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Application of Vis/NIR spectroscopy for the estimation of soluble solids, dry matter and flesh firmness in stone fruits

Running title: Use of near-infrared (NIR) absorbance to assess stone fruit quality parameters.

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Abstract

BACKGROUND: Soluble solids concentration (SSC), dry matter concentration (DMC) and flesh firmness (FF) are important fruit quality parameters in stone fruits. This study investigated the ability of a commercial Vis/NIR spectrometer to determine SSC, DMC and FF in nectarine, peach, apricot and Japanese plum cultivars at harvest. The work was conducted in summer 2019/20 on fourteen stone fruit cultivars at Tatura, Australia. Two sub-samples of 100 fruit each were collected before and after commercial maturity (± 5 days) in order to maximise sample variability.

RESULTS: Partial least square regression (PLS) models based on the 2nd derivative of the absorbance in the 729–975 nm spectral region proved accurate for the prediction of SSC and DMC ($R^2_{CV} > 0.750$). Only the model generated for SSC in 'Golden May' apricot was less precise compared to other cultivars. No Vis/NIR models were accurate enough to predict FF in the cultivars under study ($R^2_{CV} < 0.750$).

CONCLUSION: This study demonstrated that the Vis/NIR spectrometer was a reliable tool to monitor SSC and DMC in stone fruits at harvest but proved less useful for FF estimation. These results highlight the potential of Vis/NIR spectrometry to evaluate stone fruit quality both *in situ* pre-harvest and in the laboratory after harvest.

Keywords: apricot; fruit quality; near-infrared; nectarine; peach; plum

1. Introduction

Portable, rapid, non-destructive devices for the determination of objective fruit quality parameters offer improvements over traditional destructive and labour-expensive approaches to guide harvesting and marketing operations and supply chain logistics. Quality parameters provide insightful information on the ripening stage of specific fruit crops, and based on the traditional reference maturity indices, technology can be adapted for the estimation of fruit maturity. For temperate tree fruits, traditionally, sugars, dry matter, flesh firmness, starch, acidity, colour, size and shape, ethylene production and respiration rate have provided common indicators of maturity. Each fruit and/or cultivar has key maturity indices based on its genetic, morphological and physiological characteristics, or a combination. In stone fruit, several maturation indices can be used to determine the best harvest time. Maximising sugars, specifically soluble solids concentration (SSC), is a strategy of some fruit growers to improve quality and to determine harvest time. Flesh firmness (FF) is commonly used in apricot, nectarine, peach and plum as an indicator of ripeness.[1] However, a high degree of variability in SSC and FF is found among different cultivars[2, 3] making them not universal parameters for stone fruit maturity assessment, if used alone. Dry matter concentration (DMC) has been efficiently used to determine maturity in crops that accumulate oil in their fruit such as avocado[4] and olive,[5] and more recently for quality determination in mango,[6] kiwifruit,[7] apple[8] and cherry.[9]

Besides being used as maturity indices, SSC, FF and DMC can be determined prior to harvest as quality parameters to anticipate the marketability of the produce and to improve harvest logistics. Typical SSC, FF and DMC determination requires sample destruction and can be expensive as specific equipment and labour are required. Therefore, a non-destructive device that can accurately predict multiple fruit quality parameters is highly sought after by industry. Visible/Near Infrared (Vis/NIR) spectrometry is one of the most established non-destructive technology for the prediction of several quality and maturity indicators in temperate fruit crops and has been successfully used in apple,[10,11] stone fruits,[12,13,14,15] pear[16,17] and several other crops. Many commercial in-line grader systems come fully equipped with near infrared spectrometers that quickly assess quality parameters after harvest[18], but there is a need to assess the usefulness of Vis/NIR spectrometers for field and laboratory monitoring of stone fruit quality indices. Golic and Walsh validated the suitability of NIR spectroscopy in commercial graders to estimate SSC in stone fruits.[19] A range of handheld NIR devices is currently commercially available and their performance for the estimation of fruit DMC was compared by Kaur *et al.*[20]. Donis-González *et al.* compared two portable devices for the estimation of SSC and DMC in peach, finding an overall better ability to predict the latter, and a reduced estimation power for the former.[21]

With the goal of improving harvest logistics and labour efficiency, this study aimed to investigate the suitability of a portable Vis/NIR spectrometer as a smart tool for the estimation of SSC, DMC and FF in nectarine, peach, apricot and Japanese plum cultivars at harvest.

MATERIALS AND METHODS

Experimental site and cultivar characteristics

The experiment was carried out in the summer of 2019/20 in a stone fruit orchard at the Tatura SmartFarm, Agriculture Victoria, Australia (36°26'7" S and 145°16'8" E, 113 m a.s.l.). The stone fruit orchard (3.0 ha) at the farm comprises agronomic experiments on apricot, nectarine, peach and plum. A total of fourteen cultivars, i.e. one apricot (*Prunus armeniaca* L., 'Golden May'), one Japanese plum (*P. salicina* L., 'Angeleno'), four nectarine (*P. persica* L. Batsch, 'August Bright', 'Autumn Bright', 'Rose Bright' and 'September Bright'), four yellow peach (*P. persica* L. Batsch, 'August Flame', late 'O'Henry', 'Redhaven' and 'September Sun') and four white peach (*P. persica* L. Batsch, 'Ice Princess', 'Snow Fall', 'Snow Flame 23' and 'Snow Flame 25') were selected for this study. The harvest time of all the cultivars stretched from December 2019 to April 2020, with the first to reach commercial maturity being the apricot 'Golden May' (i.e. early December), and the last being the white peach 'Snow Fall' (i.e. start of April). The orchard was planted in 2013–2015, the soil had a clay loam soil texture and trees were irrigated, fertigated, thinned, pest/disease-managed and pruned based on commercial practices.

Fruit sampling and preparation

Fruit from each cultivar were collected at two different times, one slightly before (1st batch) and one slightly after commercial harvest (2nd batch), within a window of ten days. Each batch of fruit included specimens with diverse size and colour. This sample collection method was applied to target fruit at different maturity stages and increase sample variability. Commercial harvest time was assessed by a DA-meter (TR Turoni, Forlì, Italy) based on the index of absorbance difference (I_{AD}) thresholds provided by the HIN (Victorian Horticulture Industry Network).[22] The only exception occurred for 'Redhaven', of which the two batches of fruit were harvested after commercial harvest because the DA-meter was temporarily unavailable. Each batch of fruit consisted of 100 fruit, leading to a total sample size of 200 fruit for each of the fourteen cultivars collected over a total of 28 days of measurements between December 2019 and April 2020.

Fruit were harvested in the early morning from different canopy sides and heights (i.e. to pool together fruit that received different amounts of sunlight), immediately brought to the laboratory, numbered and weighed, and then left on the laboratory bench for two hours in order to adjust to a standard temperature of 25 °C prior to measurement.

