Effects of variety, region and season on near infrared reflectance spectroscopic analysis of quality parameters in red wine grapes

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The wine industry requires practical methods for objectively measuring the composition of both red wine grapes on the vine to determine optimal harvest time; and of freshly harvested grapes for efficient allocation to winery process streams for particular red wine products, and to determine payment of contract grapegrowers. To be practical for industry application these methods must be rapid, inexpensive and accurate. In most cases this restricts the analyses available to measurement of TSS (total soluble solids, predominantly sugars) by refractometry and pH by electropotentiometry. These two parameters, however, do not provide a comprehensive compositional characterisation for the purpose of winemaking.

The concentration of anthocyanin pigment in red wine grapes is an accepted indicator of potential wine quality and price. However, routine analysis for total anthocyanins is not considered as a practical option by the wider wine industry because of the high cost and slow turnaround time of this multi-step wet chemical laboratory analysis.

Recent work by this group^{1,2} has established the capability of near infrared (NIR) spectroscopy to provide rapid, accurate and simultaneous measurement of total anthocyanins, TSS and pH in red wine grapes. The analyses may be carried out equally well using either research grade scanning spectrometers or much simpler reduced spectral range portable diode-array based instrumentation.

We have recently expanded on this work by collecting thousands of red wine grape samples in Australia. The sample set spans two vintages (1999 and 2000), five distinct geographical winegrowing regions and three main red wine grape varieties used in Australia (Cabernet Sauvignon, Shiraz and Merlot). Homogenised grape samples were scanned in diffuse reflectance mode on a FOSS NIRSystems6500 spectrometer and subject to laboratory analysis by the traditional methods for total anthocyanins, TSS and pH.

We report here an analysis of the correlations between the NIR spectra and the laboratory data using standard chemometric algorithms within *The Unscrambler* software package. In particular, various subsets of the total data set are considered in turn to elucidate the effects of vintage, geographical area and grape variety on the measurement of grape composition by NIR spectroscopy. The relative ability of discrete calibrations to predict within and across these differences is considered. The results are then used to propose an optimal calibration strategy for red wine grape analysis.

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¹ M. Gishen and R.G. Dambergs, "Some preliminary trials in the application of scanning near infrared spectroscopy (NIRS) for determining the compositional quality of grape, wine and spirits", *Australian Grapegrower and Winemaker*, 414a, 43-45.47 (1998).

² M. Gishen, R.G. Dambergs, A. Kambouris, M. Kwiatkowski, W.U. Cynkar, P.B. Høj and I.L Francis, "Application of near infrared spectroscopy for quality assessment of grapes, wine and spirits", in *Near Infrared Spectroscopy:* Proceedings of the 9th International Conference, Verona Italy 1999, Ed by A.M.C. Davies and R. Giangiacomo, NIR Publications, Chichester, UK (2000).