

**Prediction of ‘Nules Clementine’ mandarin susceptibility to rind breakdown
disorder using Vis/NIR spectroscopy.**

ABSTRACT

The use of diffuse reflectance visible and near infrared (Vis/NIR) spectroscopy was explored as a non-destructive technique to predict ‘Nules Clementine’ mandarin fruit susceptibility to rind breakdown disorder (RBD) by detecting rind physico-chemical properties of individual intact fruit from different canopy positions. Vis/NIR spectra were obtained using a LabSpec® spectrometer. Reference physico-chemical data of the fruit were obtained after 8 weeks of storage at 8°C using conventional methods and included RBD, H°, colour index, fruit mass loss, rind dry matter, sugar (sucrose, glucose, fructose, total sugars), phenolic acid concentrations. Principal component analysis (PCA) was applied to analyse spectral data to identify clusters in the PCA score plots and outliers. Partial least squares regression (PLSR) was applied to spectral data after PCA to develop prediction models for each quality attribute. The spectra were subjected to a test set validation by randomly dividing the data into calibration (60%) and validation (40%) sets. PLS-discriminant analysis (PLS-DA) models were developed to sort fruit based on canopy position and RBD susceptibility. Fruit position within the canopy had a significant influence on rind biochemical properties. Outside fruit had higher rind sugar, phenolic acids and dry matter content and lower RBD index than inside fruit. The data distribution in the PCA and PLS-DA models displayed four clusters that could easily be identified. These clusters allowed distinction between fruit from different preharvest treatments. NIR calibration and validation results demonstrated that sugars, dry matter,

colour index and mass loss were predicted with significant accuracy. The good correlation between spectral information and sugar content demonstrated the potential of Vis/NIR as a non-destructive tool to predict fruit susceptibility to RBD.

Keywords: Non-destructive technique · Vis/near infrared spectroscopy· Rind breakdown disorder (RBD) · Citrus · ‘Nules Clementine’ Mandarin · Canopy position.

1. Introduction

South Africa produces approximately 100 000 tons of Clementine mandarins per annum, making it the third largest producer and exporter of Clementine mandarins in the world after Spain and Morocco (Barry and Rabe, 2004). The development of various types of physiological disorders limits the postharvest storage capability and causes commercial losses. A lack of understanding the physiological mechanism underlying these disorders affects both supply and profits. The challenge is significant regarding rind breakdown disorder (RBD) of ‘Nules Clementine’ mandarins (*Citrus reticulata* Blanco.) that do not manifest during harvest grading and postharvest treatments but develop about 3 to 5 weeks after harvest.

RBD is initially manifested on the equatorial plane as small, irregular, slightly sunken and colourless patches of about 3 to 6 mm in diameter scattered about the flavedo (the outer-most, pigmented part of citrus rind) of the fruit (Cronje et al., 2011). These sunken areas, occurring directly above and among the oil glands of the flavedo, coalesce

47 producing larger affected areas, turning redish-brown to dark-brown, become dry and
48 necrotic in the severe stages of the disorder with extended storage period (Cronje, 2007,
49 2009). According to Agustí et al. (2001) browning of affected rind surface appears to be
50 the result of oxidative processes.

51
52 Intensive research has been conducted towards determining factors triggering RBD. As a
53 result, it has been established by several research groups that different microclimates are
54 influencing sensitivity of fruit to RBD and similar rind disorders such as rind pitting on
55 oranges (Alferez and Zacarias, 2001) and grapefruit (Alferez and Burns, 2004) and peteca
56 spots on lemons (Wild, 1991). In a study conducted in Spain (northern hemisphere),
57 Almela et al. (1992) reported that these fluctuations could also be observed among fruits
58 from the same tree and the incidence being by exposure of individual fruit to the sun.
59 These investigators further showed that fruit oriented to the north-west (NW) in canopy
60 were most affected by the disorder. In a later study conducted in the same country, Agustí
61 et al. (2001) corroborated that fruit positioned in the NW face of the tree to be more
62 prone to develop the rind pitting disorder and this was reported to be consistent over five
63 seasons. Similar observations were reported in ‘Fortune’ (Duarte and Guardiola, 1995)
64 and ‘Encore’ (Chikaizumi, 2000) mandarin fruit, where it was maintained that the
65 disorder affects mainly the exposed fruit from the north-west quadrant of the tree.

66
67 In a study conducted in South Africa (southern hemisphere), fruit position, and therefore
68 exposure to high (outside) or low (inside) light levels in the canopy, affect the flavedo
69 concentration of carbohydrates during fruit development (Cronje, 2009; Cronje et al.

2011). The latter authors reported the flavedo from fruit borne on the outside of the canopy to have significantly higher sucrose, glucose and fructose content than the fruit borne inside the canopy. Interestingly, the results obtained by this group of investigators revealed a correlation between fruit position, rind sugar content and ultimately development of RBD. The incidence of rind breakdown was higher on inside fruit compared with the outside fruit and this was consistent from season to season and could be attributed to their exclusion from adequate sunlight during their fruit development. In addition, fruit borne inside the canopy had lower chlorophyll and carotenoid contents, and therefore poorer rind colour (Khumalo, 2006), and lower carbohydrates rendered them susceptible to the disorder (Cronje, 2009). Although intensive research aimed at appreciating RBD has been conducted, the disorder still occurs frequently and unpredictably, reducing the quality of the fruit (Almela et al., 1992; Cronje, 2005).

There is therefore a need to develop an objective, fast and non-destructive assessment that can be used to determine/predict citrus fruit susceptibility to rind disorders accurately. Non-visible information, such as that provided by near infrared (NIR) region of the spectrum can improve the inspection by detecting rind biochemical profile and hence the detection of non-visible physiological disorders (Blasco et al., 2007). Most current non-destructive quality measurement using NIR spectroscopy (NIRS) has been developed to assess fresh fruit according to their internal quality attributes (Butz et al., 2005). Very limited research work has been conducted to develop a technology that can assess, predict and monitor the physiological disorders and rind physiological disorders of citrus fruit in particular. Nevertheless, NIRS has been used successfully to detect

surface bruising in apple (Geeola et al., 1994), surface defects in peach (Miller and Delwiche, 1991), storage disorders in kiwifruit (Clark et al., 2004) and drying internal disorder in Tangerine citrus (Peiris et al., 1998). Recently, Teerachaichayut and co-workers (2011) successfully used NIR spectroscopy to non-destructively predict pericarp hardening disorder in magosteen fruit. The trend has constantly shifted towards developing reliable and cost effective technologies to non-destructively screen fruit physiological disorders. Recently, Zheng et al. (2010) used NIR in the reflectance mode to predict oleocellosis sensitivity in citrus fruit. A review by Magwaza et al. (2011) discusses the recent developments and application of Vis/NIR spectroscopy to non-destructively evaluate internal and external fruit quality.

