**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

53 ITB, internal tissue browning

54 KNN, K-nearest neighbors

55 LDA, linear discriminant analysis

56 LV, latent variables

57 MIR, med-infrared

58 MLR, multiple linear regression

59 MSC, multiplicative scatter correction

60 OSC, orthogonal signal correction

61 PCR, principal component regression

62 PLS, partial least square

63 PLS-DA, partial least squares-discriminant analysis

64 QDA, quadratic discriminant analysis

65 QS, quantitative starch

66 r, correlation coefficient

67 $r_p$, correlation coefficient for prediction

68 $R^2$, coefficient of determination

69 RMSE, root mean square error

70 RMSECV, root mean square error of cross-validation

71 RMSEP, root mean square error of prediction

72 $R_P^2$, determination coefficient for prediction

73 RPD, ratio of performance to deviation

74 SEP, square error of prediction

75 SIMCA, soft independent modeling of class analogy

76 SNV, standard normal variate

77 SPI, starch pattern index

78    SSC, soluble solids content

79    SVM, support vector machine

80    SWIR, short-wavelength near-infrared

81    SWS, standardized weighted sum

82    TA, titratable acidity

83    TDIS, time-delayed integration method

84    TPC, content of total phenolic compounds

85    VIS-NIR, visible and near-infrared

86

**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

103      of applications using VIS-NIR and chemometrics to measure the quality and properties

104      of products. Giovenzana *et al.* (2015) presented an overview of spectroscopy

105      applications on fruit and vegetables, in this case focused on different moments

106      throughout the production and distribution process. Cozzolino *et al.* (2011) surveyed the

107      diverse steps and procedures that should be taken into account when calibrations based

108      on NIR spectrometry are developed for the assessment of chemical properties in fruits.

109      Magwaza *et al.* (2012) and Jha *et al.* (2010), respectively, have also reviewed other

110      specific applications of VIS-NIR spectroscopy for certain agro-food products, such as

111      citrus fruit and mango.

112      Generally, reviews on this topic have been focused on off-line and laboratory

113      applications. This is probably because, until recently, little in-line or real-time research

114      had been conducted with the aim of measuring, controlling, or predicting the quality of

115      fruits and vegetables at the industrial or semi-industrial level. Working in-line requires

116      special equipment to move the products in a manner that is synchronized with the

117      measurements, and presents a series of restrictions that makes them different from ideal

118      static measurements. Some previous research carried out by Huang *et al.* (2008) was

119      focused on NIR on/in-line applications for monitoring quality in food and beverages,

120      but without going deeper into the agro-food sector and without making any comparisons

121      between off/in-line applications for the same product.

122      Therefore, this work reviews for the first time the implementation of VIS-NIR

123      spectroscopy applications for the in-line inspection of agro-food products under semi-

124      industrial conditions, and establishes comparisons between these and other similar

125      studies with the same products based on static measurements under laboratory

126      conditions. Moreover, the main differences between the two types of implementations

127     are highlighted, the advantages and disadvantages of each system are emphasized, and

128     the problems and practical solutions adopted are reviewed.

129

130     **2. VIS-NIR technology**

131     Infrared spectroscopy is based on the absorbance of radiation at molecular

132     vibrational frequencies occurring for the O-H, N-H, and C-H groups and for the C-C,

133     C-O, C-N, and N-O groups in organic materials (Soriano-Disla *et al.*, 2014). Overtone

134     and combination vibrations of the first group dominate the NIR region (4,000–14,286

135     $cm^{-1}$; 700–2,500 nm), while those of the second group absorb in the mid-infrared region

136     (MIR) (400–4,000 $cm^{-1}$; 2,500–25,000 nm). Electronic transitions absorb in the visible

137     region (14,286–25,000 $cm^{-1}$; 400–700 nm) and in the ultraviolet region (25,000–40,000

138     $cm^{-1}$; 250–400 nm) (Rossel *et al.*, 2006; Coates, 2000). Figure 1 shows the

139     electromagnetic spectrum, with the location of the different spectral regions.

140     A varied selection of spectroscopic instruments is accessible and there are around

141     sixty NIR spectrometer manufacturers around the world (McClure & Tsuchikawa,

142     2007). These instruments can be divided into three groups: (i) laboratory devices, (ii)

143     sorting and grading, and (iii) portable devices. The main differences between these

144     types of NIR devices and an overview of spectroscopy applications on fruits and

145     vegetables based on the instrumental characteristics of the NIR devices employed for

146     the studies can be found in Beghi *et al*. (2017). The literature shows that many

147     applications of VIS-NIR spectroscopy involve the use of benchtop and portable full

148     spectra devices, but recent studies have been conducted using simplified optical systems

149     based on a small number of wavelengths (Beghi *et al*., 2013; Giovenzana *et al*., 2014;

150     Civelli *et al*., 2015). This topic is discussed in Beghi *et al*. (2017). Regardless of the

151     type of instrument, the principal components are a sample holder, where the sample is

152  placed, a light source, a detector to record the received light intensity, and a computer

153  unit to register and process the spectral information obtained (Siesler *et al.*, 2008). The

154  use of fiber-optic probes is often desirable, as many current applications are based on

155  their intensive use in order to simplify data acquisition procedures due to their capacity

156  for multiplexing, thus allowing them to monitor many points (Pasquini, 2003).

