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Additional Information

28 on the comparison between **the two processes** for the same agro-food product,
29 highlighting the main advantages and disadvantages, problems, solutions, and
30 differences.

31 *Key Findings and Conclusions*

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

42

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

45

46 NOMENCLATURE

47 ANN, artificial neural network

48 BC, background colour

49 CA, cluster analysis

50 CDA, canonical discriminant analysis

51 CR², squared canonical correlation

52 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

87 **1. Introduction**

88 The current demands in an increasingly competitive and globalized framework
89 [call for](#) the agri-food sector to produce higher quality products, which requires an in-line
90 inspection of the entire production. For this reason, the research and development of
91 fast, accurate and non-destructive tools [that are](#) capable of evaluating each individual
92 product is increasing at high speed (Porep *et al.*, 2015). [Among them, VIS-NIR](#)
93 [spectroscopy appears as a promising alternative. This technology allows easy, fast,](#)
94 [accurate, non-destructive, and inexpensive quality assessments to be performed without](#)
95 [previous sample preparation, and the potential exists to develop instruments for in-line](#)
96 [measurements. However, as it is based on indirect measurements that produce highly](#)
97 [complex data, VIS-NIR spectroscopy needs the support of chemometrics to take full](#)
98 [advantage of the corresponding spectra](#) (Porep *et al.*, 2015; Huang *et al.*, 2008; Siesler,
99 2008).

100 The versatile applications of VIS-NIR spectroscopy for fruit quality assessment
101 have [already](#) been reviewed, for instance by Cen and He (2007) and Kumaravelu and
102 Gopal (2015). [Wang *et al.* \(2015\) and Nicolai *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 al.*
183 *al.* (1998), Berrueta *et al.* (2007), Liu *et al.* (2011), Lorente *et al.* (2015), and Wang *et al.*
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

202 of VIS-NIR models for fruit quality prediction is usually evaluated by means of the R^2
203 or r , the RMSE, and the RPD (Bobelyn *et al.*, 2010). Generally, a good model should
204 achieve a low RMSE and a high R^2 or r . Additionally, a satisfactory model should have
205 an RPD value of more than 2.5, a value above 3.0 being very good (Kamruzzaman *et*
206 *al.*, 2016; Cortés *et al.*, 2016). Other statistical parameters reflecting a good model are
207 low average difference between predicted and measured values (Bias) and a small
208 difference between RMSEC and RMSEP. Moreover, a good model should have as few
209 LV as possible.

210

211 **4. Monitoring strategies in the postharvest stage**

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

215 - off-line: analyzes the sample away from the production line, classically in a
216 laboratory.

217 - at-line: random samples are manually extracted from the production line and
218 examined in a place very close to the process line.

219 - on-line: samples are diverted from the production line to be analyzed directly in
220 the recirculation loop (by-pass) and are returned to the production line after analysis.

221 - in-line: analyzes the sample within the running production line (*in situ*).

222

223 The terms on-line and in-line are seemingly used similarly and so, for the
224 publications cited in this review, the term employed in the original article is **the one**
225 used. An exhaustive review of the literature shows that the VIS-NIR technique has been
226 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; Nicolai *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; Shenderay *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 Shenderay *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 Shenderoy *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 45°. 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 °Brix for off-
360 line and RMSEP=0.39 °Brix 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 ($R^2_{\text{fat content}} =$
397 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
398 analyzed off-line ($R^2_{\text{fat content}} = 0.87$; $R^2_{\text{free acidity}} = 0.76$; and $R^2_{\text{moisture content}} = 0.89$).

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 Nicolai *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

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447

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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.