In summary, the knowledge of biochemical changes in the rind of citrus fruit that could be used to precisely predict fruit rind condition and therefore susceptibility to rind disorders is limited. However, previous research by Cronje et al. (2011) indicated that fruit position within the canopy affects rind biochemical profile, particularly carbohydrate concentration and hence susceptibility of fruit to RBD. This study aims to explore the use of diffuse reflectance Vis/NIR spectroscopy in the wavelength range of 350-2500 nm as a non-destructive tool to predict susceptibility to RBD by detecting rind physico-chemical properties of individual intact fruit from different canopy positions.

2. Material and methods

115 2.1. *Site, fruit sampling and postharvest handling*

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117 A total of 15 ‘Nules Clementine’ mandarin trees in an orchard at Stellenbosch University
118 experimental farm, Western Cape Province, South Africa (33°53’4.56’’S, 18°37’36.84’’E)
119 were identified and marked based on their health and fruit setting ability. On each tree,
120 200 fruit from sun-exposed and 200 from shaded canopy positions were randomly
121 selected and tagged. To increase our success of having fruit with RBD, a method of
122 enhancing the disorder demonstrated by [Cronje \(2009\)](#) was adopted. Briefly, during
123 January 2011 (after physiological drop about four months until commercial maturity),
124 half of the selected fruit from each position was covered with brown paper bags without
125 removing or covering subtending leaves. The study consisted of four preharvest
126 treatments, viz., outside, outside bagged, inside and inside bagged.

127
128 Upon reaching commercial maturity, on 16 May, individual fruit were harvested
129 according to industry practice, coded according to treatment and canopy position and
130 underwent all commercial postharvest practices, including drenching (Thiabendazole, 500
131 mg/L; Imazalil, 500 mg/L and 2,4-dichlorophenoxyacetic acid, 125 mg/L) and waxing
132 (polyethylene citrus wax, Citrushine®, Johannesburg, South Africa). After which they
133 were brought to the postharvest evaluation laboratory, sorted to remove any defective
134 fruit and weighed. A total of 80 blemish free fruit (20 fruit from each treatment) were
135 selected to provide fruit samples for non-destructive and destructive measurements. After
136 phytosanitary inspection and certification, these fruit were separately packed in boxes

marked, sent at room temperature via a courier service to Cranfield University (CU) in the United Kingdom, where postharvest storage took place.

2.2. *Spectral acquisition*

Vis/NIR spectra were obtained upon arrival at CU using a method described by Kuang and Mouazen (2011). Spectral acquisition from intact fruit samples was carried out using a mobile fibre-optic Vis/NIR spectrophotometer (350-2500nm) (LabSpec2500(r) Near Infrared Analyzer, Analytical Spectral Devices Inc., USA) in diffuse reflectance mode equipped with one Si array (350-1000nm) and two Peltier cooled InGaAs detectors (1000-1800 nm and 1800-2500 nm). The sampling interval of the instrument was 1 nm. However, the spectral resolution was 3 nm at 700 nm and 10 nm at 1400 nm and 2100 nm. A high intensity probe with an in-built light source was used. A quartz-halogen bulb of 3000 Kelvin light source and a detection fibre are gathered in the high intensity probe enclosing a 35° angle.

Prior to scanning the fruit samples, and periodically at intervals of 30min, white reference measurements were taken. Fruit samples were placed in direct contact with the high intensity probe. Reflectance spectral data was acquired from 8 position of the fruit; 4 from equatorial spots of the fruit and 2 from the stem-end and 2 from the stylar-end of the fruit, averaged and used for spectral pre-processing and multivariate analysis.

2.3. Physico-chemical measurements to obtain reference values

2.3.1. Storage conditions, RBD rating, weight and rind colour

After scanning, fruits were stored in a cold room with delivery air temperature of 8°C, a temperature which is known to cause the highest degree of RBD incidence (Khumalo, 2006). During cold storage, fruit were scored weekly, for the incidence of RBD for the duration of 8 weeks. RBD was scored on a subjective scale from 0 = no breakdown to 3 = severe breakdown. RBD was then expressed as RBD index (RBDI), estimated as previously described (Alf  rez et al., 2003) and calculated according to the following formula previously reported for chilling injury and peel pitting by Lafuente et al. (1997) and Lafuente and Sala (2002):

$$RBDI = \frac{\sum \{RBD(0 - 3) \times \text{No. of fruit in each class}\}}{\text{Total number of fruit}} \quad (1)$$

Fruit were weighed weekly using a calibrated balance (Mettler Toledo, ML3002E / 01, Switzerland). Rind colour components were measured in L*a*b* colour space using Minolta CR-400 colourimeter (Chroma Meter CR-400, Konica Minolta Sensing Inc., Japan) after calibration using standard white tile (CR-A43; Y = 93.1, x = 0.3138; y = 0.3203). From L*, a* and b* colour parameters, colour index (CI) was calculated according to Jimenez-Cuesta et al. (1981) using the following formula:

$$CI = \frac{1000 \times a}{L \times b} \quad (2)$$

182

183 2.3.2. *Sample preparation*

184

185 After 8 weeks in storage, fruit samples were destructed where rind was peeled from the
 186 rest of the fruit. The pulp was juiced and the juice used for fresh TSS analysis. TSS was
 187 measured with a digital hand-held refractometer (Palette, PR-32 α , Brix 0.0-32.0, Atago,
 188 Co. LTD, Japan) using 1 mL of freshly squeezed juice and expressed as °Brix. The rind
 189 from each sample was snap frozen in liquid nitrogen, separated into two portions, of
 190 which one portion was stored at -40°C and the other at -80°C freezer until further
 191 analysis.

192

193 Fresh frozen rind samples were freeze-dried in Edwards Modulyo freeze drier (W.
 194 Sussex, UK) for 7 days at 0.015 kPa and -55°C. Lyophilized samples were weighed and
 195 water content was calculated from freeze dried samples and expressed as a percentage of
 196 fresh weight. Samples were then ground using pestle and mortar into fine powder and
 197 returned into the freezer prior to being used for sugar and phenolic acids determination by
 198 HPLC.

