Available online at www.sciencedirect.com

ScienceDirect

Food Chemistry 106 (2008) 781–786

Food Chemistry

www.elsevier.com/locate/foodchem

Analytical, Nutritional and Clinical Methods

Preliminary study on the application of visible–near infrared spectroscopy and chemometrics to classify Riesling wines from different countries

L. Liu [a,b,1,2], D. Cozzolino [b,c,*], W.U. Cynkar [b,c,2], R.G. Dambergs [b,c,2], L. Janik [b,c,2], B.K. O'Neill [a,1], C.B. Colby [a,1], M. Gishen [b,c,2]

[a] *School of Chemical Engineering, Engineering North Building, The University of Adelaide, SA 5005, Australia*
[b] *The Australian Wine Research Institute, Waite Road, Urrbrae, P.O. Box 197, Adelaide, SA 5064, Australia*
[c] *Cooperative Research Centre for Viticulture, P.O. Box 154, SA 5064, Australia*

Received 29 January 2007; received in revised form 20 April 2007; accepted 18 June 2007

Abstract

Visible (VIS) and near infrared (NIR) spectroscopy combined with chemometrics was used in an attempt to classify commercial Riesling wines from different countries (Australia, New Zealand, France and Germany). Commercial Riesling wines ($n = 50$) were scanned in the VIS and NIR regions (400–2500 nm) in a monochromator instrument, in transmission mode. Principal component analysis (PCA), partial least squares discriminant analysis (PLS-DA) and stepwise linear discriminant analysis (SLDA) based on PCA scores were used to classify Riesling wines according to their country of origin. Full cross validation (leave-one-out) was used as the validation method when classification models were developed. PLS-DA models correctly classified 97.5%, 80% and 70.5% of the Australian, New Zealand and European (France and Germany) Riesling wines, respectively. SLDA calibration models correctly classified 86%, 67%, 67% and 87.5% of the Australian, New Zealand, French and German Riesling wines, respectively. These results demonstrated that the VIS and NIR spectra contain information that when used with chemometrics allow discrimination between wines from different countries. To further validate the ability of VIS–NIR to classify white wine samples, a larger sample set will be required.

Keywords: Visible; Near infrared; Spectroscopy; Principal component analysis; Discriminant partial least squares; Stepwise linear discriminant analysis; Riesling; Wine; Country origin

1. Introduction

Riesling is considered to be one of the world's greatest white grape varieties and produces some of the best white wines. It is a native variety of Germany, where it is believed to have been cultivated for at least 500 years and possibly as long as 2000 years. As well as in Germany, it has been planted in California, in the Alsace region of France, in Austria, Australia, Canada and New Zealand. The Riesling grape's ability to retain its acidity while achieving high sugar levels is what creates wines with considerable aging potential. Wines made from Riesling grapes are usually characterized as of a light to medium body, floral and fruity, and an implicit sweetness (Iland & Gago, 2002).

Wine has become a commodity of significant commercial value and consumer expectations depend on many factors, such as grape variety and maturity, geographic origin, country of origin and vinification techniques (Cordella, Moussa, Martel, Sbirrazzuoli, & Lizzani-Cuvelier, 2002). In most wine producing countries in Europe, wine quality value is associated with both climate and soil characteristics, in particular defined by geographical classification or

---

[*] Corresponding author. Address: The Australian Wine Research Institute, Waite Road, Urrbrae, P.O. Box 197, Adelaide, SA 5064, Australia. Tel.: +61 8 8303 6600; fax: +61 8 8303 6601.
E-mail address: Daniel.cozzolino@awri.com.au (D. Cozzolino).
[1] Fax: +61 8 8303 4373.
[2] Fax: +61 8 8303 6601.