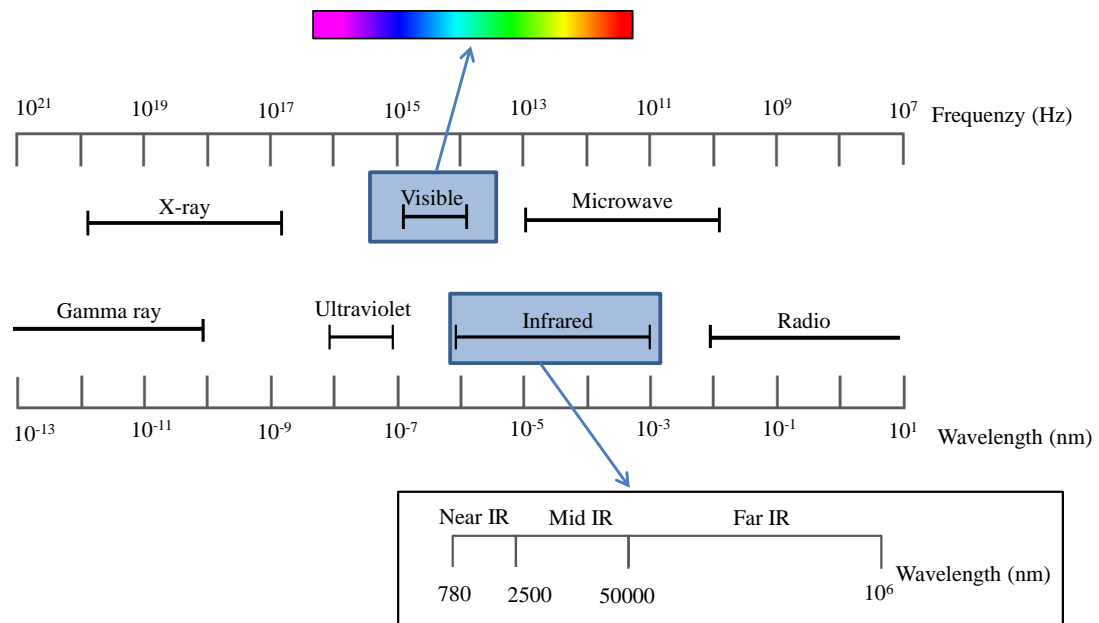


Figure 1. V. Cortés et al.

