Classification of Smoke Tainted Wines Using Mid-Infrared Spectroscopy and Chemometrics

Anthea L. Fudge,[†] Kerry L. Wilkinson,[†] Renata Ristic,[†] and Daniel Cozzolino*,[‡]

[†]School of Agriculture, Food and Wine, The University of Adelaide, PMB 1, Glen Osmond, SA 5064, Australia
[‡]The Australian Wine Research Institute, P.O. Box 197, Glen Osmond, SA 5064, Australia

ABSTRACT: In this study, the suitability of mid-infrared (MIR) spectroscopy, combined with principal component analysis (PCA) and linear discriminant analysis (LDA), was evaluated as a rapid analytical technique to identify smoke tainted wines. Control (i.e., unsmoked) and smoke-affected wines (260 in total) from experimental and commercial sources were analyzed by MIR spectroscopy and chemometrics. The concentrations of guaiacol and 4-methylguaiacol were also determined using gas chromatography−mass spectrometry (GC-MS), as markers of smoke taint. LDA models correctly classified 61% of control wines and 70% of smoke-affected wines. Classification rates were found to be influenced by the extent of smoke taint (based on GC-MS and informal sensory assessment), as well as qualitative differences in wine composition due to grape variety and oak maturation. Overall, the potential application of MIR spectroscopy combined with chemometrics as a rapid analytical technique for screening smoke-affected wines was demonstrated.

KEYWORDS: classification, guaiacol, linear discriminant analysis, mid-infrared spectroscopy, principal component analysis, smoke taint, wine

INTRODUCTION

Spectroscopic techniques in the mid-infrared (MIR) region have been applied to the analyses of a diverse range of agricultural products, for example, olive oils,[1,2] honey,[3,4] meat products,[5] cheese,[6] and fruits and vegetables,[7−9] for purposes including authentication, classification, quality control, and compositional determinations. Infrared (IR) spectroscopy measures changes in the absorption of IR radiation by organic compounds due to the vibration of fundamental frequencies (in particular C−H, N−H, and O−H bonds) within different functional groups.[1,10] Spectra in the MIR region (4,000 to 400 cm^{-1}) comprise well-defined bands that can be used for qualitative analysis to identify organic constituents or to differentiate samples.[1,10]

Wine is a complex medium, and the diverse nature of its chemical constituents, many of which are present at only trace concentrations, can complicate its analysis. Traditional analytical techniques, such as those using gas (GC) or liquid chromatography (LC), are often time-consuming and costly due to sample preparation requirements. By comparison, spectroscopic techniques are rapid and nondestructive, thereby offering significant time and cost savings.[10] Not surprisingly, numerous studies have therefore applied MIR spectroscopy to te analysis of wine. Some recent examples describe the classification of wines on the basis of geographical origin;[11,12] red wine fermentation monitoring;[13] analysis of red wine tannins;[14] the use of red wine phenolic extracts to discriminate between different cultivars;[15,16] and the authentication of wine[17] and organic grape production systems.[18]

The objective of this study was to evaluate the suitability of MIR spectroscopy as a rapid analytical technique for the detection of smoke taint in wine. Vineyard exposure to smoke from bushfires occurring in close proximity to wine regions can result in the uptake of smoke-derived volatile compounds by grapes, and in some cases, unpalatable smoke-related sensory attributes in the resulting wines.[19,20] A number of volatile phenols have been identified in smoke-affected grapes and wine.[19−23] Since these compounds can be readily quantified by existing gas chromatography−mass spectrometry (GC-MS) based methods,[24] they have been used as marker compounds for assessing the smoke exposure of grapes and wine, but they are not considered to be solely responsible for smoke taint.[19] Furthermore, recent studies have shown that smoke-derived phenols can accumulate in glycoconjugate precursor forms.[25,26] A comparison of methods for the determination of glyco-conjugate derivatives of smoke-derived volatile phenols has recently been reported.[27] Wineries typically rely on commercial laboratories for smoke taint related analyses, and during periods of high demand, winemakers can experience delays in results being returned. As such, there is clearly a need for a rapid analytical method for differentiating smoke-affected grapes and wine, to give winemakers the opportunity to make informed processing decisions, within the time constraints of vintage.

