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Evaluation of handheld NIR spectrometers for quantitative purposes on whole table grape berries

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Lord Charles, Somerset West

Introduction

- Table grape berries are individual fruit – non-climacteric
- Within which metabolic processes
- Such as the accumulation of sugar and degradation of acids
- Occur completely separately and at a different rate
- From those next to it on a bunch
- The accumulation of sugar in the form of total soluble solids (TSS)
- Or soluble solid content (SCC)
- And color are the main factors that determine the berry readiness for harvest
- These TSS levels at which a specific cultivar may be harvested
- Are defined by thresholds for the specific exporting country
- In South Africa, these thresholds are guided by
- Section 4(3) (a) (ii) of the Agricultural Product Standards Act, 1990 (Act No. 119 of 1990).
- This means that grape harvest may be selective
- By requiring either early harvest
- Or storage on the vines up until reaching the desired threshold
- The first problem with this is the negative effects of post-harvest treatments or pests and diseases by harvesting early or late
- The second problem is that it is time and labour intensive
- To do individual TSS measurements of grape berries through the traditional use of a refractometer
- Thirdly it is creating a lot of waste and destroying the integral structure and shape of the bunch
- Seeing that many berries would have to be removed and measured from a lot of bunches and vines

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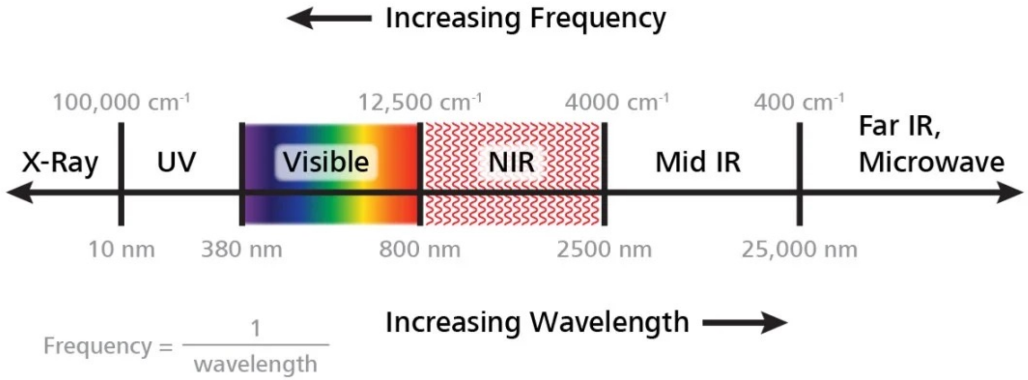
- This is crucial since not all berries on a bunch, not all bunches on a vine, and not all vines in a block are at the same maturity level for harvest
- The need for technology or an instrument that can help to overcome this problem
- So that TSS can be measured fast, in real-time on the bunch and on the vine is, therefore, vital



- Near-infrared (NIR) spectroscopy has proven to be such a technique/technology
- That combines many sought-after characteristics such as
- Speed, convenience, flexibility, and precision and safety,
- With cheap and non-destructive measurement/analysis of different fruit quality attributes with no harm to the environment
- Its incorporation into any industry will thus greatly help with various decision-making steps
- Through continuous monitoring of essential attributes such as TSS in the pre-harvest, harvest, and post-harvest periods of table grapes

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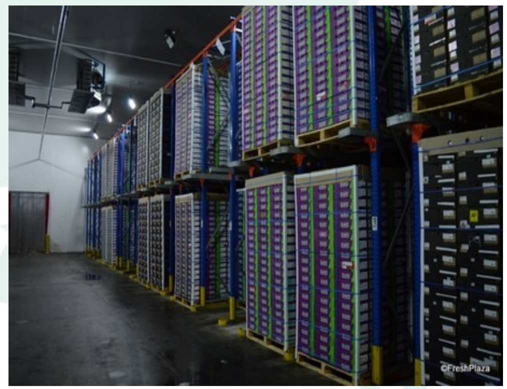
Different levels of table grape quality measurement

Before harvest

Post harvest



Introduction

- ❖ A wide range of portable or handheld NIR instruments is now available,
- ❖ Which offers other great advantages that includes variability in size, weight, robustness, spectral range and optical design options when choosing which instrument to use for the analysis
- ❖ Portable or handheld visible (VIS)-NIR spectrometers
- ❖ Just like their benchtop counterparts
- ❖ Have been used to non-destructively estimate a wide variety of attributes on a wide variety of products.