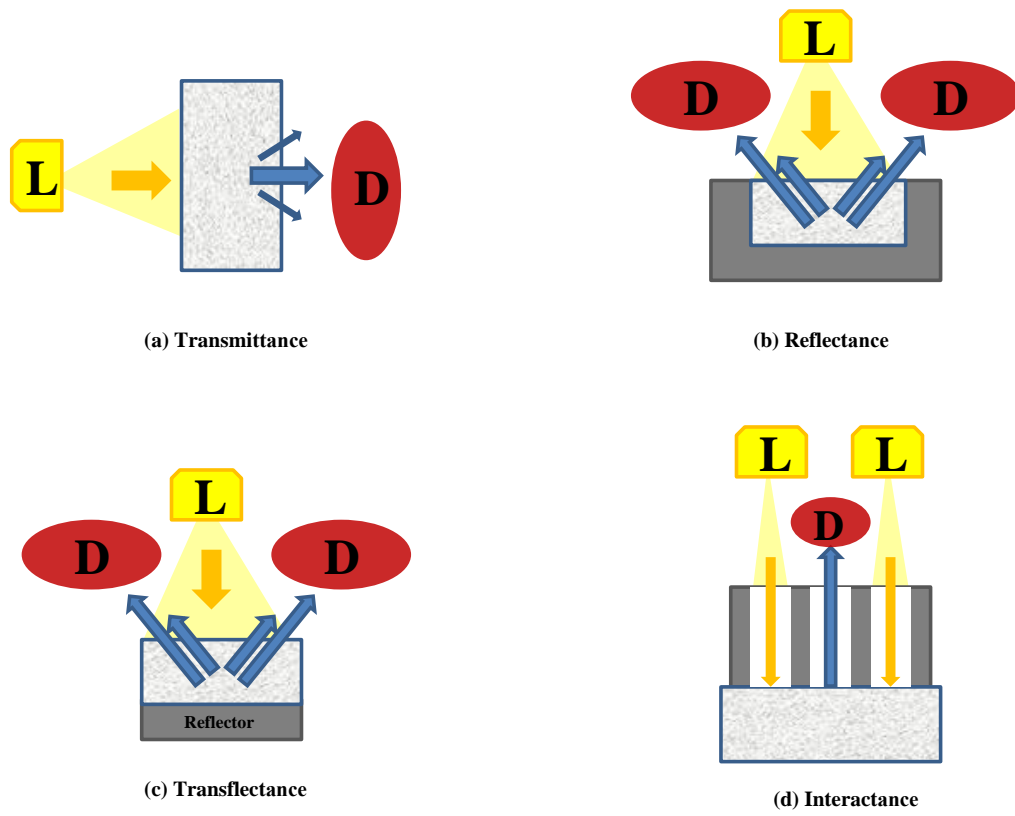


Figure 2. V. Cortés et al.

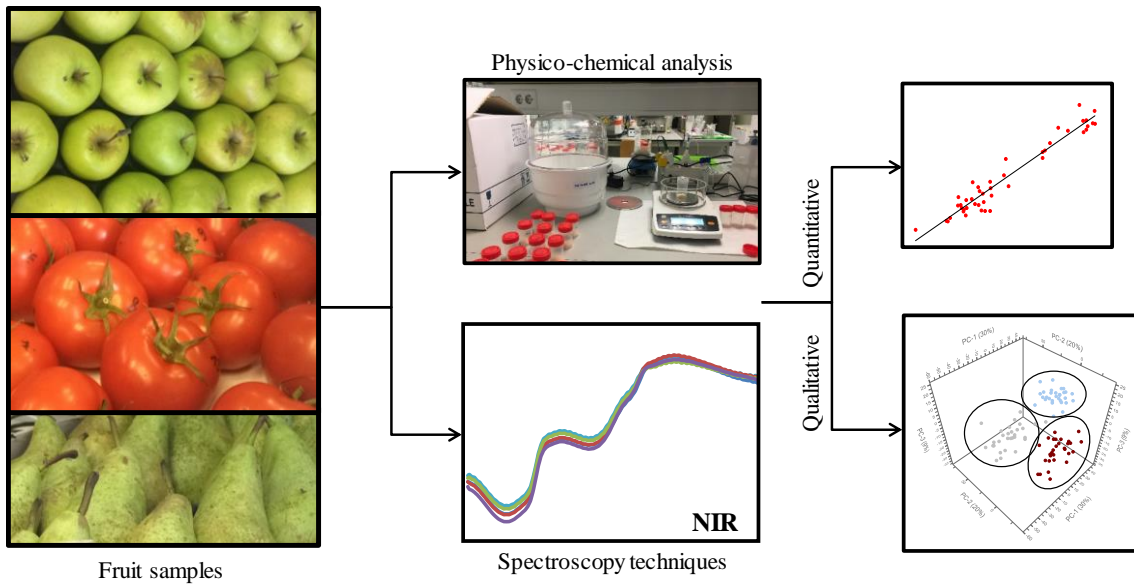


Figure 3. V. Cortés et al.