0308-8146/$ - see front matter © 2007 Elsevier Ltd. All rights reserved.
doi:10.1016/j.foodchem.2007.06.015

denomination of origin systems (Fischer, Roth, & Christmann, 1999). Today, the determination of food authenticity and the detection of adulteration are major issues in the food industry and are attracting an increasing amount of attention for wine producers, researchers and consumers. Wine quality is related to an obvious commercial value, determining that adulteration is possible to be practiced, which may bring an unfair competition in the wine industry and harm the rights of consumers (Cordella et al., 2002; Fischer et al., 1999; Reid, O'Donnell, & Downey, 2006). Thus, there is significant interest in accurate methods for wine characterization that could be used to prevent adulteration and to classify wine from different geographical origins or countries (Cordella et al., 2002; Fischer et al., 1999; Reid et al., 2006). The differentiation of wines from different countries has been successfully achieved by measuring chemical compounds present in the wine matrix (e.g. volatiles, phenolic compounds, minerals) using various analytical techniques such as high liquid performance chromatography (HPLC), gas chromatography (GC) and inductively coupled plasma mass spectrometry (Alvarez, Aleixandre, Garcia, Casp, & Zenica, 2003; Baxter, Crews, Dennis, Goodall, & Anderson, 1996; Castiñeira, Feldmann, Jakubowski, & Andersson, 2004; Cordella et al., 2002; de Villiers et al., 2005; Fischer et al., 1999; Frias, Conde, Rodriguez-Bencomo, Garcia-Montelongo, & Perez-Trujillo, 2003; Latorre, Garcia-Jares, Medina, & Herrero, 1994; Maarse, Slump, Tas, & Schaefer, 1987).

The wine industry needs analytical tools to verify the authenticity of high value products in order to protect their brands and ideally these tools should allow rapid and inexpensive analysis at any point of the distribution chain (Francis et al., 2005). Near infrared (NIR) spectroscopy has the potential to meet these requirements. NIR spectroscopy utilises the spectral range from 750 to 2500 nm and provides compositional information related to the vibrational behaviour of combinations of bonds compared to those obtained using mid infrared (MIR) (Reid et al., 2006). The NIR spectra are composed of absorption bands due to overtones and combinations of fundamental bond stretching or bending vibrations occurring in the MIR region of the electromagnetic spectrum. Molecules containing hydrogen will have measurable NIR spectra and given the ubiquitous distribution of hydrogen this means that a very large number of analytes are amenable to NIR analysis (Davies, 1998). It is well known that simple visual examination of the NIR spectra cannot discriminate between authentic and adulterated product (Cozzolino, Smyth, & Gishen, 2003; Kemsley, 1996; Naes, Isaksson, Fearn, & Davies, 2002). Therefore, the application of multivariate data analysis techniques like principal component (PCA) or discriminant analysis (e.g. partial least squares discriminant analysis, PLS-DA) opens the possibility to unravel and interpret the spectral properties of the sample and allow a classification without the use of chemical reference data. The use of visible (VIS) and NIR spectroscopy in the Australian wine industry has mainly been restricted to the measurement of the concentration of total anthocyanins (colour), total soluble solids and pH in red grapes (Dambergs et al., 2001; Gishen et al., 2002), methanol in spirits (Dambergs, Kambouris, Francis, & Gishen, 2002) and ethanol content in wines (Gishen et al., 2002). Some preliminary work has demonstrated the ability of VIS–NIR spectroscopy to predict overall 'quality grade' in both red and fortified wines (Gishen et al., 2000).

The objective of this study was to explore the use of VIS and NIR spectroscopy, combined with chemometrics, to classify Riesling wines from four different countries: Australia, New Zealand, France and Germany.

2. Materials and methods

2.1. Wine samples and reference analysis

A total of 50 bottles (4 labels × 3 bottle replicates and 19 labels × 2 bottle replicates) of 23 different commercially available Australian ($n = 10$), New Zealand ($n = 5$) and European (France and Germany) ($n = 8$) Riesling wines were collected and analysed in 2006. The wines showed a diversity of sensory (data not presented) and chemical characteristics and ranged from 2001 to 2004 vintages. Vintage 2001 ($n = 1$) from France, vintage 2002 ($n = 1$) from France, vintage 2003 ($n = 2$) from France, ($n = 2$) from New Zealand, ($n = 2$) from Germany and ($n = 1$) from Australia, vintage 2004 ($n = 3$) from New Zealand, ($n = 2$) from Germany and ($n = 9$) from Australia. Samples were analysed for alcohol, pH, titratable acidity (TA), glucose plus fructose (G+F), volatile acidity (VA) and total phenolics (TP) (Table 1) using standard industry methods (Iland, Ewart, & Sitters, 1993).