MATERIALS AND METHODS

Wine Samples. Samples (260 in total) included experimental wines sourced from several previous studies,[20,28,29] smoke tainted wines provided by industry, and commercial wines (i.e., without smoke taint). Experimental wine samples (Table 1) comprised (i) 27 smoke-affected Shiraz wines from a winemaking trial involving the addition of oak or tannin to fermentations of grapes harvested from a Victorian vineyard exposed to smoke from bushfires that occurred between 7 February and 14 March, 2009 (9 treatments each conducted in

Table 1. Concentration of Guaiacol and 4-Methylguaiacol in Control and Smoke-Affected Experimental Wines

	wine samples	guaiacol (μg/L)	4-methylguaiacol (μg/L)
Shiraz	smoke-affected[a] (n = 27)	19–27	1–5
Viognier	control (n = 12)	na[c]	na
	smoke-affected[b] (n = 12)	na	na
Grenache	control (n = 30)	nd[c]	nd
	smoke-affected[b] (n = 30)	2–9	nd – 2
Chardonnay	control (n = 6)	nd	nd
	smoke-affected[b] (n = 9)	1–5	nd
Shiraz	control (n = 3)	9	nd
	smoke-affected[b] (n = 3)	26	2
Cabernet Sauvignon	control (n = 3)	2	nd
	smoke-affected[b] (n = 3)	20	3
Merlot	control (n = 3)	2	nd
	smoke-affected[b] (n = 3)	18	3
Pinot Noir	control (n = 3)	nd	nd
	smoke-affected[b] (n = 3)	6	1
Pinot Gris	control (n = 3)	nd	nd
	smoke-affected[b] (n = 3)	10	2
Chardonnay	control (n = 3)	nd	nd
	smoke-affected[b] (n = 3)	1	nd
Sauvignon Blanc	control (n = 3)	nd	nd
	smoke-affected[b] (n = 3)	1	nd

[a]Bushfire smoke. [b]Experimental smoke. [c]na, not available; nd, not detected; n, number of samples.

Table 2. Concentration of Guaiacol and 4-Methylguaiacol in Smoke-Affected Industry Wines

wine samples	guaiacol (μg/L)	4-methyl-guaiacol (μg/L)	sensory description	sensory score[a]
Red Blend 1	51	29	smoked meat aroma; ashy AT[b]	4.3
Red Blend 2	34	17	fruit and oak aroma; drying palate	6.8
Red Blend 3	48	33	barnyard and wood smoke aromas; ashy and bitter AT	4.5
Red Blend 4	6	nd[b]	toasty, smoke aroma; sour and drying palate	6.7
Shiraz 1	55	23	wood smoke and gamey palate	4.8
Shiraz 2	28	8	plum, spice and oak aromas; metallic AT	9.0
Shiraz 3	6	nd	smoky, gamey aroma; ashy AT	5.0
Cabernet Sauvignon 1	2	nd	fruit aromas; astringent palate	7.8
Merlot 1	3	nd	fruit aromas; metallic palate	6.7
Pinot Noir 1	15	4	unpleasant AT; bandaid palate	5.7
Pinot Noir 2	7	3	subdued fruit; smoky aroma; dusty, ashy palate	6.8
Pinot Noir 3	21	7	fruit, burnt sugar and bandaid aromas; ashy palate	6.0
Graciano	4	nd	barnyard aroma	6.5
White Blend 1	11	3	yeast and rancid aromas; smoky AT	5.3
Sauvignon Blanc 1	2	nd	fruit aromas; lacks fruit on palate; AT	8.3
Sauvignon Blanc 2	nd	nd	fruit and perfume aromas; sour finish	7.3
Semillon 1	2	nd	fruit aromas; flat finish	8.7
Semillon 2	2	nd	fruit aromas; slightly sour; 9.2	9.2
Pinot Grigio 1	5	nd	fruit and oak aromas; sour palate; 7.0	7.0
Pinot Grigio 2	1	nd	fruit and yeast aromas; 8.7	8.7

[a]Mean scores from three judges using a 10 point scale where 1 = "unacceptable, tainted" and 10 = "acceptable". [b]nd, not detected; AT, aftertaste.

triplicate); (ii) 12 control and 12 smoke-affected Viognier wines from a winemaking trial involving the fermentation of control and smoke-affected grapes by indigenous yeast (2 treatments each with 12 replicates), where smoke-affected grapes were harvested from grapevines exposed to smoke for 30 min under experimental conditions and control grapes were harvested from unsmoked grapevines; (iii) 30 control and 30 smoke-affected Grenache wines from winemaking trials involving either different skin contact times (4 treatments each conducted in triplicate) or selection of different yeast strains for fermentation (16 treatments each conducted in triplicate) where smoke-affected grapes were harvested from grapevines exposed to smoke for 20 min under experimental conditions, and control grapes were harvested from unsmoked grapevines; (iv) 6 control and 9 smoke-affected Chardonnay wines from a viticultural trial involving defoliation and/or smoke exposure of grapevines (5 treatments each conducted in triplicate) where smoke-affected grapes were harvested from grapevines exposed to smoke for 60 min under experimental conditions, and control grapes were harvested from unsmoked grapevines; and (v) 21 control and 21 smoke-affected wines from a varietal trial involving Shiraz, Cabernet Sauvignon, Merlot, Pinot Noir, Pinot Gris, Chardonnay, and Sauvignon Blanc grapevines (2 treatments per variety each conducted in triplicate) where smoked-affected grapes were harvested from grapevines exposed to smoke for 60 min under experimental conditions, and control grapes were harvested from unsmoked grapevines. Experimental smoke treatments involved grapevines being enclosed in purpose-built smoke tents and exposed to straw-derived smoke using methodology described previously.[21] Twenty wines were provided by industry (Table 2); these wines were made from grapes harvested from vineyards thought to be exposed to smoke during bushfires that occurred between 7 February and 14 March, 2009 and/or were considered by their respective winemakers to exhibit the smoke-related sensory attributes typically associated with smoke taint; i.e., smoky, ashy, medicinal, and smoked meat aroma and flavor attributes.[19,20] Sixty-eight commercial wines were also included as examples of control (i.e., unsmoked) wines. Finally, two cask wines, one white and one red, were also included, with and without the addition of guaiacol (at approximately 30 mg/L). The presence/absence of smoke taint in industry and commercial wines was determined by informal sensory assessment by a panel of three experienced tasters using a 10 point scale where 1 = unacceptable, tainted, and 10 = acceptable. Wines were stored at constant temperature (15 °C) prior to analysis.

