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Additional Information

1 **Sweet and nonsweet taste discrimination of nectarines using visible and near-**  
2 **infrared spectroscopy**

3  
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26 **ABSTRACT**

27 The feasibility of using visible and near-infrared spectroscopy technology combined  
28 with multivariate analysis to discriminate cv. 'Big Top' and cv. 'Diamond Ray'  
29 nectarines has been studied. These varieties are very difficult to differentiate visually  
30 on the production line but show important differences in taste that affects the  
31 acceptance by final consumers. The relationship between the diffuse reflectance  
32 spectra and the two nectarine varieties was established. Five hundred nectarine  
33 samples (250 of each variety) were used for the study. Tests were performed by  
34 using a spectrometer capable of measuring in two different spectral ranges (600 –  
35 1100 nm and 900 – 1700 nm). These spectral ranges were used to develop two  
36 accurate classification models based on linear discriminate analysis (LDA) and partial  
37 least squares discriminate analysis (PLS-DA). Later, selection techniques were  
38 applied to select the most effective wavelengths. The results showed that the PLS-  
39 DA model achieved better accuracy and less latent variables than LDA model, and  
40 specifically, good results with 100 % classification accuracy were obtained using only  
41 the 600 – 1100 nm spectral range for the two models and eight selected  
42 wavelengths. These results places visible and near-infrared spectroscopy as an  
43 accurate classification tool for nectarine varieties with a very similar appearance but  
44 different tastes that could be potentially used in an automated inspection system.

45

46 **Keywords:** nectarine, sweet taste, nonsweet taste, visible and near-infrared  
47 spectroscopy, discrimination, chemometrics

48

49 **1. INTRODUCTION**

50 Nectarine and peach fruit [*Prunus persica* (L.) Batch] are the second most important  
51 fruit crop in the European Union (EU) after apple (Iglesias & Echeverría, 2009).  
52 Recently, significant innovations have been made in the field of fruit varieties that  
53 seek improvements in colour and size, consistency of pulp, texture, taste and flavour  
54 (Jha *et al.*, 2012; Jha *et al.*, 2006; Picha, 2006; Jha *et al.*, 2005; Jha *et al.*, 2004).  
55 New varieties obtained show an attractive range of colours, tastes and forms as well  
56 as having an extended maturity schedule, which have given rise to excellent  
57 acceptance by consumers in both national and international markets (Iglesias, 2013;  
58 Iglesias & Casals, 2014).

59 The most appreciated attributes among fruit consumers have been described as  
60 being taste, food safety (absence of pesticides), ease of consumption and cost  
61 (Wandel & Bugge, 1997; Radman, 2005; Dragsted, 2008). Regarding taste  
62 consumers generally prefer sweet and balanced tastes, except in some countries like  
63 Germany or England, where there is preference for nonsweet tastes (Cembalo *et al.*,  
64 2009). In fact, the introduction of 'Big Top' nectarine variety into the market  
65 represented a remarkable innovation for its sweet taste (< 6 g L<sup>-1</sup> of malic acid) and  
66 excellent consistency, and has been widely accepted by national and international  
67 markets.

68 Recently, new varieties of nectarines completing the collection period from late May  
69 to late September have been introduced into the market. This varietal range is  
70 complemented by new or existing varieties showing a similar appearance, but a  
71 balanced or nonsweet taste (> 6 g L<sup>-1</sup> of malic acid), as occurs in the case of the  
72 'Diamond Ray' variety. In nectarine fruit, it is essential to differentiate the varieties  
73 from in processing line, which would allow the consumer to choose the ones that best  
74 adapt to their preferences.

75 The application of visible and near-infrared spectroscopy for the analysis of fruit has  
76 allowed the prediction of chemical composition, notably sugar content (Li *et al.*, 2013;  
77 Reita *et al.*, 2008), and textural parameters (Lee *et al.*, 2012; Sánchez *et al.*, 2011),  
78 as well as the identification of varieties (Li *et al.*, 2016; Guo *et al.*, 2016) and the  
79 measurement of quality-related parameters (Pérez-Marín *et al.*, 2011). This  
80 technique is relatively rapid, simple, cost-effective, non-destructive, and  
81 environmentally friendly. Its application in combination with chemometrics has been  
82 successfully used in non-destructive discrimination between varieties of agricultural  
83 products such as peach (Guo *et al.*, 2016), bayberry (Li *et al.*, 2007), orange  
84 (Suphamitmongkol *et al.*, 2013), and pummelos (Li *et al.*, 2016).

85 This study aimed to evaluate the ability of visible and near-infrared spectroscopy to  
86 discriminate between two varieties of nectarine (cv. 'Big Top' and cv. 'Diamond Ray'),  
87 which, because there are similar in colour and appearance, are very difficult to  
88 differentiate visually on the production line but show important differences in taste,  
89 thereby affecting the acceptance by the final consumers. Two supervised methods  
90 such as linear discriminate analysis (LDA) and partial least squares discriminate  
91 analysis (PLS-DA) were used for this purpose.

92

## 93 **2. MATERIALS AND METHODS**

### 94 **2.1. Experimental procedure**

95 A total of 500 nectarines with commercial maturity and uniform size and the absence  
96 of any external damage were harvested in a commercial orchard in Lérida, Spain.  
97 They were then stored at 0.1 °C with 87 % relative humidity to prevent the evolution  
98 of maturity during the experiment and to extend their shelf-life (Gorny *et al.*, 1998).  
99 Half of the total samples belonged to the variety 'Big Top' and the other half to the

100 variety 'Diamond Ray'. These varieties were selected because they are grown in the  
101 same period and have a similar evolution and physical appearance, although they  
102 differ critically in some of their organoleptic properties.