2.2. Visible and near infrared measurements

Wine samples taken from freshly opened bottles were scanned in transmission mode (400–2500 nm) using a scanning monochromator FOSS NIRSystems 6500 (FOSS NIRSystems, Silver Spring, MD, USA). Spectral data were collected using Vision software (version 1.0). Samples were scanned in a rectangular cuvette with a 1 mm path length and equilibrated at 33 °C for 3 min before scanning. Spectral data were stored as the logarithm of the reciprocal of transmittance [log $(1/T)$] at 2 nm intervals. The spectrum of each sample was obtained in triplicate and the mean of the three measurements was used for multivariate analysis and classification. Instrument performance was checked daily following the diagnostic protocols provided by the manufacturer.

2.3. Multivariate data analysis

Spectra were exported from the Vision software in NSAS format into The Unscrambler software (version 9.2, CAMO ASA, Norway) for chemometric analysis. Principal component analysis (PCA) was used to reduce the

Table 1
Chemical composition for Riesling wines from different countries

	Australia ($n = 21$)				New Zealand ($n = 12$)				Europe ($n = 17$)			
	Mean	SD	Max	Min	Mean	SD	Max	Min	Mean	SD	Max	Min
Alcohol (%)	12.0^{a}	0.54	12.9	11.1	11.5^{a}	1.4	13.2	8.8	11.9^{a}	1.02	13.2	10.1
pH	3.01^{a}	0.13	3.2	2.9	2.95^{a}	0.21	3.25	2.57	3.26^{b}	0.17	3.76	3.07
VA (g/L)	0.44^{a}	0.06	0.59	0.38	0.49^{a}	0.11	0.67	0.40	0.46^{a}	0.13	0.81	0.34
TA (g/L)	7.32^{b}	0.65	8.64	6.14	8.35^{a}	1.43	10.81	7.14	6.97^{b}	0.73	7.96	5.87
G+F (g/L)	1.74^{b}	1.94	5.38	0.01	20.1^{a}	4.45	56.49	17.1	12.4^{a}	12.7	41.4	2.15
TP(A.U.)	8.51^{a}	1.18	11.6	6.8	8.12^{a}	1.96	12.18	6.58	8.9^{a}	1.11	11.91	7.68

TA: titratable acidity; VA: volatile acidity; G+F: glucose plus fructose; TP: total phenolics; Europe: France plus Germany. ^{a,b}Levels not connected by same letter are significantly different, $p < 0.05$.

dimensionality of the data to a smaller number of components, to examine any possible grouping of samples according to their country and to visualise the presence of outliers (Naes et al., 2002). PCA models were developed using both raw and pre-processed data. The spectra were pre-processed using the standard normal variate (SNV) method (Barnes, Dhanoa, & Lister, 1989) to correct for scatter, followed by second derivative transformation using Savitzky-Golay derivation and smoothing (10 point and 2nd order filtering operation) to reduce baseline variation and enhance the spectral features (Naes et al., 2002). Discrimination models were developed using partial least squares discriminant analysis regression (PLS-DA) and stepwise linear discriminant analysis (SLDA), respectively (Adams, 1995; Naes et al., 2002; Otto, 1999). PLS-DA is a variant of partial least squares regression (PLS). The principle is very simple, for each class, a model [$\boldsymbol{C} = \boldsymbol{T} \cdot \boldsymbol{q}$], where $\boldsymbol{T}$ are the PLS scores obtained from the original data using the PLS algorithm, $\boldsymbol{q}$ is the vector and $\boldsymbol{C}$ is the class membership function. This is obtained by PLS regression from an original $\boldsymbol{C}$ vector whose elements have values of 1 if an object is a member of a class and 0 otherwise (Naes et al., 2002; Otto, 1999). In this technique, a dummy variable that describes the group membership is used (values of zero and one were used). Due to the fact that we have more than two variable groups, the PLS2 algorithm was used as the regression method to develop the classification models. The PLS2 regression uses the dummy variable as the dependent variable Y and the wavelengths as the independent X variables. Group membership of a new unknown sample is determined by its predicted value with PLS-DA (Naes et al., 2002).