❖ **Reliance on old manual methods is not necessary anymore**

- **Time-consuming, laborious and destructive**
- **APPLICATION OF PRESENT-DAY STRATEGIES TO MONITOR FRUIT QUALITY PROVEN TO BE MORE ACCURATE**

AIM:

To evaluate the quality of TSS prediction models constructed using two NIR instruments: a handheld Micro-NIR device ideal for measuring intact fruits on the vine and a benchtop spectrometer well suited for measuring any sample that does not need sample preparation over two different harvest years.

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Materials and Methods – Sampling and scanning

- Regal Seedless & Thompson Seedless bunches were randomly selected from the vines on both sides of the canopy from two different vineyards located in the Wellington and the Hex River Valley regions
- Every berry on the selected bunches was numbered with a permanent marker and scanned while still on the vine (Figure a)
- These bunches were then harvested for scanning in the laboratory (Figure b & c).
- Spectral data of the intact table grape berries was collected in reflectance mode (log 1/R) using a handheld Micro-NIR Pro 1700 ES Lite spectrometer (Figure a&b)
- And the solid probe benchtop multi-purpose analyzer (MPA) (Figure c)
- The Micro-NIR was used to scan individual whole berries in the vineyard and the laboratory and the MPA was used only in the laboratory
- The TSS (in °Brix) for each berry was measured and recorded according to the number assigned to it on the bunch with a handheld digital refractometer


(a)


(b)


(c)

Materials and Methods – Data analysis

- Partial least squares (PLS)
- Which is a bilinear modelling strategy
- Was applied to find the correlation between the spectra of the intact table grape berries and the reference values
- PLS regression was implemented in the R statistical environment
- Using the PLS package
- The data matrix, therefore,
    - consisted of a set of independent X variables (NIR spectral data)
    - and a dependent Y variable (TSS)

Materials and Methods – Models Construction

- Several different models were constructed
- The 1st was with data collected from samples in 2016 with the Micro-NIR in the laboratory
- The 2nd with the same 2016 samples, but with data collect-ed with the MPA in the laboratory
- The 3rd with samples collected in 2017 in the vineyard with the Micro-NIR
- The 4th with the same samples but collected with the Micro-NIR in the laboratory
- The 5th by combining the samples collected in 2016 and 2017 with the Micro-NIR in the laboratory
- The 6th and final model was constructed using the 2016 data collected with the Micro-NIR in the laboratory as the training set and the 2017 data collected with the Micro-NIR in the laboratory as the test set
- With the final model where the datasets for 2016 and 2017 were combined (n=3559), the entire dataset was randomly divided into two sub-datasets
- The training set contained 2/3 of the data (n=2373)
- And the test set contained 1/3 of the total dataset (n=1186) for TSS
- A full cross-validation process was applied to build the PLS regression models using the training dataset

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Materials and Methods – Model Evaluation

- Evaluation of all the models was performed through several different statistical indicators
- The coefficient of determination (R^2)
- The Root Mean-Square Error of Calibration (RMSEC)
- The Root Mean-Square Error of Prediction (RMSEP)
- The Standard Error of Calibration (SEC)
- The Standard Error of Performance (SEP)
- Limit Control for SEP (LC_SEP)
- Limit Control for bias (LC_bias)
- And the Residual Prediction Deviation (RPD)
- The R^2 value needs to be as close as possible to 1 for a good model
- The RMSEC, RMSEP, as well as SEC, SEP, LC_SEP and LC bias
- Must be as close as possible to zero to give good working models
- While the RPD needs to adhere to the following values to show the efficacy of the models;
  - between 2.5 and 3 or above to show good and excellent prediction accuracy,
  - between 2 and 2.5 to indicate that robust quantitative predictions are possible
  - And between 1.5 and 2 for the model to discriminate low from high values of the response variable