Determination of Smoke Taint Marker Compounds. The concentrations of guaiacol and 4-methylguaiacol were quantified in experimental and industry wines, as markers of smoke taint, according to stable isotope dilution assay methods reported previously.[24] This publication describes the preparation of internal standards and instrument operating conditions used herein. Analyses were performed by the Australian Wine Research Institute's Commercial Services Laboratory (Adelaide, Australia) using an Agilent 6890N gas chromatograph coupled to a 5975 inert source mass spectrometer (Agilent, Palo Alto, CA, USA).

MIR Spectroscopy Measurements. Wine samples (ca. 20 mL) taken from freshly opened bottles were centrifuged (4300g for 5 min) and scanned in transmission mode using a UV–vis flow cell (1 and 0.2 mm path length) in the MIR region (400–4000 cm^{-1}; 25 μm path length) in a Multispec system Bacchus/Multispec System equipped with a Thermo Nicolet, Avatar 380 FT-MIR spectrometer (Microdom, Taverny, France). The fingerprint range was 1000–1500 cm^{-1}. Spectral data and instrument diagnostics were collected using

Bacchus acquisition software (Quant, version 4, 2001) as described previously.[18]

Multivariate Data Analysis and Wine Classification. Multivariate data analysis was performed using The Unscrambler software (version 9.5, Camo ASA, Oslo, Norway). Spectral data were examined for unusual outlier samples before classification methods were used by applying principal component analysis (PCA). Discrimination models were developed using linear discriminant analysis (LDA), a supervised classification technique by which the number of categories and the samples that belong to each category are previously defined.[30] The criterion of LDA for the selection of latent variables is the maximum differentiation between the categories and minimizes the variance within categories. This method produces a number of orthogonal linear discriminant functions, equal to the number of categories minus one, that allow samples to be classified in one or another category. LDA was carried out using the score values of the first three principal components which gave the highest level of separation (high variance) in the PCA models developed (JMP, v. 5.01, SAS Institute, Inc., Cary, NC). In this technique, each sample is assigned with a dummy variable as a reference value, which is an arbitrary number designating whether the sample belongs to a particular group. In the current study, smoke-affected wines were assigned a numeric value of 1 and control wines with the value 2; the cutoff was set at 0.5. Both LDA and PCA models were developed using full cross-validation (leave-one-out). The MIR spectra were preprocessed using standard normal and variate transformation (SNV).[30]

■ RESULTS AND DISCUSSION

The intensity of smoke-related sensory attributes and concentrations of smoke-derived volatile phenols in wine have been shown to be influenced by the duration of grapevine exposure to smoke.[22,27] Therefore, a diverse sample set was sourced for this study, comprising wines derived from (i) unsmoked grapes, i.e., commercial and experimental control wines; (ii) grapes exposed to smoke for short durations (20 to 60 min) under experimental conditions, i.e., experimental smoke-affected wines; and (iii) grapes exposed to bushfire smoke for longer (but unknown) durations, i.e., industry wines. The guaiacol and 4-methylguaiacol concentrations of experimental and industry wines were determined by GC-MS to evaluate the extent of smoke taint (Tables 1 and 2).

For experimental wines (Table 1), guaiacol and 4-methylguaiacol were not detected in the majority of control wines; the exceptions were Shiraz, Cabernet Sauvignon, and Merlot control wines, which contained 2 or 9 μg/L of guaiacol as a natural grape component, in agreement with previous studies.[31] The highest volatile phenol levels were observed in Shiraz wines made from bushfire smoke-affected grapes; lower levels were observed in wines made from grapes exposed to smoke under experimental conditions. This was as expected, given the different durations of smoke exposure. The variation in guaiacol and 4-methylguaiacol concentrations for experimental smoke-affected wines was attributed to different winemaking practices; specifically, the different durations of skin contact for red and white winemaking, which has previously been shown to influence the intensity of smoke taint.[20] However, it is acknowledged that these results may also reflect varietal differences.