Stepwise linear discriminant analysis (SLDA) is a supervised classification technique, where the number of categories and the samples that belong to each category are previously defined (Adams, 1995; Naes et al., 2002; Otto, 1999). The criterion of SLDA for selection of latent variables is maximum differentiation between the categories and minimise the variance within categories (Adams, 1995; Naes et al., 2002; Otto, 1999). The method produces a number of orthogonal linear discriminant functions, equal to the number of categories minus one, that allow the samples to be classified in one or another category. SLDA was carried out using JMP software (version 5.01, SAS Institute Inc., Cary, NC, USA) on the scores of principal components (PCs) 1–3, which gave the highest level of separation (high variance) in the PCA models developed. The PCA, SLDA and PLS-DA calibration models were developed using full cross validation (CV) (leave-one-out method). The number of latent variables (LV) used to develop the calibration models were selected by the software as indicated by the PRESS function (predicted residual error sum-of-squares) (Naes et al., 2002). Statistical analysis of the chemical composition was performed by JMP statistical software with a general linear model (GLM) procedure.

3. Results and discussion

3.1. Chemical analysis

Table 1 shows the descriptive statistics (mean, standard deviation and range) for the chemical composition of the Riesling wine samples. No statistically significant differences between wines from different countries were observed for alcohol content, TP and VA in the set of wines analysed. However, statistically significant differences were observed in pH, TA and glucose plus fructose content. A PCA analysis was carried out using the chemical composition of the Riesling wines analysed (data not shown) and the first two PCs accounted for 98% of the total variance in the set of Riesling wines analysed. The first PC was mainly associated with TA, VA and alcohol content, and the second PC was related to pH and TP. Although differences were observed in the G+F content of individual wines, no clear discrimination, by country, between samples was observed.

3.2. Visible and near infrared spectra interpretation

Fig. 1 shows the VIS and NIR mean raw spectra of Riesling wines. The VIS and NIR mean spectra of the Riesling wines after SNV and second derivative transformations did not show obvious differences from visual inspection according to the different countries. The absorption band at 1450 nm was related to the second O–H overtone of both

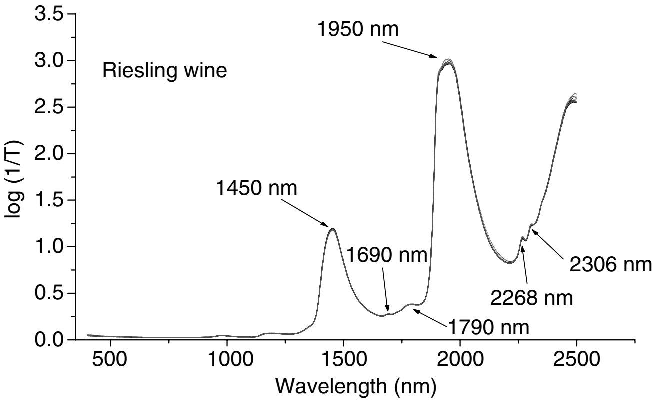

Fig. 1. Visible and near infrared mean spectra of Riesling wine samples.

water and ethanol (Osborne, Fearn, & Hindle, 1993). Absorptions were observed at 1690 nm and 1750 nm, related to C–H stretch first overtones, and at 2268 nm, and 2306 nm, due to C–H combination vibrations (Cozzolino et al., 2003; Dambergs et al., 2002; Osborne et al., 1993). The absorption band at 1790 nm is related to O–H bonds and has been associated with sucrose, fructose and glucose in fruit juices (Giangiacomo & Dull, 1986).

3.3. Principal component analysis (PCA)

The pre-processed spectra (SNV and 2nd derivative) of the Riesling wine samples were analysed by means of PCA. Fig. 2 shows the score plot of the first two PCs, which account for 94% of the variation in the VIS and NIR spectra of the wine samples. A grouping was observed among the wines from Australia, however, the separation was not clear for other countries and some overlap was observed between the groups. The overlapped samples were mainly from New Zealand and Europe. The eigenvectors for the first three PCs were investigated in order to find specific regions in the VIS and NIR spectra that explain the separation between samples (Fig. 3). PC1 accounts for 91% of the total variance in the spectra of the Riesling samples, and the highest eigenvectors were found at around 2250–2350 nm, related to C–H combinations and O–H stretch overtones. Additional absorption bonds were observed around 1400–1460 nm and around the 1660–1760 nm region, related to O–H first overtones and C–H first overtones, respectively. The highest eigenvectors in PC2 (3%) were observed at around 1400–1460 nm and 2250–2350 nm, respectively and the highest eigenvectors in PC3 (2%) were observed in the VIS region at around 410–540 nm. In an attempt to achieve a better classification, separate PCA models were developed using only two groups of samples. Therefore, the PCA models were developed for Australian and European wines, Australian and New Zealand wines, and New Zealand and European wines, respectively. Subsequently, the PCA scores were used as input data for SLDA.