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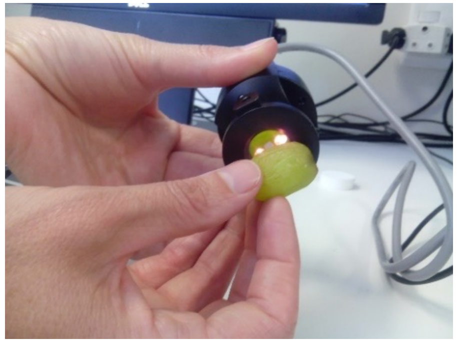
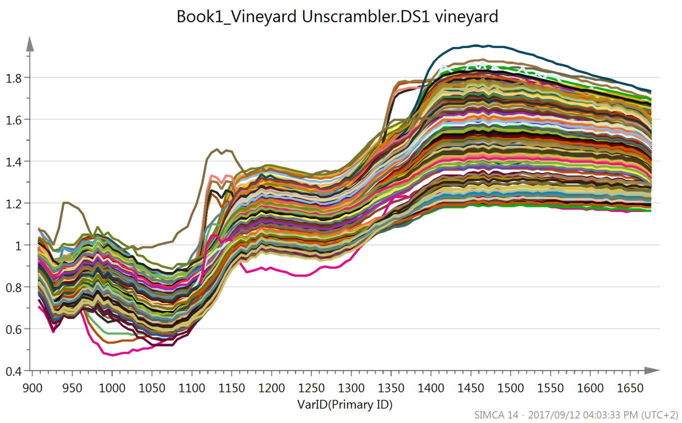
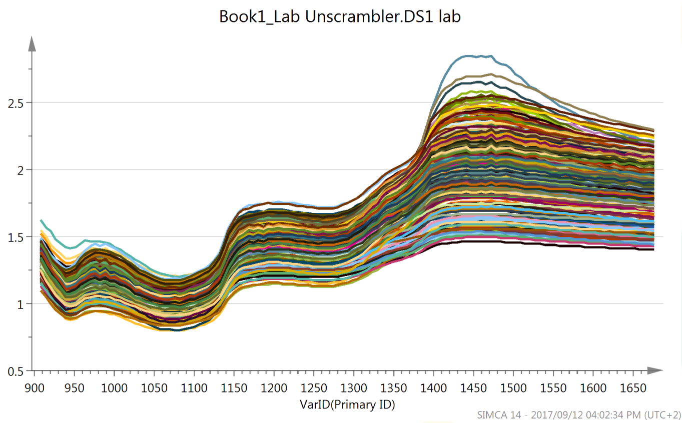
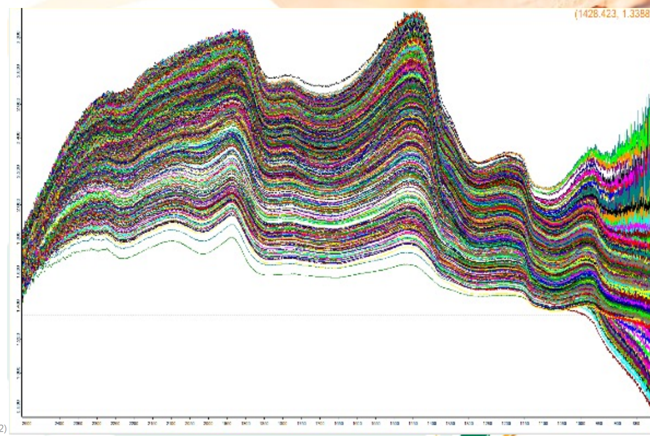
Results – Intact berry spectral features









Results - Reference data statistics (Training Set)

Statistical analysis of the training dataset for TSS[a] collected in 2016 in the laboratory with the MicroNIR an[d] MPA and in 2017 in the vineyard and the laboratory with the MicroNIR only, as well as these combined

Training Statistic	2016 MicroNIR Laboratory	2016 MPA Laboratory	2017 MicroNIR Vineyard	2017 MicroNIR Laboratory	2016 MicroNIR combined 2017 MicroN[IR] Laboratory
N	3120	2110	381	381	3559
Mean	17.56	17.28	20.72	20.74	17.93
Median	17.60	17.30	20.80	20.80	18.00
Min[b]	10.10	10.10	16.60	16.60	10.10
Max[c]	25.20	26.70	25.50	25.50	26.70
Range	15.10	16.60	8.90	8.79	16.60
Standard Deviation	2.38	2.56	1.45	1.47	2.57
Coefficient of Variation	0.14	0.15	0.07	0.07	0.14