For industry wines (Table 2), the volatile phenol content varied considerably. Guaiacol was detected in all but one wine, at concentrations between 1 and 55 μg/L; while 4-methylguaiacol was detected in only half the wines, at concentrations ranging from 3 to 33 μg/L. Again, this is likely to be attributable to differences in the duration of grapevine exposure to smoke, but it was not possible to ascertain the exact

timing, duration, and density of smoke exposure by commercial vineyards. As such, the occurrence of smoke taint in industry wines was further evaluated by informal sensory analysis. Seven wines received scores of 6.0 or less: Red Blend 1, Red Blend 3, Shiraz 1, Shiraz 3, Pinot Noir 1, Pinot Noir 3, and White Blend 1. These wines generally contained the highest volatile phenol levels and were also considered to exhibit apparent smoke-related sensory attributes (Table 2), i.e., they were considered to be heavily smoke tainted. Red Blend 2 and Shiraz 2 also contained high concentrations of guaiacol and 4-methylguaiacol, but from oak maturation, since these wines were described by fruit and oak-related sensory attributes, rather than smoky characters, albeit drying and metallic characters were reported. Smoke-related aromas were also identified in Red Blend 4 and Pinot Noir 2. These wines contained moderate volatile phenol levels and received sensory scores of 6.7 and 6.8, respectively, indicative of moderate levels of smoke taint. The remaining industry wines contained low levels of guaiacol and 4-methylguaiacol, and were not described by specific sensory attributes associated with smoke taint. That said, these wines were considered to lack fruit intensity and/or to exhibit drying, sour or metallic characters, which might be indicative of low levels of smoke taint.

Commercial wines were similarly subjected to informal sensory assessment, but there was no evidence of smoke taint in these wines (data not shown). No visual differences were apparent in the MIR spectra obtained for the wine samples (data not shown); therefore, PCA was performed on the spectral data to investigate qualitative differences within the sample set. Of the 260 wine samples analyzed, three outliers were identified (data not shown): two control Viognier wines (from the winemaking trial) and one commercial Riesling wine. Spectral data collected for these samples were therefore removed prior to further chemometric analyses.

Separate PCA models were performed as follows on five sets of experimental wines, with the inclusion of commercial wines of the same variety as controls and industry wines, with the inclusion of red and white cask wines with and without the addition of guaiacol. PCA was also developed using a larger data set ($n = 245$) comprising all wines, with the exception of the previously identified outliers and the experimental control Viognier wines. Figures 1 and 2 show the score plots of the MIR spectra from the Shiraz and varietal wine sets, respectively.

For the Shiraz wine set (Figure 1), clear separation between control and smoke-affected wines was observed, i.e., samples clustered on opposite sides of the score plot. PC1 and PC2 accounted for 73% and 10% of the variation, respectively. Loadings were investigated to identify the wavenumber regions that corresponded to the PCA separation. For PC1, wavenumbers between 1000 and 1100 cm^{-1} can be assigned to C–O vibrations of residual carbohydrates, i.e., fructose and glucose[15] (Figure 3). For PC2, the highest loadings were observed around 1045 cm^{-1}, due to C–O stretching, for example, from the oxygen atom of hydroxyl groups (Figure 3). These wavenumbers could potentially be associated with the presence of smoke-derived volatile phenols, such as guaiacol and 4-methylguaiacol.

For Viognier wines, separation was observed between the smoke-affected wines, which were located in the top left quadrant (together with the two control outliers) and the remaining control wines, which clustered within PC1 in the other three quadrants (data not shown). The loading plot for Viognier (data not shown) showed a large positive peak at
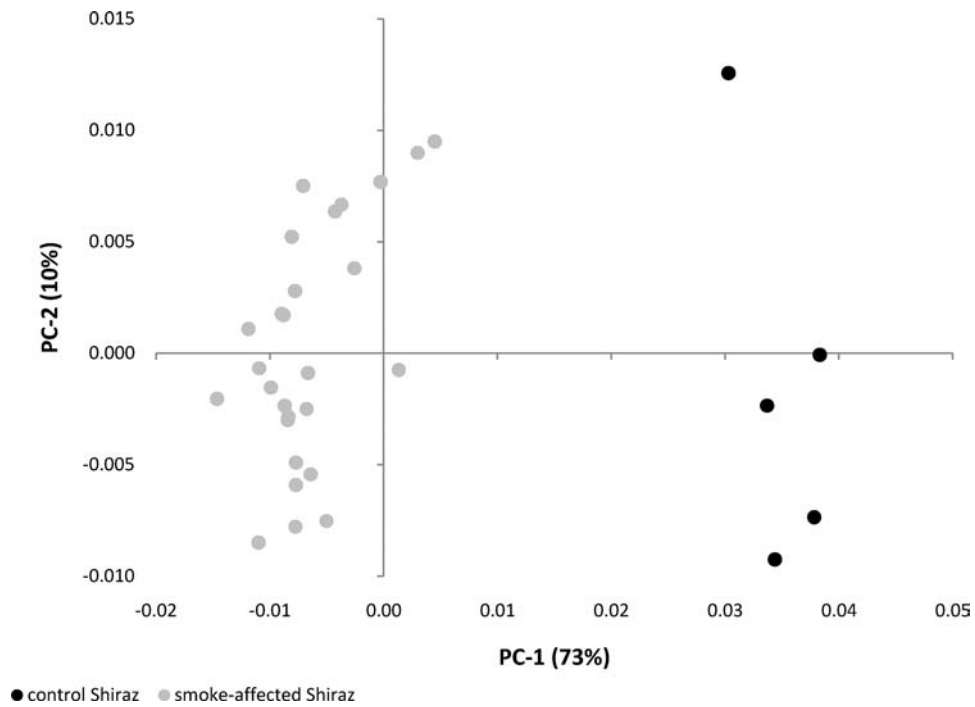
● control Shiraz ● smoke-affected Shiraz