103 On arrival at the laboratory, fruits were cleaned, individually numbered and each  
104 variety was randomly divided into five sets of 50 fruits. The visible and near-infrared  
105 spectra of the fruits in each set were collected and their physicochemical properties  
106 (soluble solids, firmness and flesh and external colour) were analysed by standard  
107 destructive methods (Cortés *et al.*, 2016; Martins *et al.*, 2016; Li *et al.*, 2013;  
108 Hernández *et al.*, 2006).

109

## 110 **2.2. Visible and near-infrared spectra acquisition**

111 Diffuse visible and near-infrared reflectance spectra of intact nectarines were  
112 collected using a multichannel spectrometer platform (AvaSpecAS-5216 USB2-DT,  
113 Avantes BV, The Netherlands) equipped with two detectors. The first detector  
114 (AvaSpec-ULS2048 StarLine, Avantes BV, The Netherlands) included a 2048-pixel  
115 charge-coupled device (CCD) sensor (SONY ILX554, SONY Corp., Japan), 50 µm  
116 entrance slit and a 600 line mm<sup>-1</sup> diffraction grating covering the visible and near-  
117 infrared range from 600 nm to 1100 nm (VNIR) with a spectral FWHM (full width at  
118 half maximum) resolution of 1.15 nm and a spectral sampling interval of 0.255 nm.  
119 The second detector (AvaSpec-NIR256-1.7 NIRLine, Avantes BV, The Netherlands)  
120 was equipped with a 256 pixel non-cooled InGaAs (Indium Gallium Arsenide) sensor  
121 (Hamamatsu 92xx, Hamamatsu Photonics K.K., Japan), with a 100 µm entrance slit  
122 and a 200 line mm<sup>-1</sup> diffraction grating covering the near-infrared range from 900 nm  
123 to 1700 nm (NIR) with a spectral FWHM resolution of 12 nm and a spectral sampling  
124 interval of 3.535 nm.

125 The measurements were performed using a bi-directional fibre-optic reflectance  
126 probe (FCR-7IR200-2-45-ME, Avantes BV, The Netherlands). The probe was  
127 configured fitted with an illumination leg which connects to a stabilised 10 W tungsten  
128 halogen light source (AvaLight-HAL-S, Avantes B0V, The Netherlands) and the other  
129 leg of the fibre-optic probe was connected to both detectors for simultaneous  
130 measurement. A personal computer equipped with software (AvaSoft version 7.2,  
131 Avantes, Inc.) was used to control both detectors and to acquire the spectra. The  
132 integration times were adjusted for each spectrophotometer using a 99 % reflective  
133 white reference tile (WS-2, Avantes BV, The Netherlands), so that the maximum  
134 reflectance value over each wavelength range was around 90 % of saturation  
135 (Lorente *et al.*, 2015). The white reference tile for reflectance measurements was a  
136 32 mm diameter and 10 mm thick block of white polytetrafluoroethylene (PTFE). The  
137 white reference tile was placed at a distance of 5 mm from the probe to make a  
138 reference measurement. The dark spectrum was obtained by turning off the light  
139 source and completely covering the tip of the reflectance probe. The integration time  
140 was set to 120 ms for the VNIR detector and 550 ms for the NIR detector due to the  
141 different features of the two detectors. For both detectors, each spectrum was  
142 obtained as the average of five scans to reduce the thermal noise of the detector  
143 (Nicolai *et al.*, 2007). The average reflectance measurements of each sample (S)  
144 were then converted into relative reflectance values (R) with respect to the white  
145 reference using dark reflectance values (D) and the reflectance values of the white  
146 reference (W), as shown in Eq. (1):

147

$$148 \quad R = \frac{S-D}{W-D} \quad (1)$$

149

150 Prior to the spectral measurements, the temperature of the nectarines was stabilised  
151 at a room temperature of  $22 \pm 1$  °C. All the measurements were taken at two points  
152 on each side of the fruit and mean values of the spectra were used for the analysis.

153

### 154 **2.3. Determination of the quality attributes**

155 Destructive methods were performed immediately after the spectral acquisition to  
156 determine the quality attributes for use as reference values. Both the external and the  
157 flesh colours were measured using a spectrophotometer (CM-700d, Minolta Co.,  
158 Tokyo, Japan) every 10 nm between 400 and 700 nm. The colour was evaluated  
159 using the  $L^*$ ,  $a^*$  and  $b^*$  space proposed by the International Commission on  
160 Illumination (CIE).  $L^*a^*b^*$  were determined from the reflectance spectra, considering  
161 standard illuminant D65 and standard observer 10°.  $L^*$  refers to the luminosity or  
162 lightness component,  $a^*$  (intensity of red (+) and green (-)) and  $b^*$  (intensity of yellow  
163 (+) and blue (-)) are the chromaticity coordinates. The total colour difference ( $\Delta E$ )  
164 between the 'Big Top' samples and the 'Diamond Ray' samples was calculated by  
165 Eq. (2).

166

$$167 \quad \Delta E = \sqrt{(L^*_{BT} - L^*_{DR})^2 + (a^*_{BT} - a^*_{DR})^2 + (b^*_{BT} - b^*_{DR})^2} \quad (2)$$

168

169 where subscript 'BT' refers to the colour reading of the 'Big Top' samples and 'DR'  
170 refers to the colour reading of the 'Diamond Ray' samples.