Vis/NIR spectrometry

In this study we used a commercial portable F-750 Produce Quality Meter (Felix Instruments, Camas, WA, USA) for Vis/NIR spectra collections in the 310–1100 nm range with a resolution of 3 nm. This device is equipped with a Carl Zeiss MMC-1 spectrometer, a xenon tungsten lamp as light source and a glass coated lens as per manufacturer specifications.

A circular area (≈ Ø 30 mm) was marked on a single side of each fruit and scanned using the F-750 meter. Each batch of 100 fruit was scanned within one hour after samples had reached 25 °C in the same morning after fruit collection. The device recorded the absorbance spectra and their second derivatives, which were subsequently smoothed using a Savitzky and Golay 10-point convolution. Data were stored in an SD card and downloaded prior to data analysis.

Reference destructive determinations

Once spectra were collected, the fruit were immediately destructed for SSC, DMC and FF determination. Fruit skin was peeled off from the area previously scanned with the F-750 meter, and flesh was exposed to a penetrometer (FT327, FACCHINI srl, Alfonsine, Italy) equipped with an 8 mm tip to measure FF on a scale from 0 to 15 kgf. Afterwards, a few drops of juice were extracted with the help of a pointy tool and SSC was measured using a digital refractometer (PR-1; ATAGO CO., LTD, Saitama, Japan) and expressed as °Brix. After SSC determination, a cylindrical core (Ø ≈ 30 mm, h ≈ 15 mm) of the pulp — where previous measurements were taken — was extracted using a fruit corer and weighed on a digital scale with four decimal places. Fresh mass was instantly recorded, cores were placed in silicone trays and dried in an oven at 55 °C until constant weight was obtained (≈ 72–96 h). Afterwards, samples were weighed to determine dry mass and DMC (%) was calculated as dry mass / fresh mass × 100.

Data analysis and prediction models

Fruit fresh weight (FW), SSC, FF and DMC were represented using boxplots to determine average values and sample variability for each cultivar. Collected Vis/NIR spectra were analysed with a partial least square regression (PLS) procedure using Minitab® Statistical Software (Minitab, LL v.19, PA, USA). The absorbance spectra between 729 and 975 nm and their second derivatives were tested and compared in terms of robustness of the prediction models for SSC, DMC and FF. The region between 729 and 975 nm was chosen as it has previously been linked to sugars, carbohydrate and water absorbance.[9,10,17] For comparison purposes, secondary FF models were built using the 500–1000 nm spectral region, in accordance with the wavelengths used by Uwadaira *et al.* for FF estimation in peach.[23] The PLS procedure used the nonlinear iterative partial least squares (NIPALS) algorithm and consisted of three steps. First, a train-sample composed of 170 fruit per cultivar (minus measurement errors and/or outliers in the sample) was used to generate the prediction model. A second step was carried out by performing a leave-one-out (LOO) cross-validation (CV) on the same sample. The third and last step consisted of testing model robustness on 30 additional fruit per cultivar (test-sample). Half of the 30 test-sample fruit originated from the 1st batch and the other half from the 2nd batch of harvested fruit. Model robustness was determined based on the number of principal components (PCs), the coefficient of determination of the model (R^2)

and the root mean square error (*RMSE*) calculated as the standard deviation of the residuals and expressed with the same units of each variable (i.e. °Brix for SSC, % for DMC and kgf for FF). The R^2 and *RMSE* were calculated for the prediction model and for the CV (R^2_{CV} and $RMSE_{CV}$, respectively) using from 1 to 10 PCs. In short, preferable models had fewer PCs, high R^2 and low *RMSE*. The best models for each cultivar were selected by looking at the lowest number of PCs used for R^2_{CV} and $RMSE_{CV}$ to reach values near their maximum and minimum, respectively. Once models were selected, the second step consisted of validating them on the test-sample and expressing their accuracy by comparing the test R^2 (R^2_{test}) to the R^2_{CV}. A large difference between the two coefficients indicated low predictive ability for an external sample. Although frequently used in PLS model comparison, the ratio of performance to deviation (i.e. RPD or residual prediction deviation) was not considered as a measure of goodness of fit in this study, as it is redundant with the use of R^2_{CV}, [24] and less known in the scientific community, making it difficult to be correctly interpreted.

RESULTS AND DISCUSSION

Fruit characteristics

Boxplots in Fig. 1 show variability and sample characteristics of FW, SSC, FF and DMC for each cultivar under study. FW provided an indication of fruit size. 'Golden May' apricot and 'Angeleno' plum trees yielded the smallest fruit and had uniform size, with means ± standard deviations equal to 46.26 ± 13.10 g and 67.33 ± 12.02 g, respectively, whereas 'September Sun' and 'Snow Fall' produced the largest fruit (192.94 ± 54.18 g and 174.41 ± 57.09 g, respectively), but also had less homogenous FW (Fig. 1A). On the one hand, 'Angeleno' plums had the highest SSC with very low variability among fruits (19.69 ± 1.35 °Brix). On the other hand, 'Golden May' apricots expressed a very large SSC variability (Fig. 1B). 'Redhaven' peach had the lowest FF (2.34 ± 1.52 kgf), followed by 'Angeleno' plum (2.97

± 0.50 kgf), with the former being affected by the late sample collection (Fig. 1C). Overall, FF was characterised by high intra-cultivar variability, except for 'Angeleno' plums that showed a very narrow distribution. DMC had low intra- and inter-cultivar variability, with only 'Angeleno' plums expressing a distinctively high mean DMC of 19.44 ± 1.36 % (Fig. 1D).

Model analysis and prediction ability

Outliers observed in the distribution analysis (Fig. 1) and erroneous device measurements (i.e. showing false spectra responses) were removed from the samples before building the PLS models. A graphical example of the methodology used for model selection is presented for the estimation of SSC in late 'O'Henry' (Fig. 2). Both the models that used Vis/NIR absorbance (Fig. 2A and C) and its 2nd derivative (Fig. 2B and D) yielded very high R^2 and R^2_{CV} with very small *RMSE* and $RMSE_{CV}$. However, the latter needed a lower number of PCs than the former. In the case of SSC in 'O'Henry', the most accurate model was built using 4 PCs that summarised the 2nd derivative of the absorbance in the 729–975 nm wavelength. The proximity of model and cross-validation lines in Fig. 2 indicated that the cross-validation efficiently reproduced the prediction model and kept a small prediction error (*RMSE*).

In line with what was observed for the prediction of SSC in 'O'Henry', when the absorbance and its 2nd derivative were compared for all the parameters (SSC, DMC and FF) and in all the cultivars under study, they both yielded very similar models, with the exception that the latter always needed less PCs to build the optimal models (3–5) when compared to the former (5–10).