Figure 1. Score plot of the first two PCs derived from the MIR spectra of control and smoke-affected Shiraz wines.

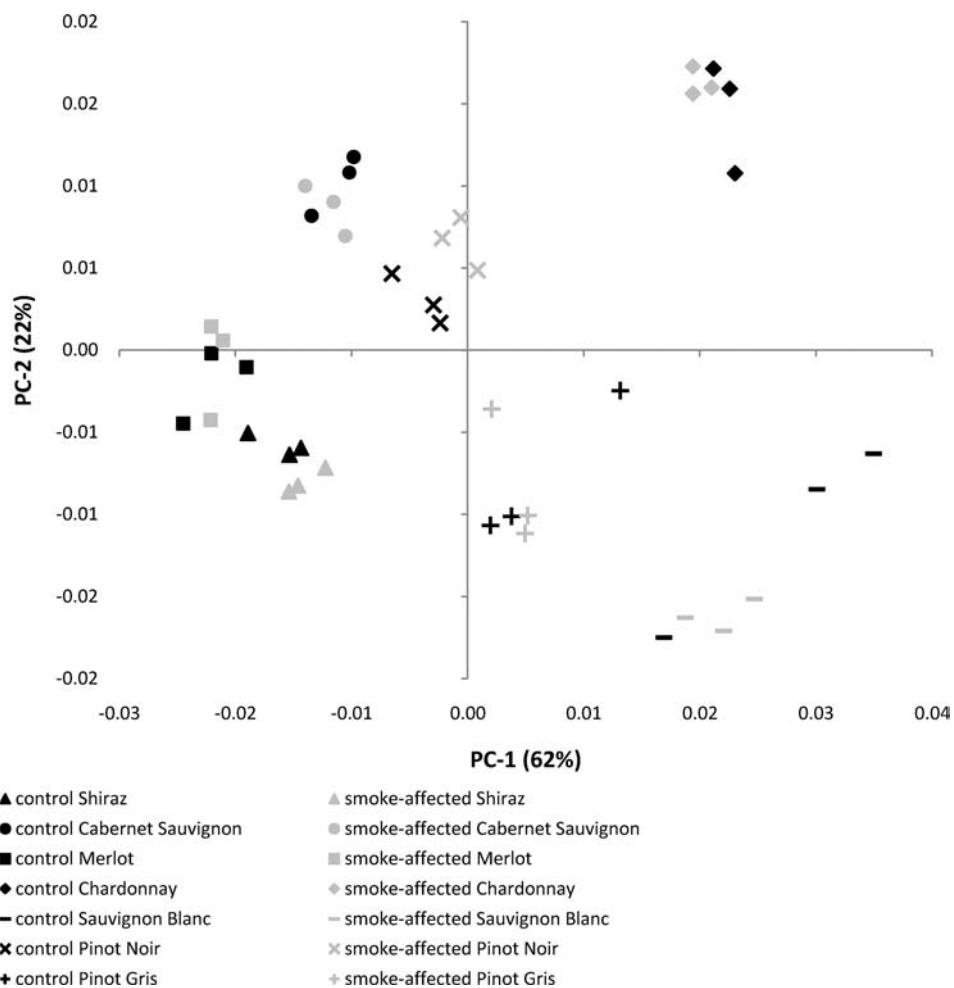▲ control Shiraz ▲ smoke-affected Shiraz
● control Cabernet Sauvignon ● smoke-affected Cabernet Sauvignon
■ control Merlot ■ smoke-affected Merlot
◆ control Chardonnay ◆ smoke-affected Chardonnay
━ control Sauvignon Blanc ━ smoke-affected Sauvignon Blanc
✕ control Pinot Noir ✕ smoke-affected Pinot Noir
✛ control Pinot Gris ✛ smoke-affected Pinot Gris