157  Several optical alternatives are available for VIS-NIR spectroscopy: 'reflectance',

158  'transmittance', 'transflectance', and 'interactance' (Alander *et al.*, 2013). Illustrations

159  of these different optical geometries are shown in Figure 2, where it can be seen how

160  the location of the detectors with respect to the sample determines the mode of

161  operation.

162  According to the mode used, light attenuation by the sample, relative to the

163  reference, is known as reflectance (R) or transmittance (T). Commonly, R and T are

164  transformed into absorbance (log 1/R or log 1/T) to perform chemometric analyses

165  (Herold *et al*., 2009).

166

167  **3. Chemometrics**

168

169  The powerful VIS-NIR instruments currently available rapidly provide large

170  amounts of information that need efficient pre-treatment and useful evaluation.

171  Chemometrics is a discipline developed for this purpose. Generally, it involves three

172  steps: (i) spectral data pre-treatment; (ii) construction of calibration models; and (iii)

173  model transfer. The main objective of spectra pre-treatment is to transform the data into

174  more useful information capable of facilitating its subsequent multivariate analysis.

175  Some of the more frequent pre-treatments for VIS-NIR spectra include: (i) smoothing

176  methods (for example, Gaussian filter, moving average, median filter, and Savitzky-

177 Golay smoothing); (ii) derivation methods (usually first and second derivative); (iii)

178 MSC; (iv) OSC; (v) SNV; (vi) wavelet transformation; (vii) normalization and/or

179 scaling; and (viii) de-trending to eliminate the baseline drift in the spectrum. Moreover,

180 different combinations of these methods applied simultaneously can also be used for

181 signal processing (Brereton, 2003). Information about the application of these

182 pretreatments to VIS-NIR spectra can be found in Savitzky and Golay (1964), Wold *et*

183 *al.* (1998), Berrueta *et al.* (2007), Liu *et al.* (2011), Lorente *et al.* (2015), and Wang *et*

184 *al.* (2015). The calibration model can be built for qualitative and/or quantitative analysis

185 of the samples. Figure 3 shows a schematic diagram of possible experimental

186 approaches using VIS-NIR spectroscopy techniques. The first step of the data analysis

187 is often principal component analysis (PCA), in order to detect patterns and outliers

188 (Cozzolino *et al.*, 2011) in the measured data. Another unsupervised pattern recognition

189 technique that can be used is CA (Næs *et al.*, 2002). Subsequently, a qualitative or

190 quantitative approach to the data will be chosen according to the objectives of the

191 particular study. Qualitative analysis involves classifying the samples according to their

192 VIS-NIR spectra based on pattern recognition methods (Roggo *et al.*, 2007). The

193 classification model is created with a training set of samples with known categories, and

194 subsequently this model is evaluated by a test set of unknown samples. In order to do

195 this, many qualitative methods are used, such as LDA (Baranowski *et al.*, 2012), QDA,

196 KNN (Derde *et al.*, 1987), PLS-DA (Liu *et al.*, 2011), SIMCA (Pontes *et al.*, 2006),

197 ANN (Mariey *et al.*, 2001), and SVM (Chen *et al.*, 2007). Of these techniques, PLS-DA

198 is often commonly selected for optimal classification. For quantitative analyses, which

199 focus on predicting some of the properties that, for example, can greatly influence fruit

200 quality, methods such as MLR, PCR, PLS, or ANN are broadly used. The best modeling

201 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

227 technology can be employed is the postharvest handling of fruit and vegetables. This

228 section summarizes the recent position of research in the above-mentioned area by

229 highlighting current investigative and exploratory studies about off-line and in-line

230 applications.

231

232 *4.1. Overview of the off-line and in-line applications*

233 When this technology is applied for an off-line quality control, random samples

234 are acquired from finished products or from reaction blends and analyzed at laboratory

235 scale (Roggo *et al.*, 2007). The main disadvantages are that this type of analysis requires

236 some time and, in the meantime, the production of a product of unknown quality

237 continues. Additionally, most commercially accessible VIS-NIR spectroscopy

238 instruments are limited to single point analysis, and therefore if the sample is

239 heterogeneous, such as fruit, a single value might not be able to characterize the bulk

240 sample (Wold *et al.*, 2011).

