[Cortés, V., Blasco, J., Aleixos, N., Cubero, S., & Talens, P. (2019). Monitoring strategies for quality control of agricultural products using visible and near-infrared spectroscopy: A review. Trends in food science & technology. 85, pp. 138-148.]

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Institut Valencià
d'Investigacions Agràries

[http://dx.doi.org/10.1016/j.tifs.2019.01.015]

# Monitoring strategies for quality control of agricultural products using visible and near-infrared spectroscopy: A review

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**ABSTRACT**

*Background*

The increasing demand for quality assurance in agro-food production requires sophisticated analytical methods for in-line quality control. One of these techniques is visible and near-infrared (VIS-NIR) spectroscopy, which has low running costs, does not need sample preparation, and is non-destructive, environmentally friendly, and fast. Despite these advantages, only a limited amount of research has been conducted on VIS-NIR in-line applications to measure, control, and predict quality in fruits and vegetables.

*Scope and Approach*

The applicability of VIS-NIR spectroscopy for the off-line and in-line monitoring of quality in postharvest products has been addressed in this review. The document focuses on the comparison between the two processes for the same agro-food product, highlighting the main advantages and disadvantages, problems, solutions, and differences.

*Key Findings and Conclusions*

VIS-NIR techniques, combined with chemometric methods, have shown great potential due to their fast detection speed, and the possibility of simultaneously predicting multiple quality parameters or distinguishing between products according to the objectives. Being able to automate processes is a great advantage compared to routine off-line analyses, mainly due to the savings achieved in time, material, and personnel. However, in numerous cases, in-line implementation has not been accomplished in the corresponding studies, hence the scarcity of real in-line applications. Recent demands, together with the advances being made in the technology and a reduction in the price of equipment, makes VIS-NIR technology an analytical alternative for continuous real-time food quality controls, which will become predominant in the next few years.

**Keywords:** VIS-NIR spectroscopy; in-line; off-line; chemometrics; quantification; qualification

NOMENCLATURE

ANN, artificial neural network

BC, background colour

CA, cluster analysis

CDA, canonical discriminant analysis

CR$^2$, squared canonical correlation

IQI, internal quality index

ITB, internal tissue browning

KNN, K-nearest neighbors

LDA, linear discriminant analysis

LV, latent variables

MIR, med-infrared

MLR, multiple linear regression

MSC, multiplicative scatter correction

OSC, orthogonal signal correction

PCR, principal component regression

PLS, partial least square

PLS-DA, partial least squares-discriminant analysis

QDA, quadratic discriminant analysis

QS, quantitative starch

r, correlation coefficient

$r_p$, correlation coefficient for prediction

$R^2$, coefficient of determination

RMSE, root mean square error

RMSECV, root mean square error of cross-validation

RMSEP, root mean square error of prediction

$R_P^2$, determination coefficient for prediction

RPD, ratio of performance to deviation

SEP, square error of prediction

SIMCA, soft independent modeling of class analogy

SNV, standard normal variate

SPI, starch pattern index

SSC, soluble solids content

SVM, support vector machine

SWIR, short-wavelength near-infrared

SWS, standardized weighted sum

TA, titratable acidity

TDIS, time-delayed integration method

TPC, content of total phenolic compounds

VIS-NIR, visible and near-infrared

## 1. Introduction

The current demands in an increasingly competitive and globalized framework call for the agri-food sector to produce higher quality products, which requires an in-line inspection of the entire production. For this reason, the research and development of fast, accurate and non-destructive tools that are capable of evaluating each individual product is increasing at high speed (Porep *et al.*, 2015). Among them, VIS-NIR spectroscopy appears as a promising alternative. This technology allows easy, fast, accurate, non-destructive, and inexpensive quality assessments to be performed without previous sample preparation, and the potential exists to develop instruments for in-line measurements. However, as it is based on indirect measurements that produce highly complex data, VIS-NIR spectroscopy needs the support of chemometrics to take full advantage of the corresponding spectra (Porep *et al.*, 2015; Huang *et al.*, 2008; Siesler, 2008).

The versatile applications of VIS-NIR spectroscopy for fruit quality assessment have already been reviewed, for instance by Cen and He (2007) and Kumaravelu and Gopal (2015). Wang *et al.* (2015) and Nicolaï *et al.* (2007) review an extensive number of applications using VIS-NIR and chemometrics to measure the quality and properties of products. Giovenzana *et al.* (2015) presented an overview of spectroscopy applications on fruit and vegetables, in this case focused on different moments throughout the production and distribution process. Cozzolino *et al.* (2011) surveyed the diverse steps and procedures that should be taken into account when calibrations based on NIR spectrometry are developed for the assessment of chemical properties in fruits. Magwaza *et al.* (2012) and Jha *et al.* (2010), respectively, have also reviewed other specific applications of VIS-NIR spectroscopy for certain agro-food products, such as citrus fruit and mango.

Generally, reviews on this topic have been focused on off-line and laboratory applications. This is probably because, until recently, little in-line or real-time research had been conducted with the aim of measuring, controlling, or predicting the quality of fruits and vegetables at the industrial or semi-industrial level. Working in-line requires special equipment to move the products in a manner that is synchronized with the measurements, and presents a series of restrictions that makes them different from ideal static measurements. Some previous research carried out by Huang *et al.* (2008) was focused on NIR on/in-line applications for monitoring quality in food and beverages, but without going deeper into the agro-food sector and without making any comparisons between off/in-line applications for the same product.