171 Nectarine firmness was measured using a Universal Testing Machine  
172 (TextureAnalyser-XT2, Stable MicroSystems, Haslemere, England) to perform  
173 puncture tests using a 6 mm diameter cylindrical probe (P/15ANAMEsignature) to a  
174 relative deformation of 30 % at a speed of 1 mm s<sup>-1</sup>. Two measurements were



175 performed for each fruit on opposite sides along the equator. The fracture strength  
176 ( $F_{max}$ ) was analysed for all samples as the maximum force applied to break up the  
177 sample, being expressed in Newtons.

178 Immediately after firmness measurements, juice samples were extracted to estimate  
179 the total soluble solids content (TSS) and titratable acidity (TA). The TSS was  
180 determined by refractometry (%) with a digital refractometer (set RFM330+, VWR  
181 International Eurolab S.L Barcelona, Spain) at 20 °C with a sensitivity of  $\pm 0.1$  %.  
182 Samples were analysed in triplicate and average values were calculated. The  
183 analysis of the TA was performed with an automatic titrator (CRISON, pH-burette 24,  
184 Barcelona, Spain) with 0.5 N NaOH until a pH of 8.1 (UNE34211:1981), using 15 g of  
185 crushed nectarine, which was diluted in 60 mL of distilled water. The TA was  
186 determined based on the percentage of citric acid, which was calculated using Eq.  
187 (3).

188

$$189 \quad TA [g \text{ citric acid} / 100 g \text{ of sample}] = (((A \times B \times C) / D) \times 100) / E \quad (3)$$

190

191 where A is the volume of NaOH consumed in the titration (in L), B is the normality of  
192 NaOH (0.5 N), C is the molecular weight of citric acid (192.1 g mol<sup>-1</sup>), D is the weight  
193 of the sample (15 g) and E is the valence of citric acid (E = 3).

194

#### 195 **2.4. Spectral pre-processing**

196 The spectral data were organised in a matrix, where the rows represent the number  
197 of samples (#N = 500 samples) and the columns represent the variables (X-variables  
198 and Y-variables). The X-variables, or predictors, were the spectral signals from the  
199 two detectors. The Y-variables, or responses, were the artificial (dummy) variables

200 created by assigning different values or letters to the different classes to be  
201 discriminated. In the case of PLS-DA, assuming a discrete numerical value (zero for  
202 the cv. 'Diamond Ray' or one for the cv. 'Big Top'), was used as Y-variable. However,  
203 for LDA the Y-variable was a categorical value created by assigning different letter to  
204 the different cultivar (*A* for the cv. 'Diamond Ray' and *B* for the cv. 'Big Top'). In  
205 addition, for LDA the number of samples in the training set must be larger than the  
206 number of variables included in the model (Kozak & Scaman, 2008; Sádecká *et al.*,  
207 2016), thus requiring a variable selection or variable reduction. This was performed  
208 using the principal component analysis (PCA) scores as input data, since the linear  
209 combinations of the original variables, called principal components, are uncorrelated  
210 (Rodríguez-Campos *et al.*, 2011).

211 The raw spectra were transformed to apparent absorbance ( $\log(1/R)$ ) values so as to  
212 be able to linearise the correlation with the concentration of the constituents  
213 (Hernández *et al.*, 2006; Shao *et al.*, 2007; Liu *et al.*, 2009) using The Unscrambler X  
214 software package (CAMO, Norway). Then, the raw spectra belonging to the two  
215 detectors were normalised (Bakeev, 2010) by dividing each variable by its standard  
216 deviation (Bouveresse *et al.*, 1996). By so doing, the spectral intensities are rescaled  
217 to a common range, thus allowing the comparison of spectra acquired using two  
218 detectors with different resolutions.

219 In addition, different pre-processing techniques were applied. Savitzky-Golay  
220 smoothing with a gap of three data points (Carr *et al.*, 2005) was applied to improve  
221 the signal-to-noise ratio in order to reduce the effects caused by the physiological  
222 variability of samples (Carr *et al.*, 2005; Beghi *et al.*, 2017). Due to the fresh light  
223 scattering in samples (Gelbukh *et al.*, 2006), the light does not always travel the  
224 same distance in the sample before it is detected. A longer light traveling path

225 corresponds to a lower relative reflectance value, since more light is absorbed. This  
226 causes a parallel translation of the spectra. This kind of variation interferes in the  
227 calibration models and need to be eliminated by the extend multiplicative scatter  
228 correction (EMSC) technique (He *et al.*, 2007; Martens *et al.*, 2003; Bruun *et al.*,  
229 2007). In addition to those two pre-processing, the second derivative with Gap-  
230 Segment (2.3) were applied for the NIR spectra because it allowed the extraction of  
231 useful information (Cortés *et al.*, 2016; Rodriguez-Saona *et al.*, 2001).

232

## 233 **2.5. Multivariate data analysis of spectral data**

234 PCA (Naes *et al.*, 2004), PLS-DA and LDA were used in this work by means of The  
235 Unscrambler X software package. PCA was selected as the method for outlier  
236 detection (through the analysis of Hotelling's T2 and squared residual statistics) and  
237 to explore the data structure and the relationship between objects (Beghi *et al.*, 2017;  
238 Beebe *et al.*, 1998), in order to pinpoint the most relevant varietal groups and  
239 spectral features. So, the use of suitable projection, e.g., PCA or partial least square  
240 regression (PLS) (Balabin *et al.*, 2007; Xiabo *et al.*, 2010) may help to minimize the  
241 large number of spectral variables in the data sets and identify variables that  
242 contribute useful information (effective wavelengths, EWs). In this study, wavelengths  
243 with large loading weight values were selected as important for the varietal  
244 discrimination. EWs were selected as only those located at the peaks or valleys of x-  
245 loading weights plots, and with an absolute x-loading weight higher than 0.1 (Liu *et*  
246 *al.*, 2008).