241 Some solutions to these disadvantages are, on the one hand, to install the

242 spectrometer very close to the production line and to perform the analysis at-line

243 immediately after sampling. This is possible due to research innovations that are

244 creating more compact and portable VIS-NIR devices (McClure *et al.*, 2007). On the

245 other hand, another solution is to use a multipoint NIR system capable of monitoring

246 different points simultaneously. In addition, the system could be installed at different

247 standoff distances adapted to the shape and size of the product, or even different light

248 sources for individual probes depending on the objectives. Other advantages that these

249 multipoint probes offer are their flexibility and the fact that they can be coupled to

250 different scenarios.

251

252        However, acquiring data from the intact product in real time is a currently being a

253    critical requirement in processing lines. Thus, the demand for strict quality controls and

254    optimization of the product is expected to increase. In-line monitoring of the food

255    production process has considered the use of specific analytical methods and in situ

256    sensors or probes, such as NIR spectroscopy (Zude, 2008), acoustics and vibration

257    (Patist & Bates, 2008), microwave resonance technology (Kim *et al.*, 1999), visible

258    imaging (Cubero *et al.*, 2016), and hyperspectral imaging (Balasundaram *et al.*, 2009;

259    Lorente *et al.*, 2012). In particular, NIR spectroscopy has proven to be a fast, non-

260    invasive and effective tool in fruit quality analysis, and its in-line application may be

261    used to substitute slow and tedious conventional methods (Ait Kaddour & Cuq, 2009;

262    Alcalà *et al.*, 2010). Therefore, the ability to collect data about the quality of the entire

263    fruit production using in-line systems based on spectroscopy could be valuable for the

264    industry. Hence, the determination of the quality traits of intact fruit in movement with

265    the use of VIS-NIR technology is a great benefit for production lines such as conveyor

266    belts, sample cups on a conveyor belt or hopper systems, and research has been

267    conducted in this regard. Figure 4 depicts the implementation of a system for automatic

268    acquisition of spectra in a line of inspection and control of fruit quality. The system

269    shows a possible solution to the problem of the acquisition of measurements at uniform

270    distances on one side of the fruit. Another solution could be to locate the probe in the

271    lower part, but there would be problems of dirt accumulation and a uniform

272    measurement distance is not guaranteed either.

273

274    *4.2. Comparison between off-line and in-line applications*

275        Although several reviews of VIS-NIR applications on intact harvest fruits and

276    vegetables have been published to date (Blanco & Villarroya, 2002; Huang *et al.*, 2008;

277  Cen & He, 2007; Su *et al.*, 2017; Wang *et al.*, 2017; López *et al.*, 2013; Lin & Ying,

278  2009; Magwaza *et al.*, 2012; Opara & Pathare, 2014; Wang *et al.*, 2015; Wiesner *et al.*,

279  2014; Porep *et al.*, 2015; Wang *et al.*, 2007; Jha *et al.*, 2010; Nicolaï *et al.*, 2007;

280  Cozzolino *et al.*, 2011; Ruiz-Altisent *et al.*, 2010), only one of them (Porep *et al.*, 2015)

281  delves into the possible applications of NIR technology on a semi-industrial and

282  industrial scale. Porep *et al.* (2015) based their review on NIR applications that follow

283  an on-line strategy. In contrast, this paper carries out the first comparative study

284  between off- and in-line strategies followed by different authors for the same type of

285  product (apples, watermelons, nectarines, olives, and pears). The implementations of

286  VIS-NIR spectroscopy that have been reviewed are summarized in Table 1.

287       In most off-line applications with fruits, the acquisition mode used is reflectance,

288  except for the study conducted by Khatiwada *et al.* (2016) and the two studies by

289  McGlone *et al.* (2002 and 2003), which were carried out in transmittance mode with

290  apples, as well as the studies by Abebe (2006) and Jie *et al.* (2013) with watermelons or

291  Xu *et al.* (2014) with pears. In the case of in-line applications the situation is similar:

292  the predominant acquisition modes are reflectance, used in all in-line applications with

293  olives (Salguero-Chaparro *et al.*, 2012, 2013 and 2014), and the transmittance mode in

294  the case of pears (Xu *et al.*, 2012; Sun *et al.*, 2016). Examples of both acquisition modes

295  were found in in-line applications with watermelon (Jie *et al.*, 2014; Tamburini *et al.*,

296  2017) and apple (McGlone *et al.*, 2005; Shenderey *et al.*, 2010; Ignat *et al.*, 2014), but

297  nectarines were the only example found that employed the interactance mode (Golic &

298  Walsh, 2006).

299       Several works have been already done to analyzed VIS-NIR spectroscopy applied

300  to the in-line analysis of intact apples. In the study by Shenderey *et al.* (2010) moldy

301  core in apples was detected by a VIS-NIR mini-spectrometer (400–1,000 nm) installed

302　in-line. The system was fitted with four cells, and in each cell rubber rings at the top and

303　bottom hold the fruit and the fiber-optic probe was connected below the fruit-cell

304　locations. The fruits were analyzed in transmittance mode, with a whole scan time of 1

305　second per fruit. The accuracy of the classification results was high: 92% recognition of

306　healthy apples and 100% detection of deterioration at levels of damage above 30%.

