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Characterization of Odor-Active Compounds in Californian Chardonnay Wines Using GC-Olfactometry and GC-Mass Spectrometry

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Nineteen commercial Californian Chardonnay wines were analyzed by gas chromatography-mass spectrometry (GC-MS). Freon extracts of wines were separated by silica gel chromatography into three fractions. Volatiles were quantified by GC analysis of each fraction using internal standards added to the wine prior to Freon extraction. Twelve of the 19 wines were evaluated by GC-Olfactometry (GC-O). Of the 81 compounds shown to be odor-active (OA) by GC/O, 74 were quantified and 61 were tentatively identified, all of which had been previously reported in grapes or wines. Overall concentrations of compounds with floral or oak-related aromas were higher in wines shown by descriptive analysis to be high in intensity of either floral or oak notes, respectively. The relationship between sensory intensity ratings from a previous descriptive analysis of the wines and 74 OA compounds was modeled by partial least-squares regression (PLS) analysis. This PLS model only explained 17% of the variation in the OA variables, whereas a PLS using a subset of 16 OA peaks explained 64 and 47% of variance in the sensory and GC data, respectively. Fruity wines high in peach, citrus, and floral terms were separated from those high in oak-related sensory attributes (oak, vanilla, caramel, spice, and butter). In both PLS models, the fruity and floral terms were associated with isoamyl acetate, 2-phenylethyl acetate, linalool and two unknowns exhibiting minty and bandaid-caramel odors; the oaky attributes were associated with vanillin, oak-lactones, 4-ethyl guaiacol, γ-nonalactone, 2-acetyl furan, eugenol, 2-methoxy phenol, and two unknowns with plastic and smoky odors.

KEYWORDS: Wine; odor-active compounds; Chardonnay; gas-chromatography- olfactometry; partial least-squares regression analysis

INTRODUCTION

In a recent consumer study, the flavor of wine was found to be one of the most important attributes to consumers when buying wine (*1*). Over eight hundred volatiles have been identified in wine aroma including alcohols, esters, organic acids, aldehydes, ketones, and monoterpenes (*2*−*5*). These compounds come from the grapes and are produced during fermentation and post fermentation treatments such as oak storage and bottle aging (*2*−*4*).

Volatiles of Chardonnay grapes and wines have been studied using a variety of techniques. Principal component analysis (PCA) of headspace volatiles of three white wine varieties (Riesling, Chardonnay, and French Colombard) clustered wines by grape varieties (*6*). Chardonnay wines were higher in esters and vitispirane, while the Rieslings were higher in terpene components, with French Colombard wines falling in between.

In studies of seven Chardonnay wines from Burgundy, dichloromethane extracts were analyzed by GC−O (*7*) by one judge using Charm analysis (*8*). Of the 32 odor-active compounds detected, the 11 compounds which had the highest "Charm values" were identified as contributing to the distinctiveness of the wines' aromas. They were vanillin (vanilla), diacetyl (butter), 4-vinylguaiacol (curry-smoked), ethyl cinnamate (cherry pits), ethyl hexanoate (green-grassy), ethyl 2-methyl butanoate (apple), ethyl butanoate (fruity), guaiacol (smoked-spicey), and three unidentified compounds, which had aromas of burnt sugar, wet ashes, and honey. In a preliminary study of white Burgundies, cyclotene, maltol, guaiacol (2-methoxy phenol), and ethyl cinnamate were claimed to be the most potent odorants (*9*).

Using a different approach to study Chardonnay aromas, volatiles that had been hydrolyzed from the glycosides of Chardonnay juice were analyzed by GC-MS (*10*). Compounds (n = 181) were identified, of which more than 70% of the metabolites were C13 compounds, norisoprenoids. Benzene derivatives accounted for 20% of the total volatile concentration, while monoterpenes made up only 5%. The potential of these Chardonnay glycosides to serve as flavor precursors was confirmed, as the intensity of tea, floral, lime, honey, oak, talc,

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Table 1. Wines and Their Regions of Origin

code	winery	region of origin
CAL[a]	Callaway	Riverside (Temecula)
CDB-A	Clos Du Bois	Sonoma
CDB-C[a]	Clos Du Bois	Sonoma
CDB-S	Clos Du Bois	Sonoma
CON[a]	Concannon	Alameda
DEL[a]	Delicato	San Joaquin
DUN	Canandaigua Wine Co.	Dunnewood, North Coast
EBE	Eberle	Paso Robles
FET	Fetzer	Mendocino
GP	Geyser Peak	Sonoma
JL[a]	J. Lohr	Monterey
MER[a]	Meridian	Paso Robles
PR	Pine Ridge	Napa-Carneros
RHP[a]	R. H. Phillips	Esparto (Dunnigan Hills)
SH[a]	Sutter Home	Napa Valley
TAFT[a]	Taft Street Winery	Sonoma
TES[a]	Monterey Vineyards	Monterey County
VME[a]	Villa Mt. Eden	Napa Valley
VMErs[a]	Villa Mt. Eden (Grand Reserve)	Napa Valley

[a] Wines analyzed by GC/O.

and pineapple aromas was increased by addition of their acid hydrolysates to base wines (*11*).