247 PLS-DA and LDA were used to classify the nectarines in terms of variety. These  
248 discriminant analyses seek to correlate spectral variations (X) with defined classes  
249 (Y), attempting to maximise the covariance between the two types of variables.

250 A training set was used and consisted in randomly selecting 80 % of the samples that  
251 were studied to develop a calibration model. Each calibration model was internally  
252 validated using the leave-one-out cross-validation technique (Huang *et al.*, 2008). In  
253 order to correct the relative influences of the different instrumental responses on a  
254 model, a standardisation technique was used, where the weight of each X-variable  
255 was the standard deviation of the variable (Bouveresse *et al.*, 1996). An independent  
256 test set composed of the remaining 20 % of the samples was used for the evaluation  
257 and comparison of the classification models (Soares *et al.*, 2013).

258

## 259 **2.6. Model performance evaluation**

260 The PLS-DA cut-off value for nectarine samples discrimination was fixed at 0.5. If the  
261 predicted value of a sample was less than 0.5, the sample was assigned to the group  
262 of the 'Diamond Ray' samples, while if the predicted value was more than 0.5, the  
263 sample was assigned to the group of the 'Big Top' samples. The determination  
264 coefficient ( $R^2$ ), root mean square error (RMSE) and the number of latent variables  
265 (LVs) were used to evaluate the accuracy of the PLS-DA calibration model to predict  
266 new samples. In the case of LDA, the criterion for the selection of LVs is maximum  
267 differentiation between the categories and minimal variance within categories  
268 (Cardoso & Silva, 2016; Naes *et al.*, 2002; Adams, 1995). The method produces a  
269 number of orthogonal linear discriminant functions, equal to the number of categories  
270 minus one, that allow the samples to be classified in one category or another (Naes  
271 *et al.*, 2002; Otto, 1999).

272

## 273 **3. RESULTS AND DISCUSSION**

### 274 **3.1. Analysis of the quality attributes**

275 Table 1 shows the minimum, maximum, mean and standard deviation of the  
 276 physicochemical characteristics (fracture strength, total soluble solids, tritatable  
 277 acidity, and flesh and external colour) analysed in the samples of both varieties of  
 278 nectarines (#N = 250 samples for each variety).

279

280 **Table 1.** Descriptive statistics for the physicochemical characteristics of nectarines  
 281 during the storage period

		TSS (%)	TA (g 100g <sup>-1</sup> )	F <sub>max</sub> (N)	Flesh colour					External colour				
					L* <sub>flesh</sub>	a* <sub>flesh</sub>	b* <sub>flesh</sub>	C* <sub>flesh</sub>	h* <sub>flesh</sub>	L* <sub>ext</sub>	a* <sub>ext</sub>	b* <sub>ext</sub>	C* <sub>ext</sub>	h* <sub>ext</sub>
	Max	17	1.07	57	76	23	35	36	100	59	38	28	42	60
	Min	8	0.36	5	52	-6	23	28	46	25	15	4	18	10
	Mean	12	0.65	33	67	2	31	32	86	37	28	14	32	26
	Sdev	2	0.12	10	4	4	2	1	8	7	4	5	4	10
	Max	22	0.57	53	75	4	36	36	103	63	34	31	39	75
	Min	7	0.20	6	60	-8	30	30	83	26	8	4	21	12
	Mean	13	0.37	35	68	-2	33	33	93	37	27	14	31	26
	Sdev	2	0.07	7	3	2	1	1	3	6	4	5	4	10

282

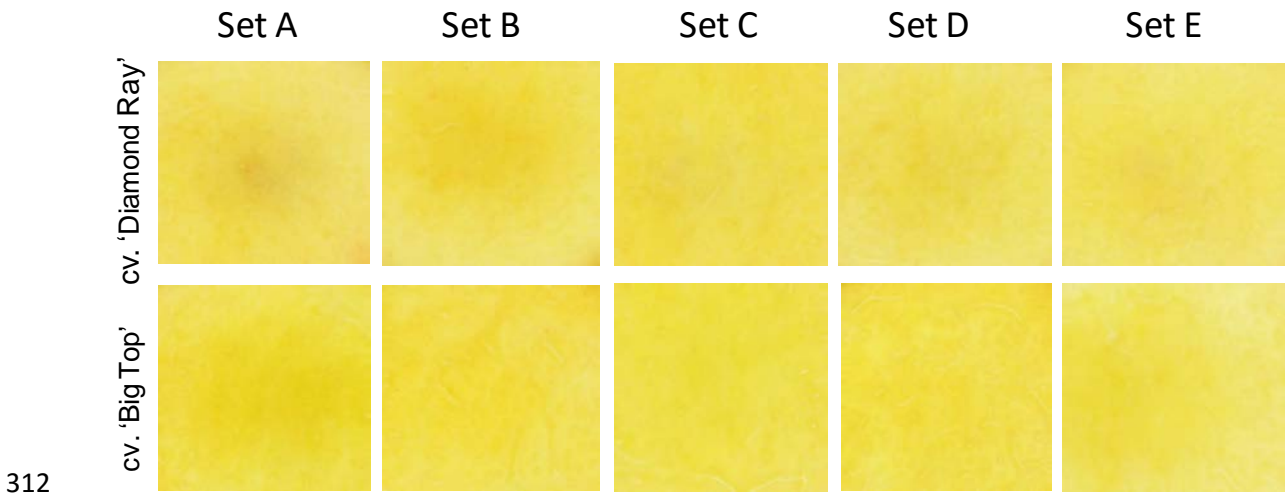
283 No differences were observed between the two varieties, and among the different  
 284 sets, in terms of soluble solids, firmness, and flesh and external colour.