199

200 2.3.3. *Extraction and HPLC quantification of non-structural sugars*

201

202 Sugar was extracted from 150 mg of fruit rind powder using 62.5% (v/v) aqueous
 203 methanol as described elsewhere by [Terry et al. \(2007\)](#). Following extraction,

concentration of fructose, glucose and sucrose was determined using an Agilent 1200 series HPLC binary pump system (Agilent, Berks., UK), equipped with an Agilent refractive index detector (RID) G1362A, based on the method described by Crespo et al. (2010). Briefly, sample extracts was diluted (1:10), and injected into a Rezex RCM monosaccharide Ca^+ (8%) column of 300 mm x 7.8 mm diameter (Phenomenex, Torrance, CA) with a Carbo- Ca^{2+} guard column of 4 mm x 3 mm diameter (Phenomenex). Temperature of the column was set at 80°C using a G1316A thermostated column compartment. The mobile phase used was HPLC-grade water at a flow rate of 0.6 ml/min (Giné Bordonaba and Terry, 2008). The presence and abundance of the selected sugars was calculated by comparison of peak area with peak of known standards using ChemStation Rev. B.02.01.

2.3.4. *Extraction and HPLC quantification of phenolic compounds*

Phenolic acids were extracted and quantified using a method described elsewhere by (Magwaza et al., 2012). Briefly, a 150 mg of freeze dried rind powder was dissolved into 3 mL 70:29.5:0.5 (methanol:H₂O:HCL). Samples were extracted at 35°C in water bath for 30 minutes, agitated for 30s every 5 minutes and the flocculate filtered through a 0.2 µm syringe filter. Phenolic acid concentrations were determined using the HPLC system equipped with an Agilent DAD G1315B/G1365G photodiode array with multiple wavelength detector.

2.3.5. Determination of antioxidant capacity

Antioxidant capacity was measured on freeze-dried samples following the method by [Crespo et al. \(2010\)](#). The absorbance of prepared sample solutions was measured spectrophotometrically at 517 nm using a Camspec M501 UV/vis spectrometer. Basically, the antioxidant capacity determination with 2,2-diphenyl-1-picrylhydrazyl (DPPH) is based on the properties of DPPH, which its radical form has an absorption band at 517 nm and disappears upon reduction by an antiradical compound.

2.4. Data analysis

2.4.1. Statistical analysis

Statistical analyses carried out using SPSS 10.0 for Windows (SPSS Inc. Chicago, USA). Data was subjected to analysis of variance (ANOVA). Least significant difference values (LSD; $P=0.05$) were calculated for mean separation ([Landahl et al., 2009](#)).

2.4.2. NIRS analysis, calibration development and validation

Before analysis, the reflectance spectra in Indico format (Indico Pro 5.6 software, Analytical Spectral Devices Inc., USA) were transformed to absorbance ($\log(1/R)$). Calculations of the average of 8 spectra obtained from each fruit, pre-processing and

248 calibration methods were executed using the Unscrambler chemometric software (The
249 Unscrambler Version 9.2, Camo Process, SA, Trondheim, Norway).

250

251 Several pre-processing methods including, smoothing using moving average and
252 Savitzky-Golay methods, full multiple scatter correction (MSC), Savitzky-Golay first
253 derivative and second derivative, minimum and maximum normalisation and vector
254 normalisation (SVN) were tested to correct light scatter and reduce the changes of light
255 path length. After pre-processing trials, the optimal model performance was obtained
256 using the Savitzky-Golay second derivative with the polynomial order of 5 and MSC.
257 Savitzky-Golay second derivative was used to correct light scattering properties while
258 MSC was used to correct for additive, multiplicative effects of the spectra, and pathlength
259 variations ([Leonardi and Burns, 1999](#); [Gómez et al., 2006](#)).

260

261 In order to determine effective wavelength, discriminate fruit from four canopy positions
262 using Vis/NIR and to detect outliers, PCA was performed using full cross validation.
263 Partial least squares regression (PLSR) was applied to spectral data to develop prediction
264 models for each quality attribute. A PLS variant known as partial least squares
265 discriminant analysis (PLS-DA) was also used in order to classify fruit from different
266 canopy positions according to the spectra. A method by [Chen et al. \(2011\)](#) was used in
267 the application of PLS-DA. Briefly, fruit from each of the canopy positions in the
268 calibration set was assigned a dummy variable as a reference value (outside = 1, outside
269 bagged = 2, inside = 3 and inside bagged = 4). In addition, due to discrete nature of RBD
270 scores, samples were assigned a binary dummy variable as a reference value, which was

an arbitrary number whether the sample belongs to a particular position or not. RBD affected fruit were set as reference data one, while unaffected fruit were assigned to 1 ([Teerachaichayut et al., 2011](#)).

To develop PLS models, the dataset was randomly separated into two subsets, 60% for calibration and 40% for test set validation. The regression statistics of developed models was described by the value of the root mean square error of calibration (RMSEC), root mean square error of validation or prediction (RMSEP), the Pearson correlation coefficients (R) between predicted and observed reference values, number of latent variables (LVs), and the residual predictive deviation (RPD), described by [Williams and Sobering \(1996\)](#) as the ratio of the standard deviation of the reference data for the validation set to the RMSEP. The ideal model should have higher R and RPD values as well as lower RMSEC and RMSEP values. The optimal number of LVs was determined as the minimum number of LVs corresponding to the first lowest value of the RMSEC or RMSEP from the plot of the RMSEC or RMSEP for increasing number of LVs ([Davey et al. 2009](#)). The stability of the calibration model was tested by interchanging validation and calibration data sets and checking that the differences in the regression statistics obtained were small ([Alvarez-Guerra et al., 2010](#)).

3. Results and discussion

3.1. Rind breakdown disorder and biochemical profile of fruit from different canopy positions.

Symptoms of rind breakdown disorder were visible on affected fruit after five weeks of continuous storage at 8°C. RBD was significantly affected by preharvest manipulation of sunlight exposure ([Table 1](#)). Outside fruit had the lowest susceptibility to develop the disorder compared to other preharvest treatments. Fruit position within the canopy on its own did not show a significant difference on fruit susceptibility to RBD. However, exclusion of sunlight by bagging fruit resulted in increased fruit susceptibility but only showed a significant difference on fruit located inside the canopy. These findings are consistent with those observed by [Almela et al. \(1992\)](#). In their study, these authors established that the sensitivity of fruit to development of rind spots related to RBD in ‘Fortune’ mandarins was influenced by different microclimates. Similar to observations reported by [Cronje et al. \(2011\)](#), fruit position within the canopy affected rind colour index (CI). Fruit borne on the outside of the tree canopy had the highest CI and hence were more orange while shaded fruit had pale, yellow rinds.

Foregoing research suggests that rind water status is a factor prevailing in the susceptibility of citrus fruit to rind physiological disorders ([Cohen et al., 1994](#); [Alfárez and Burns \(2004\)](#)). In this study, fruit from the bagged treatments, both inside and outside of the canopy, were characterized by high postharvest weight loss, and this was essentially due to water loss by transpiration, as this account for 90% of total weight loss ([Ben-Yehoshua, 1969](#)). Water loss from the fruit results from a water pressure gradient

315 prevailing between the fruit rind, which is close to saturation with water, and the less
316 saturated outer atmosphere (Ben-Yehoshua *et al.*, 1994; Macnish *et al.*, 1997).