307　Similarly, and also in transmittance mode, but in this case with a higher analysis speed

308　(approximately 5 fruits per second), McGlone *et al.* (2005) developed two prototype

309　on-line NIR systems to measure the proportion of internal tissue browning in apples in

310　the wavelength range 650–950 nm. The same motor-driven fruit conveyor with 21 fruit

311　cups was used for both prototypes. The best correlations for the measurement of ITB in

312　apples, comparing the two transmission systems that were designed, indicated that a

313　conventional large aperture approach to the spectrometry (LAS) was more precise as

314　well as more economical and less susceptible to data misses than an alternative based on

315　the recently developed TDIS. In reflectance mode, but with the same speed as that

316　employed by Shenderey *et al.* (2010) (1 sample per second), Ignat *et al.* (2014) assessed

317　the possibility of quickly determining the quality of apples of three cultivars using two

318　commercial spectrophotometers (VIS-NIR with a spectral region between 340–

319　1,014 nm and SWIR between 850–1,888 nm). The advantage of this study is that they

320　evaluated both instruments to measure the same product in a static mode (off-line) and

321　on a moving conveyor (in-line). In this case, the conveyor had 24 fruit cells and the

322　light source illuminated the sample vertically with an optical fiber at an inclination of

323　45º. The results demonstrated that in-motion measurement modes gave higher SWS

324　than static measurements in some cases. During in-motion measurement modes, the

325　scanned area of the samples is greater and, thus, it reflects the individual apples more

326　accurately compared with the static mode, where the optical fiber observes a reduced

327     area. Additionally, comparing certain quality parameters, such as SSC, in both static

328     and in-motion studies resulted in similar prediction models as regards the in-motion and

329     the static measurements. Moreover, a comparison of certain quality parameters in both

330     off-line and in-line studies resulted in similar and, in some cases, even better models for

331     in-line than for static measurements. For example, observing the prediction of the SSC

332     in studies with similar spectral ranges and the same measurement mode, an $R^2=0.86$ was

333     obtained for the in-motion study by Ignat *et al.* (2014), which is a very similar result to

334     that found in static studies by Nicolaï *et al.* (2007), with an $R^2=0.87$, Xiaobo *et al.*

335     (2007), with an $R^2=0.93$, and the studies by Pissard *et al.* (2013) and Guo *et al.* (2016),

336     with an $R^2=0.94$. Schmutzler and Huck (2014) quantified soluble solids content, total

337     acid and polyphenol content of Golden Delicious and Pink Lady apples comparing a

338     novel automated surface scanning technique to a manual measurement. They used a

339     prototype constructed to rotate samples while recording spectra. The samples were

340     analyzed in the wavelength region from 1,000 to 2,500 nm in diffuse reflectance mode.

341     The NIR-based determinations were superior to the manual measurements, for the three

342     analyses and for both varieties of apples, using surface scanning.

343         Watermelons were analyzed by Jie *et al.* (2014) using a prototype in-line

344     detection system based on the VIS-NIR technique for predicting their soluble solids

345     contents. The prototype works in transmittance mode and the spectral range studied was

346     687–920 nm. The measurements were conducted on a conveyor belt, where trays were

347     moved at a speed of 0.3 m/s. The best results were obtained using a calibration model

348     based on Monte-Carlo uninformative variable elimination (MC-UVE) jointly with

349     stepwise multiple linear regressions (SMLR) ($r_{pre}=0.66$). The spectra were pre-treated

350     using baseline offset correction (BOC). Recently, Tamburini *et al.* (2017) developed an

351     NIR in-line system to determine lycopene, β-carotene, and total soluble solids content in

352     red-flesh watermelons in the selected wavelength range from 900 to 1,700 nm in

353     reflectance mode. Watermelons were transported along a conveyor belt system at

354     different speeds (2,100, 2,400 and 2,700 rpm). Models were performed using partial

355     least squares (PLS) on pre-treated spectra (derivate and standard normal variation), and

356     the results confirmed a good predictive ability with $R^2_p$ higher than 0.70.

357         On comparing the off- and in-line studies by Jie *et al.* (2013 and 2014) in

358     transmittance mode, it is observed that off-line results are slightly better ($R^2_p$=0.845 for

359     off-line and $r_{pre}$=0.66 for in-line) but with higher RMSEP (RMSEP=0.574 ºBrix for off-

360     line and RMSEP=0.39 ºBrix for in-line). If this is compared with the other off-line study

361     (Abebe *et al.*, 2006) conducted in transmittance mode found for this type of product, a

362     higher $R^2_p$ (0.81) is also obtained but with higher RMSEP (0.42 %) than for the in-line

363     system.