Therefore, this work reviews for the first time the implementation of VIS-NIR spectroscopy applications for the in-line inspection of agro-food products under semi-industrial conditions, and establishes comparisons between these and other similar studies with the same products based on static measurements under laboratory conditions. Moreover, the main differences between the two types of implementations are highlighted, the advantages and disadvantages of each system are emphasized, and the problems and practical solutions adopted are reviewed.

## 2. VIS-NIR technology

Infrared spectroscopy is based on the absorbance of radiation at molecular vibrational frequencies occurring for the O-H, N-H, and C-H groups and for the C-C, C-O, C-N, and N-O groups in organic materials (Soriano-Disla *et al.*, 2014). Overtone and combination vibrations of the first group dominate the NIR region (4,000–14,286 $\mathrm{cm}^{-1}$; 700–2,500 nm), while those of the second group absorb in the mid-infrared region (MIR) (400–4,000 $\mathrm{cm}^{-1}$; 2,500–25,000 nm). Electronic transitions absorb in the visible region (14,286–25,000 $\mathrm{cm}^{-1}$; 400–700 nm) and in the ultraviolet region (25,000–40,000 $\mathrm{cm}^{-1}$; 250–400 nm) (Rossel *et al.*, 2006; Coates, 2000). Figure 1 shows the electromagnetic spectrum, with the location of the different spectral regions.

A varied selection of spectroscopic instruments is accessible and there are around sixty NIR spectrometer manufacturers around the world (McClure & Tsuchikawa, 2007). These instruments can be divided into three groups: (i) laboratory devices, (ii) sorting and grading, and (iii) portable devices. The main differences between these types of NIR devices and an overview of spectroscopy applications on fruits and vegetables based on the instrumental characteristics of the NIR devices employed for the studies can be found in Beghi *et al.* (2017). The literature shows that many applications of VIS-NIR spectroscopy involve the use of benchtop and portable full spectra devices, but recent studies have been conducted using simplified optical systems based on a small number of wavelengths (Beghi *et al.*, 2013; Giovenzana *et al.*, 2014; Civelli *et al.*, 2015). This topic is discussed in Beghi *et al.* (2017). Regardless of the type of instrument, the principal components are a sample holder, where the sample is placed, a light source, a detector to record the received light intensity, and a computer unit to register and process the spectral information obtained (Siesler *et al.*, 2008). The use of fiber-optic probes is often desirable, as many current applications are based on their intensive use in order to simplify data acquisition procedures due to their capacity for multiplexing, thus allowing them to monitor many points (Pasquini, 2003).

Several optical alternatives are available for VIS-NIR spectroscopy: ‘reflectance’, ‘transmittance’, ‘transflectance’, and ‘interactance’ (Alander *et al.*, 2013). Illustrations of these different optical geometries are shown in Figure 2, where it can be seen how the location of the detectors with respect to the sample determines the mode of operation.

According to the mode used, light attenuation by the sample, relative to the reference, is known as reflectance (R) or transmittance (T). Commonly, R and T are transformed into absorbance (log 1/R or log 1/T) to perform chemometric analyses (Herold *et al.*, 2009).

## 3. Chemometrics

The powerful VIS-NIR instruments currently available rapidly provide large amounts of information that need efficient pre-treatment and useful evaluation. Chemometrics is a discipline developed for this purpose. Generally, it involves three steps: (i) spectral data pre-treatment; (ii) construction of calibration models; and (iii) model transfer. The main objective of spectra pre-treatment is to transform the data into more useful information capable of facilitating its subsequent multivariate analysis. Some of the more frequent pre-treatments for VIS-NIR spectra include: (i) smoothing methods (for example, Gaussian filter, moving average, median filter, and Savitzky-

Golay smoothing); (ii) derivation methods (usually first and second derivative); (iii) MSC; (iv) OSC; (v) SNV; (vi) wavelet transformation; (vii) normalization and/or scaling; and (viii) de-trending to eliminate the baseline drift in the spectrum. Moreover, different combinations of these methods applied simultaneously can also be used for signal processing (Brereton, 2003). Information about the application of these pretreatments to VIS-NIR spectra can be found in Savitzky and Golay (1964), Wold *et al.* (1998), Berrueta *et al.* (2007), Liu *et al.* (2011), Lorente *et al.* (2015), and Wang *et al.* (2015). The calibration model can be built for qualitative and/or quantitative analysis of the samples. Figure 3 shows a schematic diagram of possible experimental approaches using VIS-NIR spectroscopy techniques. The first step of the data analysis is often principal component analysis (PCA), in order to detect patterns and outliers (Cozzolino *et al.*, 2011) in the measured data. Another unsupervised pattern recognition technique that can be used is CA (Næs *et al.*, 2002). Subsequently, a qualitative or quantitative approach to the data will be chosen according to the objectives of the particular study. Qualitative analysis involves classifying the samples according to their VIS-NIR spectra based on pattern recognition methods (Roggo *et al.*, 2007). The classification model is created with a training set of samples with known categories, and subsequently this model is evaluated by a test set of unknown samples. In order to do this, many qualitative methods are used, such as LDA (Baranowski *et al.*, 2012), QDA, KNN (Derde *et al.*, 1987), PLS-DA (Liu *et al.*, 2011), SIMCA (Pontes *et al.*, 2006), ANN (Mariey *et al.*, 2001), and SVM (Chen *et al.*, 2007). Of these techniques, PLS-DA is often commonly selected for optimal classification. For quantitative analyses, which focus on predicting some of the properties that, for example, can greatly influence fruit quality, methods such as MLR, PCR, PLS, or ANN are broadly used. The best modeling method suggested for most VIS-NIR spectra is PLS (Lin & Ying, 2009). The accuracy of VIS-NIR models for fruit quality prediction is usually evaluated by means of the $R^2$ or r, the RMSE, and the RPD (Bobelyn *et al.*, 2010). Generally, a good model should achieve a low RMSE and a high $R^2$ or r. Additionally, a satisfactory model should have an RPD value of more than 2.5, a value above 3.0 being very good (Kamruzzaman *et al.*, 2016; Cortés *et al.*, 2016). Other statistical parameters reflecting a good model are low average difference between predicted and measured values (Bias) and a small difference between RMSEC and RMSEP. Moreover, a good model should have as few LV as possible.