317

318 Fruit position within the canopy also had a significant influence on rind biochemical
319 properties. Results in Table 1 showed that outside fruit had higher TSS, dry matter
320 content, glucose and total phenolic acid concentrations compared to shaded samples. The
321 effect of canopy position on fruit quality was documented by (Barry *et al.*, 2000) who
322 reported that fruit from the south western top part of the canopy had significantly higher
323 soluble solids contents, lower titratable acid content and higher ratio than fruit borne in
324 the north east bottom position. In this study, bagged fruit from outer portion of the
325 canopy had significantly higher glucose concentration of 92.03 mg/g DW compared to
326 inside fruit, which had 66.92 mg/g DW glucose concentration. On the contrary, sucrose,
327 and total carbohydrate of bagged fruit from inside the canopy were significantly higher in
328 relation to other three positions. It was therefore noteworthy that these fruit also had
329 highest susceptibility to RBD.

330

331 In addition to carbohydrate contents, phenolic acid concentration and antioxidant
332 capacity were affected by fruit exposure to sunlight. Unbagged samples from the inside
333 and outside position had relatively higher phenolic acid content of 39.29 and 37.65 mg/g
334 DW when compared to outside bagged and inside bagged samples which had 33.48 and
335 34.68 mg/g DW, respectively. Moreover, the antioxidant activity of inside bagged
336 samples, i.e. fruit with the highest RBD, was much higher than those with low RBD
337 disorder. It has reported previously that the presence antioxidant species or the lack

thereof could be implicated to the development of various postharvest disorders including non-chilling peel pitting in ‘Navelate’ oranges (Cajuste and Lafuente, 2007). The results presented above are in accord with the notion that manipulating light levels around an individual fruit reduces rind condition and susceptibility to the disorder. Pearson correlation analysis between physico-chemical properties and RBD development had very low correlation coefficients which serve to prove the complexity of factors involved in the development of this disorder. Furthermore, the lack of a specific threshold values below or above which all fruit become affected and above or below which all fruit stay healthy suggests that several preharvest and postharvest factors also play a role.

3.2. Vis/NIR spectroscopy

3.2.1. Distribution of prediction and validation reference data

In this study, reference data set was partitioned into the calibration (60% of n) and validation (40% of n) set. **Table 2** shows the distributional statistics for reference datasets used in calibration and test validation. The reference measurements of all parameters in calibration and validation were fairly normally distributed round the means. Although the selection method for calibration and validation was random, validation data set was scrutinised to ensure that the validation data sets were confined within a boundary of the calibration set. The interpretation of calibration results depends greatly on the precision of the determined reference data and enough variation in both calibration and validation data (Lu et al. 2006). As is apparent in the range and CV% values of the data presented,

the calibration and validation values of the sample quality parameters cover a large range, which is helpful for developing calibration models for NIR spectroscopy (Clément et al. 2008). For instance, the mean concentration of sucrose values used for calibration and validation were 101.40 and 78.81 mg/g DW with standard deviation of 43.27 and 34.15 mg/g DW, respectively. The range of total sugars in the calibration set was from 121.91 to 511.11 mg/g DW and the range of validation set was from 141.91 to 492.28 mg/g DW with corresponding CV % of 29.38 and 36.31%, respectively.

3.2.2. *Spectrum description*

The absorbance spectra presented in Figure 1(a) portrays the typical spectra obtained from intact “Nules Clementine” mandarins subjected to different preharvest treatments. Each line represents the average spectra from 20 fruit in each preharvest treatment. Spectral features were similar to those obtained by Gómez and co-workers (2006). Strong absorption bands around 670, 740, 980, 1200, 1450, 1780 and 1930 nm were observed. Absorption at these wavebands were, respectively, due to red absorbing pigments, particularly chlorophyll (Clément et al. 2008), third overtone of O-H stretching, second overtone of H-O-H stretching modes of water, second and first overtones of C-H stretching as well as the third overtone of O-H, C-H and C-H₂ deformation associated with sugar solution reported by Kawano et al. (1993) and Golic et al. (2003). It should be noted that the average spectra of inside bagged fruit (with highest RBD) had a distinctly stronger absorbance in the waveband between 600 and 900 nm. This was similar to results obtained by Zheng et al. (2010) for prediction of olleocellosis disorder, where large

variations in absorbance spectra were observed among fruit with different sensitivities in the same waveband. Since the intensities of reflectance vary with concentrations of biochemical constituents of the sample (Williams and Norris, 2001) this band may possibly be related to fruit sensitivity to rind physiological disorders such as oleocellosis and RBD.

3.2.3. *Pre-processing methods*

The spectra of solid samples such as fruit are influenced by physical properties such as shape, size, path length, etc. (Leonardi and Burns 1999), which create noise and determine light scattering properties. As a common practice in NIRS, obtained spectra was subjected to several pre-processing methods and the suitable pre-processing methods were selected. Results presented in Table 3 show that Savitzky-Golay second derivative with the fifth order polynomial (Figure 1(b)) provided the best results for the PCA classification and PLS model for predicting RBD. MSC (Figure 1(c)) gave best results for PLS prediction of physico-chemical properties such as h° , CI, weight loss, dry matter content, and carbohydrate concentrations as well PLS-DA classification by preharvest treatments.

3.2.4. *Vis/NIR- based PCA and PLS classification models*

Individual spectra from 8 positions within the fruit and the average spectra were tested to develop PCA and PLD-DA classification models. Average spectra showed better models than individual spectra; and thus subsequent analyses were based on average spectra.

PCA was performed on Vis/NIR spectra to compare spectral characteristics of fruit from different preharvest treatments. The PCA applied to the spectra using Savitzky Golay second derivative pre-processing revealed better grouping of the samples than other tested pre-processing methods. The data distribution in the PCA score plot presented in **Figure 2** displayed four clusters that could easily be identified. These clusters allowed distinction between fruit from different preharvest treatments. The first two principal components (PC) accounted for 68.0 % of the total variability, PC1 explains the 53.0 % of the variance and PC2 explained 15.0 % of the variance. The effective wavelength band for this classification was from 350 to 1200 nm with a strong absorption at 670 nm influenced by chlorophyll and three at 740, 980, 1200 nm corresponding to water (O-H) functional groups. From this, it could be concluded that a combination of colour and moisture content of the rind play an important role in discriminating from different positions of the canopy.

Spectral data was further subjected to discriminant analysis by assigning fruit from each canopy positions to a dummy variable (1, 2, 3 and 4 for outside, outside bagged, inside bagged and inside, respectively). **Figure 3** depicts performance of the PLS-DA model to classify fruit based on their origin within the tree canopy using full spectral range (350-2500 nm) and MSC spectral pre-processing. The prediction accuracy determined using 24 test set for validation was high ($r = 0.971$, $RMSEP = 0.304$).