364         In the case of nectarines, only one study conducted with an in-line application has

365     been found. In this case, Golic and Walsh (2006) employed an NIR spectrometer (735–

366     930 nm). In contrast to the rest of the in-line systems, this prototype was designed to

367     acquire the fruit spectra in interactance mode (or partial transmittance configuration).

368     The SSC of nectarines were determined above the cup in the conveyor belt by passing

369     each cup at approximately 0.7 m/s, or 6 cups per second. The prediction performance of

370     the model was good in terms of $R^2$>0.8. Comparing the prediction results of SSC of the

371     in-line system (Golic & Walsh, 2006) with the off-line studies, although the mode of

372     data acquisition was different, it was shown how the in-line system achieved, with a

373     smaller spectral range, results as good as or even better than those obtained by Pérez-

374     Marín *et al.* (2009), with an $R^2$=0.89, and Sánchez *et al.* (2011), with an $r^2$=0.47–0.68.

375         Intact olives were also measured by VIS-NIR reflectance spectroscopy in both

376     off-line and in-line applications by a research group at the University of Córdoba

377 (Salguero-Chaparro *et al.*, 2012, 2013 and 2014). Salguero-Chaparro *et al.* (2012)

378 studied and optimized some parameters, such as focal distance and integration time,

379 prior to implementing the system at factory level. The spectrometer was fitted on a

380 structure designed expressly to support it and to achieve on-line analysis on a conveyor

381 belt in the spectral range of 380–1,690 nm. With the same semi-industrial scale

382 development line on a conveyor belt, Salguero-Chaparro *et al.* (2013) determined the

383 moisture, fat content and acidity in intact olives. The predictive performance achieved

384 varied depending on spectra pre-treatment and validation strategies. However, the

385 authors determined that the in-line NIR estimate results were adequate with $R^2 > 0.74$ for

386 the three parameters analyzed in samples in movement. Additionally, Salguero-

387 Chaparro *et al.* (2014) compared on-line versus off-line NIR systems to analyze the

388 same properties as in the previous study. The parameters used were characterized in

389 Salguero-Chaparro *et al.* (2012) and were the focal distance, the speed of the conveyor

390 belt, and the integration time. The values were 13 mm, 0.1 m/s and 5 s, respectively.

391 Similar accuracy for the determination of physicochemical composition in intact olives

392 was obtained for the on-line analysis and using the traditional off-line methodology.

393 More specifically, on comparing the prediction by the PLS method of certain

394 quality parameters such as fat content, free acidity, and moisture content for the same

395 mode of acquisition (reflectance), it is observed how the predictions achieved in the

396 in-line studies (Salguero-Chaparro *et al.*, 2013 and 2014) were as good ($R^2_{fat\ content} =$

397 0.79 and 0.86; $R^2_{free\ acidity} = 0.74$ and 0.77; and $R^2_{moisture\ content} = 0.87$ and 0.89) as those

398 analyzed off-line ($R^2_{fat\ content} = 0.87$; $R^2_{free\ acidity} = 0.76$ ; and $R^2_{moisture\ content} = 0.89$).

399 In the same way as in two studies dealing with apple and one with watermelon,

400 the in-line systems developed for pears have been used in transmission mode. Xu *et al.*

401 (2012) investigated the determination of sugar content in pears between 533–930 nm in

402   an on-line system. The on-line measuring system included a tray conveyor with a

403   circular hole in the back of the tray to fit a collimating lens and an optical fiber used to

404   connect the collimating lens and spectrometer. The halogen lamps were attached to two

405   sides of the tray. The speed of the conveyor belt was 0.5 m/s and the integration time

406   was 100 ms. Similarly, Sun *et al.* (2016) developed on-line VIS-NIR transmittance

407   system to measure soluble solids content and also brown core in pears. Like Xu *et al.*

408   (2012), VIS-NIR spectra were collected using a very similar wavelength range (from

409   600 to 904 nm) and at a moving speed of 5 samples per second. Furthermore, the

410   system also consisted of a transmission chain, light source, detector, sorting device, and

411   fruit cup.

412       A comparison of both systems in in-line applications allowed very good results to

413   be obtained for SSC predictions, with an $R^2$ between 0.82 and 0.99. Compared with the

414   SSC analysis off-line and also in transmission mode (Xu *et al.*, 2014), the in-line results

415   are better than those performed off-line ($r_p$=0.96). With respect to off-line analyses but

416   in reflectance mode (Li *et al.*, 2013 and Nicolaï *et al.*, 2008), in-line results were still

417   better than those performed off-line ($r_p$=0.91 and $R^2$=0.60, respectively).