In addition, FF models were similar for both the 729–975 and 500–1000 nm regions in terms of R^2, R^2_{CV}, *RMSE* and $RMSE_{CV}$ (data not shown). Therefore, only models based on the 2nd derivative of the 729–975 nm absorbance were considered for the following results on SSC, DMC and FF.

Model and cross-validation fits for SSC, DMC and FF were plotted against the actual responses to graphically assess model linearity (Fig. 3, 4 and 5) and data dispersion. In the case of SSC, model fits responded linearly to actual values and the points were tightly distributed around the y = x regression line, except for 'Golden May', whose fits were uniformly scattered farther away (Fig. 3) from the line. This was likely to be due to the high variability of SSC values highlighted in Fig. 1B. Similar results were obtained for DMC (Fig. 4), although in this case, model fits in 'Golden May' had a tighter linearity with actual responses than for SSC, as foreseeable from the lower variability of DMC observed in Fig. 1D. FF responses of model fits to actual responses were rather erratic (Fig. 5), with high point dispersion in all the cultivars, suggesting that the absorbance in the 729–975 nm spectra poorly predicts FF in stone fruit. Cross-validation fits showed almost identical responses to actual responses (Fig. 3, 4 and 5), in line with the model fits, thus, providing a promising indication of model robustness.

To confirm model linearity and assumptions from observations in Figs. 3–5, *RMSE*, $RMSE_{CV}$, R^2 and R^2_{CV} were analysed (Table 1). For all the cultivars, $RMSE_{CV}$ was always higher than *RMSE*, as expected, but the difference between the two errors was very small for all the observed parameters (< 0.13 °Brix for SSC, < 0.10 % for DMC and < 0.13 kgf for FF). Similarly, R^2 was expectedly higher than R^2_{CV} but the delta between them was negligible (< 0.04 for SSC and DM and < 0.09 for FF). However, assuming a threshold of $R^2_{CV} = 0.75$ — equivalent to RPD = 2, a common threshold of goodness of fit [24] — prediction efficiency was consistently high for SSC and DMC models, but always low for FF models (Table 1). The only exception occurred for SSC prediction in 'Golden May' apricot, whose model generated a lower prediction ability ($R^2_{CV} = 0.688$), as foreseen from the preliminary observations in Fig. 3. Overall, the best prediction models for SSC were obtained for 'August Bright' nectarine and 'August Flame' peach, whereas the most accurate DMC estimation was found in 'September Sun' and 'Ice Princess' peaches (Table 1). The SSC and DMC models with lowest R^2_{CV} were found in 'Golden May' apricot, followed by 'Redhaven' peach. The low R^2_{CV} found in 'Redhaven' might have been influenced by late fruit sampling that led to slightly overripened fruit. As mentioned above, none of the models robustly predicted actual FF responses, regardless of sample variability. Indeed, the two lowest R^2_{CV} were found in 'Angeleno' plum and in 'Ice Princess' peach (Table 1), which had very different sample variabilities (Fig. 1C).

Model validation on the further test-sample (i.e. 30 fruit) corroborated model robustness for SSC and DMC in all the cultivars (Table 1). Indeed, R^2_{test} was always very similar to R^2_{CV} (Table 1), with the highest delta (0.134) obtained in the DMC model for 'Ice Princess' peach. In the case of FF, given that R^2_{CV} was always low, it was not needed to further test the model on the test-sample, as there was enough evidence of poor robustness. However, R^2_{test} of FF models are reported in Table 1 for completeness.

A first preliminary analysis could lead to associating poor Vis/NIR prediction ability to high sample variability. Nevertheless, models built on accurate readings would benefit from high sample variability if spectra were truly related to specific variables (i.e. sugars, water, etc.). Indeed, very poor prediction ability was obtained for FF in 'Angeleno' plums (R^2 and R^2_{CV} < 0.30), probably due to highly homogenous FF, in line with previous findings on the same cultivar,[25] suggesting that there is likely a physiological explanation that justifies the lack of accuracy for FF prediction. The strong association between NIR spectra and SSC and DMC found in peach is not in line with the findings of Donis-González *et al.*, who observed poor SSC prediction.[21] This was likely to be due to different sample characteristics (e.g. size and cultivars) and post-harvest handling (i.e. fruit stored at 0 °C after harvest in Donis-González *et al.* [21]) as very low temperatures might significantly alter SSC and FF.[26] Other studies have successfully predicted SSC and DMC using Vis/NIR wavelengths like the one used in this work (i.e. 729–975 nm).[9,10,17] The spectral region between 880 and 970 nm was particularly useful for DMC estimation in pear [27] since it contains the absorbance bands of starch, cellulose, sucrose and water. FF is influenced by cell wall degradation, which is in turn regulated by organic acids, pectins and water content.[23] Fruit may also soften due to the indirect effect of external impacts (wind, sunburn, insects, birds and pathogens) that trigger internal biochemical changes. This multitude of factors affect FF in a combined way, though not unique, meaning that, for example, while one fruit might mainly soften up due to cell water content changes, the FF of a second fruit might be lower because of a sudden pest or pathogen occurrence, and a third because of high light exposure and sunburn. Therefore, it is particularly hard to estimate FF using a predefined combination of the absorbance at different wavelengths. The fact that Udawaira *et al.* obtained a more robust model to predict FF in the peach 'Akatsuki' [23] was probably due to the different sample characteristics, as they used a lower amount of fruit and they progressively ripened fruit post-harvest. Indeed, there might be a significant increase of FF prediction ability in overripening peach, as indicated by the highest R^2_{CV} observed in 'Redhaven' (Table 1), the only cultivar that was harvested later than commercial maturity. Nonetheless, post-harvest experiments on the same cultivars should be conducted to verify this assumption.

The models built for all the cultivars proved robust for the estimation of SSC and DMC, even in the case of the late harvested 'Redhaven', indicating that these two parameters can be estimated with Vis/NIR spectrometers before and after ‘commercial harvest’ with a high degree of confidence. However, the R^2cv of SSC and DMC in 'Redhaven' was lower than other peaches, suggesting that an optimal prediction of these two parameters becomes more difficult as fruit reach and exceed physiological maturity. The prediction of SSC in 'Golden May' apricot was not as accurate as for the other stone fruit and further studies on other apricot cultivars need to be conducted to determine if this strictly depends on genotype characteristics and sugar variability among fruits.