3.2.5. Vis/NIR- based PLS prediction models

431 **Table 3** shows summary statistics for calibration and validation results for the prediction
432 of different physico-chemical properties with PLS models. After testing different
433 wavelength ranges based on observed peaks and information provided in the literature,
434 wavelength bands that gave the lowest RMSEC and RMSEP were selected to develop
435 calibration models for each physico-chemical property. As would be expected, models
436 for colour parameters (h° and CI) were developed using visible range (350-700 nm) of
437 the spectrum, whereas RBD model was developed with the region between 350-1000 nm.
438 This was in accordance with the range used by [Zheng et al. \(2010\)](#) to develop models for
439 predicting susceptibility of citrus fruit to oleocellosis, another rind physiological disorder.
440
441 Prediction models for sucrose, fructose, glucose, total sugars, TSS, dry matter and water
442 loss were developed using wavelength range between 900 to 1800 nm. According to the
443 absorption bands of common foods constituents provided by [Williams and Norris \(2001\)](#),
444 all these biochemical components have absorption bands in this spectral region. Results
445 obtained in this study are similar to previous studies suggesting that the range from 350-
446 1800 nm is suitable for predicting colour parameters ([Sun et al., 2009](#)), dry matter
447 ([Guthrie et al., 2005a, b](#)), sucrose, fructose, glucose ([Tewari et al., 2008](#)) and sugar
448 content ([Liu et al., 2010](#)).
449
450 Models for predicting quality parameters such as colour index, h° , DM and water loss
451 showed significantly high performance, with predictive R values ranging from 0.91 to
452 0.98 and RPD ranging from 2.34 to 4.13 for water loss and CI, respectively (**Figure 5**).
453 NIR calibration and validation results demonstrated that sugars, dry matter, colour index

and mass loss were predicted with significant accuracy. The prediction performance for sugars (sucrose, fructose, glucose, and total sugars) was high with R of 0.88, 0.94, 0.95, and 0.95 and corresponding RMSEP values of 24.36, 11.41, 11.58, 31.04 mg/g DW, respectively (Figure 6). Although the accuracy is slightly lower, these results were comparable to those reported in the literature by Tewari et al. (2008) for the prediction of sucrose, fructose and glucose of grapefruit.

As suggested by Davey et al. (2009) and Saeys et al. (2005), although the correlation between NIR predicted and reference values is high, it is also very critical to verify the accuracy of the model by referring to the RPD values. These authors stated that RPD values below 1.5 are considered unusable, those between 1.5 and 2.0 are suitable for rough prediction, those between 2.0 and 2.5 are suitable for quantitative predictions, while RPD values between 2.5 and above 3.0 are respectively considered good and excellent prediction models. The low RPD values, 0.30 and 1.40 for RBD and sucrose, respectively, clearly indicate poor accuracy of these models. The poor accuracy of these models could be attributed to high variation of these parameters in both calibration and test set data. Furthermore, the low predictability of sucrose could possibly results due to the difference in molecular weight of sucrose (MW=342.30 g/mol) compared to fructose and glucose (MW=180.16) (Golic et al., 2003). This difference in molecular weight is such that there are 1.89 times fewer number of sucrose molecules than glucose and fructose in the same weight of sample. Therefore, the intensity of the bands associated with hydrogen bonding is smaller in sucrose than in glucose and fructose.

The complexity of biological factors involved in the development of RBD complicated the development of an acceptable model for predicting the disorder. However, the high ability of Vis/NIR to classify fruit based on their origin within the canopy using PLS-DA could have online practical interest for online application. Another reason for the poor prediction model for RBD is that calibration and test set also contained a large proportion of samples in which RBD didn't develop. The inability to generate the disorder due to unfavourable conditions to develop the disorder under this type of study occurs. To correct this problem in future studies, it will be necessary to increase sample size for both calibration and validation sets. This is to ensure that the distribution of the disorder is wide, normal around the mean and that it represents distribution present in a harvested population of mandarin fruit (Davey et al. 2009).

4. Conclusions

In this study, the positional effects within the canopy and bagging were significant in altering rind biochemical properties. Outside unbagged fruit had higher rind sugar, phenolic acids and dry matter content and lower RBD index than inside and bagged fruit. The data distribution in the PCA and PLS-DA models displayed four clusters that could easily be identified. These clusters allowed distinction between fruit from different preharvest treatments. NIR calibration and validation results demonstrated that sugars, dry matter, colour index and mass loss were predicted with significant accuracy. The exploration of the statistics of the developed models revealed the high potential that Vis/NIR spectroscopy has to non-destructively detect rind biochemical profile and hence susceptibility to RBD. The good correlation between spectral information and

biochemical information demonstrated the potential of Vis/NIR as a non-destructive tool to predict fruit susceptibility to RBD.

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676 **Table 1:** Physico-chemical profile of fruit from different canopy positions. Different
677 alphabets next to figures (mean and standard error of the mean) in the same row are
678 significantly different.

Quality Parameter	Canopy position			
	Outside	Outside bagged	Inside	Inside bagged
h°	67.34±0.58ns	75.50±1.46ns	62.94±11.32ns	74.01±0.97ns
CI	6.12±0.19b	3.62±0.38a	3.65±0.57a	3.99±0.27a
Mass (g)	107.63±4.68b	104.89±4.28b	89.29±4.95a	107.61±6.38b
RBDI	0.00±0.00a	0.05±0.03a	0.04±0.04a	0.19±0.05b
WL (g)	9.51±0.42ab	13.02±1.76bc	7.76±0.58a	13.62±1.67c
TSS (°Brix)	13.71±0.24b	11.89±0.28a	12.11±0.27a	11.94±0.25a
DMC (%)	30.00±0.78b	26.98±0.51a	28.78±0.96a	26.99±0.79ab
Sucrose (mg/g DW)	95.31±6.07b	93.59±9.51b	63.30±8.65a	114.94±12.51b
Glucose (mg/g DW)	92.03±5.29b	85.44±8.94ab	66.92±6.97a	77.09±8.50ab
Fructose (mg/g DW)	126.48±5.19ab	130.21±9.76b	100.65±8.52a	122.26±9.71ab
Total Sugars (mg/g DW)	313.82±11.58b	309.23±25.05b	230.88±22.82a	314.29±27.70b
Total phenolic acids (mg/g DW)	39.29±0.86b	33.48±1.10a	37.65±0.85b	34.68±1.25a
DPPH (μmol trolox eq./g DW)	0.95±0.04b	1.23±0.18b	0.50±0.11a	1.36±0.17b

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687 **Table 2:** Mean, standard deviation (SD), range and coefficient of variation (CV %) for
688 calibration (60% of n) and validation (40% of n) subsets of mandarin fruit.