418

419   **4. Conclusions and future directions**

420       Visible and near-infrared reflectance spectroscopy has become a powerful tool for

421   the non-destructive monitoring and prediction of multiple quality and safety attributes

422   of agro-food products. This technique, combined with chemometric methods, has

423   proven to be an alternative to destructive analysis due to its fast detection speed, no

424   need for sample disposal, relative lower cost, and potential to predict multiple quality

425   parameters at the same time, and therefore to distinguish the products according to

426   different characteristics.

427  Most applications carried out to date have been based on static measurements

428 under controlled laboratory conditions. In these arrangements, the product is placed

429 appropriately and the probe is carefully moved toward the sample to take the

430 measurement. However, recent demands from industry and consumers, together with

431 the advances being made in the technology, makes VIS-NIR spectroscopy a promising

432 analytical tool for routine and real-time food safety and quality controls in the coming

433 years. This would allow all the production to be monitored instead of just choosing

434 some random samples as being representative of the whole batch, as occurs at present.

435  However, the creation of practical in-line applications running on industrial

436 prototypes is still challenging and requires extensive research to overcome problems

437 such as: i) the negative influence of the high-speed movement of the samples; ii)

438 maintaining the same distance between the probe and the samples regardless of the size

439 or shape of the samples; iii) measuring on different points of the fruit at the same time

440 to avoid the natural distribution of the compounds inside the fruits; and iv) reducing the

441 integration and data processing time to allow the speed of the system to be increased.

442

447

448 **References**

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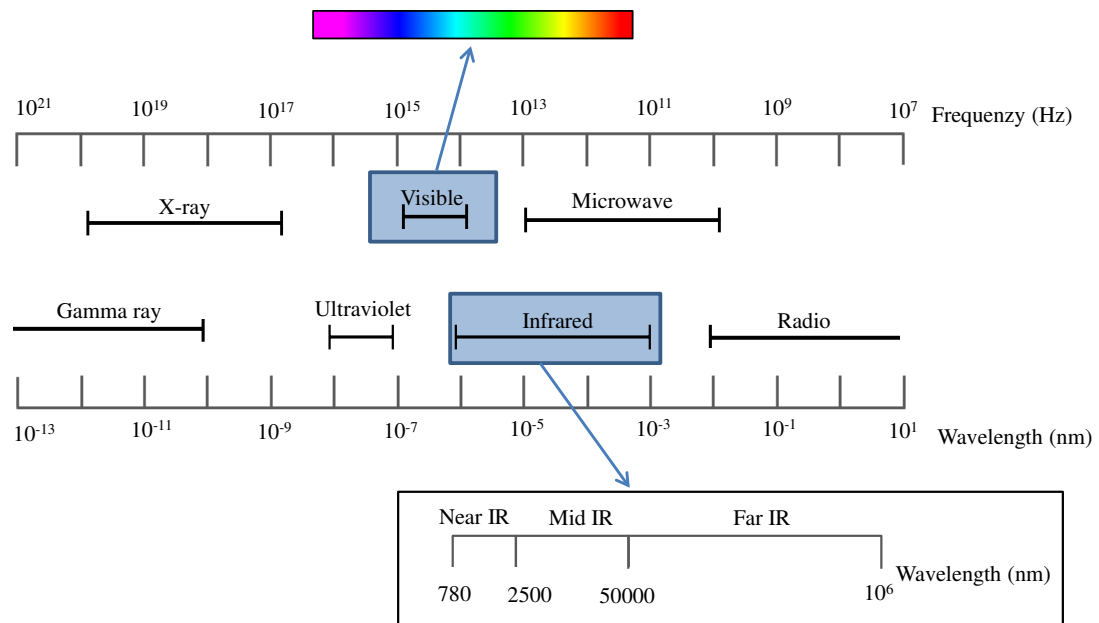
**Figure captions**

