The Australian Wine Research Institute

White wine varietal discrimination using near infrared reflectance spectroscopy

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Introduction

In the last 30 years, near infrared spectroscopy (NIR) has attracted interest as a method for authenticating different foods and agricultural products due to the inherent speed of analysis, possibility of minimal sample preparation and relatively low cost. The aim of this work was to investigate the potential of NIR as a technique to discriminate between samples of two varieties of commercial dry white wine, namely Riesling and unwooded Chardonnay, using NIR spectral properties alone.

Materials and methods

The samples used in the study were three bottles each of 20 different brand labels of commercial unwooded Chardonnay (n=122) and Riesling (n=144) wines from a number of Australian regions, and while most were from the 2001 and 2002 vintages, included wines up to ten years old. Samples were scanned (400 – 2500 nm) in transmission in a 1 mm path length cuvette in a FOSS *NIRSystems6500* monochromator instrument. Spectral data collection and manipulation were achieved using the *VISION* software. Principal component analysis (PCA) and discriminant partial least squares (DPLS) models were developed using *The Unscrambler* software. The sample set was randomly split in two with half being used for development of the discrimination model, and the other half for validation.

Figure 1. Score plots for the first two principal components for the spectra of the wines, labeled by variety (1 = Riesling, 2 = Chardonnay).

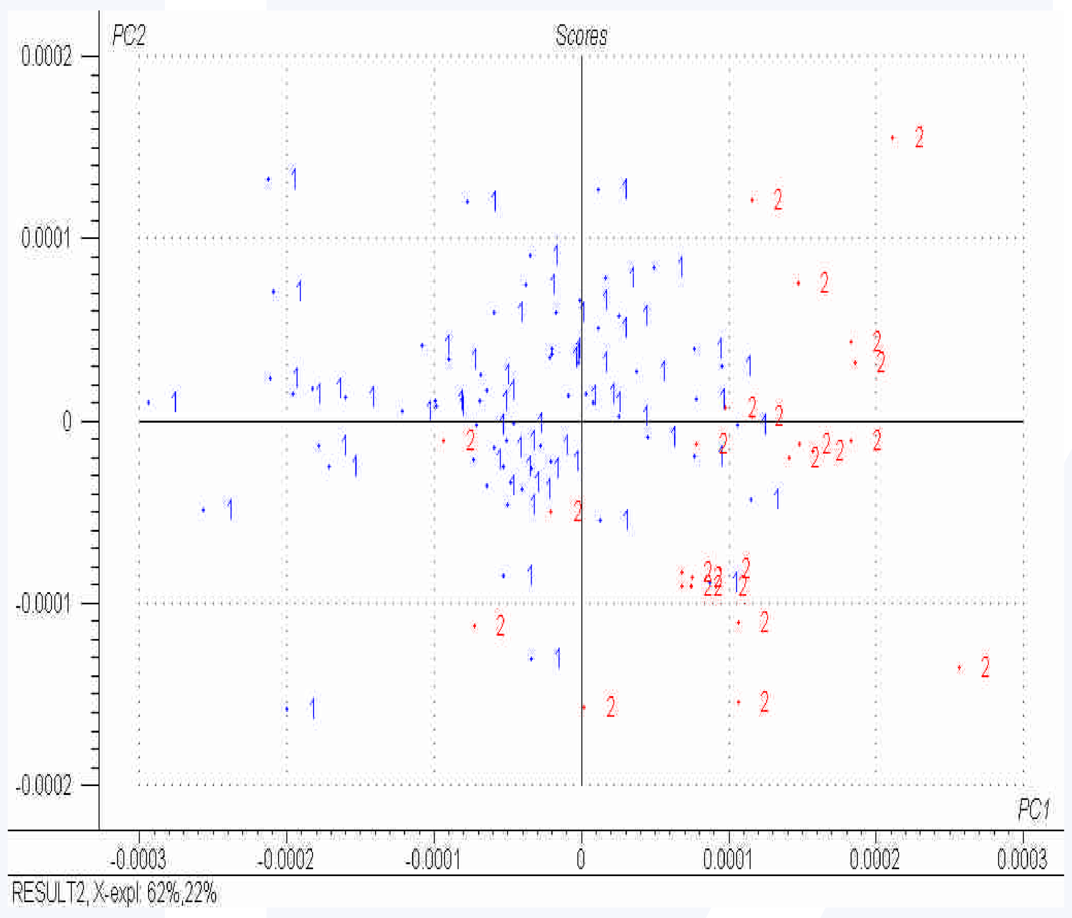
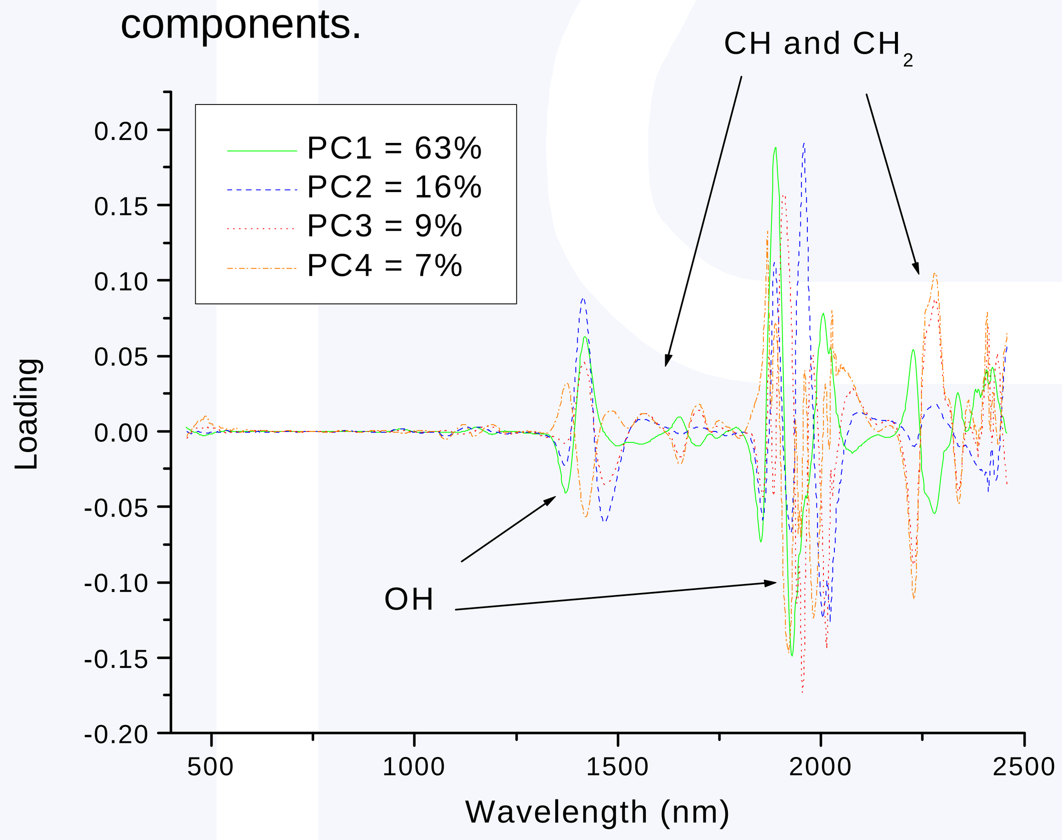