Figure 2. Score plot of the first two PCs derived from the MIR spectra of control and smoke-affected Shiraz, Cabernet Sauvignon, Merlot, Chardonnay, Sauvignon Blanc, Pinot Noir, and Pinot Gris wines.
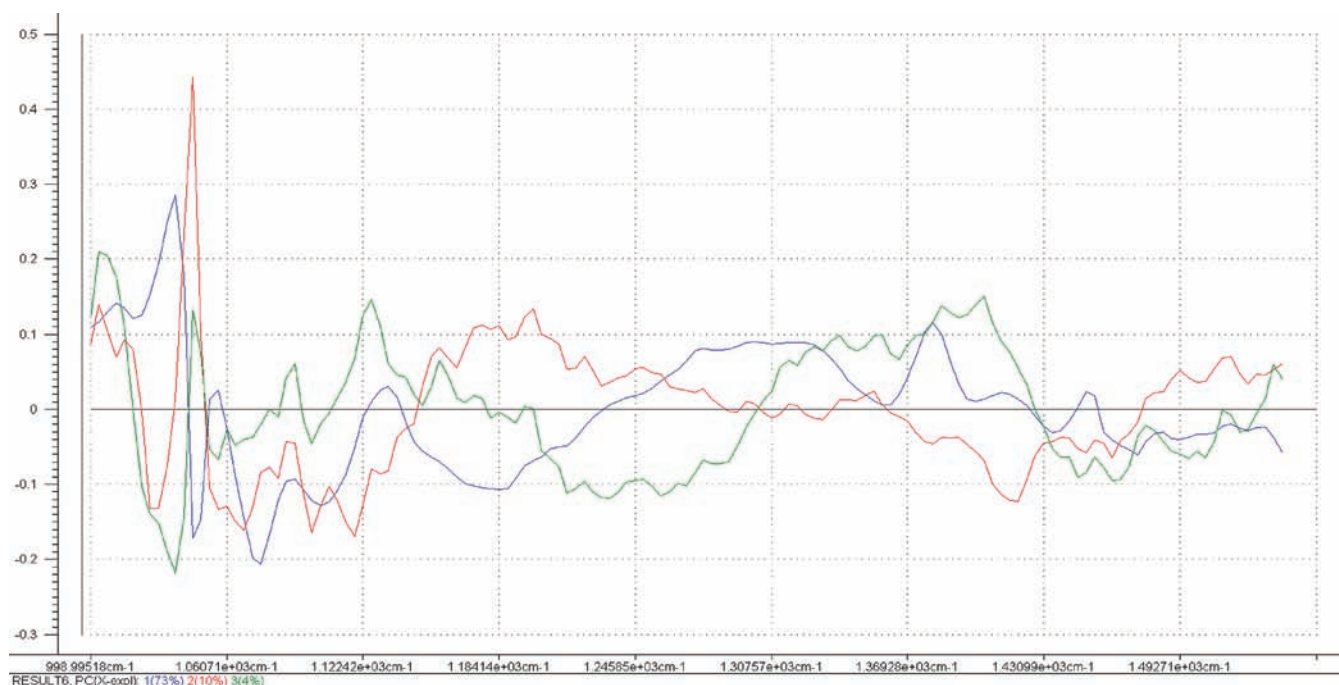
Figure 3. Loadings for the first three PCs of the fingerprint region derived from Shiraz MIR spectra.

1045 cm^{-1} wavenumbers for PC1, which accounted for 90% of variation. Negatively correlated peaks due to PC3 (which explained only 2% of variation) were observed at approximately 1130 cm^{-1} and 1415 cm^{-1} wavenumbers, respectively. The latter peak occurs in the 1500 to 1400 cm^{-1} region typically associated with aromatic C−C stretching, and so these wavenumbers could also be associated with the presence of volatile phenols.

Control and smoke-affected Grenache wines showed reasonable separation (data not shown). Control wines were generally positively correlated with PC2, while smoke-affected wines were negatively correlated with PC2. The Grenache loadings (Figure 4) also showed the influence of the 1500 to 1400 cm^{-1} region, again due to aromatic C−C stretching. The wavenumbers observed around 1080 cm^{-1} and 1045 cm^{-1} could be attributed to the C−O and C−C bonds of ethanol and other alcohols.[32] Wavenumbers at 1470 and 1380 cm^{-1} could be associated with vibrations of phenolic hydroxyl groups,[33] i.e., signals which volatile phenols would influence.

The PCA models developed for Chardonnay wines (data not shown) did not show separation between control and smoke-affected experimental wines. Smoke-affected wines clustered in the top right quadrant, whereas experimental and control wines were distributed throughout the other quadrants. Significant variation was observed between control Chardonnay wines, which likely reflects differences in geographical origin, vintage and/or production methods, as reported in previous studies.[15−18] The loadings plot also showed broader peaks and thus less defined information. The C−O stretch for primary alcohols[34] at 1050 cm^{-1} was prominent for both PC1 and PC2 (which explained 79% total variation). Characteristic bands due to C−O−C bonds were observed at 1218 and 1108 cm^{-1},[35] suggesting the presence of substituted phenols such as syringol and its derivatives, compounds which have also been identified as components of smoke-affected wines.[26] Bands in the fingerprint region between 1500 and 1200 cm^{-1} were attributed to deformations of −CH$_2$ and also C−C−H and H−C−O,

whereas bands between 1200 and 950 cm^{-1} were attributed to stretching modes of C−C and C−O.[36] These regions were observed in all of the data sets analyzed.