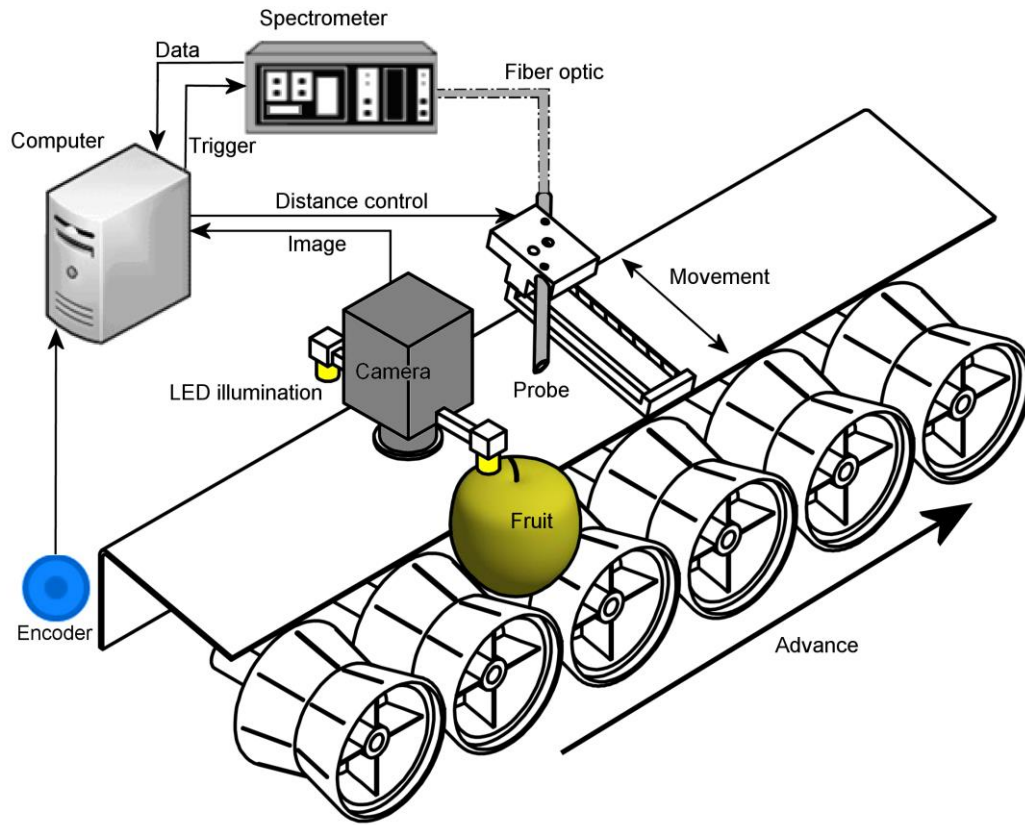


Figure 4. V. Cortés et al.

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	$R_p^2=0.49$, $SEP=1.14^\circ\text{Brix}$	Ventura <i>et al.</i> (1998)	
		Transmittance	PLS	500-750 nm	BC	$R^2_{(\text{on the harvest})}=0.78$; $R^2_{(\text{on the storage})}=0.71$	McGlone <i>et al.</i> (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 <i>et al.</i> (2003)
						SSC	$R^2_{(\text{at harvest time})}=0.79$ and $RMSEP=0.52\%\text{brix}$; $R^2_{(\text{post-storage})}=0.94$ and $RMSEP=0.30\%\text{brix}$;	
			Reflectance	PLS	300-1100 nm	SSC	$RMSEP_{\text{corr}}=0.65^\circ\text{Brix}$ $\text{Bias}=-0.35 - 0.39^\circ\text{Brix}$	Roger <i>et al.</i> (2003)
	Reflectance	CDA	400-1700 nm	Impact bruises and non-bruised tissue Compression bruises and sound tissue	$CR^2=0.68$ $CR^2=0.68$	Xing <i>et al.</i> (2003)		