CONCLUSIONS

Overall, we demonstrated that Vis/NIR can be a reliable tool to monitor SSC and DMC in stone fruits at harvest. This study showed that the 2nd derivative of the absorbance in the 729–975 nm spectral region generated robust models for SSC and DMC. The influence of temperature on Vis/NIR spectra is well known, thus the models in this study are suitable for measurements carried out at temperatures close to the one used in this study (25 °C). However, Vis/NIR spectrometry appears to be not accurate enough for FF determinations in stone fruits and the use of a more direct physical non-destructive method would be advisable (e.g. impact, acoustic or vibration sensors). Based on findings in this study, the Felix F-750 portable device offers the potential for the industry to routinely and rapidly take non-destructive field measurements of SSC and DMC in apricots, Japanese plum, peach and nectarine to improve harvest timing, determine destination markets and match consumers' expectations.

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REFERENCES

1 Crisosto CH, Stone fruit maturity indices: a descriptive review. *Postharvest News and Information 5*(6): 65N-68N (1994).

2 Byrne DH, Nikolic AN and Burns EE, Variability in sugars, acids, firmness, and color characteristics of 12 peach genotypes. *J Amer Soc Hort Sci* **116**: 1004-1006 (1991). https://doi.org/10.21273/jashs.116.6.1004

3 Lopresti J, Goodwin I, McGlasson B, Holford P and Golding J. Variability in size and soluble solids concentration in peaches and nectarines, in *Horticultural Reviews,* ed. by Janick J, 42 pp. 253-312 (2014). https://doi.org/10.1002/9781118916827.ch05

4 Lee SK, Young RE, Schiffman PM and Coggins CW. Maturity studies of avocado fruit based on picking dates and dry weight. *J Amer Soc Hort Sci* **108**: 390-394 (1983).

5 Mickelbart MV and James D, Development of a dry matter maturity index for olive (*Olea europaea*). *New Zeal J Crop Hort Sci* **31**: 269-276 (2003). https://doi.org/10.1080/01140671.2003.9514261

6 Subedi PP, Walsh KB and Owens G, Prediction of mango eating quality at harvest using short-wave near infrared spectrometry. *Postharvest Biol Tec* **43**: 326-334 (2007). https://doi.org/10.1016/j.postharvbio.2006.09.012

7 Harker FR, Carr BT, Lenjo M, MacRae EA, Wismer WV, Marsh KB, Williams M, White A, Lund CM, Walker SB, Gunson FA and Pereira RB, Consumer liking for kiwifruit flavour: A meta-analysis of five studies on fruit quality. *Food Qual Prefer* **20**: 30-41 (2009). https://doi.org/10.1016/j.foodqual.2008.07.001

8 Palmer JW, Harker FR, Tustin DS and Johnston J, Fruit dry matter concentration: a new quality metric for apples. *J Sci Food Agric* **90**: 2586-2594 (2010). https://doi.org/10.1002/jsfa.4125

9 Escribano S, Biasi WV, Lerud R, Slaughter DC and Mitcham EJ, Non-destructive prediction of soluble solids and dry matter content using NIR spectroscopy and its relationship with sensory quality in sweet cherries. *Postharvest Biol Tec* **128**: 112-120 (2017). https://doi.org/10.1016/j.postharvbio.2017.01.016

10 McGlone VA, Jordan RB and Martinsen PJ, Vis/NIR estimation at harvest of pre- and post-storage quality indices for 'Royal Gala' apple. *Postharvest Biol Tec* **25**: 135-144 (2002). https://doi.org/10.1016/s0925-5214(01)00180-6

11 Fan G, Zha J, Du R and Gao L, Determination of soluble solids and firmness of apples by Vis/NIR transmittance. *J Food Eng* **93**: 416-420 (2009). https://doi.org/10.1016/j.jfoodeng.2009.02.006

12 Ziosi V, Noferini M, Fiori G, Tadiello A, Trainotti L, Casadoro G and Costa G, A new index based on vis spectroscopy to characterize the progression of ripening in peach fruit. *Postharvest Biol Tec* **49**: 319-329 (2008). https://doi.org/10.1016/j.postharvbio.2008.01.017

13 Bureau S, Ruiz D, Reich M, Gouble B, Bertrand D, Audergon JM and Renard CM, Rapid and non-destructive analysis of apricot fruit quality using FT-near-infrared spectroscopy. *Food Chem* **113**: 1323-1328 (2009). https://doi.org/10.1016/j.foodchem.2008.08.066

14 Pérez-Marín D, Paz P, Guerrero JE, Garrido-Varo A and Sánchez MT, Miniature handheld NIR sensor for the on-site non-destructive *J Food Eng* **99**: 294-302 (2010). https://doi.org/10.1016/j.jfoodeng.2010.03.002

15 Munera S, Amigo JM, Blasco J, Cubero S, Talens P and Aleixos N, Ripeness monitoring of two cultivars of nectarine using VIS-NIR hyperspectral reflectance imaging. *J Food Eng* **214**: 29-39 (2017). https://doi.org/10.1016/j.jfoodeng.2017.06.031

16 Li J, Huang W, Zhao C and Zhang B, A comparative study for the quantitative determination of soluble solids content, pH and firmness of pears by Vis/NIR spectroscopy. *J Food Eng* **116**: 324-332 (2013). https://doi.org/10.1016/j.jfoodeng.2012.11.007

17 Goke A, Serra S and Musacchi S, Postharvest dry matter and soluble solids content prediction in d'Anjou and Bartlett pear using near-infrared spectroscopy. *HortScience*, **53**: 669-680 (2018). https://doi.org/10.21273/hortsci12843-17

18 Walsh KB, Long RL and Middleton SG, Use of near infra-red spectroscopy in evaluation of source-sink manipulation to increase the soluble sugar content of stonefruit. *J Hort Sci Biotec* **82**: 316-322 (2007). https://doi.org/10.1080/14620316.2007.11512235

19 Golic M and Walsh KB, Robustness of calibration models based on near infrared spectroscopy for the in-line grading of stonefruit for total soluble solids content. *Anal Chim Acta* **555**: 286-291 (2006). https://doi.org/10.1016/j.aca.2005.09.014

20 Kaur H, Künnemeyer R and McGlone A, Comparison of hand-held near infrared spectrophotometers for fruit dry matter assessment. *J Near Infrared Spec* **25**: 267-277 (2017). https://doi.org/10.1177/0967033517725530

21 Donis-González IR, Valero C, Momin MA, Kaur A and Slaughter DC, Performance evaluation of two commercially available portable spectrometers to non-invasively determine table grape and peach quality attributes. *Agronomy* **10**: 148 (2020). https://doi.org/10.3390/agronomy10010148

22 HIN (Horticulture Industry Network). [Online]. Available: http://www.hin.com.au/networks/profitable-stonefruit-research/stonefruit-maturity-and-fruit-quality/da-meter-iad-maturity-classes-database [30 November 2019]

23 Uwadaira Y, Sekiyama Y and Ikehata A, An examination of the principle of non-destructive flesh firmness measurement of peach fruit by using VIS-NIR spectroscopy. Heliyon, **4**: e00531 (2018). https://doi.org/10.1016/j.heliyon.2018.e00531

