



Preliminary study on the use of near infrared spectroscopy to assess wine composition in a bottle

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Introduction

An ideal technique to analyse bottled wine would be one that is non-destructive, non-intrusive and allows the determination of chemical composition in real time. Visible (VIS) combined with near infrared (NIR) spectroscopy is one such possible technique. NIR spectroscopy provides a global signature of composition, which can be used by advanced pattern recognition software techniques to infer particular characteristics not readily detected by traditional analytical techniques. Glass wine bottles are transparent to NIR radiation and hence it is possible that measurements on wine might be made directly in unopened wine bottles. The aim of this study was to explore the use of VIS-NIR spectroscopy to measure wine composition non-destructively in the bottle.

Figure 1. A FOSS NIRSystems6500 spectrophotometer

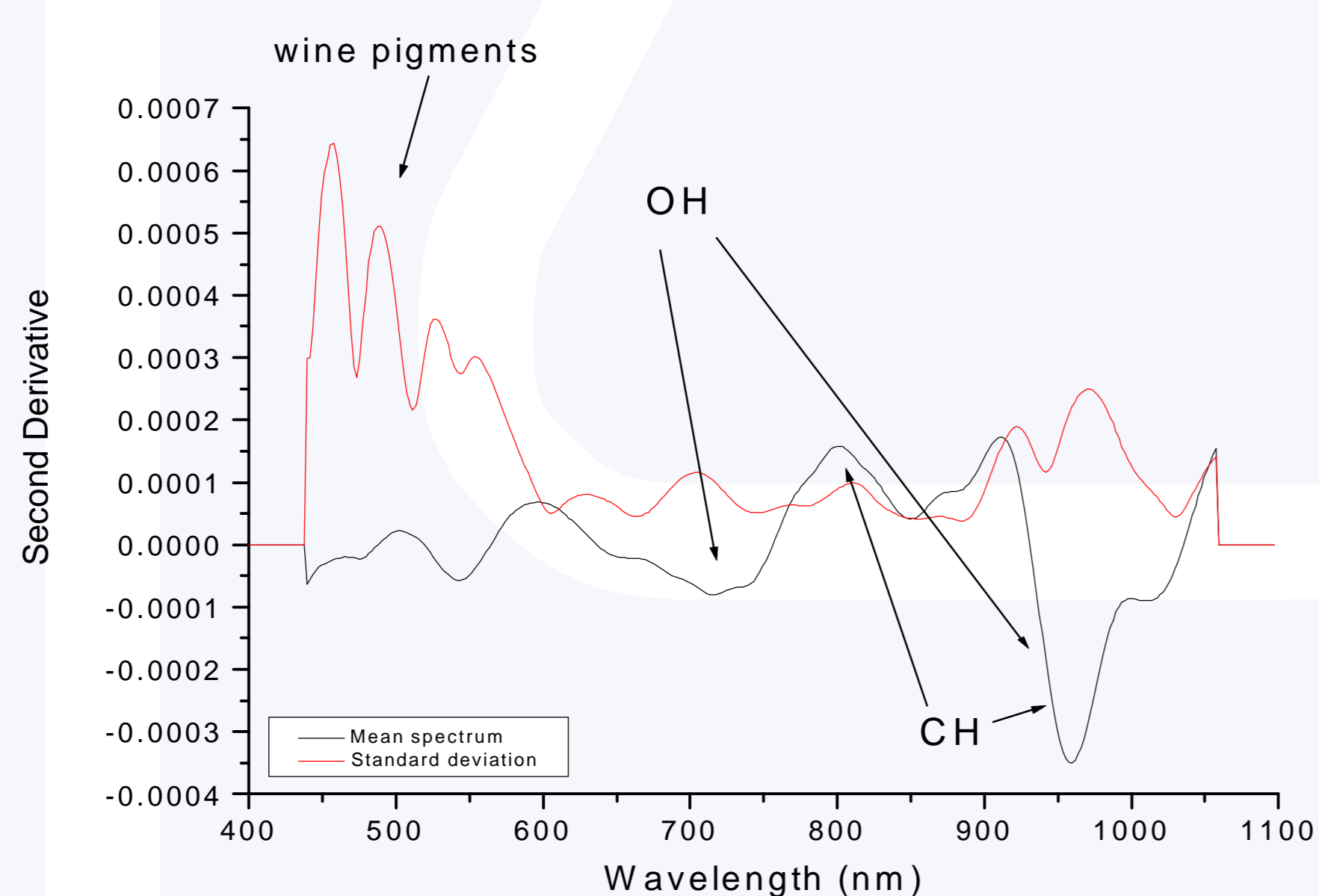


Materials and methods

A FOSS NIRSystems6500 spectrophotometer (Figure 1A) was used to obtain transmittance spectra over the wavelength range 400 – 1150 nm (VIS-NIR) without opening the wine bottle. This was achieved by placing the bottle against the detectors of the instrument and using a backing of aluminium foil on the opposite side of the bottle (Figures 1B and 1C). Approximately 200 samples of bottled wine from the Australian Wine Research Institute Analytical Service (~70% of the total) and Wine and Oxygen project (~30%) were used to build calibration models for the concentration of alcohol, free and total sulfur dioxide (SO₂) and pH. Spectral data collection was achieved using VISION software. Modified partial least square (MPLS) with cross validation were used to develop the calibration models using WinISI software. Reference analyses were conducted using standard laboratory methods by the AWRI Analytical Service.