Quality parameter	Calibration data set			Validation data set		
	Mean±SD	Range	CV%	Mean±SD	Range	CV%
h°	73.14±5.11	63.53-89.27	7.05%	72.28±6.27	64.51-85.71	8.54%
CI	4.52±1.47	1.25-7.49	32.59%	4.29±1.76	0.07-7.04	41.12%
RBDI	0.09±0.18	0.00-0.56	205.84%	0.05±0.10	0.00-0.33	187.75%
Mass (g)	107.90±22.87	67.40-153.60	21.20%	94.58±15.07	70.7-123.1	15.93%
WL (g)	11.33±5.21	4.51-28.53	45.99%	10.83±6.45	4.87-25.84	59.52%
DMC (%)	27.85±3.14	22.84-35.41	11.28%	28.56±3.29	23.54-35.71	11.50%
Sucrose (mg/g DW)	101.40±43.27	35.17-207.91	42.66%	78.81±34.15	42.85-144.30	43.34%
Glucose (mg/g DW)	83.87±30.11	22.19-152.1	35.91%	75.69±32.59	36.01-127.60	43.06%
Fructose (mg/g DW)	124.30±33.52	53.72-195.9	26.96%	114.70±37.38	59.38-182.48	32.62%
Total Sugars (mg/g DW)	309.60±90.97	121.91-511.11	29.38%	269.17±97.74	141.91-492.28	36.31%
PLS-DA dummy variables	2.34±1.07	1.00-4.00	45.79%	2.63±1.17	1.00-4.00	44.67%

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Table 3: An overview of statistics obtained during calibration and validation of models for individual quality parameters.

Quality parameter	Calibration model					Validation model			
	LV	Prepr	R	RMSEC	RPD	R	RMSEP	RPD	Info. Region (nm)
h°	3	MSC	0.97	1.31	3.91	0.97	1.66	3.78	350-700
CI	3	MSC	0.98	0.37	3.93	0.98	0.43	4.13	350-700
RBD (binary scores)	5	2nd der	0.77	0.27	0.67	0.70	0.34	0.30	350-1000
WL (g)	10	MSC	0.92	2.01	2.59	0.91	2.76	2.34	900-1700
DMC (%)	8	MSC	0.98	0.68	4.65	0.96	0.92	3.57	900-1700
Sucrose (mg/g DW)	10	MSC	0.96	12.38	3.50	0.88	24.36	1.40	900-1700
Glucose (mg/g DW)	10	MSC	0.95	9.18	3.28	0.94	11.41	2.86	900-1700
Fructose (mg/g DW)	14	MSC	0.98	6.33	5.30	0.95	11.58	3.23	900-1700
Total Sugars (mg/g DW)	10	MSC	0.94	30.42	2.99	0.95	31.04	3.15	900-1700
PLS-DA dummy variables	10	MSC	0.98	0.20	5.25	0.97	0.30	3.85	350-2500

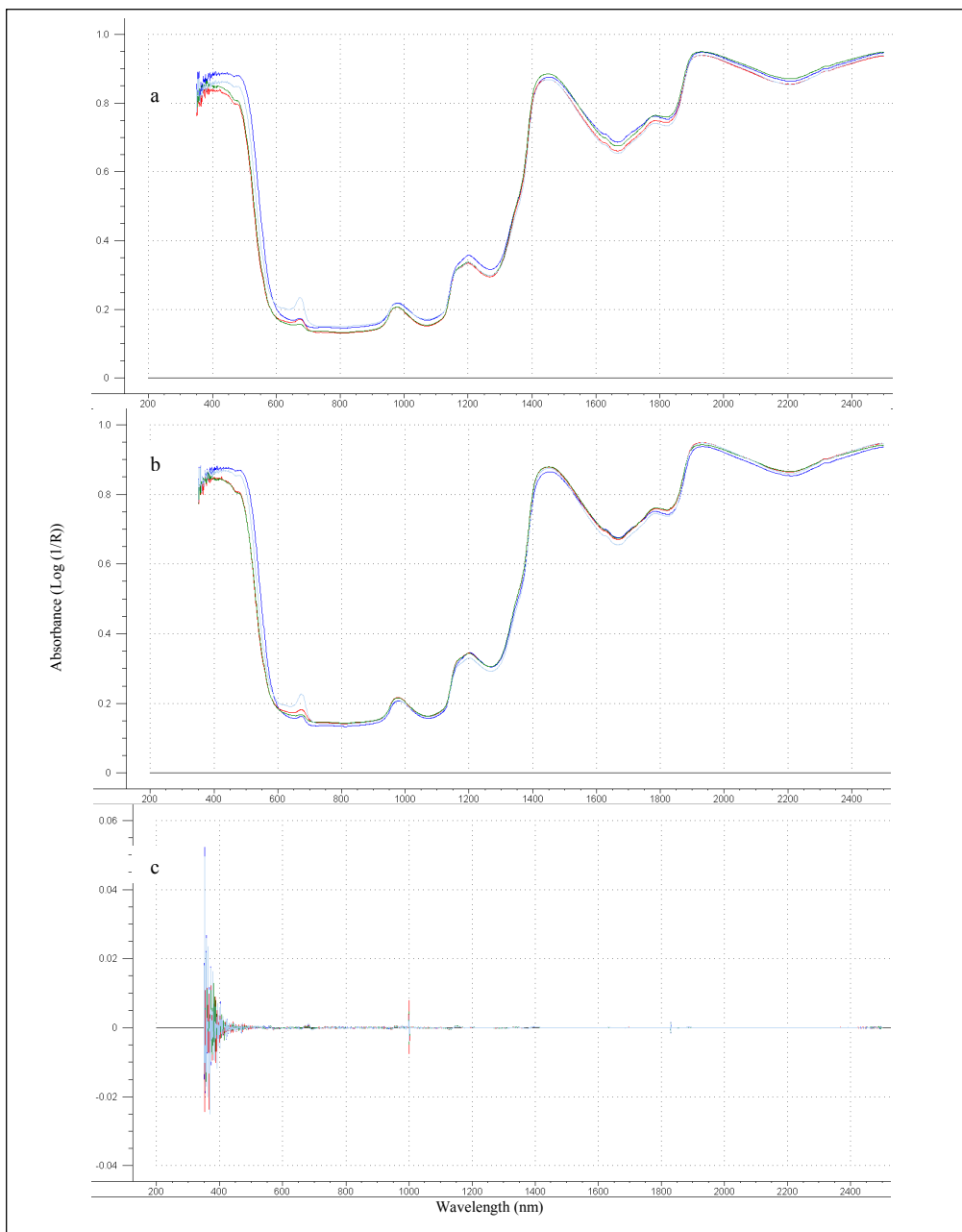


Figure 1: Typical average Vis/NIR spectra (350-2500 nm) of intact “Nules Clementine” mandarins obtained from fruit harvested from four different preharvest treatments; outside (*deep blue line*), outside bagged (*red line*), inside (*inside*), and inside bagged (*light blue line*). **(a)** Without pre-processing; **(b)** multiple scatter correction; **(c)** Savitsky-Golay first derivative of the spectra.