24 Minasny B and McBratney A Why you don't need to use RPD. *Pedometron*, **33**: 14-15 (2013).

25 Louw ED and Theron KI. Robust prediction models for quality parameters in Japanese plums (*Prunus salicina* L.) using NIR spectroscopy. *Postharvest Biol Tec*, **58**: 176-184 (2010). https://doi.org/10.1016/j.postharvbio.2010.07.001

26 Brizzolara S, Hertog M, Tosetti R, Nicolai B, Tonutti P. Metabolic responses to low temperature of three peach fruit cultivars differently sensitive to cold storage. *Front Plant Sci* **9**: 1-16 (2018). https://doi.org/10.3389/fpls.2018.00706

27 Travers S, Bertelsen MG, Petersen KK and Kucheryavskiy SV, Predicting pear (cv. Clara Frijs) dry matter and soluble solids content with near infrared spectroscopy. *LWT-Food Sci Tec* **59**: 1107-1113 (2014). https://doi.org/10.1016/j.lwt.2014.04.048

Figure legends

Figure 1. Fruit weight (FW, A), soluble solids concentration (SSC, B), flesh firmness (FF, C) and dry matter concentration (DMC, D) in fourteen stone fruit cultivars at harvest time (± 5 days). Boxplots display interquartile range boxes (1st to 3rd quartile), with horizontal median lines, highest and lowest observations (whiskers) and outliers (dots). Cultivar name abbreviations: 'Golden May' (GM), 'Angeleno' (AN), 'August Bright' (AGB), 'Autumn Bright' (ATB), 'Rose Bright' (RB), 'September Bright' (SB), 'Ice Princess' (IP), 'Snow Fall' (SF), 'Snow Flame 23' (FL23), 'Snow Flame 25' (FL25), 'August Flame' (AF), 'O'Henry' (OH), 'Redhaven' (RH) and 'September Sun' (SS).

Figure 2. Coefficients of determination (R^2) and root mean square errors (*RMSE*) of partial least square regression models for the prediction of soluble solids concentration (SSC) with 1–10 principal components in the peach 'O'Henry'. Model and cross-validation R^2 and *RMSE* reported for the 729–975 nm absorbance (A and C) and for its second derivative (B and D). Grey dashed vertical lines show the number of principal components selected for SSC prediction.

Figure 3. Scatter plots of model and cross-validation (CV) prediction fits against actual responses of soluble solids concentration (SSC). Dashed lines represent reference linear fits where SSC prediction = SSC actual response. Cultivar name abbreviations: 'Golden May' (GM), 'Angeleno' (AN), 'August Bright' (AGB), 'Autumn Bright' (ATB), 'Rose Bright' (RB), 'September Bright' (SB), 'Ice Princess'

(IP), 'Snow Fall' (SF), 'Snow Flame 23' (FL23), 'Snow Flame 25' (FL25), 'August Flame' (AF), 'O'Henry' (OH), 'Redhaven' (RH) and 'September Sun' (SS).

Figure 4. Scatter plots of model and cross-validation (CV) prediction fits against actual responses of dry matter concentration (DMC). Dashed lines represent reference linear fits where DMC prediction = DMC actual response. Cultivar name abbreviations: 'Golden May' (GM), 'Angeleno' (AN), 'August Bright' (AGB), 'Autumn Bright' (ATB), 'Rose Bright' (RB), 'September Bright' (SB), 'Ice Princess' (IP), 'Snow Fall' (SF), 'Snow Flame 23' (FL23), 'Snow Flame 25' (FL25), 'August Flame' (AF), 'O'Henry' (OH), 'Redhaven' (RH) and 'September Sun' (SS).

Figure 5. Scatter plots of model and cross-validation (CV) prediction fits against actual responses of flesh firmness (FF). Dashed lines represent reference linear fits where FF prediction = FF actual response. Cultivar name abbreviations: 'Golden May' (GM), 'Angeleno' (AN), 'August Bright' (AGB), 'Autumn Bright' (ATB), 'Rose Bright' (RB), 'September Bright' (SB), 'Ice Princess' (IP), 'Snow Fall' (SF), 'Snow Flame 23' (FL23), 'Snow Flame 25' (FL25), 'August Flame' (AF), 'O'Henry' (OH), 'Redhaven' (RH) and 'September Sun' (SS).

Table 1. Partial least square regression model statistics for the prediction of soluble solids concentration (SSC), dry matter concentration (DMC) and flesh firmness (FF) using the 2nd derivative of the 729–975 nm absorbance.

Crop	Cultivar	Variable	PCs†	$RMSE^{y}$	$RMSE_{CV}{}^{x}$	R^{2w}	$R^2_{CV}{}^{v}$	$R^2_{test}{}^{u}$	$n_{train}{}^{t}$	$n_{test}{}^{s}$
Apricot	Golden May	SSC	5	1.861	1.983	0.725	0.688	0.759	165	30
		DMC	5	1.074	1.168	0.793	0.756	0.811	165	30
		FF	5	1.272	1.379	0.581	0.508	0.438	165	30
Plum	Angeleno	SSC	3	0.361	0.377	0.928	0.922	0.931	162	30
		DMC	3	0.479	0.498	0.877	0.867	0.881	162	30
		FF	3	0.442	0.459	0.225	0.163	0.336	162	30
Nectarine	August Bright	SSC	5	0.541	0.575	0.955	0.949	0.933	166	30
		DMC	5	0.665	0.700	0.915	0.906	0.928	166	30
		FF	5	1.416	1.537	0.529	0.445	0.423	166	30
	Autumn Bright	SSC	4	0.557	0.589	0.880	0.865	0.938	169	30
		DMC	4	0.546	0.577	0.887	0.874	0.932	168	30
		FF	4	1.020	1.079	0.467	0.402	0.496	169	30
	Rose Bright	SSC	5	0.574	0.614	0.939	0.930	0.919	166	30
		DMC	5	0.602	0.650	0.914	0.900	0.954	166	30
		FF	5	1.327	1.399	0.499	0.443	0.000	166	30
	September Bright	SSC	4	0.650	0.692	0.903	0.890	0.919	163	30
		DMC	4	0.647	0.695	0.914	0.901	0.945	163	30
		FF	4	0.989	1.032	0.449	0.399	0.177	162	30
White peach	Ice Princess	SSC	3	0.715	0.755	0.918	0.909	0.922	164	30
		DMC	3	0.640	0.683	0.930	0.920	0.786	164	30
		FF	3	1.262	1.332	0.300	0.220	0.254	164	30
	Snow Fall	SSC	4	0.638	0.686	0.894	0.877	0.796	162	30
		DMC	4	0.712	0.767	0.876	0.856	0.844	162	30
		FF	4	1.286	1.368	0.449	0.377	0.039	162	30
	Snow	SSC	5	0.761	0.812	0.892	0.877	0.865	160	30