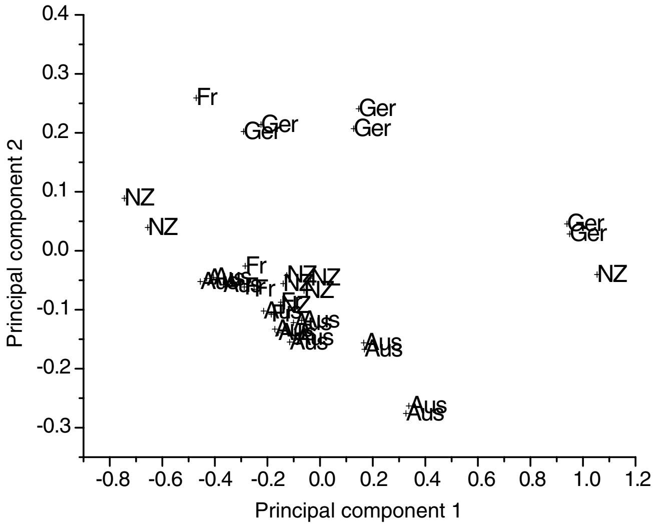

Fig. 2. Principal component score plot based on VIS and NIR spectra of Riesling wine samples grouped according to country of origin (Fr = France; Ger = Germany; NZ = New Zealand; Aus = Australia).

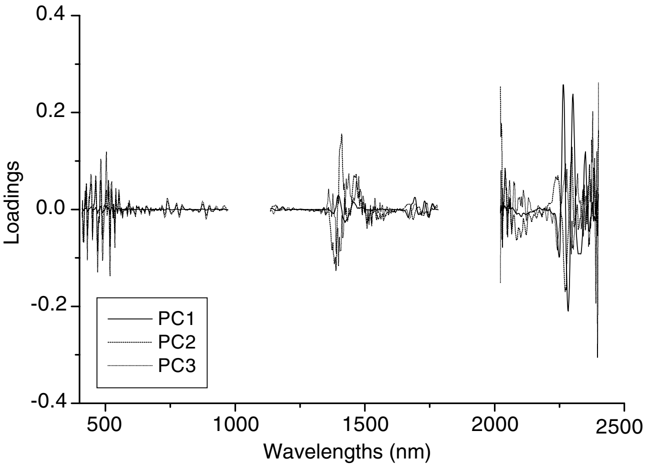

Fig. 3. Eigenvectors of the three principal components of Riesling wine samples analysed by visible and near infrared.

3.4. Stepwise linear discriminant analysis (SLDA)

SLDA was performed on the first six PCs from PCA, which accounted for 98% variation of the spectral data. The SLDA correctly classified 86%, 67%, 67% and 87.5% of the Australian, New Zealand, French and German Riesling wines, respectively. SLDA models were developed using specific pairs from different geographical origins. This resulted in 95% correct classification between wines from Australia and Europe and 86% correct classification between Australia and New Zealand. It was more difficult to discriminate between Riesling wines from Europe and New Zealand, compared with those from Australia. The low classification rate might indicate style similarities of the Riesling wines from New Zealand and Europe compared to those produced in Australia (see Table 2).

Table 2
Stepwise linear discriminant (SLDA) classification results of Riesling wines using VIS–NIR pre-processed spectra (6 PCs)

	Australia ($n = 21$)	New Zealand ($n = 12$)	France ($n = 9$)	Germany ($n = 8$)	Overall classification
Australia	18 (86%)	3	0	0	
New Zealand	3	8 (67%)	0	1	
France	2	1	6 (67%)	0	
Germany	0	1	0	7 (87.5%)	39 (78%)

Table 3
Partial least squares discriminant (PLS–DA) classification results of Australian, New Zealand and European Riesling wines using VIS–NIR pre-processed spectra

	% CC as Australia	% CC as New Zealand	% CC as Europe
Australia ($n = 21$)	97.5	–	–
New Zealand ($n = 17$)	–	80	–
Europe ($n = 12$)	–	–	70.5

CC = Correct Classification, Europe = France and Germany.