## 4. Monitoring strategies in the postharvest stage

Regarding the implementation process used, off-line, at-line, on-line, and in-line measurements can be differentiated. The definitions of these terms are as follows (Dickens, 2010):

- off-line: analyzes the sample away from the production line, classically in a laboratory.
- at-line: random samples are manually extracted from the production line and examined in a place very close to the process line.
- on-line: samples are diverted from the production line to be analyzed directly in the recirculation loop (by-pass) and are returned to the production line after analysis.
- in-line: analyzes the sample within the running production line (*in situ*).

The terms on-line and in-line are seemingly used similarly and so, for the publications cited in this review, the term employed in the original article is the one used. An exhaustive review of the literature shows that the VIS-NIR technique has been used with a wide range of agro-food applications. One of the major areas where the technology can be employed is the postharvest handling of fruit and vegetables. This section summarizes the recent position of research in the above-mentioned area by highlighting current investigative and exploratory studies about off-line and in-line applications.

### *4.1. Overview of the off-line and in-line applications*

When this technology is applied for an off-line quality control, random samples are acquired from finished products or from reaction blends and analyzed at laboratory scale (Roggo *et al.*, 2007). The main disadvantages are that this type of analysis requires some time and, in the meantime, the production of a product of unknown quality continues. Additionally, most commercially accessible VIS-NIR spectroscopy instruments are limited to single point analysis, and therefore if the sample is heterogeneous, such as fruit, a single value might not be able to characterize the bulk sample (Wold *et al.*, 2011).

Some solutions to these disadvantages are, on the one hand, to install the spectrometer very close to the production line and to perform the analysis at-line immediately after sampling. This is possible due to research innovations that are creating more compact and portable VIS-NIR devices (McClure *et al.*, 2007). On the other hand, another solution is to use a multipoint NIR system capable of monitoring different points simultaneously. In addition, the system could be installed at different standoff distances adapted to the shape and size of the product, or even different light sources for individual probes depending on the objectives. Other advantages that these multipoint probes offer are their flexibility and the fact that they can be coupled to different scenarios.

However, acquiring data from the intact product in real time is a currently being a critical requirement in processing lines. Thus, the demand for strict quality controls and optimization of the product is expected to increase. In-line monitoring of the food production process has considered the use of specific analytical methods and in situ sensors or probes, such as NIR spectroscopy (Zude, 2008), acoustics and vibration (Patist & Bates, 2008), microwave resonance technology (Kim *et al.*, 1999), visible imaging (Cubero *et al.*, 2016), and hyperspectral imaging (Balasundaram *et al.*, 2009; Lorente *et al.*, 2012). In particular, NIR spectroscopy has proven to be a fast, non-invasive and effective tool in fruit quality analysis, and its in-line application may be used to substitute slow and tedious conventional methods (Ait Kaddour & Cuq, 2009; Alcalà *et al.*, 2010). Therefore, the ability to collect data about the quality of the entire fruit production using in-line systems based on spectroscopy could be valuable for the industry. Hence, the determination of the quality traits of intact fruit in movement with the use of VIS-NIR technology is a great benefit for production lines such as conveyor belts, sample cups on a conveyor belt or hopper systems, and research has been conducted in this regard. Figure 4 depicts the implementation of a system for automatic acquisition of spectra in a line of inspection and control of fruit quality. The system shows a possible solution to the problem of the acquisition of measurements at uniform distances on one side of the fruit. Another solution could be to locate the probe in the lower part, but there would be problems of dirt accumulation and a uniform measurement distance is not guaranteed either.

### *4.2. Comparison between off-line and in-line applications*

Although several reviews of VIS-NIR applications on intact harvest fruits and vegetables have been published to date (Blanco & Villarroya, 2002; Huang *et al.*, 2008;

Cen & He, 2007; Su *et al.*, 2017; Wang *et al.*, 2017; López *et al.*, 2013; Lin & Ying, 2009; Magwaza *et al.*, 2012; Opara & Pathare, 2014; Wang *et al.*, 2015; Wiesner *et al.*, 2014; Porep *et al.*, 2015; Wang *et al.*, 2007; Jha *et al.*, 2010; Nicolaï *et al.*, 2007; Cozzolino *et al.*, 2011; Ruiz-Altisent *et al.*, 2010), only one of them (Porep *et al.*, 2015) delves into the possible applications of NIR technology on a semi-industrial and industrial scale. Porep *et al.* (2015) based their review on NIR applications that follow an on-line strategy. In contrast, this paper carries out the first comparative study between off- and in-line strategies followed by different authors for the same type of product (apples, watermelons, nectarines, olives, and pears). The implementations of VIS-NIR spectroscopy that have been reviewed are summarized in Table 1.