	Flame 23	DMC	5	0.683	0.734	0.900	0.884	0.862	160	30
		FF	5	0.908	0.971	0.567	0.505	0.580	160	30
	Snow Flame 25	SSC	5	0.587	0.627	0.877	0.860	0.820	166	30
		DMC	5	0.502	0.542	0.891	0.872	0.824	166	30
		FF	5	0.940	0.991	0.625	0.583	0.656	165	30
Yellow peach	August Flame	SSC	4	0.532	0.571	0.943	0.935	0.845	162	30
		DMC	4	0.598	0.643	0.909	0.895	0.864	163	30
		FF	4	1.287	1.363	0.459	0.393	0.488	161	30
	OHenry	SSC	4	0.524	0.566	0.942	0.932	0.951	161	30
		DMC	4	0.650	0.693	0.889	0.873	0.945	161	30
		FF	4	1.234	1.299	0.652	0.614	0.328	161	30
	Redhaven	SSC	4	0.570	0.606	0.790	0.762	0.754	167	30
		DMC	4	0.568	0.601	0.805	0.782	0.820	167	30
		FF	4	0.795	0.848	0.715	0.676	0.629	167	30
	September Sun	SSC	5	0.637	0.683	0.913	0.900	0.945	162	30
		DMC	5	0.513	0.558	0.943	0.932	0.923	162	30
		FF	5	1.187	1.237	0.459	0.383	0.208	162	30

[z]Number of principal components; [y]root mean square error (*RMSE*) of the model; [x]*RMSE* of the cross-validation; [w]coefficient of determination (R^2) of the model; [v]R^2 of the cross-validation; [u]R^2 of the validation test; [t]train-sample size and [s]test-sample size.

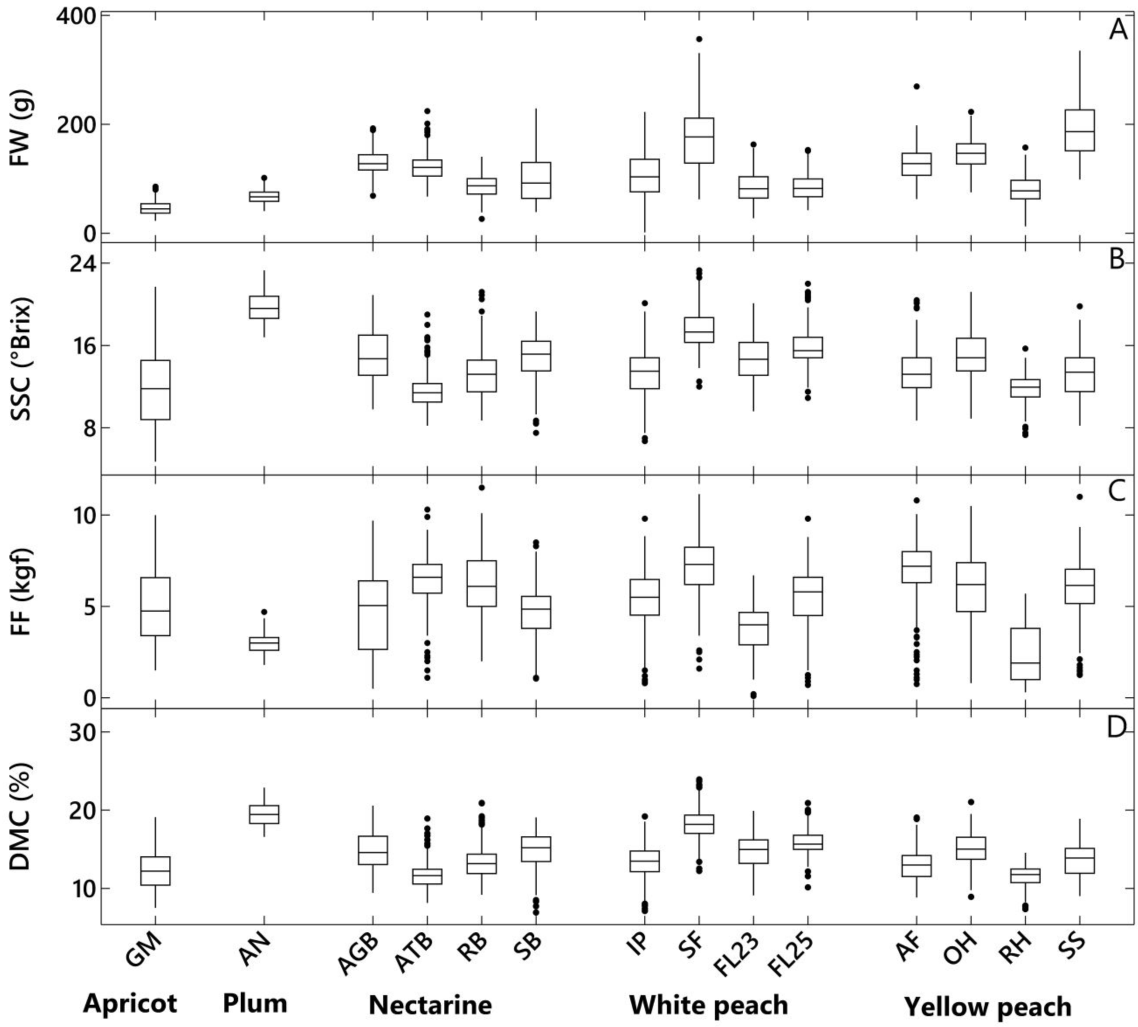

Figure 1. Fruit weight (FW, A), soluble solids concentration (SSC, B), flesh firmness (FF, C) and dry matter concentration (DMC, D) in fourteen stone fruit cultivars at harvest time (± 5 days). Boxplots display interquartile range boxes (1^{st} to 3^{rd} quartile), with horizontal median lines, highest and lowest observations (whiskers) and outliers (dots). Cultivar name abbreviations: 'Golden May' (GM), 'Angeleno' (AN), 'August Bright' (AGB), 'Autumn Bright' (ATB), 'Rose Bright' (RB), 'September Bright' (SB), 'Ice Princess' (IP), 'Snow Fall' (SF), 'Snow Flame 23' (FL23), 'Snow Flame 25' (FL25), 'August Flame' (AF), 'O'Henry' (OH), 'Redhaven' (RH) and 'September Sun' (SS).