3.5. Partial least squares discriminant analysis (PLS-DA)

PLS-DA was used also to classify Riesling wine samples according to their country of origin. Table 3 shows the classification results obtained for Riesling wine samples from the three different countries. Correct classification rates of 97.5%, 80% and 70.5% were obtained for Australian, New Zealand and European Riesling wines, respectively. These results were better to the classification rates obtained using SLDA.

The results obtained in this study shows that the VIS and NIR spectra of Riesling wines contain information that allows us to classify such wines according to their country of origin. The spectral loadings in the NIR region are related to C–H combination and O–H stretch overtones, suggesting that the differences caused by the phenolic profiles as well as other organic compounds present in the wine matrix (e.g. organic acids, sugars), might contribute to the variations among the wines according to the country of origin (Somers, 1998). Based on these data, it was possible to discriminate between Australian Riesling and Riesling wines produced in New Zealand, France or Germany. It was noticed that seven out of eight Riesling samples originating from Germany were classified correctly, indicating that samples of this country were highly characteristic. The misclassification results obtained for samples from New Zealand and France could be attributed to the small number of wine samples, lack of varietal integrity and possibly other factors such as similarities in the grape growing or winemaking process. A question that must be answered is whether the regional differences observed in the spectra are due to fundamental differences in the grapes or due to differences in winemaking methods or the yeast used to ferment the wine.

White wine classification was achieved between the samples from three countries. Riesling wines from Australia were correctly classified with an overall classification rate of 90% using various multivariate methods when compared with samples from New Zealand or Europe. However, lower classification rates were achieved for wine samples from New Zealand and Europe. The similarity among wines from New Zealand and Europe might explain the low classification results obtained. Overall, the interpretation of conclusions from this particular study were limited by the relatively small number of wine samples and the characteristics of the sample variables in terms of vintage, diversity of origin, among others. To further validate the ability of VIS–NIR to classify white wine samples, a larger sample set will be required.

Acknowledgements

We thank G. Cowey and M. Holdstock of the Industry Development and Support team of the AWRI for helping to collect the wine samples. Staff of the Analytical Service Laboratory of the AWRI is thanked for providing the chemical analysis. Suggestions and comments made in the manuscript by Dr. M. Herderich are also acknowledged. This project is supported by Australia's grapegrowers and winemakers through their investment body the Grape and Wine Research and Development Corporation, with matching funds from the Australian government and by the Commonwealth Cooperative Research Centres Program. The work was conducted by The Australian Wine Research Institute and formed part of the research portfolio of the Cooperative Research Centre for Viticulture.

References

Adams, M. J. (1995). *Chemometrics in analytical spectroscopy*. RSC, Analytical spectroscopy monographs. The Royal Society of Chemistry, Cambridge, UK.

Alvarez, I., Aleixandre, J. L., Garcia, M. A. J., Casp, A., & Zenica, L. (2003). Geographical differentiation of white wines from three subzones of the designation of origin Valencia. *European Journal of Food Research and Technology, 217*, 173–179.

Barnes, R. J., Dhanoa, M. S., & Lister, S. J. (1989). Standard normal variate transformation and de-trending of near infrared diffuse reflectance spectra. *Applied Spectroscopy, 43*, 772–777.

Baxter, M. J., Crews, H. M., Dennis, M. J., Goodall, I., & Anderson, D. (1996). The determination of the authenticity of wine from its trace element composition. *Food Chemistry, 60*, 443–450.

Castiñeira, M. M., Feldmann, I., Jakubowski, N., & Andersson, J. T. (2004). Classification of German white wines with certified brand of origin by multielement quantification and pattern recognition techniques. *Journal of Agriculture and Food Chemistry, 52*, 2962–2974.

Cordella, C., Moussa, I., Martel, A.-C., Sbirrazzuoli, N., & Lizzani-Cuvelier, L. (2002). Recent developments in food characterization and adulteration detection: Technique-oriented perspectives. *Journal of Agriculture and Food Chemistry, 50*, 1751–1764.

Cozzolino, D., Smyth, H. E., & Gishen, M. (2003). Feasibility study on the use of visible and near infrared spectroscopy together with chemometrics to discriminate between commercial white wines of different varietal origins. *Journal of Agriculture and Food Chemistry, 51*, 7703–7708.