**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.

**Figure 1.** V. Cortés et al.

**(a) Transmittance**

**(b) Reflectance**

**(c) Transflectance**

**(d) Interactance**

**Figure 2.** V. Cortés et al.

Physico-chemical analysis

Spectroscopy techniques

**NIR**

Quantitative

Qualitative

Fruit samples
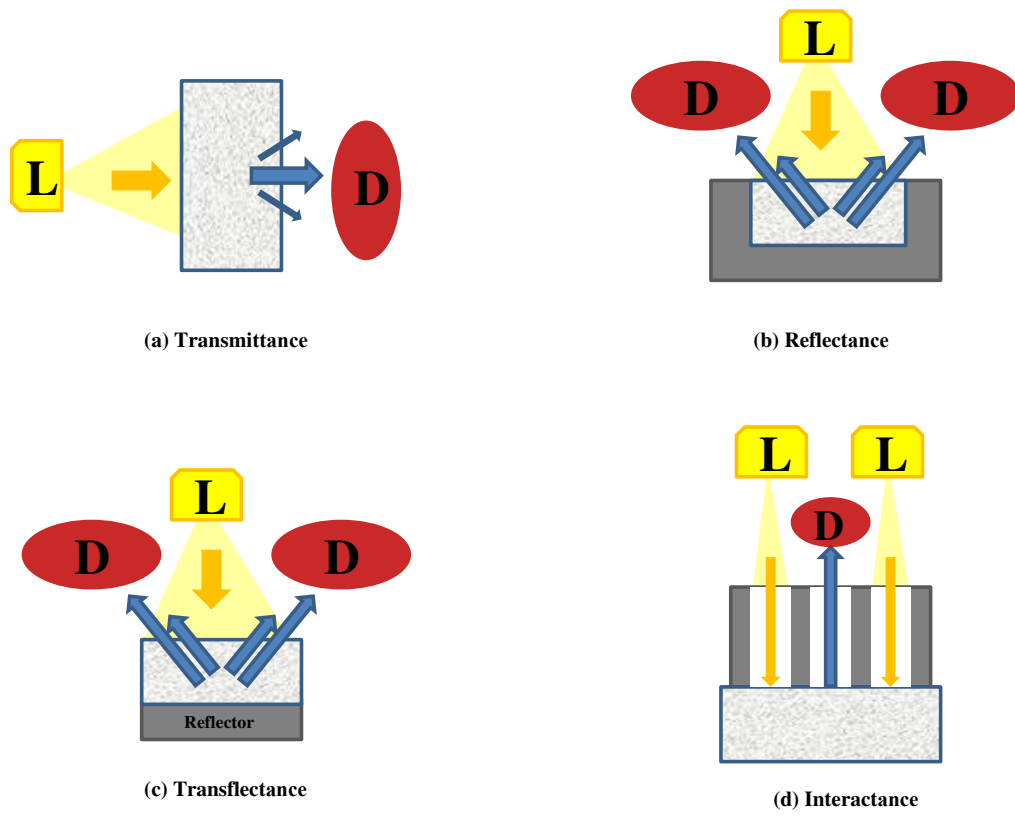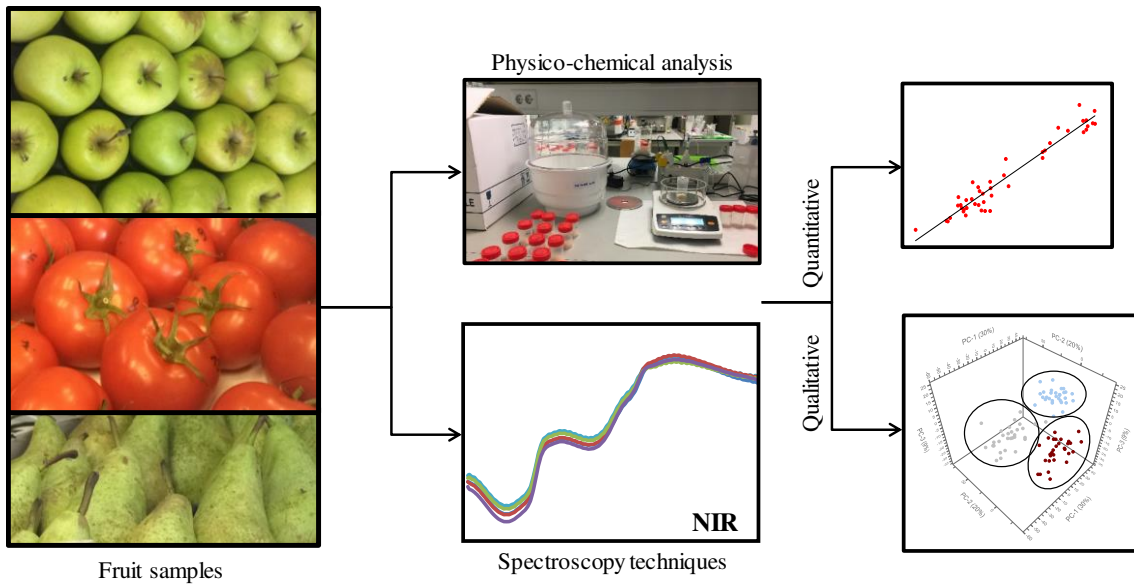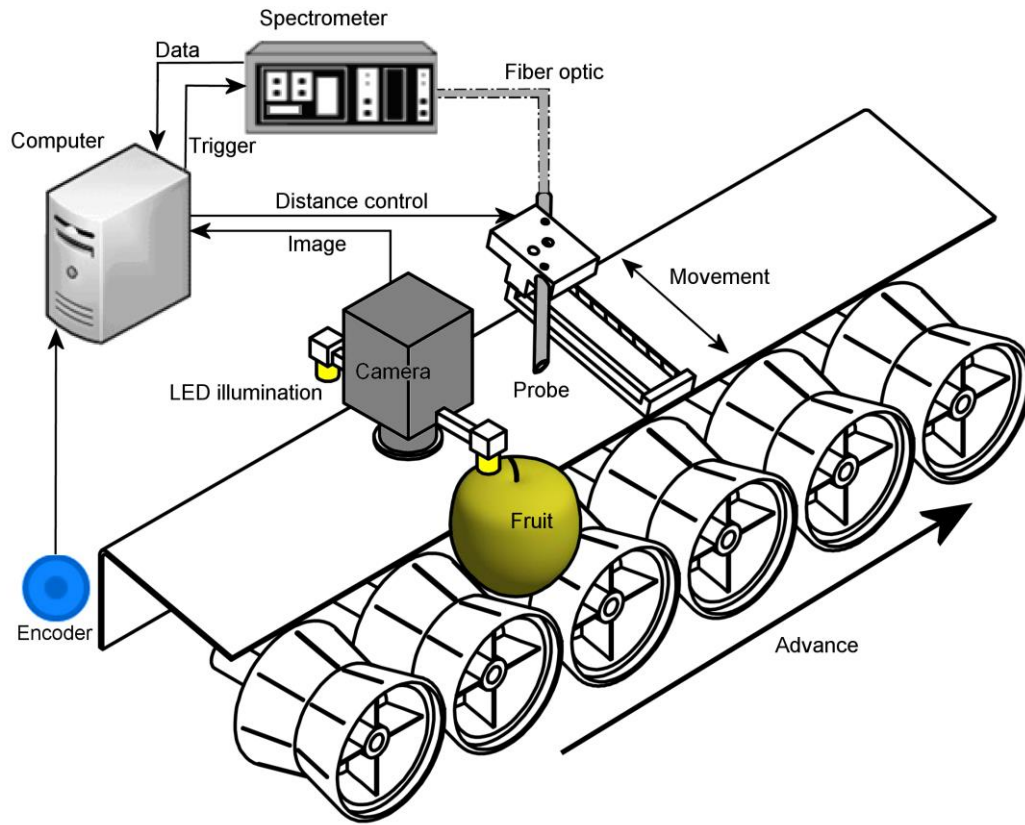
**Figure 3.** V. Cortés et al.