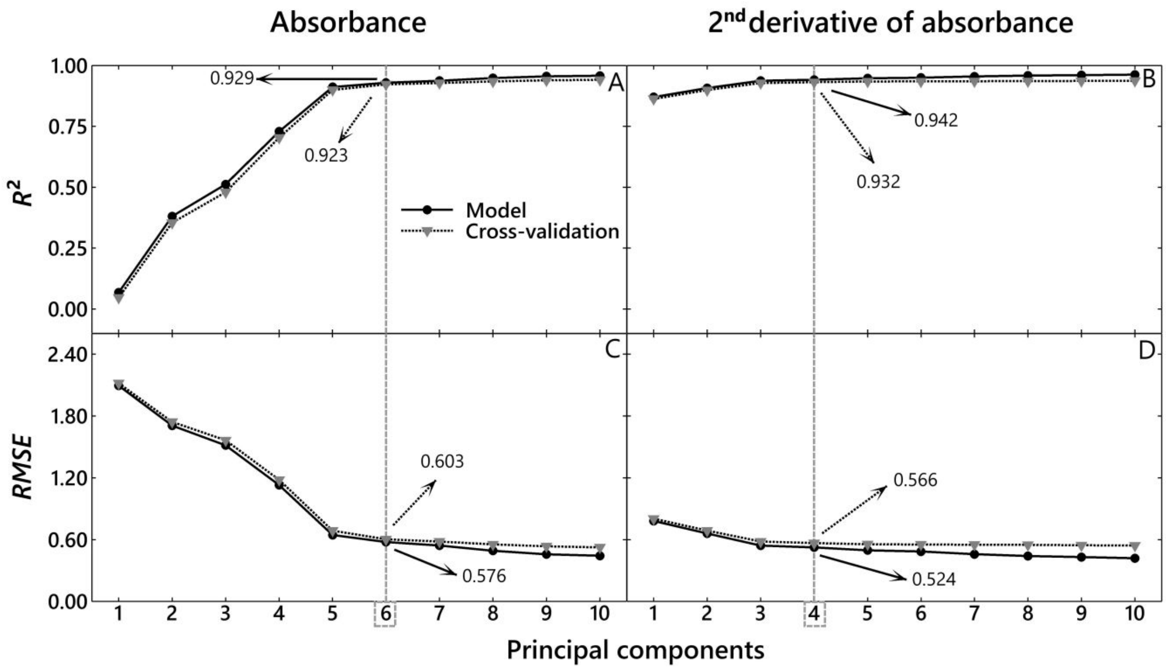

Figure 2. Coefficients of determination (R^2) and root mean square errors (*RMSE*) of partial least square regression models for the prediction of soluble solids concentration (SSC) with 1–10 principal components in the peach 'O'Henry'. Model and cross-validation R^2 and *RMSE* reported for the 729–975 nm absorbance (A and C) and for its second derivative (B and D). Grey dashed vertical lines show the number of principal components selected for SSC prediction.

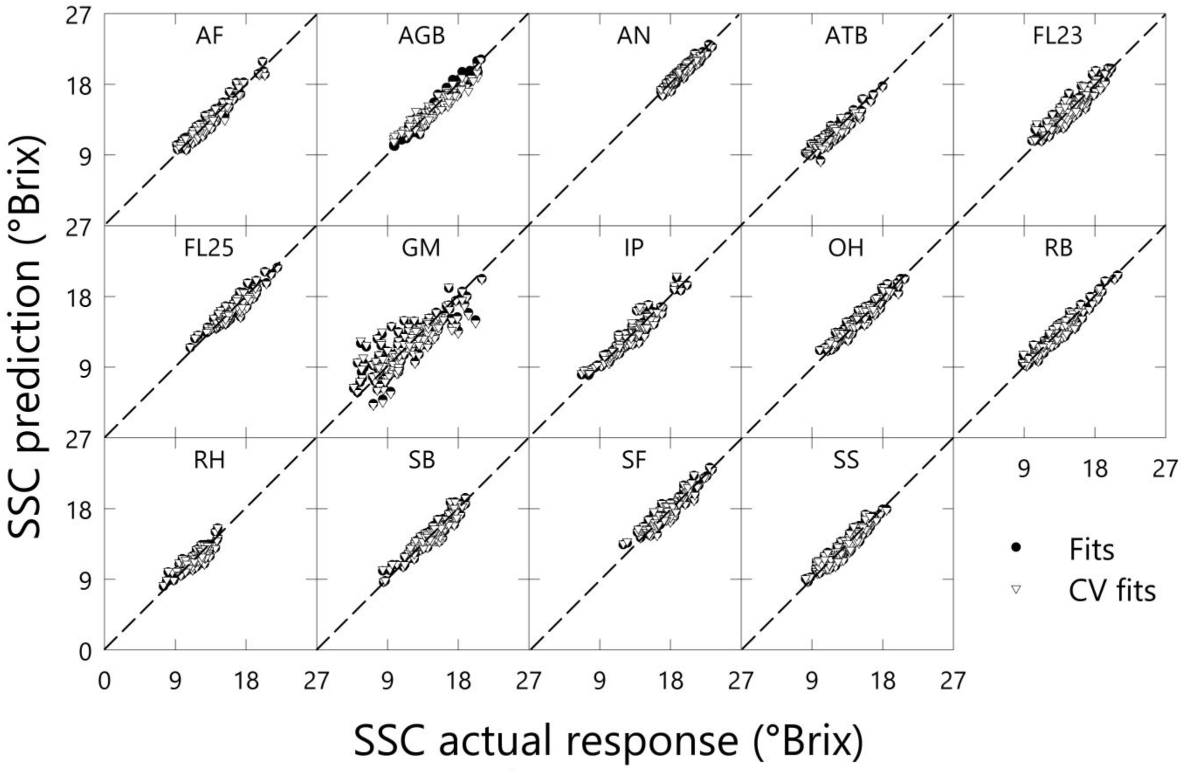

Figure 3. Scatter plots of model and cross-validation (CV) prediction fits against actual responses of soluble solids concentration (SSC). Dashed lines represent reference linear fits where SSC prediction = SSC actual response. Cultivar name abbreviations: 'Golden May' (GM), 'Angeleno' (AN), 'August Bright' (AGB), 'Autumn Bright' (ATB), 'Rose Bright' (RB), 'September Bright' (SB), 'Ice Princess' (IP), 'Snow Fall' (SF), 'Snow Flame 23' (FL23), 'Snow Flame 25' (FL25), 'August Flame' (AF), 'O'Henry' (OH), 'Redhaven' (RH) and 'September Sun' (SS).