In most off-line applications with fruits, the acquisition mode used is reflectance, except for the study conducted by Khatiwada *et al.* (2016) and the two studies by McGlone *et al.* (2002 and 2003), which were carried out in transmittance mode with apples, as well as the studies by Abebe (2006) and Jie *et al.* (2013) with watermelons or Xu *et al.* (2014) with pears. In the case of in-line applications the situation is similar: the predominant acquisition modes are reflectance, used in all in-line applications with olives (Salguero-Chaparro *et al.*, 2012, 2013 and 2014), and the transmittance mode in the case of pears (Xu *et al.*, 2012; Sun *et al.*, 2016). Examples of both acquisition modes were found in in-line applications with watermelon (Jie *et al.*, 2014; Tamburini *et al.*, 2017) and apple (McGlone *et al.*, 2005; Shenderey *et al.*, 2010; Ignat *et al.*, 2014), but nectarines were the only example found that employed the interactance mode (Golic & Walsh, 2006).

Several works have been already done to analyzed VIS-NIR spectroscopy applied to the in-line analysis of intact apples. In the study by Shenderey *et al.* (2010) moldy core in apples was detected by a VIS-NIR mini-spectrometer (400–1,000 nm) installed in-line. The system was fitted with four cells, and in each cell rubber rings at the top and bottom hold the fruit and the fiber-optic probe was connected below the fruit-cell locations. The fruits were analyzed in transmittance mode, with a whole scan time of 1 second per fruit. The accuracy of the classification results was high: 92% recognition of healthy apples and 100% detection of deterioration at levels of damage above 30%. Similarly, and also in transmittance mode, but in this case with a higher analysis speed (approximately 5 fruits per second), McGlone *et al.* (2005) developed two prototype on-line NIR systems to measure the proportion of internal tissue browning in apples in the wavelength range 650–950 nm. The same motor-driven fruit conveyor with 21 fruit cups was used for both prototypes. The best correlations for the measurement of ITB in apples, comparing the two transmission systems that were designed, indicated that a conventional large aperture approach to the spectrometry (LAS) was more precise as well as more economical and less susceptible to data misses than an alternative based on the recently developed TDIS. In reflectance mode, but with the same speed as that employed by Shenderey *et al.* (2010) (1 sample per second), Ignat *et al.* (2014) assessed the possibility of quickly determining the quality of apples of three cultivars using two commercial spectrophotometers (VIS-NIR with a spectral region between 340–1,014 nm and SWIR between 850–1,888 nm). The advantage of this study is that they evaluated both instruments to measure the same product in a static mode (off-line) and on a moving conveyor (in-line). In this case, the conveyor had 24 fruit cells and the light source illuminated the sample vertically with an optical fiber at an inclination of 45°. The results demonstrated that in-motion measurement modes gave higher SWS than static measurements in some cases. During in-motion measurement modes, the scanned area of the samples is greater and, thus, it reflects the individual apples more accurately compared with the static mode, where the optical fiber observes a reduced area. Additionally, comparing certain quality parameters, such as SSC, in both static and in-motion studies resulted in similar prediction models as regards the in-motion and the static measurements. Moreover, a comparison of certain quality parameters in both off-line and in-line studies resulted in similar and, in some cases, even better models for in-line than for static measurements. For example, observing the prediction of the SSC in studies with similar spectral ranges and the same measurement mode, an $R^2$=0.86 was obtained for the in-motion study by Ignat *et al.* (2014), which is a very similar result to that found in static studies by Nicolaï *et al.* (2007), with an $R^2$=0.87, Xiaobo *et al.* (2007), with an $R^2$=0.93, and the studies by Pissard *et al.* (2013) and Guo *et al.* (2016), with an $R^2$=0.94. Schmutzler and Huck (2014) quantified soluble solids content, total acid and polyphenol content of Golden Delicious and Pink Lady apples comparing a novel automated surface scanning technique to a manual measurement. They used a prototype constructed to rotate samples while recording spectra. The samples were analyzed in the wavelength region from 1,000 to 2,500 nm in diffuse reflectance mode. The NIR-based determinations were superior to the manual measurements, for the three analyses and for both varieties of apples, using surface scanning.

Watermelons were analyzed by Jie *et al.* (2014) using a prototype in-line detection system based on the VIS-NIR technique for predicting their soluble solids contents. The prototype works in transmittance mode and the spectral range studied was 687–920 nm. The measurements were conducted on a conveyor belt, where trays were moved at a speed of 0.3 m/s. The best results were obtained using a calibration model based on Monte-Carlo uninformative variable elimination (MC-UVE) jointly with stepwise multiple linear regressions (SMLR) ($r_{pre}$=0.66). The spectra were pre-treated using baseline offset correction (BOC). Recently, Tamburini *et al.* (2017) developed an NIR in-line system to determine lycopene, β-carotene, and total soluble solids content in red-flesh watermelons in the selected wavelength range from 900 to 1,700 nm in reflectance mode. Watermelons were transported along a conveyor belt system at different speeds (2,100, 2,400 and 2,700 rpm). Models were performed using partial least squares (PLS) on pre-treated spectra (derivate and standard normal variation), and the results confirmed a good predictive ability with $R^2_p$ higher than 0.70.