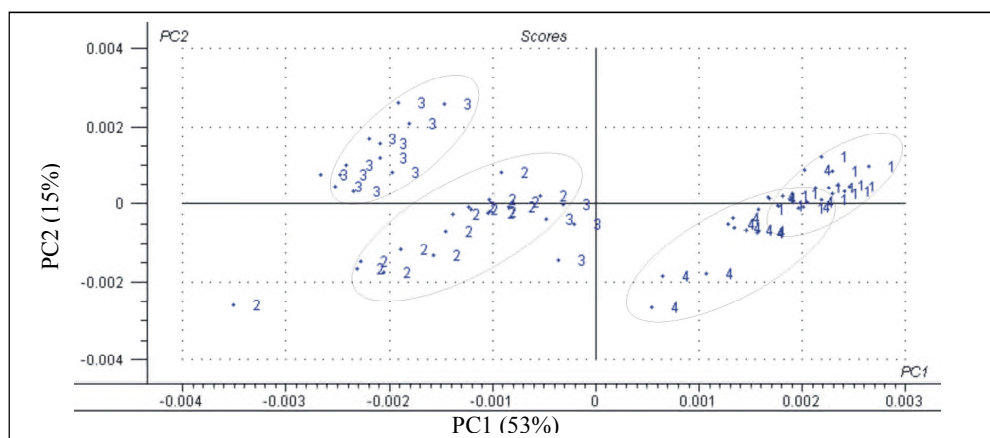


Figure 2: PCA plot for the two PC factors showing spectral ability to sort based on their origin within the tree canopy.

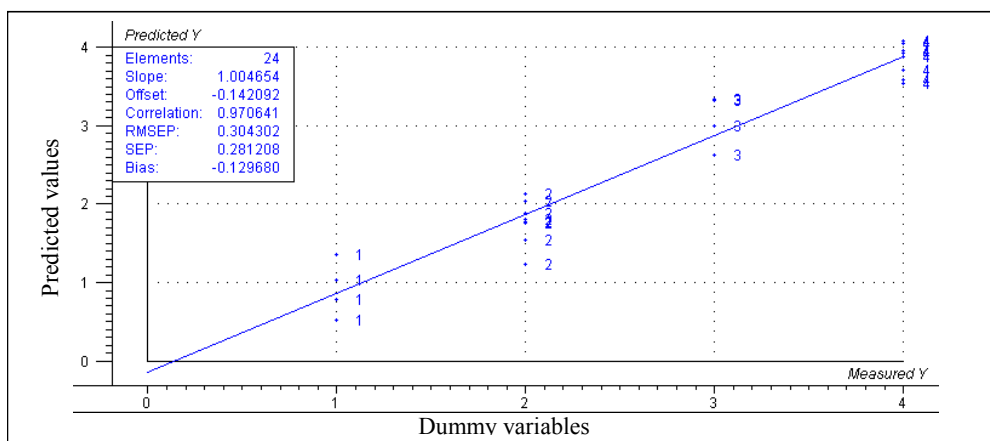


Figure 3: PLS-DA models showing Vis/NIR spectral ability to predict fruit origin within the tree canopy.

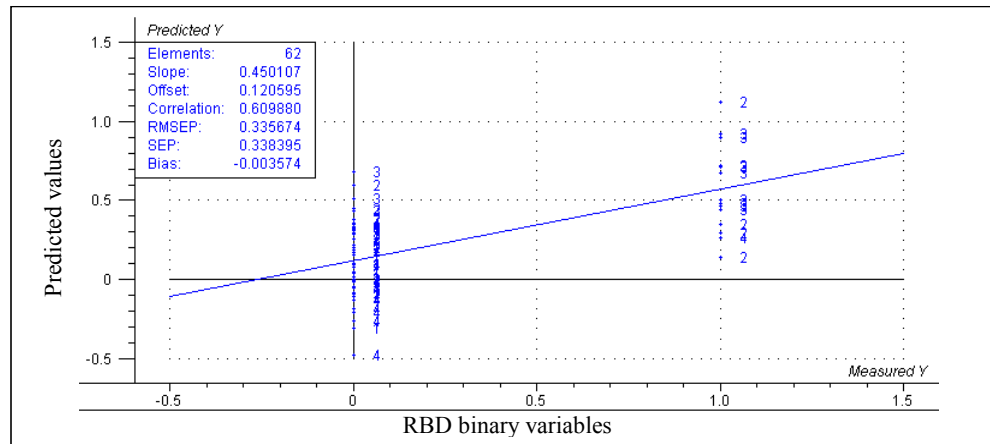


Figure 4: PLS scatter plot showing Vis/NIR model performance to classify fruit based on the occurrence of RBD.

