# Wine quality grading by near infrared spectroscopy

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## Introduction

The ability to accurately assess wine quality is an important part of the wine making process, particularly when allocating batches of wines to styles determined by consumer requirements. Also, grape pricing is often determined by the quality category of the resulting wine—so called "end use" payment. Wine quality, in terms of sensory characteristics, is normally a subjective measure, performed by experienced winemakers, wine competition judges or winetasting panellists. By nature, such assessments can be biased by individual preferences and may be subject to day-to-day variation. An objective quality grading method would therefore be of great assistance.

Flavour compounds are often present in concentrations below the detection limit of near infrared spectroscopy but the more abundant organic compounds offer potential for objective quality grading by this technique.

## Materials and methods

Samples were drawn from one of Australia's major wine shows and from BRL Hardy's post-vintage wine quality allocation tastings. Turbid samples were clarified by centrifugation. The samples were scanned in transmission mode with a Foss NIRSystems 6500 spectrometer, over the wavelength range 400–2500 nm, using a 1 mm pathlength.

Data analysis was performed with the Vision chemometrics package (Foss NIRSystems). For the quality allocation samples, the reference values used for calibration development were based on sensory assessments from a panel of winemakers, with a consensus grading into five categories (i.e. discrete values from 1 to 5, with category 1 being the lowest quality grade). For the wine show samples, the average score from a panel of judges was used as the reference value. The scores were based on a standard Australian wine show system with three points for appearance (colour intensity, hue, clarity), seven points for aroma and ten points for palate characteristics, resulting in a combined maximum score of 20 points.

## Results and discussion

### Wine quality allocation

With samples from wine quality allocation tastings, the best correlations between near infrared (NIR) spectra and tasting data were obtained with dry red wines. Figure 1 shows a correlation plot of the quality grading *vs* the NIR predicted values for a Cabernet Sauvignon dry red wine. The reference



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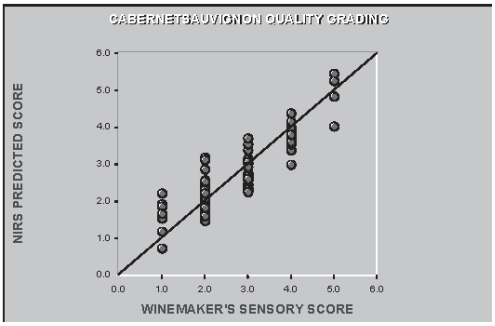


**Figure 1. NIR calibration for Cabernet Sauvignon wine quality grading. *N* = 89. PLS 1st derivative, three factors, $R^2$ = 0.76, *SEC* = 0.49 and *SECV* = 0.55**

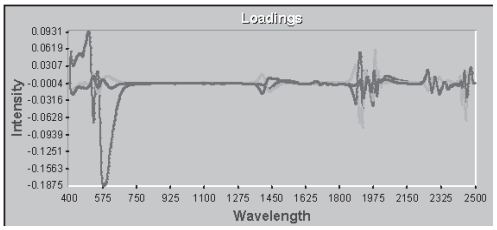


**Figure 2. Factor loadings for Cabernet Sauvignon wine quality calibration.**

quality scores were discrete values, whereas the NIR values were on a continuous scale: this would have reduced the $R^2$ value (0.76). Due to this discrete categorisation, the theoretical minimum error is a grade score of 0.5—the *SECV* of the NIR predicted values was 0.6 grade points.

The Cabernet Sauvignon dry red calibration used PLS factor loadings in the wavelengths related to anthocyanins, ethanol and possibly phenolic compounds (Figure 2).[1–3] Only a small number of factors were required and the strongest loadings were in the anthocyanin spectral region (400–700 nm). Anthocyanins are a group of compounds responsible for colour in red wines.[4] Restricting the wavelengths to a region dominated by anthocyanins produced calibrations of similar accuracy to those using the full available wavelength range. Note, however, that this region can also be used to predict pH, another important wine analytical parameter and it has been suggested that NIR prediction of pH may be related to pH-induced shifts in anthocyanin chromophores.[1] One consequence of the NIR predictions being based predominantly on anthocyanin levels may be that a wine could have high anthocyanin levels but may be downgraded because of a major sensory fault, caused by compounds that have a strong sensory effect at very low concentrations (for example, taints of microbial origin). In this situation the NIR predicted value would tend to be higher than the reference value. This appeared to be the case with grade 1 wines in particular (grade 1 being the lowest quality level).

For dry white wines, calibrations were less significant and appeared to be more dependent on the ethanol-related regions of the spectrum (1700–2400 nm), implying that the quality parameters that could be predicted by NIR correlated with fruit maturity.

## Wine show grading

The correlations between NIR spectra and sensory data obtained using the wine show samples were less significant in general. The difficulty may have been due to excessive sample matrix variation. With most classes in the show, the samples may span vintages, growing areas and winemaking styles, even though they may be made from only one grape variety. For dry red wines, the best calibrations were obtained with a class of Pinot Noir—a variety that tends to be produced in limited areas in Australia and would represent the least matrix variation. Again, the loadings relied predominantly on anthocyanins.

Strong correlations were also obtained with a tawny port class (Figure 3). The sample set was small but the *SECV* represented a 6% error, relative to the mean score. These were sweet, fortified wines, that were aged for long periods in wooden barrels. During the ageing process, Maillard browning compounds are formed and the water is lost through the barrels in preference to ethanol, producing "concentrated", darkly-coloured wines with high alcohol content. The tawny port quality calibrations

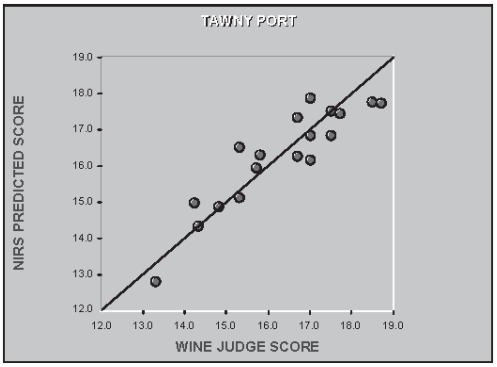


**Figure 3. NIR calibration for Tawny port wine show score. *N* = 20. PLS 1st derivative, three factors, $R^2$ = 0.84, *SEC* = 0.67 and *SECV* = 0.97.**

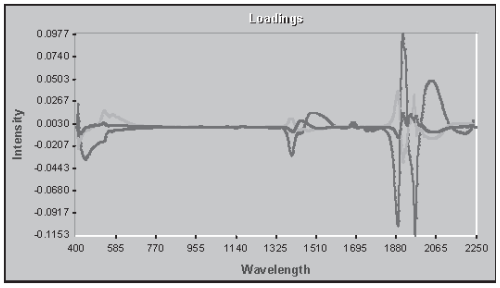


**Figure 4. Factor loadings for Tawny port wine show score calibration.**

indicated strongest loadings in the water regions of the spectrum, suggesting that "concentration" of the wines was important, whilst the visible and alcohol regions of the spectrum also featured as important factors (Figure 4). It has previously been demonstrated that NIR can predict alcohol and total dry extract in this type of wine[5]—the wine calibrations suggest that these are both important quality parameters.

NIR calibrations based on sensory scores will tend to be difficult to obtain due to variation between individual winetasters and may not pick up compounds at low concentrations, yet with strong sensory properties. Nevertheless, these results warrant further investigation and may provide valuable insight into the main parameters affecting wine quality.

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