On comparing the off- and in-line studies by Jie *et al.* (2013 and 2014) in transmittance mode, it is observed that off-line results are slightly better ($R^2_p$=0.845 for off-line and $r_{pre}$=0.66 for in-line) but with higher RMSEP (RMSEP=0.574 ºBrix for off-line and RMSEP=0.39 ºBrix for in-line). If this is compared with the other off-line study (Abebe *et al.*, 2006) conducted in transmittance mode found for this type of product, a higher $R^2_p$ (0.81) is also obtained but with higher RMSEP (0.42 %) than for the in-line system.

In the case of nectarines, only one study conducted with an in-line application has been found. In this case, Golic and Walsh (2006) employed an NIR spectrometer (735–930 nm). In contrast to the rest of the in-line systems, this prototype was designed to acquire the fruit spectra in interactance mode (or partial transmittance configuration). The SSC of nectarines were determined above the cup in the conveyor belt by passing each cup at approximately 0.7 m/s, or 6 cups per second. The prediction performance of the model was good in terms of $R^2$>0.8. Comparing the prediction results of SSC of the in-line system (Golic & Walsh, 2006) with the off-line studies, although the mode of data acquisition was different, it was shown how the in-line system achieved, with a smaller spectral range, results as good as or even better than those obtained by Pérez-Marín *et al.* (2009), with an $R^2$=0.89, and Sánchez *et al.* (2011), with an $r^2$=0.47–0.68.

Intact olives were also measured by VIS-NIR reflectance spectroscopy in both off-line and in-line applications by a research group at the University of Córdoba

(Salguero-Chaparro *et al.*, 2012, 2013 and 2014). Salguero-Chaparro *et al.* (2012) studied and optimized some parameters, such as focal distance and integration time, prior to implementing the system at factory level. The spectrometer was fitted on a structure designed expressly to support it and to achieve on-line analysis on a conveyor belt in the spectral range of 380–1,690 nm. With the same semi-industrial scale development line on a conveyor belt, Salguero-Chaparro *et al.* (2013) determined the moisture, fat content and acidity in intact olives. The predictive performance achieved varied depending on spectra pre-treatment and validation strategies. However, the authors determined that the in-line NIR estimate results were adequate with $R^2>0.74$ for the three parameters analyzed in samples in movement. Additionally, Salguero-Chaparro *et al.* (2014) compared on-line versus off-line NIR systems to analyze the same properties as in the previous study. The parameters used were characterized in Salguero-Chaparro *et al.* (2012) and were the focal distance, the speed of the conveyor belt, and the integration time. The values were 13 mm, 0.1 m/s and 5 s, respectively. Similar accuracy for the determination of physicochemical composition in intact olives was obtained for the on-line analysis and using the traditional off-line methodology.

More specifically, on comparing the prediction by the PLS method of certain quality parameters such as fat content, free acidity, and moisture content for the same mode of acquisition (reflectance), it is observed how the predictions achieved in the in-line studies (Salguero-Chaparro *et al.*, 2013 and 2014) were as good ($R^2_{\text{fat content}} = 0.79$ and 0.86; $R^2_{\text{free acidity}} = 0.74$ and 0.77; and $R^2_{\text{moisture content}} = 0.87$ and 0.89) as those analyzed off-line ($R^2_{\text{fat content}} = 0.87$; $R^2_{\text{free acidity}} = 0.76$ ; and $R^2_{\text{moisture content}} = 0.89$).

In the same way as in two studies dealing with apple and one with watermelon, the in-line systems developed for pears have been used in transmission mode. Xu *et al.* (2012) investigated the determination of sugar content in pears between 533–930 nm in an on-line system. The on-line measuring system included a tray conveyor with a circular hole in the back of the tray to fit a collimating lens and an optical fiber used to connect the collimating lens and spectrometer. The halogen lamps were attached to two sides of the tray. The speed of the conveyor belt was 0.5 m/s and the integration time was 100 ms. Similarly, Sun *et al.* (2016) developed on-line VIS-NIR transmittance system to measure soluble solids content and also brown core in pears. Like Xu *et al.* (2012), VIS-NIR spectra were collected using a very similar wavelength range (from 600 to 904 nm) and at a moving speed of 5 samples per second. Furthermore, the system also consisted of a transmission chain, light source, detector, sorting device, and fruit cup.

A comparison of both systems in in-line applications allowed very good results to be obtained for SSC predictions, with an $R^2$ between 0.82 and 0.99. Compared with the SSC analysis off-line and also in transmission mode (Xu *et al.*, 2014), the in-line results are better than those performed off-line ($r_p$=0.96). With respect to off-line analyses but in reflectance mode (Li *et al.*, 2013 and Nicolaï *et al.*, 2008), in-line results were still better than those performed off-line ($r_p$=0.91 and $R^2$=0.60, respectively).

## 4. Conclusions and future directions

Visible and near-infrared reflectance spectroscopy has become a powerful tool for the non-destructive monitoring and prediction of multiple quality and safety attributes of agro-food products. This technique, combined with chemometric methods, has proven to be an alternative to destructive analysis due to its fast detection speed, no need for sample disposal, relative lower cost, and potential to predict multiple quality parameters at the same time, and therefore to distinguish the products according to different characteristics.