Dambergs, R. G., Kambouris, A., Francis, I. L., & Gishen, M. (2002). Rapid analysis of methanol in grape derived distillation products using near infrared transmission spectroscopy. *Journal of Agriculture and Food Chemistry, 50*, 3079–3084.

Dambergs, R. G., Kambouris, A., Schumacher, N., Francis, I. L., Esler, M. B., & Gishen, M. (2001). Wine quality grading by near infrared spectroscopy. In *Proceedings of the 10th international near infrared spectroscopy conference* (pp. 187–189). Chichester, UK: NIR Publications.

Davies, A. M. C. (1998). The history of near infrared spectroscopic analysis: Past, present and future – from sleeping technique to the morning star of spectroscopy. *Analusis Magazine, 26*, 17–19.

de Villiers, A. D., Majek, P., Lynen, F., Crouch, A., Lauer, H., & Sandra, P. (2005). Classification of South African red and white wines according to grape variety based on the non-coloured phenolic content. *European Journal of Food Research and Technology, 221*, 520–528.

Fischer, U., Roth, D., & Christmann, M. (1999). The impact of geographic origin, vintage and wine estate on sensory properties of *Vitis vinifera cv. Riesling wines*. *Food Quality and Preferences, 10*, 281–288.

Francis, I. L., Høj, P. B., Dambergs, R. G., Gishen, M., Lopes, M. A., Pretorius, I. S., et al. (2005). Objective measures of grape quality – are they achievable? In R. J. Blair, P. J. Williams, I. S. Pretorius, (Eds.), *Proceedings 12th Australian wine industry technical conference.* (pp. 85–89). (Melbourne Victoria, Australia).

Frias, S., Conde, J. E., Rodriguez-Bencomo, J. J., Garcia-Montelongo, F., & Perez-Trujillo, J. P. (2003). Classification of commercial wines from the Canary Islands (Spain) by chemometric techniques using metallic contents. *Talanta, 59*, 335–344.

Giangiacomo, R., & Dull, G. G. (1986). Near infrared spectrophotometric determination of individual sugars in aqueous mixtures. *Journal of Food Science, 51*, 679–683.

Gishen, M., Iland, P. G., Dambergs, R. G., Esler, M. B., Francis, I. L., Kambouris, A., et al. (2002). Objective measures of grape and wine quality. In *Proceedings 11th Australian wine industry technical conference, 7–11 October 2001* (pp. 188–194). Adelaide, Australia (Australian Wine Industry Technical Conference Inc: Adelaide, SA).

Iland, P., Ewart, A., & Sitters, J. (1993). *Techniques for chemical analysis and stability test of grapes juice and wine*. Patrick Iland Wine Promotions.

Iland, P., & Gago, P., (2002). *Australian wine: Styles and tastes.* (Patrick Iland Wine Promotions).

Kemsley, E. K. (1996). Discriminant analysis of high-dimensional data: A comparison of principal components analysis and partial least squares data reduction methods. *Chemometrics and Intelligent. Laboratory Systems, 33*, 47–61.

Latorre, M. J., Garcia-Jares, C., Medina, B., & Herrero, C. (1994). Pattern recognition analysis applied to classification of wines from Galicia (Northwestern Spain) with certified brand of origin. *Journal of Agriculture and Food Chemistry, 42*, 1451–1455.

Maarse, H., Slump, P., Tas, A. C., & Schaefer, J. (1987). Classification of wines according to type and region based on their composition. *European Journal of Food Research and Technology, 184*, 198–203.

Naes, T., Isaksson, T., Fearn, T., & Davies, T. (2002). *A user-friendly guide to multivariate calibration and classification*. Chichester, UK: NIR Publications.

Osborne, B. G., Fearn, T., & Hindle, P. H. (1993). *Practical NIR spectroscopy with applications in food and beverage analysis*. Harlow, Essex, UK: Longman Scientific and Technical.

Otto, M. (1999). *Chemometrics*. Hemsbach, Germany: Wiley-VCH.

Reid, L. M., O'Donnell, C. P., & Downey, G. (2006). Recent technological advances for the determination of food authenticity. *Trends in Food Science and Technology, 17*, 344–353.

Somers, C. (1998). *The wine spectrum: An approach towards objective definition of wine quality*. Adelaide: Winetitles.