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Results - Reference data statistics (Testing Set)

Statistical analysis of the testing dataset for TSS[a] collected in 2016 in the lab with the MicroNIR and the MPA in 2017 in the vineyard and the lab with the MicroNIR only as well as these combined

Training Statistic	2016 MicroNIR Laboratory	2016 MPA Laboratory	2017 MicroNIR Vineyard	2017 MicroNIR Laboratory	2016 MicroNIR combined 2017 MicroN Laboratory
N	2078	1404	251	251	2371
Mean	17.53	17.29	20.76	20.73	17.93
Median	17.60	17.30	20.80	20.80	17.90
Min[b]	10.10	10.10	16.60	16.60	10.10
Max[c]	26.70	25.30	25.50	24.80	25.50
Range	16.60	15.20	8.90	8.20	15.40
Standard Deviation	2.43	2.55	1.45	1.41	2.57
Coefficient of Variation	0.14	0.15	0.07	0.07	0.14

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Results - Performance of calibration models

Performance of PLS models for table grape quality parameter collected in 2016 with the MicroNIR and the MPA in the laboratory and with the MicroNIR only in 2017 in the vineyard and the laboratory. Construction of a calibration model of the combined MicroNIR data collected in the laboratory for 2016 and 2017 also occurred. The dataset obtained with the MicroNIR in the laboratory in 2016 acted as the training set to construct a calibration model validated using MicroNIR in the laboratory in 2017 dataset as a testing set.

Statistic	2016 MicroNIR Laboratory	2016 MPA	2017 MicroNIR Vineyard	2017 MicroNIR Laboratory	2016 MicoNIR Laboratory combined with 2017 MicroNIR Laboratory	2016 Laboratory Calibration 2017 Laboratory Validation
LVs[a]	21.00	9.00	14.00	16.00	17.00	21.00
R^2_c[b]	0.54	0.31	0.52	0.67	0.76	0.76
R^2_{cv}[c]	0.49	0.26	0.28	0.53	0.76	0.75
R^2_p[d]	0.50	0.26	0.39	0.39	0.74	0.29
Sec[e]	1.61	2.11	0.99	0.85	1.25	1.18
Sep[f]	1.71	2.19	1.30	1.13	1.31	1.74
LC_Sep[g]	2.09	2.74	1.29	1.11	1.63	1.54
LC_bias[h]	0.97	1.26	0.60	0.51	0.75	0.71
$RMSE_c$[i]	1.61	2.11	0.99	0.85	1.25	1.18
$RMSE_p$[j]	1.71	2.19	1.31	1.13	1.31	2.49
RPD_c[k]	1.48	1.21	1.45	1.73	2.06	2.05
RPD_p[l]	1.39	1.17	1.10	1.31	1.97	0.97

[a]Latent variables, [b]Coefficient of determination for the calibration set, [c]Coefficient of determination for cross-validation, [d]Coefficient of determination for prediction, [e]Standard error of calibration, [f]Standard error of performance, [g]Limit control for SEP (LC_SEP), [h]Limit control for bias, [i]Root mean square error of calibration), [j]Root mean square error for prediction, [k]Residual prediction deviation for calibration, [l]Residual prediction.n deviation for prediction