Most applications carried out to date have been based on static measurements under controlled laboratory conditions. In these arrangements, the product is placed appropriately and the probe is carefully moved toward the sample to take the measurement. However, recent demands from industry and consumers, together with the advances being made in the technology, makes VIS-NIR spectroscopy a promising analytical tool for routine and real-time food safety and quality controls in the coming years. This would allow all the production to be monitored instead of just choosing some random samples as being representative of the whole batch, as occurs at present.

However, the creation of practical in-line applications running on industrial prototypes is still challenging and requires extensive research to overcome problems such as: i) the negative influence of the high-speed movement of the samples; ii) maintaining the same distance between the probe and the samples regardless of the size or shape of the samples; iii) measuring on different points of the fruit at the same time to avoid the natural distribution of the compounds inside the fruits; and iv) reducing the integration and data processing time to allow the speed of the system to be increased.

## Acknowledgments

This work was partially funded by INIA and FEDER funds through research project RTA2015-00078-00-00. Victoria Cortés López thanks the Spanish Ministry of Education, Culture and Sports for the FPU grant (FPU13/04202).

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## Figure captions

**Figure 1**. The electromagnetic spectrum with the location of the visible and infrared spectral regions.

**Figure 2.** Modes for the acquisition of spectra. L: light source, D: detector.

**Figure 3.** Schematic overview of the different chemometric approaches using VIS-NIR spectra.

**Figure 4.** System for taking measurements of fruits in-line using a spectrophotometer, ensuring uniform distance between the probe and the sample through a computer vision-based system.

**Table 1.** Off-line and in-line applications of VIS-NIR spectroscopy in the assessment of quality in agricultural products.

| Sample | Application | Acquisition mode | Statistic method | Spectral range (range used) | Attributes analyzed | Performance | Ref. |
|---|---|---|---|---|---|---|---|
| **Apples** | **Off-line** | Reflectance | MLR | 350-850 nm; 810-999 nm | SSC | $R_P^2$=0.49, SEP=1.14ºBrix | Ventura *et al.* (1998) |
| | | Transmittance | PLS | 500-750 nm | BC | $R^2_{\text{(on the harvest)}}$=0.78; $R^2_{\text{(on the storage)}}$=0.71 | McGlone *et al.* (2002) |
| | | | | 500-750 nm | Firmness | $R^2_{\text{(on the harvest)}}$=0.63; $R^2_{\text{(on the storage)}}$=0.59 | |
| | | | | 500-750 nm | QS | $R^2_{\text{(on the harvest)}}$=0.66 | |
| | | | | 500-750 nm | SPI | $R^2_{\text{(on the harvest)}}$=0.78 | |
| | | | | 600-1000 nm; 800-1000 nm | SSC | $R^2_{\text{(on the harvest)}}$=0.63; $R^2_{\text{(on the storage)}}$=0.70 | |
| | | | | 500-1100 nm | TA | $R^2_{\text{(on the harvest)}}$=0.38 | |
| | | Transmittance | PLS | 800-1000 nm | Dry matter | $R^2_{\text{(at harvest time)}}$=0.95 and RMSEP=0.29; $R^2_{\text{(post-storage)}}$=0.97 and RMSEP=0.24; | McGlone *et al.* (2003) |
| | | | | | SSC | $R^2_{\text{(at harvest time)}}$=0.79 and RMSEP=0.52%brix;$R^2_{\text{(post-storage)}}$=0.94 and RMSEP=0.30%brix; | |
| | | Reflectance | PLS | 300-1100 nm | SSC | $RMSEP_{corr}$=0.65 ºBrix | Roger *et al.* (2003) |
| | | | | | | Bias=-0.35 – 0.39 ºBrix | |
| | | Reflectance | CDA | 400-1700 nm | Impact bruises and non-bruised tissue | $CR^2$=0.68 | Xing *et al.* (2003) |
| | | | | | Compression bruises and sound tissue | $CR^2$=0.68 | |

**Table 1.** *(Continued)*

| Sample | Application | Acquisition mode | Statistic method | Spectral range (range used) | Attributes analyzed | Performance | Ref. |
|---|---|---|---|---|---|---|---|
| **Apples** | **Off-line** | Reflectance | PLS | 380-2000 nm | Streif index | RMSEP=0.14-0.20 log kg $cm^{-2}$ $\%brix^{-1}$ | Peirs *et al.* (2005) |
| | | | | | Respiratory maturity | RMSEP=4.4-7.9 days | |
| | | | | | Physiological maturity | RMSEP=5.7-8.8 days | |
| | | Reflectance | Conceptual model | 400–800 nm | Flavonol content | $r^{2=}0.92$; RMSEP=20 $nmol/cm^2$ | Merzlyak *et al.* (2005) |
| | | Reflectance | PLS-DA | 400-1700 nm | Bruise detection | Classification accuracy >90% | Xing *et al.* (2005) |
| | | Reflectance | Kernel PLS regression | 800-1690 nm | SSC | $R^2$=0.87; RMSEP=0.44 ºBrix | Nicolaï *et al.* (2007) |
| | | Reflectance | PLS | 11000–3800 $cm^{-1}$ | SSC | $r_{p(\text{full spectrum})}$=0.811; $RMSEP_{(\text{full spectrum})}$=1.1522; $R_{p(\text{optimal selected intervals})}$=0.93; $RMSEP_{(\text{optimal selected intervals})}$=0.4424 | Xiaobo *et al.* (2007) |
| | | Reflectance | PLS-DA | 500-1600 nm | Softening index | Classification accuracy >95% | Xing *et al.* (2007) |
| | | | PLS | 804-1294 nm | E-modulus | $r_p$=0.77-0.80 | |
| | | Reflectance | LS-SVM | 400-2500 nm | Vitamin C | $R^2$=0.80; SEP=4.9 | Pissard *et al.* (2013) |
| | | | | | Total polyphenol | $R^2$=0.94; SEP=140 | |
| | | | | | SSC | $R^2$=0.94; SEP=0.37 | |
| | | Reflectance | ICA-SVM | 500-1100 nm | SSC | $r_p$=0.94; RMSEP=0.39 % | Guo *et al.* (2016) |
| | | Reflectance | PLS-DA | 400-1000nm; 1100-2100 nm | Influence of packaging on apple slices | 86.7 % – 100 % | Beghi *et al.* (2016) |