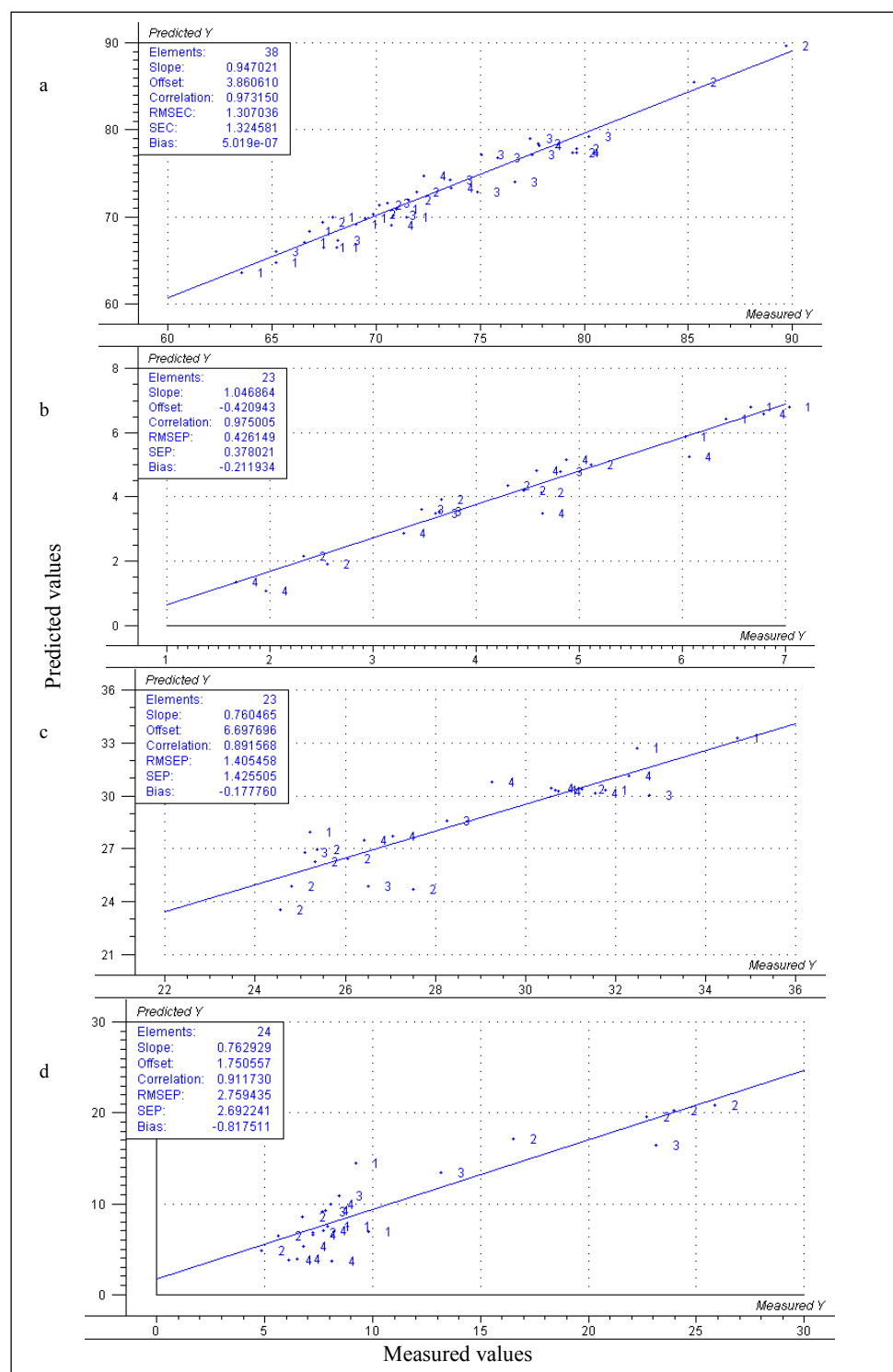


Figure 5: Scatter plots of Vis/NIR predicted versus measure values of hue angle (a), colour index (b), dry matter (%) (c), and weight/water loss (grams) (d).

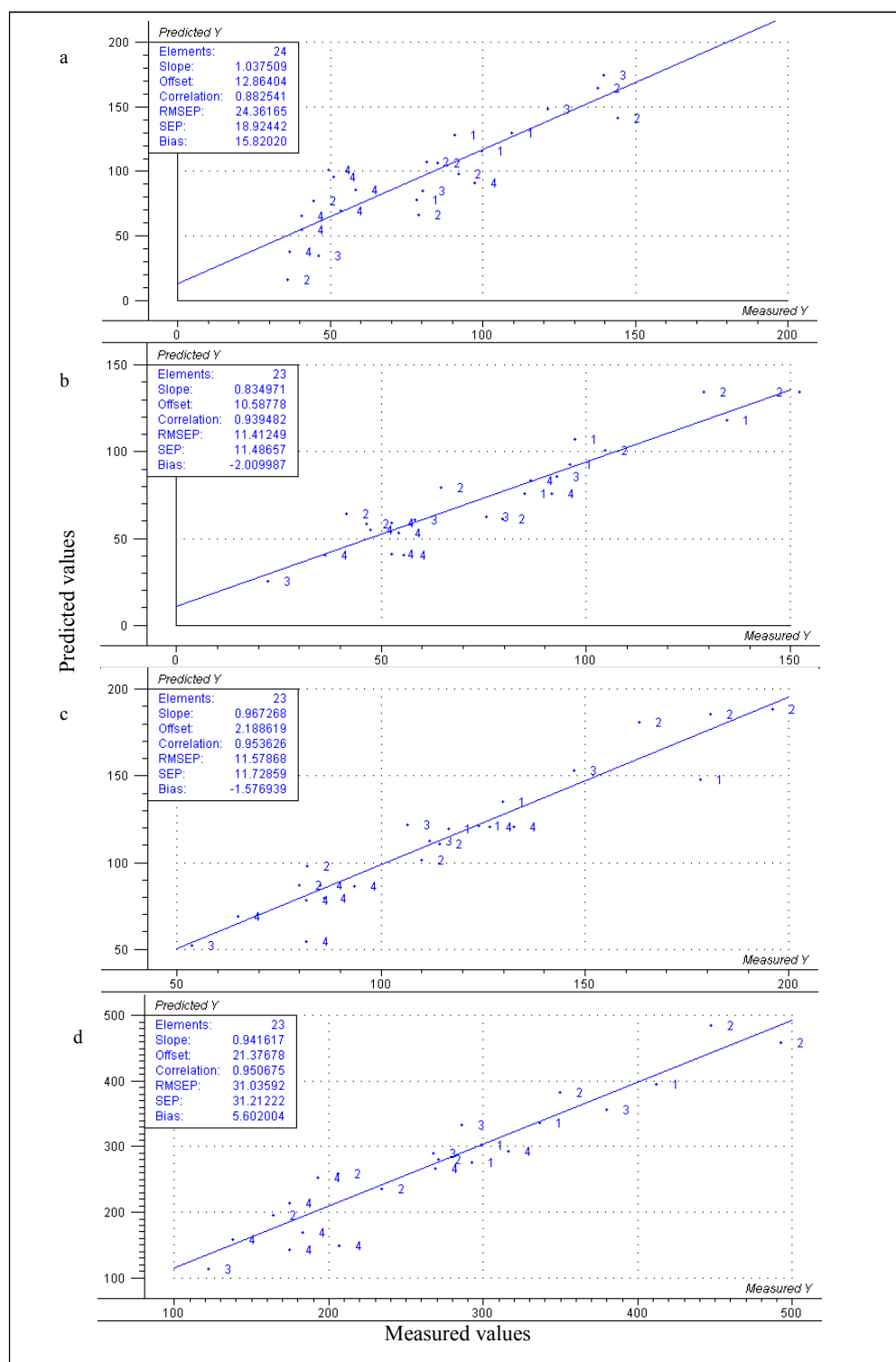


Figure 6: Scatter plots for Vis/NIR predicted versus measure values of sucrose (a), glucose (b), fructose (c), and total sugars (d). All results are expressed in mg/g DW.



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Prediction of 'Nules Clementine' mandarin susceptibility to rind breakdown disorder using Vis/NIR spectroscopy

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