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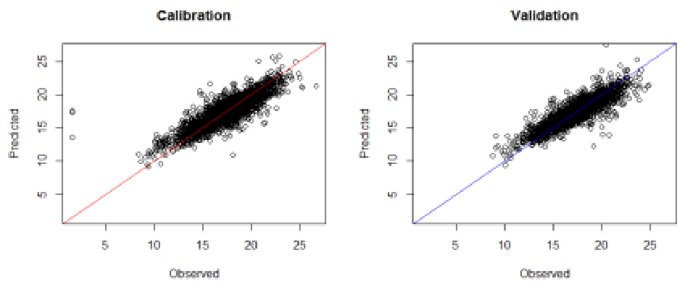
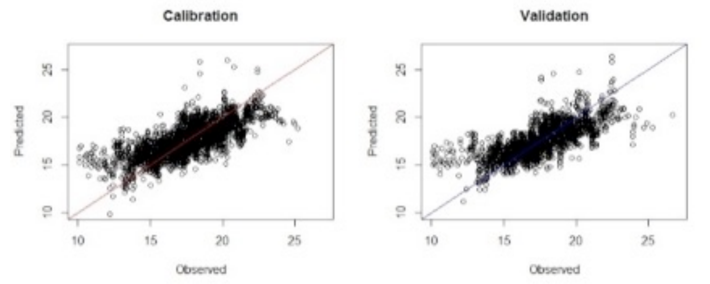
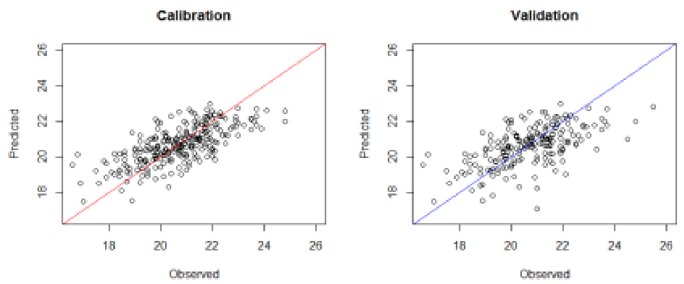
Results - Performance of calibration models