**Table 1.** *(Continued)*

| Sample | Application | Acquisition mode | Statistic method | Spectral range (range used) | Attributes analyzed | Performance | Ref. |
|---|---|---|---|---|---|---|---|
| **Apples** | **Off-line** | Transmittance | PLS | 302-1150 nm and 600-973 nm | Defect level (visual score) | $R^2$=0.83, RMSEP=0.63 | Khatiwada *et al.* (2016) |
| | | | PLS-DA, LDA and SVM | | Internal flesh browning | Classification accuracy>95% | |
| | | Reflectance | QDA, SVM | 800-2500 nm | Bitter pit detection | Average accuracy in the range of 78-87 %, | Kafle *et al.* (2016) |
| | | Reflectance | PLS | 6267-4173 $cm^{-1}$ | Total antioxidant capacity | $R^2$=0.85, SEP=0.13% gallic acid equivalents, RPD=2.8 | Schmutzler *et al.* (2016) |
| | | | | | SSC | $R^2$=0.76, SEP=0.55ºBrix, RPD=2.5 | |
| | | Reflectance | PLS | 408-2498 nm | Dry matter | $R^2_{(peel)}$=0.94; $RPD^{(peel)}$=4.8;<br>$R^2_{(flesh)}$=0.94; $RPD^{(flesh)}$=4.9 | Pissard *et al* (2018) |
| | | | | | TPC | $R^2_{(peel)}$=0.91; $R^2_{(flesh)}$=0.84 | |
| | | | | | | | |
| | **In-line** (sample cups on conveyor) | Transmittance | PLS | 650-950 nm | ITB | $R^2$=0.9; RMSECV=4.1 % | McGlone *et al.* (2005) |
| | (simulated conveyer) | Transmittance | PLS | 400-1000 nm | Moldy core | $r^2$=0.71; SEP=0.036; RPD=1.71 | Shenderey *et al.* (2010) |
| | (cell conveyer) | Reflectance | PLS | 340-1014 nm and 850-1888 nm | SSC | $R^2$=0.86, RMSEP=0.80 | Ignat *et al.* (2014) |
| | | | | | TA | $R^2$=0.66, RMSEP=0.04 | |
| | | | | | Firmness | $R^2$=0.76, RMSEP=6.60 | |
| | | | | | Starch | $R^2$=0.91, RMSEP=0.86 | |

**Table 1.** *(Continued)*

| Sample | Application | Acquisition mode | Statistic method | Spectral range (range used) | Attributes analyzed | Performance | Ref. |
|---|---|---|---|---|---|---|---|
| **Watermelons** | **Off-line** | Transmittance | PLS | 700-1100 nm | SSC | $R^2$=0.81; RMSEP=0.42 % | Abebe (2006) |
| | | Transmittance | MC-UVE-GA-PLS | 220-102 nm (680-950 nm) | SSC | $R^2$=0.845; RMSEP=0.574 ºBrix | Jie *et al.* (2013) |
| | | | | | | | |
| | **In-line** (conveyor belt) | Transmittance | MC-UVE-SMLR | 687-920 nm (200-1100 nm) | SSC | $r_{p=}$0.66; RMSEP=0.39 ºBrix | Jie *et al.* (2014) |
| | | Reflectance | PLS | 900-1700 nm | Lycopene | $R^2$=0.805; SECV=16.19 mg/kg | Tamburini *et al.* (2017) |
| | | | | | B-Carotene | $R^2$=0.737; SECV=0.96 mg/kg | |
| | | | | | SSC | $R^2$=0.707; SECV=1.4 % | |
| **Nectarines** | **Off-line** | Reflectance | PLS | 360-1760 nm | IQI | $R^2$= 0.909-0.927; RMSEP=0.235-0.238 | Cortés *et al.* (2017a) |
| | | | PLS-DA and LDA | 360-1760 nm | Varietal discrimination | Classification accuracy of 100% and 97.44% | |
| | | Reflectance | PLS-DA and LDA | 600-1100 nm | Varietal discrimination | Classification accuracy of 100% | Cortés *et al.* (2017b) |
| | | Reflectance | MPLS | 1600-2400 nm; 400-1700 nm | SSC | $r^2$=0.89;SEP=0.75-0.81% | Pérez-Marín *et al.* (2009) |
| | | | | | Flesh firmness | $r^2$=0.84-0.86; SP=11.6-12.7 N | |
| | | | | | Weight | $r^2$=0.98; SEP=5.40 g | |
| | | | | | Diameter | $r^2$=0.75; SEP= 0.46 cm | |
| | | Reflectance | PLS2-DA | 1600-2400 nm | Shelf-life discrimination | 86-96% | Pérez-Marín *et al.* (2011) |
| | | | | 400-1700 nm | | 66-89% | |
| | | Reflectance | MPLS;LOCAL algorithm | 1600-2400 nm | Weight | $r^2$=0.53;0.59 | Sánchez *et al.* (2011) |
| | | | | | Diameter | $r^2$=0.53;0.56 | |
| | | | | | Flesh firmness | $r^2$=0.85;0.87 | |
| | | | | | SSC | $r^2$=0.47;0.68 | |