285 The TSS ranged from 8 to 17 % with an average value of  $12 \pm 2$  % for cv. 'Diamond  
286 Ray' and from 7 to 22 % with an average value of  $13 \pm 2$  % for cv. 'Big Top'. In all  
287 cases, the values of TSS were greater than 8 %, which is the minimum established  
288 by the European Union to market peaches and nectarines (R-CE No. 1861/2004).  
289 Several authors have reported a linear relationship between TSS and consumer  
290 acceptance (Crisosto & Crisosto, 2005), a TSS below 10 % generally being  
291 unacceptable to consumers (Clareton, 2000).

292 The firmness of 'Diamond Ray' samples ranged from 5 to 57 N with an average value  
293 of  $33 \pm 10$  N, and 'Big Top' samples ranged from 6 to 53 N with an average value of  
294  $35 \pm 7$  N. According to Crisosto (2002) and Valero *et al.* (2007), these firmness  
295 values are in the commercial range considered 'ready to buy'.

296 For flesh colour,  $L^*$ ,  $a^*$ ,  $b^*$ ,  $C^*$  and  $h^*$  ranged from 52 to 76, -6 to 23, 23 to 35, 28 to  
297 36 and 46 to 100 for cv. 'Diamond Ray' and from 60 to 75, -8 to 4, 30 to 36, 30 to 36  
298 and 83 to 105 for cv. 'Big Top', with average values of  $67 \pm 4$ ,  $2 \pm 4$ ,  $31 \pm 2$ ,  $32 \pm 1$ ,  
299  $86 \pm 8$  and  $68 \pm 3$ ,  $-2 \pm 2$ ,  $33 \pm 1$ ,  $33 \pm 1$ ,  $93 \pm 3$  respectively. These values indicated  
300 that the flesh of both varieties has a high luminosity, low chroma and yellow hue. No  
301 differences were observed in luminosity and chroma between sets and between  
302 varieties, whereas slight differences in hue were observed between varieties. Despite  
303 these differences, the overall perception of flesh colour would make it very difficult to  
304 discriminate both varieties, especially during any industrial process where fruits must  
305 be inspected quickly, as shown in the images in Figure 1 with examples of each of  
306 the sets analysed. According to ISO 12647-2, colour differences ( $\Delta E$ ) lower than  $\pm 5$   
307 units make the human eye unable to discriminate two samples. In this case, the  $\Delta E$   
308 between both varieties measured with the colorimeter was  $\pm 4.5$ . Furthermore,  
309 differentiating nectarine varieties by the flesh colour requires the destruction of the

310 sample, and therefore this destructive analysis results in high costs and does not  
311 allow the whole production to be analysed (Torres *et al.*, 2013).



313 **Fig. 1.** Example of the internal appearance of both cultivars on each day of analysis.

314

315 Regarding the external colour of the nectarines, no significant differences were found  
316 in the values of luminosity, chroma and hue for the sets and the varieties studied.  
317 The  $L^*$ ,  $a^*$ ,  $b^*$ ,  $C^*$  and  $h^*$  ranged from 25 to 59, 15 to 38, 4 to 28, 18 to 42 and 10 to  
318 60 for cv. 'Diamond Ray' and from 26 to 63, 8 to 34, 4 to 31, 21 to 39 and 12 to 75 for  
319 cv. 'Big Top', with average values of 37 for luminosity, 31.3 for chroma and  $25.9^\circ$  for  
320 hue, for both varieties. These values indicated that, externally, both varieties had low  
321 luminosity, low chroma and red-orange hue. The  $\Delta E$  of external colour between  
322 varieties was 1.5, and therefore barely perceptible. Hence, this non-destructive  
323 analysis was not valid for varietal discrimination.

324 The main difference between the two varieties of nectarine was TA, the 'Diamond  
325 Ray' variety being more acid than the 'Big Top' variety or, according to the definition  
326 of Reig *et al.* (2013), the are a nonsweet and sweet variety, respectively. All sets of  
327 the cv. 'Diamond Ray' had an average value of  $0.65 \pm 0.1$  g 100g<sup>-1</sup>, unlike the  
328 average value of the sets of the cv. 'Big Top' which was  $0.37 \pm 0.1$  g 100g<sup>-1</sup>. These

329 results are in accordance with the sensorial profile performed by Iglesias (2012). The  
330 study concluded that the only difference between these two varieties is in the  
331 perception of acidity. Similarly, Reig *et al.* (2013) and Liverani *et al.* (2002) compared  
332 sweet cultivars (such as 'Big Top', 'Gardeta' and 'Luciana') with nonsweet cultivars  
333 (such as 'Diamond Ray', 'Amiga' and 'Rose Diamond'), and determined that they  
334 differed mainly in their TA value and the perception of acidity, the rest of their  
335 physicochemical characteristics being similar among the cultivars.