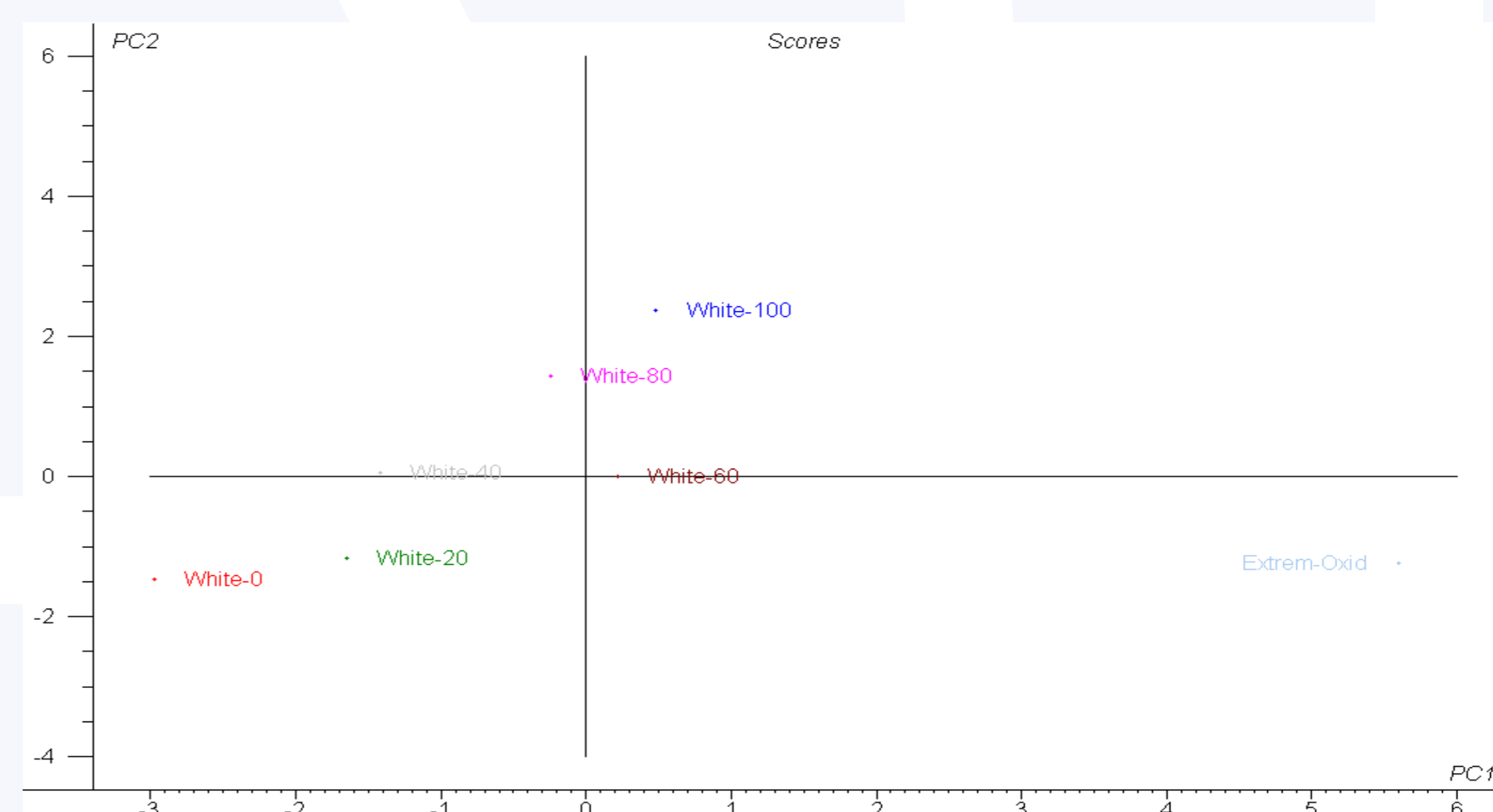
Results

Figure 2. Mean and standard deviation of the second derivative of the VIS-NIR spectra.



The standard deviation (sd) highlights the regions of the spectrum having the greatest variation for the bottle samples analysed (Figure 2). The highest sd were observed around the regions related to pigments, OH and CH tones. This indicates that it is possible to obtain calibrations for wine chemical components that contain these functional groups (OH, CH), such as alcohol.

Figure 3. Plot of the first two principal components of the spectra for the white wine samples labeled by degree of oxidation.



Samples of wine with varying degrees of oxidation (20, 40, 60, 80, 100%) were prepared by addition of various amounts of an un-oxidised wine to a highly oxidised wine (stored in the AWRI storage cellar for 8 years). In addition, another sample from a bottle that was visually even more oxidised was also scanned. The degree of oxidation was differentiated as shown in the principal component plot (Figure 3) predominantly along PC1.

Table 1. The statistics for the VIS-NIR calibrations.

	Alcohol (%)	Free SO ₂ (mg/L)	Total SO ₂ (mg/L)	pH	VA (g/L)
N	85	95	117	55	30
R ²	0.74	0.67	0.73	0.50	0.57
SECV	0.7	6	28	0.19	0.13
RPD	1.3	1.2	1.4	1.0	1.5

Note: N=number of samples; R²=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 three are considered as acceptable for analytical purposes.

Conclusions

For this limited sample set, the RPD for the calibrations indicated that they were not acceptable for analytical purposes (Table 1). However, the results demonstrated the potential of NIR spectroscopy to provide a simple non-invasive and non-destructive method for analysis of wine in-bottle that could be used in quality monitoring applications where only relative changes rather than absolute accuracy is required.

Further studies are in progress to determine the optimal sample presentation to the instrument and its influence on the calibrations, as well as to validate the robustness and accuracy of the new calibration models developed.