**Table 1.** *(Continued)*

| Sample | Application | Acquisition mode | Statistic method | Spectral range (range used) | Attributes analyzed | Performance | Ref. |
|---|---|---|---|---|---|---|---|
| **Nectarines** | **In-line** (the cup conveyor belt) | Interactance | PLS | 735-930 nm | SSC | $R^2 > 0.88$; RMSECV=0.53–0.88 %SSC | Golic & Walsh (2006) |
| **Olives** | **Off-line** | Reflectance | PLS | 400-2500 nm | Fat content | $R^2=0.87$ ; RMSEP=2.50 | Salguero-Chaparro *et al.* (2014) |
| | | | | | Free acidity | $R^2=0.76$ ; RMSEP=3.07 | |
| | | | | | Moisture content | $R^2=0.89$ ; RMSEP=3.48 | |
| | | | LS-SVM | | Fat content | $R^2=0.82$ ; RMSEP=2.28 | |
| | | | | | Free acidity | $R^2=0.69$ ; RMSEP=2.95 | |
| | | | | | Moisture content | $R^2=0.88$ ; RMSEP=3.30 | |
| | **In-line** (conveyor belt) | Reflectance | ANOVA and LSD | 380-1690 nm | Focal distance and integration time | RMS (5s)=28.753 - 66.028 | Salguero-Chaparro *et al.* (2012) |
| | | Reflectance | PLS | 380-1690 nm | Free acidity | $R^2=0.74$ ; RMSEP=2.53 | Salguero-Chaparro *et al.* (2013) |
| | | | | | Moisture content | $R^2=0.87$ ; RMSEP=2.98 | |
| | | | | | Fat content | $R^2=0.79$ ; RMSEP=2.15 | |
| | | Reflectance | PLS | 380-1690 nm | Fat content | $R^2=0.86$ ; RMSEP=2.02 | Salguero-Chaparro *et al.* (2014) |
| | | | | | Free acidity | $R^2=0.77$ ; RMSEP=2.64 | |
| | | | | | Moisture content | $R^2=0.89$ ; RMSEP=3.33 | |
| | | | LS-SVM | | Fat content | $R^2=0.83$ ; RMSEP=2.19 | |

**Table 1.** *(Continued)*

| Sample | Application | Acquisition | Statistic | Spectral range | Attributes | Performance | Ref. |
|---|---|---|---|---|---|---|---|

|  |  | mode | method | (range used) | analyzed |  |  |
|---|---|---|---|---|---|---|---|
| **Pears** | **Off-line** | Reflectance | MLR | 1100-2500 nm | Pectin constituents | R=0.93, SEP=0.62 for alcohol insoluble solids in the fresh weight (for AIS in the FW) | Sirisomboon *et al.* (2007) |
|  |  |  |  |  |  | R=0.95, SEP=8.48 for oxalate soluble pectin content in the alcohol insoluble solids (OSP in the AIS) |  |
|  |  | Reflectance | PLS | 780-1700 nm;<br>875-1030 nm | SSC | RMSEP=0.44°Brix; $R^2$=0.60 | Nicolaï *et al.* (2008) |
|  |  |  |  |  | Firmness | - |  |
|  |  | Reflectance | EW-LS-SVM | 380-1800 nm<br>(400-1800 nm) | SSC | $r_p$=0.9164; RMSEP=0.2506 | Li *et al.* (2013) |
|  |  |  |  |  | pH | $r_p$=0.8809; RMSEP=0.0579 |  |
|  |  |  |  |  | Firmness | $r_p$=0.8912; RMSEP=0.6247 |  |
|  |  | Reflectance | PLS | 300-1100 nm and 1000-2500 nm (680-1000 nm and 1100-2350 nm) | Dry matter | $R^2$=0.78; RMSECV=0.78 | Travers *et al.* (2014) |
|  |  |  |  |  | SSC | $R^2$=0.84; RMSECV=0.44 |  |
|  |  | Transmittance | PLS | 465 - 1150 nm | SSC | $r_p$=0.96; RMSEP=0.29 | Xu *et al.* (2014) |
|  |  |  |  |  |  |  |  |
|  | **In-line** | Transmittance | SMLR | 200-1100 nm<br>(533-930 nm) | SSC | $R^2$=0.8296 | Xu *et al.* (2012) |
|  |  |  | GA-PLS |  |  | $R^2$=0.8781 |  |
|  |  |  | iPLS |  |  | $R^2$=0.8396 |  |
|  |  |  | GA-SPA-MLR |  |  | $R^2$=0.880 |  |
|  |  | Transmittance | PLS | 200-1100 nm<br>(600-904 nm) | Brown core | 98.30 % | Sun *et al.* (2016) |
|  |  |  |  |  | SSC | 97.8 % – 99 % |  |