**Figure 4.** V. Cortés et al.

**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 | $R^2_{(on\ the\ harvest)}$=0.78; $R^2_{(on\ the\ storage)}$=0.71 | McGlone *et al.* (2002) |
| | | | | 500-750 nm | Firmness | $R^2_{(on\ the\ harvest)}$=0.63; $R^2_{(on\ the\ storage)}$=0.59 | |
| | | | | 500-750 nm | QS | $R^2_{(on\ the\ harvest)}$=0.66 | |
| | | | | 500-750 nm | SPI | $R^2_{(on\ the\ harvest)}$=0.78 | |
| | | | | 600-1000 nm; 800-1000 nm | SSC | $R^2_{(on\ the\ harvest)}$=0.63; $R^2_{(on\ the\ storage)}$=0.70 | |
| | | | | 500-1100 nm | TA | $R^2_{(on\ the\ harvest)}$=0.38 | |
| | | Transmittance | PLS | 800-1000 nm | Dry matter | $R^2_{(at\ harvest\ time)}$=0.95 and RMSEP=0.29; $R^2_{(post-storage)}$=0.97 and RMSEP=0.24; | McGlone *et al.* (2003) |
| | | | | | SSC | $R^2_{(at\ harvest\ time)}$=0.79 and RMSEP=0.52%brix; $R^2_{(post-storage)}$=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$_{p(full\ spectrum)}$=0.811; RMSEP$_{(full\ spectrum)}$=1.1522; R$_{p(optimal\ selected\ intervals)}$=0.93; RMSEP$_{(optimal\ selected\ intervals)}$=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; $R^2_{(flesh)}$=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 mode | Statistic method | Spectral range (range used) | Attributes analyzed | Performance | Ref. |
|---|---|---|---|---|---|---|---|
| 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) R=0.95, SEP=8.48 for oxalate soluble pectin content in the alcohol insoluble solids (OSP in the AIS) | Sirisomboon *et al.* (2007) |
| | | Reflectance | PLS | 780-1700 nm; 875-1030 nm | SSC | RMSEP=0.44ºBrix; $R^2$=0.60 | Nicolaï *et al.* (2008) |
| | | | | | Firmness | - | |
| | | Reflectance | EW-LS-SVM | 380-1800 nm (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 (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 (600-904 nm) | Brown core | 98.30 % | Sun *et al.* (2016) |
| | | | | | SSC | 97.8 % – 99 % | |