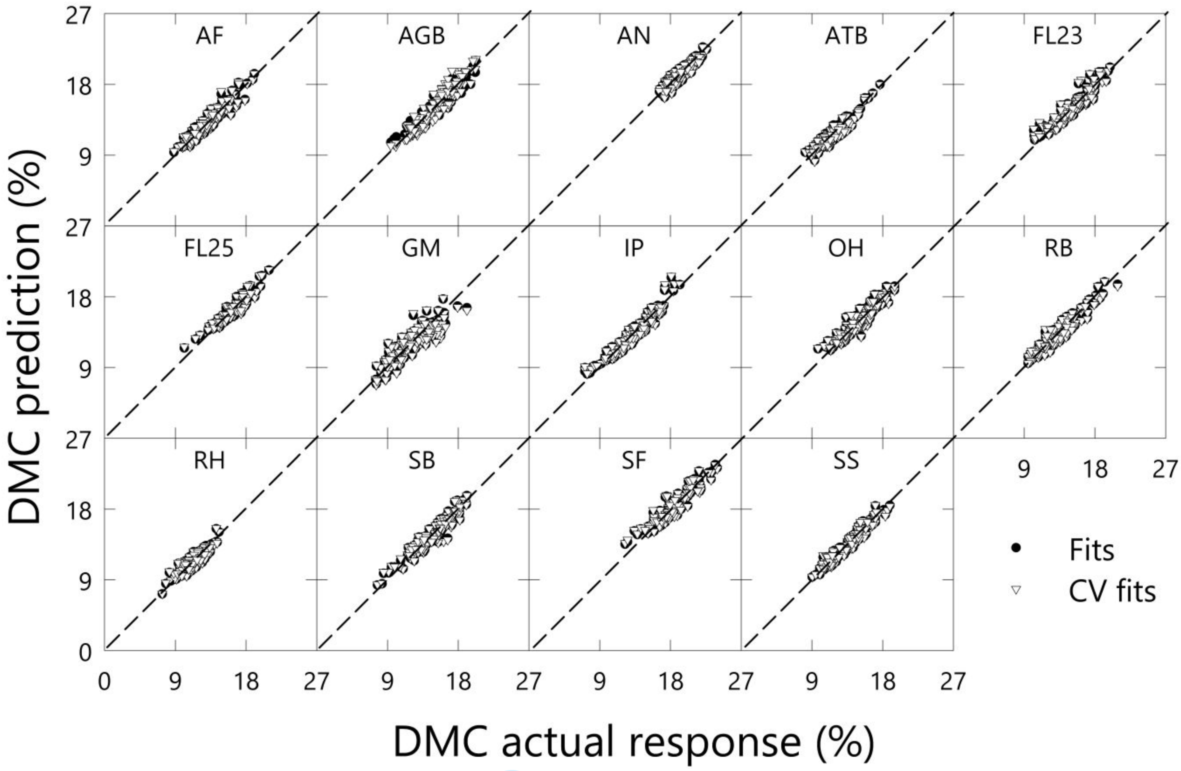

Figure 4. Scatter plots of model and cross-validation (CV) prediction fits against actual responses of dry matter concentration (DMC). Dashed lines represent reference linear fits where DMC prediction = DMC actual response. Cultivar name abbreviations: 'Golden May' (GM), 'Angeleno' (AN), 'August Bright' (AGB), 'Autumn Bright' (ATB), 'Rose Bright' (RB), 'September Bright' (SB), 'Ice Princess' (IP), 'Snow Fall' (SF), 'Snow Flame 23' (FL23), 'Snow Flame 25' (FL25), 'August Flame' (AF), 'O'Henry' (OH), 'Redhaven' (RH) and 'September Sun' (SS).

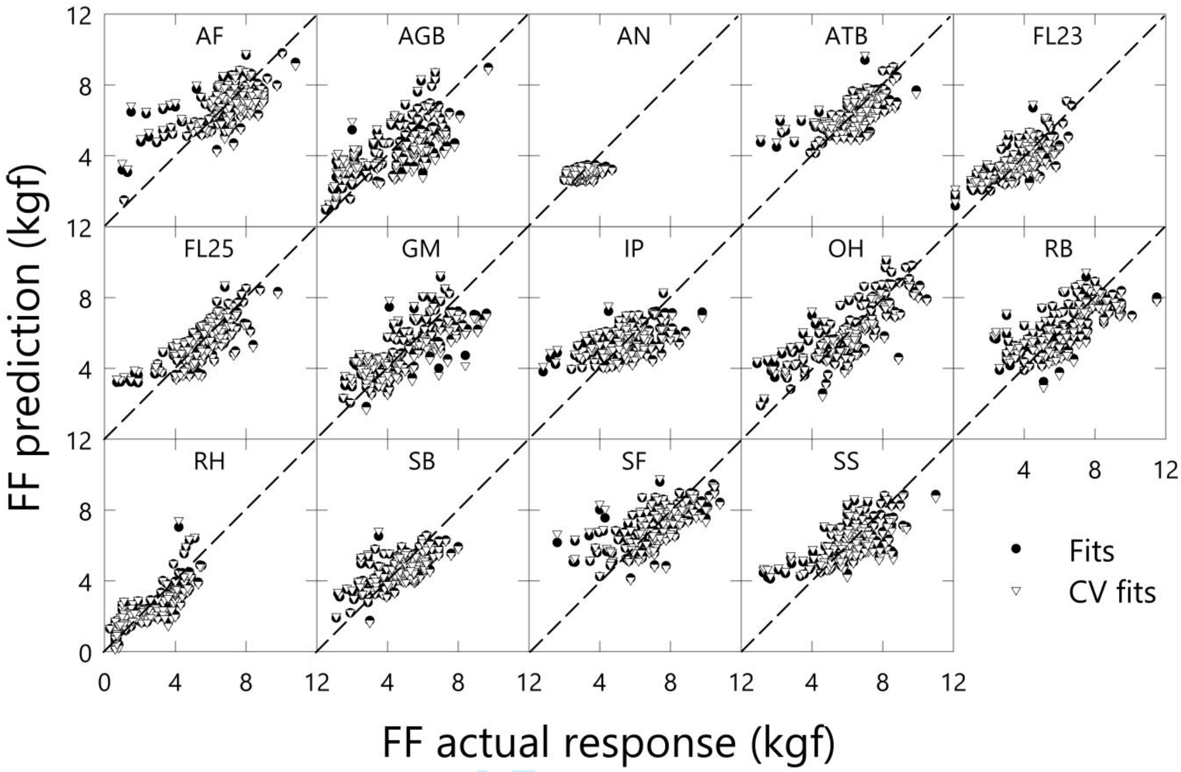

Figure 5. Scatter plots of model and cross-validation (CV) prediction fits against actual responses of flesh firmness (FF). Dashed lines represent reference linear fits where FF prediction = FF actual response. Cultivar name abbreviations: 'Golden May' (GM), 'Angeleno' (AN), 'August Bright' (AGB), 'Autumn Bright' (ATB), 'Rose Bright' (RB), 'September Bright' (SB), 'Ice Princess' (IP), 'Snow Fall' (SF), 'Snow Flame 23' (FL23), 'Snow Flame 25' (FL25), 'August Flame' (AF), 'O'Henry' (OH), 'Redhaven' (RH) and 'September Sun' (SS).