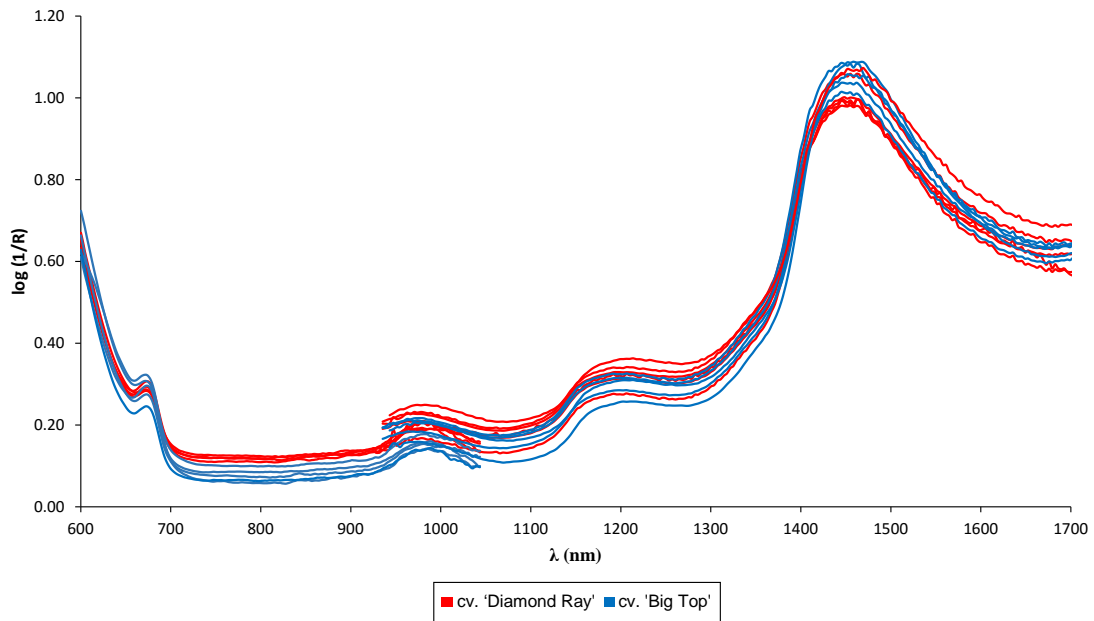
336

### 337 **3.2. Visible and Near-infrared spectra of the two nectarine varieties**

338 Figure 2 represents the mean raw VNIR and NIR spectra for the 'Diamond Ray' and  
339 'Big Top' samples at different sets of analysis. The trend and absorbance bands of  
340 the spectral curves were similar. Previous studies have documented similar values  
341 (Pérez-Marín *et al.*, 2009; Pérez-Marín *et al.*, 2011; Martins *et al.*, 2016). The  
342 varieties analysed showed the same absorbance bands around 670 nm, 970 nm,  
343 1160 nm and 1450 nm. Authors such as Tijssens *et al.* (2007) confirmed that the  
344 absorption at 670 nm allowed the maturity of nectarine to be evaluated because it is  
345 indicative of the presence of chlorophyll, with its characteristic green colour (Merzlyak  
346 *et al.*, 2003; Hernández *et al.*, 2006). The peak centred at 970 nm is present in the  
347 signal recorded by the two detectors. This peak and the one present at 1450 nm are  
348 related to pure water (Williams & Norris, 1987; McGlone & Kawano, 1998). A  
349 characteristic absorption band at around 1160 nm related to second overtone C-H  
350 stretching (Osborne *et al.*, 1993; Walsh *et al.*, 2004).

351





352

353 **Fig. 2.** Averaged raw VNIR and NIR spectra for the two varieties of nectarines at  
 354 different sets of analysis.

355

### 356 **3.3. Varietal classification**

357 Classification models were built based on supervised PLS-DA and LDA with the full  
 358 spectral range, with only the VNIR and NIR spectral ranges separately, and with the  
 359 effective wavelengths selected (EWs) from the original ranges. Table 2 shows the  
 360 predictive ability for each validation set for the twelve models developed. Similar  
 361 results were obtained to PLS-DA models for each spectral ranges and with the most  
 362 important EWs. However, the LDA models were less accurate with higher number of  
 363 LV and EWs than PLS-DA models. The optimal number of LVs was chosen  
 364 according to the lowest RMSE cross-validation (RMSECV) by internal validation  
 365 using the leave-one-out cross validation technique, in combined analysis with the  
 366 cumulative variance in the X and Y blocks (Bachion de Santana *et al.*, 2016). The x-  
 367 loading weights obtained for the different spectral ranges with only the EWs selected  
 368 are shown in Figure 3.

369

370 **Table 2.** Varietal classification results for each methods, presented both as a  
 371 percentage and an absolute number of correctly classified samples in the validation  
 372 sets.

373

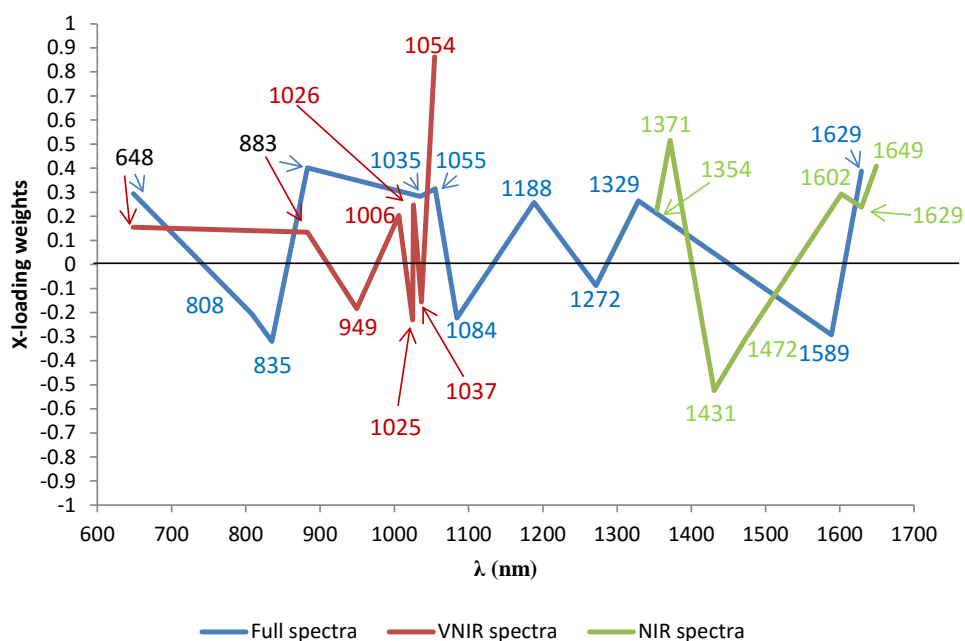
<b>Classification accuracy</b>						
<b>Methods</b>		EWs	LVs	cv.	cv.	Total
				'Diamond Ray'	'Big Top'	
<b>PLS-DA</b>	Full	2189	5	100 % (50/50)	100 % (50/50)	100 %
		12	4	94 % (47/50)	86 % (43/50)	90 %
	VNIR	1838	6	100 % (50/50)	100 % (50/50)	100 %
		8	5	100 % (50/50)	100 % (50/50)	100 %
	NIR	213	8	100 % (50/50)	100 % (50/50)	100 %
		7	4	92 % (46/50)	98 % (49/50)	95 %
<b>LDA</b>	Full	2189	14	100 % (50/50)	100 % (50/50)	100 %
		12	10	94 % (47/50)	86 % (43/50)	90 %
	VNIR	1838	12	98 % (49/50)	100 % (50/50)	99 %
		8	7	100 % (50/50)	100 % (50/50)	100 %
	NIR	213	5	84 % (42/50)	76 % (38/50)	80 %
		7	6	98 % (49/50)	96 % (48/50)	97 %

