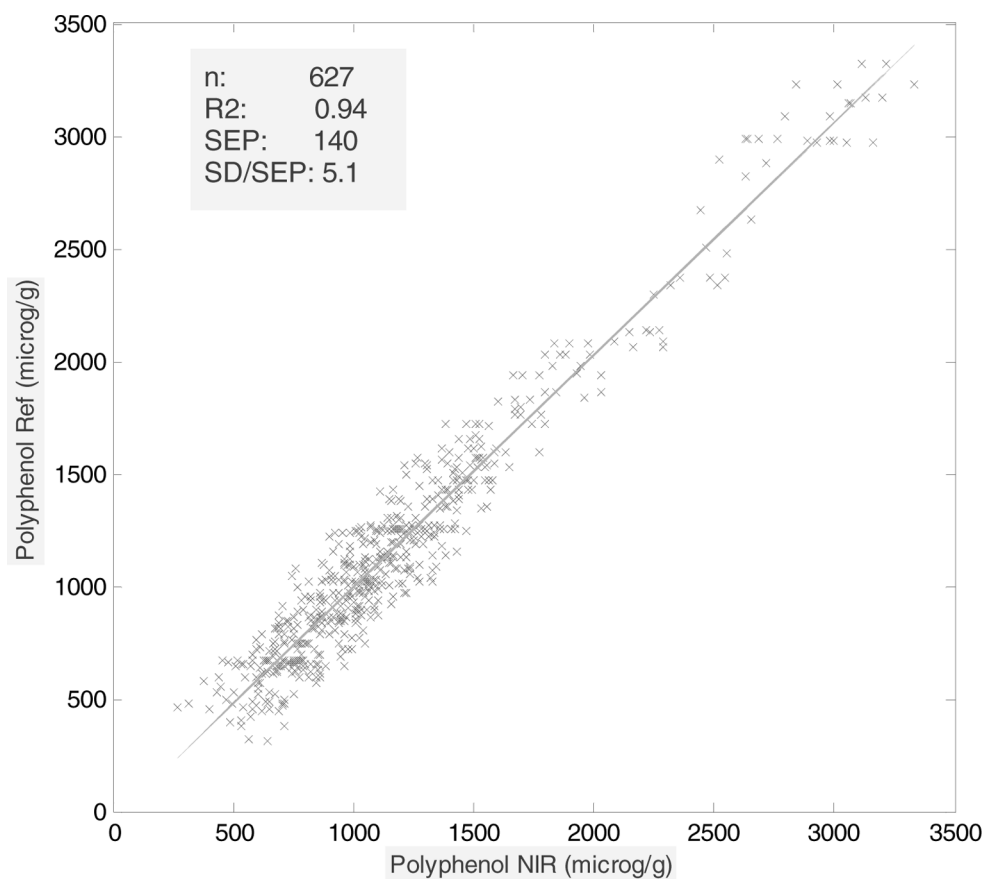
Figure 2. Scatter plot obtained for the total Polyphenol content.

order to place the fruit directly on the detector's window. To integrate the variability of the fruit, 4 measurements have been performed by rotating the apple.

Data teatment

The Winisi III package was used for collecting the spectra and for the exploratory analysis by Principal Component Analysis (PCA). Calibration models have been developed by using the Least Squares Support Vector Machine (LS-SVM) algorithm built in a Matlab environment (Matlab 7.5.0 R20e07b).[1] The database has been split into calibration and test sets. The LS-SVM models have been constructed using the calibration set and validated using the test set.
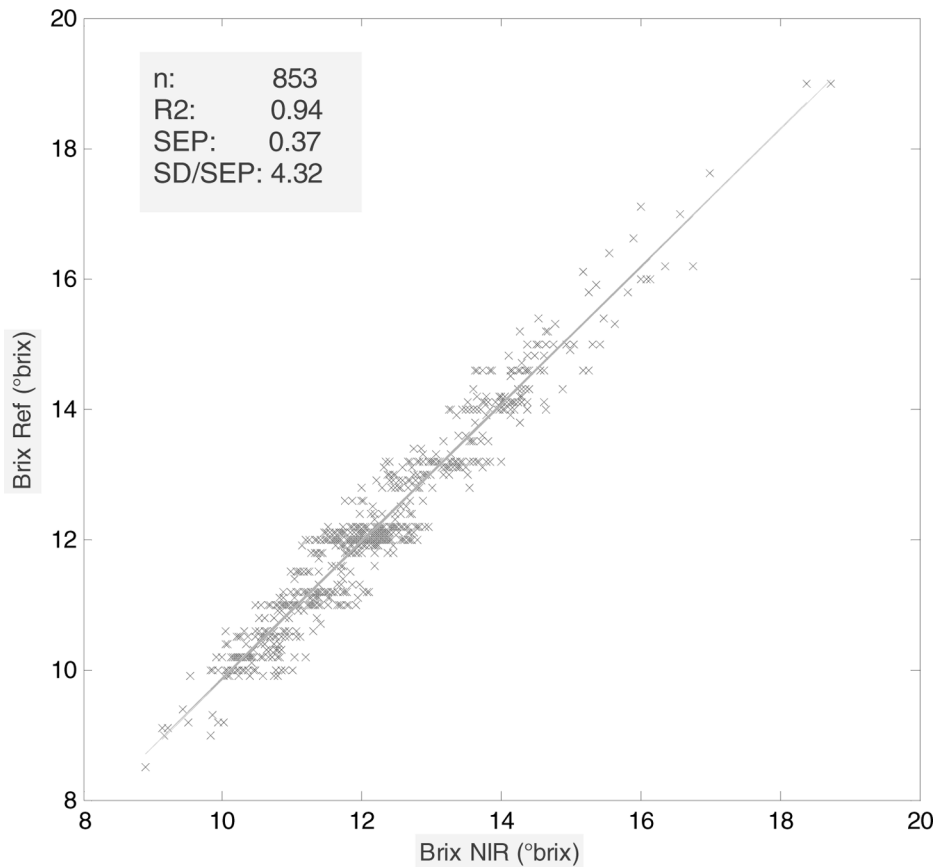
Figure 3. Scatter plot obtained for the sugar content (Brix).

Results

The best results have been obtained with a Savitsky–Golay first derivative (9,2,1) as preprocessing treatment. The accuracy obtained with the LS - SVM regression technique (see table 1) allows a good estimate of the internal quality of entire apples. Figures 1, 2 and 3 shows the scatter plots obtained on the validation sets for the criteria under investigation.

With a *SD/SEP* ratio of 2.0, the Vitamin C concentrated in the outer layer of the fruits can be estimated to at least provide a three groups assignment (Figure 1).

The best results are achieved for the prediction of the total polyphenol content as obtained by the Folin–Ciocalteu reagent.[2] With a *SD/SEP* value of 5.1, it is possible to have a quantitative determination of the total phenolics (Figure 2).

A *SD/SEP* value of 4.3 allows a quantitative determination of the total sugar content (brix) of entire apples.

Conclusion

From the study, the following outputs have been gathered:

The results indicate that NIR spectroscopy and reflection mode could be used in breeding programs to assess the internal quality of entire apples.

Although the vitamin C content is rather low, as it is concentrated in the outer layer of the fruits, NIR spectroscopy in reflectance mode can be used to have an estimate of low total concentration levels of Vitamin C.

The total polyphenols as determined by the Folin-Ciocalteu method can be predicted by NIRS. This means that NIRS can be used to analyze huge apple collections, in order to identify the varieties showing the highest polyphenol content by the prediction of polyphenols.

The sugar content can also be determined by predicting the Brix of entire fruits, using NIR spectroscopy.

References

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