Table 3 shows the classification of wines as control or smoke-affected, according to the LDA of MIR spectra. Classification was performed on both individual wine sets and the larger data set (i.e., all wines, as described above).

For the Shiraz wine set, 100% correct classification rates were obtained for both control and smoke-affected wines. This indicates qualitative differences in the composition of smoke-affected wines that enabled the classification model to differentiate these samples from control wines, i.e., differences presumably attributable to smoke taint. One hundred percent correct classification rates were also obtained for experimental Viognier wines; however, two commercial Viognier wines were incorrectly classified as being smoke-affected. These wines were fermented and matured in oak barrels, so misclassification might be due to the presence of oak derived volatile compounds, which include guaiacol and 4-methylguaiacol.[24]

Classification rates of 68% and 87% were obtained for control and smoke-affected Grenache wines, respectively. The wines incorrectly classified as controls comprised three replicate wines from the winemaking trial that involved different durations of skin contact and one wine from the yeast selection trial. The wines incorrectly classified as being smoke-affected were all control wines from the yeast selection trial. For these wines, PCA showed separation according to both wine production methods, (e.g., duration of skin contact and winemaking yeast) and smoke taint (data not shown). This further indicates factors besides grapevine exposure to smoke influence classification.

Smoke-affected Chardonnay wines were 100% correctly classified, but only 75% of control Chardonnay wines were correctly classified. However, the misclassified wines were experimental control wines rather than commercial wines. As indicated above, PCA showed significant separation of commercial
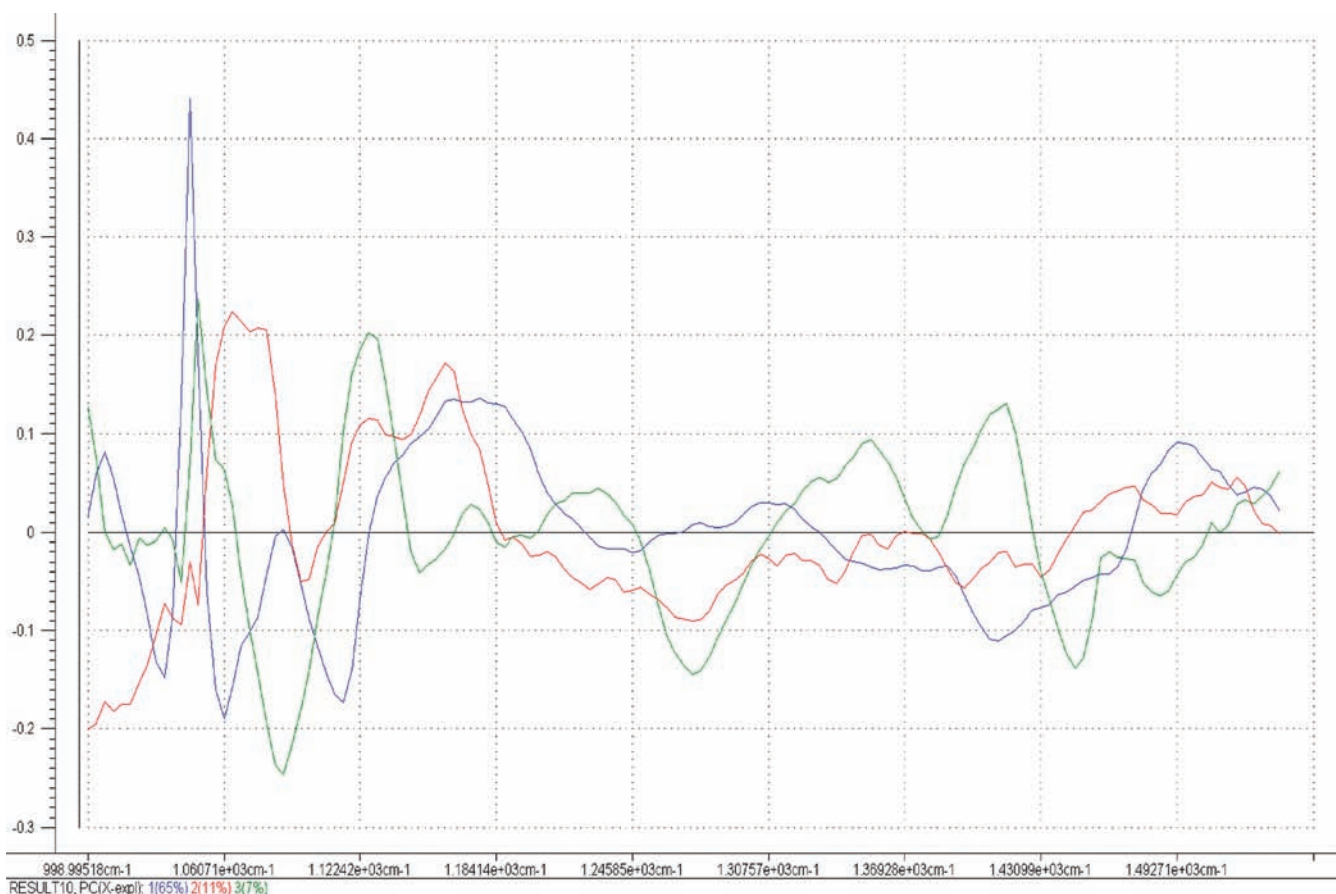
Figure 4. Loadings for the first three PCs of the fingerprint region derived from Grenache MIR spectra.