Figure 2. Eigenvectors for the first four principal components.



Results

Figure 1 shows the scores of the first two principal components that describe the variation in the second derivative of the spectra and shows a general separation of the samples by the indicated varieties. Figure 2 shows the eigenvectors for the wavelengths of the first four principal components that explain 95% of the variation in the spectra of the samples, indicating the functional groups responsible for the separation. Therefore, it is suggested that particular chemical constituents, such as ethanol, water, sugars (glucose and fructose), phenolic compounds, lactic acid, oxidation products, either in combination or alone, contribute the strongest influences that explain the basis for the observed separation between the two varieties. The results in Table 1 show that more than 90% of the wines were correctly classified by the DPLS models based on the VIS- NIR spectra.

Conclusion

This study demonstrates the potential of NIR for use as a technique to discriminate between white wine varietal origin. It also suggests that the necessary information for discrimination by NIR techniques is not simply provided by a single specific constituent (e.g. ethanol, sugars, phenolic compounds), but rather the compositional characteristics of the wine as a whole. Further studies will be conducted in order to validate and assess the robustness and accuracy of the models developed.

Table 1. DPLS discrimination model for prediction of white wine varietal origin.

Pre-processing of spectral data	Wavelength range used (nm)	Variety	Number of samples **correctly** classified	Number of samples incorrectly classified	SEP [a]
None	400 - 750	Riesling [b]	**72**	0	0.11
	400 - 1100	Riesling	**72**	0	0.13
	400 - 750	Chardonnay [c]	**60**	1	0.13
	400 - 1100	Chardonnay	**61**	0	0.11
2nd Derivative	400 - 750	Riesling	**72**	0	0.11
	400 - 750	Chardonnay	**59**	2	0.18

Notes:
(a) SEP: standard error of prediction; (b) N = 72 samples in the validation set; (c) N = 61 samples in the validation set

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