Measurement of colour, total soluble solids and pH in whole red grapes using visible and near infrared spectroscopy

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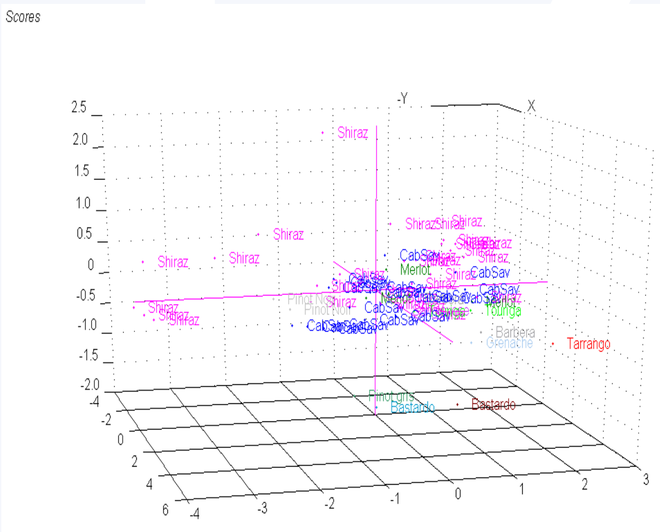
Figure 1. Rectangular cuvette

Figure 2. Score plot for the first three principal components in red grapes, labeled by variety.



Introduction

The presentation of the sample and how it affects both the calibration and prediction is a key point in near infrared (NIR) spectroscopy analysis. Previous work at the AWRI has demonstrated the ability of NIR technology to analyse red grape homogenates for the determination of the concentration of total anthocyanins (colour), total soluble solids (TSS) and pH. The objective of this study was to examine the feasibility of NIR spectroscopy to analyse intact whole berries and avoid the need for homogenisation.

Materials and methods

Whole fresh red grape berries (approximately 100 single berries per sample) were scanned (400–2500 nm) in reflectance mode in a large rectangular cuvette (50 mm by 200 mm, Figure 1) using a monochromator spectrophotometer (FOSS *NIRSystems6500)*. Spectral data were collected, manipulated, and then calibration equations developed for total anthocyanins, TSS and pH using modified partial least squares regression (MPLS) with cross validation using the *WinISI* software.

Results and conclusions

Figure 2 shows the first three principal components of the NIR spectra for the samples of whole grape berries and shows that the samples did not appear to be separated by variety. The relationship between reference and NIR predicted data for the concentration of total anthocyanins, TSS and pH, respectively is shown in Figure 3. Although the standard error of cross validation (SECV) for total anthocyanins was increased by 40% compared to that obtained on homogenised red grape samples (Dambergs et al. 2003), these results suggest that NIR spectroscopy might have potential applications in the analysis of intact whole berries. The lower accuracy might be offset by gains in productivity and increased sample throughput due to the removal of the need to homogenise samples in the laboratory. This might allow rapid measurement of samples from vineyards for 'streaming' purposes to assist in scheduling harvest dates.

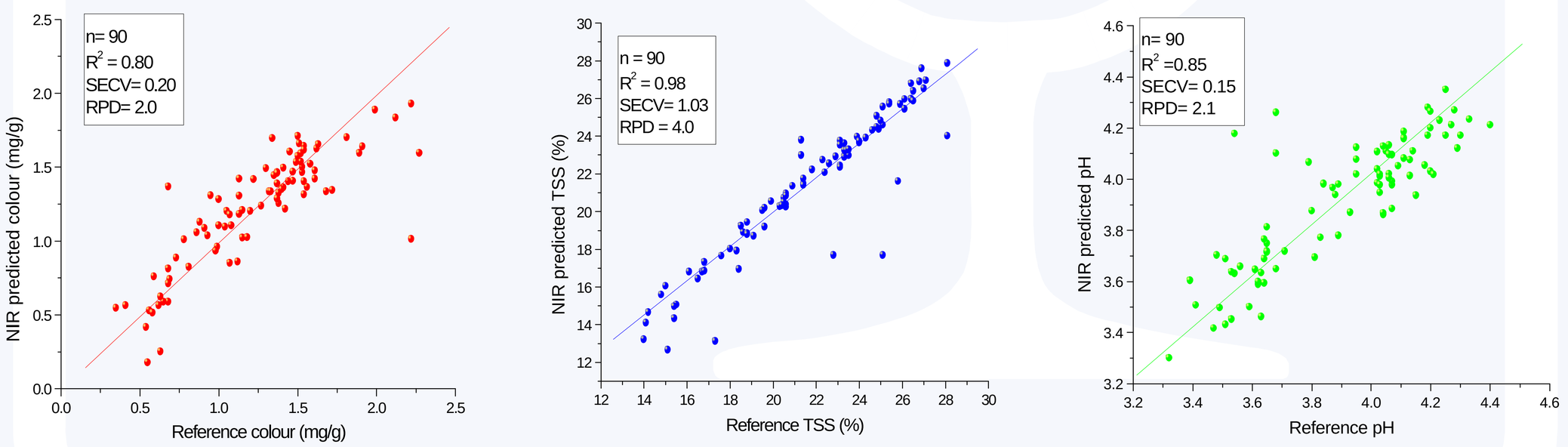


Figure 3. The relationship between reference and NR predicted values for total anthocyanins, TSS and pH, respectively.
n= number of samples; R^2 = coefficient of determination in calibration; SECV= standard error in cross validation; RPD= SD/SECV (where SD = standard deviation of the sample set) values greater than two are considered useful in screening applications, and greater than three as acceptable for analytical purposes.

Reference
Dambergs, R.G.; Cozzolino, D.; Esler, M.B.; Cynkar, W.U.; Kambouris, A.; Francis, I.L.; Høj, P.B.; Gishen, M. (2003) *Australian and New Zealand Grapegrower and Winemakers Journal*. Annual Technical Issue, 69–75.

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