Table 3. Classification of Control and Smoke-Affected Wines Using LDA

	wine samples	no. of wines classified as the control	no. of wines classified as smoke-affected	correct classification
Shiraz	control (n^b = 5)	5	0	100%
	smoke-affected (n = 27)	0	27	100%
Viognier	control (n = 14)	12	2	86%
	smoke-affected (n = 10)	0	10	100%
Grenache	control (n = 31)	21	10	68%
	smoke-affected (n = 30)	4	26	87%
Chardonnay	control (n = 16)	12	4	75%
	smoke-affected (n = 9)	0	9	100%
varietal	control (n = 21)	8	13	38%
	smoke-affected (n = 21)	8	13	62%
industry wines[a]	control (n = 2)	1	1	50%
	smoke-affected (n = 22)	7	15	68%
all wines	control (n = 126)	77	49	61%
	smoke-affected (n = 119)	36	83	70%

[a]Includes red and white cask wines with and without the addition of 30 mg/L guaiacol. [b]n, number of samples.

Chardonnay wines, likely due to a combination of vintage, regionality, and production effects.

The poorest classification rates were obtained for experimental wines from the varietal trial, being 38% and 62% for control and smoke-affected wines, respectively. For this sample set, it was observed that the PCA results were influenced more by grape variety than grapevine exposure to smoke (Figure 2). Previous studies have demonstrated the use of MIR spectroscopy to discriminate wines on the basis of grape variety.[16,17] Classification rates are also likely to be influenced by the intensity of smoke taint, with limits of detection for analysis by

MIR spectroscopy, as for analysis by GC-MS. As such, wines with low levels of smoke taint might be classified as controls.

Six industry wines were classified as controls, being Red Blend 3, Shiraz 2, Cabernet Sauvignon 1, and Pinot Noir 1, 2, and 3. The classification of Shiraz 2 and Cabernet Sauvignon 1 as control wines is not unreasonable, given that neither wine exhibited any apparent smoke related sensory attributes; Cabernet Sauvignon 1 contained only 2 μg/L of guaiacol, while the guaiacol and 4-methylguaiacol present in Shiraz 2 derived from oak maturation, rather than grapevine exposure to smoke. As such, the presence of smoke taint in these wines is

questionable, and so they might be more appropriately classified as control wines. In contrast, Red Blend 3 and Pinot Noir 1, 2, and 3 did exhibit smoke related sensory attributes and contained guaiacol and 4-methylguaiacol, so the reason for their misclassification is unclear. In the case of Red Blend 3, the presence of high levels of 4-ethylguaiacol and 4-ethylphenol (data not shown), which are indicative of *Brettanomyces/Dekkera* spoilage,[37] may have confounded classification. The industry wine set also included red and white cask wines with and without the addition of guaiacol. Both white cask wines were classified as controls, indicating that the presence of guaiacol alone does not determine classification. Both red cask wines were classified as smoke-affected; again misclassification was attributed to oak maturation of this wine.

When all wines were analyzed, correct classification rates of 61% and 70% were obtained for control and smoke-affected wines, respectively. These results demonstrate qualitative differences exist between wines made from unsmoked grapes and wines made from smoke-affected grapes; differences that can be observed by MIR spectroscopy and, when combined with chemometrics, used to screen wines for the presence of smoke taint. Some limitations were identified with the classification model developed in the current study, in particular that compositional differences due to grape variety and oak maturation may override differences resulting from grapevine exposure to smoke (especially at low levels of smoke exposure). However, further refinement of the model using a sample set that represents a broader range of grape varieties, production methods, vintages, and levels of smoke taint would enable improved classification rates.

■ AUTHOR INFORMATION

Corresponding Author
*Tel: + 61 8 8303 6600. Fax: + 61 8 8303 6601. E-mail: Daniel.Cozzolino@gmail.com.

■ ACKNOWLEDGMENTS

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