374

375 Using all 2189 spectrum features, PLS-DA and LDA achieved external validation  
 376 accuracies of 100 %. Selecting 12 wavelenghts, PLS-DA and LDA achieved  
 377 classification accuracy of 90% with four and ten LVs, respectively. PLS-DA was able

378 to correctly classify all samples in the validation set by using the 213 wavelengths of  
 379 NIR detector and with only seven EWs and four LVs attained 95 %, although LDA  
 380 achieved better results with only seven EWs and six LVs (97 % of accuracy) than  
 381 with all wavelengths of the NIR detector (80 % of accuracy). However, selecting only  
 382 eight EWs out 1838 available features of VNIR detector, PLS-DA and LDA model  
 383 attained 100 % validation accuracies with five and seven LVs, respectively. These  
 384 eight EWs were selected including 648, 883, 949, 1006, 1025, 1026, 1037, and 1054  
 385 nm. So, with only these eight EWs obtained by VNIR detector was possible achieved  
 386 better accuracy classification results (100 %) than the other models developed with  
 387 the other spectral ranges. An explanation for this result would be that visible  
 388 spectroscopy is more suitable for the characterization of nectarine colours, which are  
 389 very similar in both varieties, while near infrared spectra provides complementary  
 390 information (Liu *et al.*, 2003) related to the macronutrients and the interactions that  
 391 they can develop with other constituents (Lucas *et al.*, 2008).

392

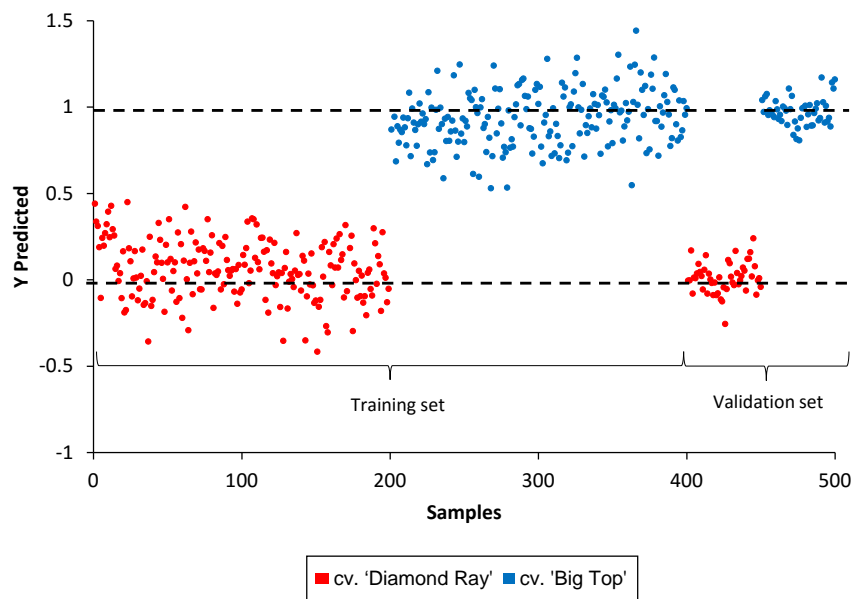


393

394 **Fig. 3.** The x-loading weights for the EWs selected at different spectral ranges.

395

396 Figure 4 shows that all the training set and validation samples were correctly  
397 classified by the best PLS-DA model obtained with eight EWs. In this situation, all  
398 'Big Top' samples have predictive values close to 1, thus classifying these as  
399 belonging to class '1', and 'Diamond Ray' samples have predictive values close to 0,  
400 thereby classifying these as belonging to class '0'. The values of the RMSE were  
401 0.179 and 0.183 for calibration and validation respectively, which exhibit good  
402 agreement, thus indicating that the calibration error is a good estimation of the  
403 standard error of prediction observed in samples of the test set. Moreover, the test  
404 set yielded similar results to those of the calibration set, with  $R^2$  of 0.872 and 0.866  
405 respectively, which indicates a good performance of the model for varietal  
406 classification.