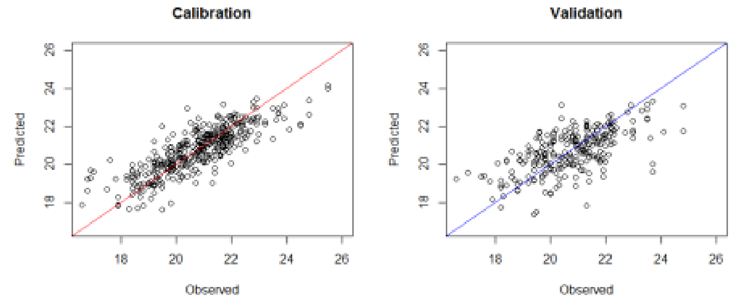
(A) 2016 MicroNIR lab



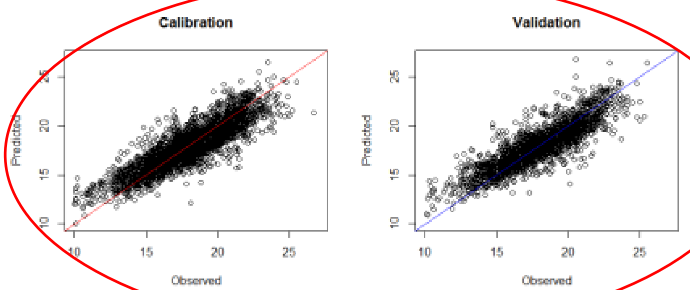
(B) 2016 MPA



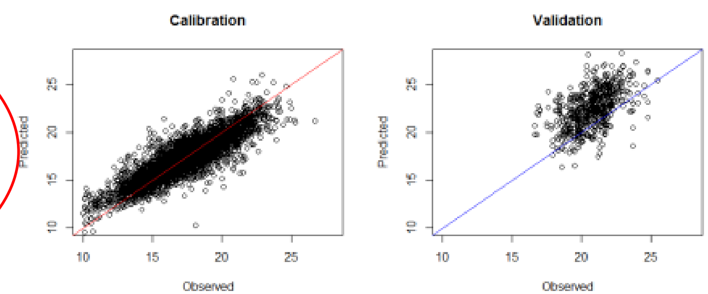
(C) 2017 MicroNIR vineyard



(D) 2017 MicroNIR lab



(E) 2016 lab combined with 2017 lab



(F) 2016 lab cal 2017 lab val

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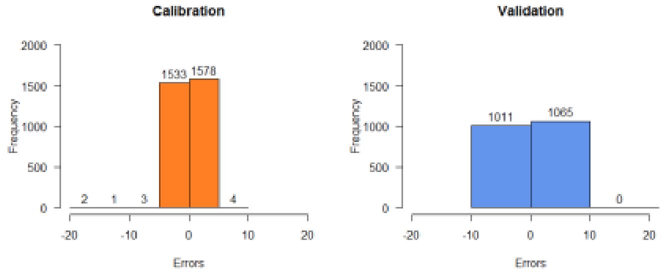
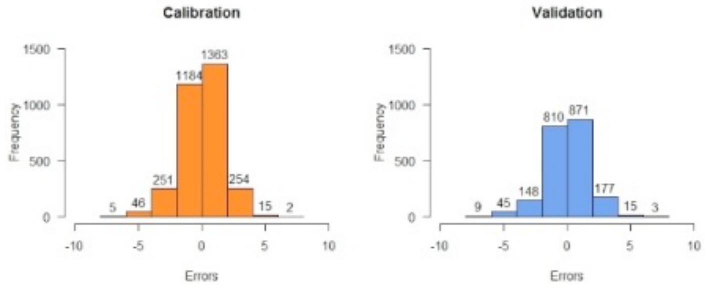
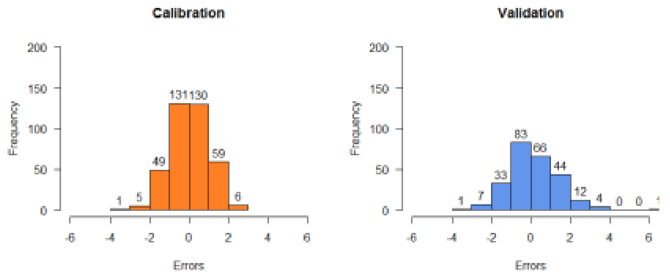
Results - Performance of calibration models