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 <i>et al.</i> (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 <i>et al.</i> (2005)
			Reflectance	PLS-DA	400-1700 nm	Bruise detection	Classification accuracy >90%	Xing <i>et al.</i> (2005)
			Reflectance	Kernel PLS regression	800-1690 nm	SSC	R ² =0.87; RMSEP=0.44 °Brix	Nicolaï <i>et al.</i> (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 <i>et al.</i> (2007)
			Reflectance	PLS-DA	500-1600 nm	Softening index	Classification accuracy >95%	Xing <i>et al.</i> (2007)
			Reflectance	PLS	804-1294 nm	E-modulus	r _p =0.77-0.80	Pissard <i>et al.</i> (2013)
			Reflectance	LS-SVM	400-2500 nm	Vitamin C	R ² =0.80; SEP=4.9	
					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 <i>et al.</i> (2016)	
		Reflectance	PLS-DA	400-1000nm; 1100-2100 nm	Influence of packaging on apple slices	86.7 % – 100 %	Beghi <i>et al.</i> (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 <i>et al.</i> (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 <i>et al.</i> (2016)	
		Reflectance	PLS	6267-4173 cm ⁻¹	Total antioxidant capacity	R ² =0.85, SEP=0.13% gallic acid equivalents, RPD=2.8	Schmutzler <i>et al.</i> (2016)	
					SSC	R ² =0.76, SEP=0.55°Brix, 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 <i>et al.</i> (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 <i>et al.</i> (2005)
		(simulated conveyor)	Transmittance	PLS	400-1000 nm	Moldy core	r ² =0.71; SEP=0.036; RPD=1.71	Shenderay <i>et al.</i> (2010)
		(cell conveyor)	Reflectance	PLS	340-1014 nm and 850-1888 nm	SSC	R ² =0.86, RMSEP=0.80	Ignat <i>et al.</i> (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 °Brix	Jie <i>et al.</i> (2013)
	In-line (conveyor belt)	Transmittance	MC-UVE-SMLR	687-920 nm (200-1100 nm)	SSC	r _p =0.66; RMSEP=0.39 °Brix	Jie <i>et al.</i> (2014)
		Reflectance	PLS	900-1700 nm	Lycopene B-Carotene SSC	R ² =0.805; SECV=16.19 mg/kg R ² =0.737; SECV=0.96 mg/kg R ² =0.707; SECV=1.4 %	Tamburini <i>et al.</i> (2017)
Nectarines	Off-line	Reflectance	PLS	360-1760 nm	IQI	R ² = 0.909-0.927; RMSEP=0.235-0.238	Cortés <i>et al.</i> (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 <i>et al.</i> (2017b)	
			MPLS	1600-2400 nm; 400-1700 nm	SSC	r ² =0.89; SEP=0.75-0.81%	Pérez-Marín <i>et al.</i> (2009)
		Flesh firmness	Weight	Diameter	Shelf-life discrimination	r ² =0.84-0.86; SP=11.6-12.7 N	Pérez-Marín <i>et al.</i> (2011)
						r ² =0.98; SEP=5.40 g	
						r ² =0.75; SEP= 0.46 cm	
		Reflectance	PLS2-DA	1600-2400 nm	Weight	86-96%	Sánchez <i>et al.</i> (2011)
400-1700 nm	66-89%						
1600-2400 nm	r ² =0.53;0.59						
Reflectance	MPLS;LOCAL algorithm	1600-2400 nm	Diameter	r ² =0.53;0.56	Sánchez <i>et al.</i> (2011)		
				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)
	Off-line	Reflectance	PLS	400-2500 nm	Fat content	$R^2=0.87$; RMSEP=2.50	Salguero-Chaparro <i>et al.</i> (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		
Olives	In-line (conveyor belt)	Reflectance	ANOVA and LSD	380-1690 nm	Focal distance and integration time	RMS (5s)=28.753 - 66.028	Salguero-Chaparro <i>et al.</i> (2012)
		Reflectance	PLS	380-1690 nm	Free acidity	$R^2=0.74$; RMSEP=2.53	Salguero-Chaparro <i>et al.</i> (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 <i>et al.</i> (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 <i>et al.</i> (2007)
		Reflectance	PLS	780-1700 nm; 875-1030 nm	SSC Firmness	RMSEP=0.44°Brix; R ² =0.60 -	Nicolaï <i>et al.</i> (2008)
		Reflectance	EW-LS-SVM	380-1800 nm (400-1800 nm)	SSC pH Firmness	r _p =0.9164; RMSEP=0.2506 r _p =0.8809; RMSEP=0.0579 r _p =0.8912; RMSEP=0.6247	Li <i>et al.</i> (2013)
		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 <i>et al.</i> (2014)
		Transmittance	PLS	465 - 1150 nm	SSC SSC	R ² =0.84; RMSECV=0.44 r _p =0.96; RMSEP=0.29	Xu <i>et al.</i> (2014)
	In-line	Transmittance	SMLR GA-PLS iPLS GA-SPA-MLR	200-1100 nm (533-930 nm)	SSC	R ² =0.8296 R ² =0.8781 R ² =0.8396 R ² =0.880	Xu <i>et al.</i> (2012)
		Transmittance	PLS	200-1100 nm (600-904 nm)	Brown core SSC	98.30 % 97.8 % – 99 %	Sun <i>et al.</i> (2016)