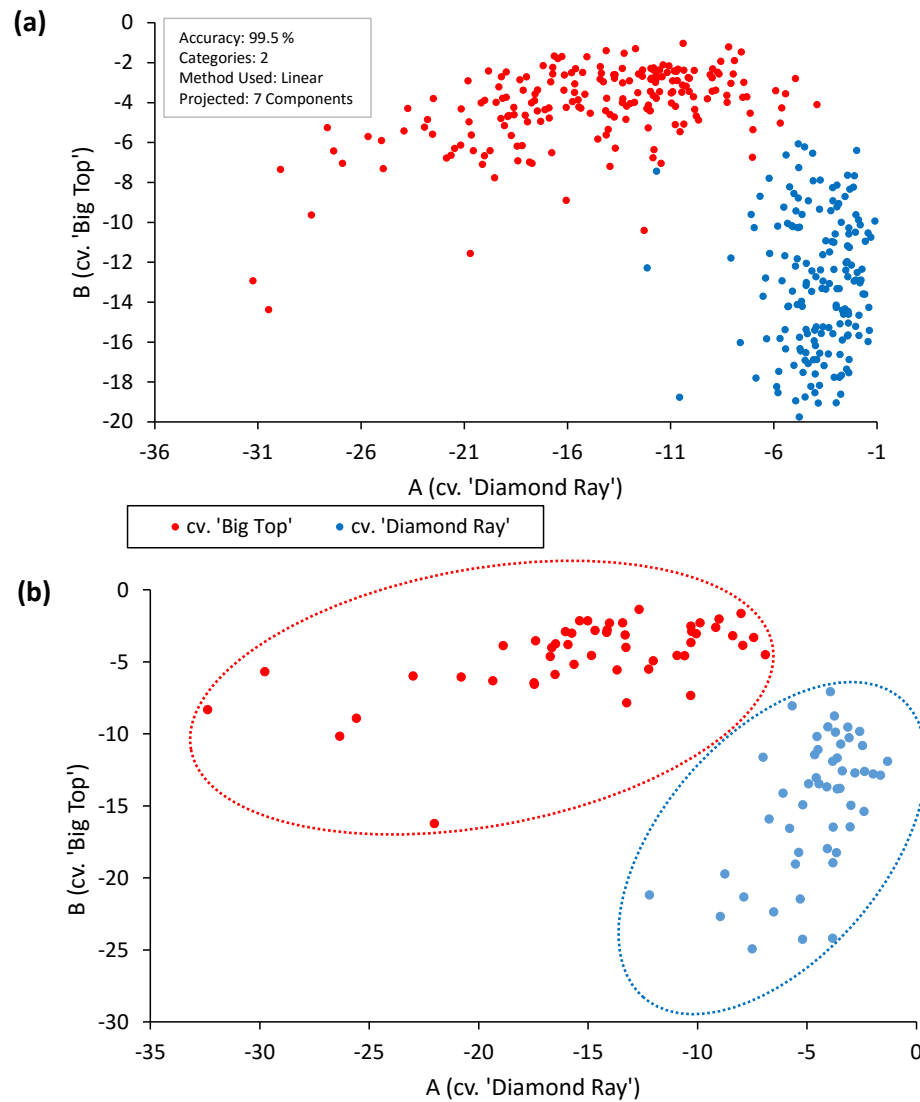
407

408 **Fig. 4.** Estimated class values for training and validation sets for varietal  
409 discrimination by the best PLS-DA model.

410

411 Regarding LDA, Figure 5 shows the results of the external validation by test set (20  
412 %) of each variety. Validation samples of the cv. 'Big Top' are displayed in blue while

413 samples of the cv. 'Diamond Ray' are in red. There were not misclassified samples,  
414 so the classification accuracy was 100 % using only eight wavelengths of the VNIR  
415 spectral region.



416

417 **Fig. 5.** Discrimination plot of the best LDA model for (a) the training samples and (b)  
418 the validation samples.

419

420 Several authors (Balabin *et al.*, 2010; Liu *et al.*, 2006; Sinelli *et al.*, 2007) have  
421 reported that the PLS-DA method is more effective than LDA. Indeed the LDA  
422 method suffers from several limitations, for example, the number of variables cannot

423 exceed the number of samples (Roggo *et al.*, 2003) and it is not able to cope with  
424 highly collinear data, which are quite common. To overcome some limitations, over  
425 the years other techniques, in particular PLS-DA, have been devised (Marini, 2010).  
426 Similarly, to us, Long *et al.* (2015) combined near-infrared spectroscopy with PLS-DA  
427 for the discrimination of transgenic rice and they achieved a classification rate of 100  
428 % in the validation test. Additionally, a considerable effort has been made in this  
429 work towards the development of models that objectively identify variables that  
430 provide useful information and eliminate those that contain unnecessary data.

431

#### 432 **4. CONCLUSIONS**

433 Classification models were developed in order to discriminate two nectarine varieties  
434 (cv. 'Big Top' and cv. 'Diamond Ray') in different spectral ranges (VNIR, NIR, and the  
435 whole spectra combined). Two classification methods including PLS-DA and LDA  
436 were evaluated based on all wavelengths or the EWs selected for the spectral  
437 regions considered. The best models were obtained using only eight EWs out of the  
438 1838 available features of the VNIR detector, identified from the x-loading weights as  
439 the most important ones. PLS-DA and LDA models attained an accuracy of 100 % for  
440 the validation set with five and seven LVs, respectively. Therefore, PLS-DA and LDA  
441 resulted as robust models for discriminating varieties of nectarine with a satisfactory  
442 level of accuracy. The comparison of the different analysis performed indicated that  
443 both detectors were able to achieve a good varietal classification, being the detector  
444 sensible in the VNIR range the one that achieved better results identifying the studied  
445 varieties of nectarines, almost identical in external and internal appearance but very  
446 different in taste and organoleptic properties..

447

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454

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