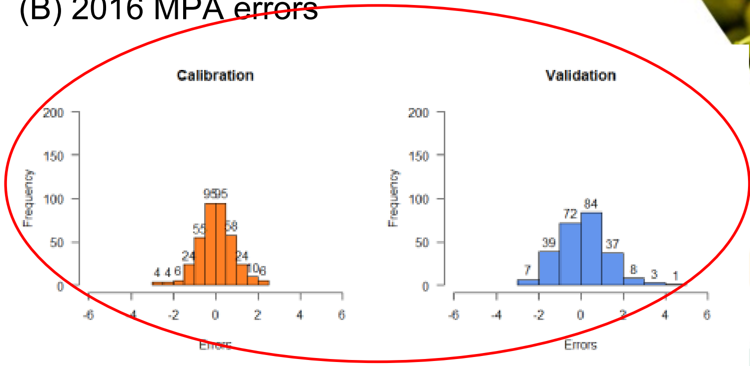
(A) 2016 MicroNIR lab errors



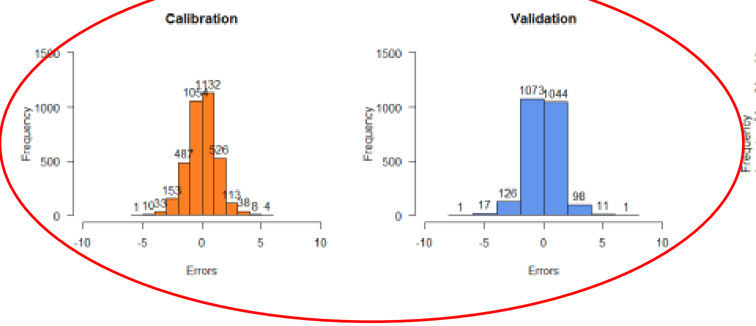
(B) 2016 MPA errors



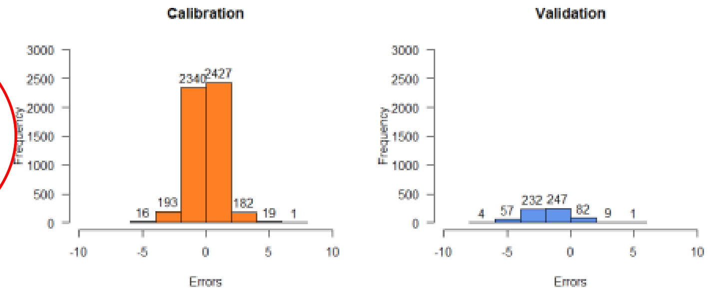
(C) 2017 MicroNIR vineyard errors



(D) 2017 MicroNIR lab errors



(E) 2016 lab combined with 2017 lab errors



(F) 2016 lab cal 2017 lab val errors

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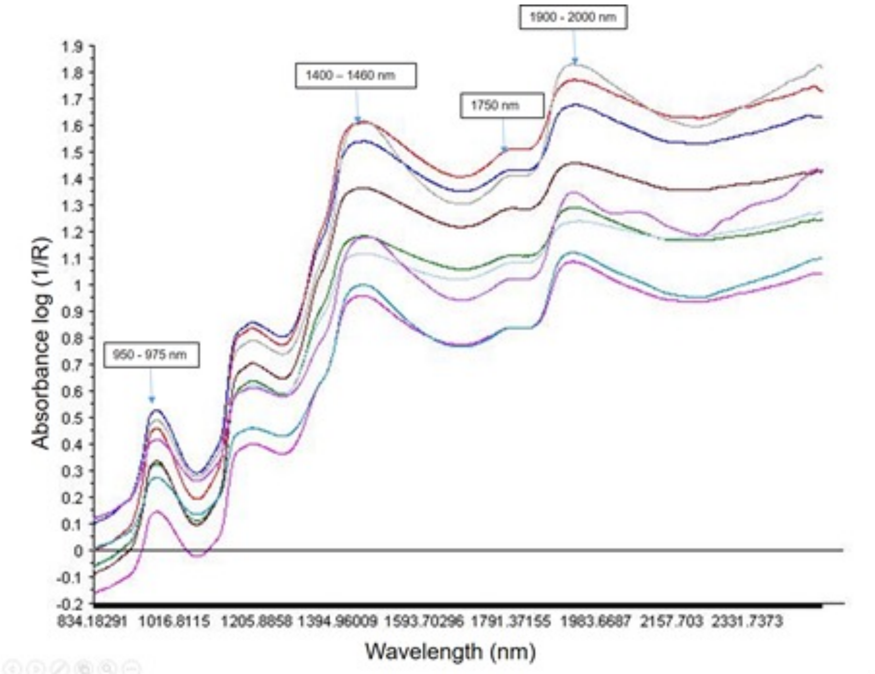
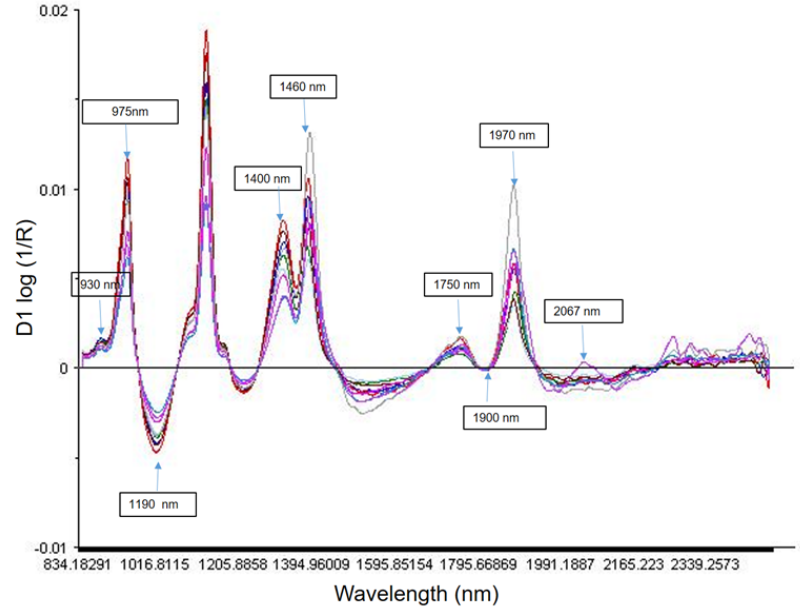
CONCLUSIONS

- These results illustrate that although obtaining good quality spectra with both the MicroNIR and the MPA spectrometers, the ability to measure the TSS content of whole table grape berries accurately in the laboratory and/or the vineyard was better with the MicroNIR than with the MPA.
- The application of spectral pre-processing techniques as well as the selection of specific wavelengths strongly associated with TSS should occur during model building to obtain higher accuracy of prediction models.





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- Also, in terms of practicability, the MicroNIR is the better instrument because of its ease of use in both the vineyard and the laboratory.

Acknowledgements

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Exploring the Impact of Local Research on a Global Scale

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