To investigate the relationships between sensory profiles and wine volatiles, multivariate statistical methods have been used, including principal component analysis of instrumental variables (PCA-IV) (*12*), generalized procrustes analysis (*13*), and partial least squares regression (PLS) (*14*, *15*), and have been compared (*16*). In previous studies of Chardonnay wines, including those cited above, hundreds of volatiles have been identified. However, with the exception of studies of the aroma of white Burgundy wines by Moio et al. (*7*) and Le Fur et al. (9, *13*), neither the odor activity of volatiles nor the sensory significance of compounds identified in Chardonnay wines have been systematically investigated. The objectives of the present study were to identify and quantify odor-active compounds in Chardonnay wines using GC−O and GC-MS and relate the OA compounds to the sensory properties of the wines using partial least squares regression analysis.

MATERIALS AND METHODS

Wines. Nineteen 1997 Californian Chardonnay wines were analyzed in 2000, all of which had been profiled by descriptive analysis (DA) 6−10 months before this study (*17*). Details about the wines, which were held at 10 °C during the studies, are shown in **Table 1**.

Chemicals. Diethyl ether, pentane, and silica gel 60 (particle size 0.063−0.200 mm, 70−230 mesh) were purchased from EM Science, a division of EM Industries, Inc (New Jersey). Trichlorofluoromethane (Freon 11), absolute ethanol, and compounds used as internal standards (IS) (methyl octanoate, 2-methyl-1-pentanol, and 3-methyl-3-hydroxy-2-butanone) were obtained from Sigma-Aldrich Chemical Co. (St. Louis, MO). The IS stock solution was prepared by adding 5 μg of each internal standard to 100 mL of absolute ethanol.

Extraction and Fractionation of Wine Volatile Compounds. Volatiles were extracted using a modification of a procedure described elsewhere (*18*). Before extraction, 45 g of NaCl and 3 mL of IS stock solution were added to 150 mL of wine, which was then extracted three times with 50 mL of trichlorofluoromethane (Freon 11) using a liquid−liquid extractor at 28∼30 °C. The extract was concentrated to ∼2 mL by distilling off the solvent on a Vigreux column (40 × 2 cm). The solvent was further removed under a purified nitrogen stream until the volume was reduced to 1 mL. The aroma extracts were fractionated by silica gel chromatography to provide better GC resolution, using a modification of Guth's method (*19*). The Freon extract (1 mL) was placed in a glass column (30 × 1.9 cm i.d.) packed with silica gel 60. The sample was fractionated by elution with 200 mL of pentane and diethyl ether (Fraction 1, 85/15; Fraction 2, 70/30) and 200 mL of diethyl ether (Fraction 3). The eluates were dried over sodium sulfate overnight and concentrated to a final volume of 1 mL, as described above, and stored at −5 °C for subsequent analyses.

The recovery of internal standards after sample preparation (extraction, fractionation, and GC analysis) was evaluated for five wines (JL, CDB−C, CAL, DEL and SH) to determine the recovery of the method. Recovery ranged from 82% for methyl octanoate in fraction 1 to 73% for 2-methyl-1-pentanol (fraction 2) and to 61% for 3-methyl-3-hydroxy-2-butanone in fraction 3. Reproducibility of the sample preparation method was examined for one wine (SH), which was extracted in duplicate, with each fraction's extract analyzed in duplicate by GC. A two-way analysis of variance (extraction, injection) for each peak showed no significant differences due to extraction for all but two peaks and no significant differences due to injection for all but two peaks.

Gas Chromatography-Mass Spectrometry (GC-MS). A 1-μL sample of each concentrated fraction of the wines was analyzed in duplicate on a Hewlett-Packard (HP) gas chromatograph model 6890 equipped with a split/splitless injector and a DB-WAX bonded fused capillary column (30 m × 0.25 mm i.d., film thickness = 0.25 μm, J&W scientific Inc., Folsom, CA). The detector was a mass spectrometer (MS 6890 series Mass selective detector, Hewlett-Packard, Palo Alto, CA). Temperature of the inlet was 220 °C. Splitless time was 1 min. Purge flow to split vent was 50 mL/min for 1 min. Column head pressure was 14.14 psi and the helium carrier gas flow rate was 1.3 mL/min. Average helium gas velocity was 30 cm/s. The oven temperature was held at 40 °C for 4 min and programmed at 4 °C/min to 185 °C and held for 20 min isothermally. Mass spectra in the electron impact mode (MS-EI) were generated at 70 eV and ion source temperature was 230 °C. Mass spectra were taken over the *m*/*z* range 45−300. The total ion chromatogram (TIC) acquired by GC-MS was used for peak area integration. HP MS chemstation software G1701BA ver.B.01.00 was used for data acquisition.

To determine the reproducibility of the duplicate injections and determine which peaks varied across wines, two-way analyses of variance (wines, injection) were performed for each odor-active peak. All peaks varied highly significantly across wines, with only four varying significantly across replications.

GC-Olfactometry (GC-O). All analyses were performed at E & J Gallo Winery, (Modesto, CA). For GC-O analysis, 1 μL of the concentrated fractions were injected on a HP GC model 6890 equipped with a split/splitless injector. At the end of the capillary, the effluent was split into the HP MS Mass selective detector described above and a sniffing port (Gerstel, Germany). The sniffing port was held at 250 °C to prevent any condensation of volatile compounds. Humidified air was added at 100 mL/min in the sniffing cone to reduce fatigue and drying of the judge's nasal passage. The column and operating conditions were the same as those used for GC-MS.

For determination of odor-active (OA) compounds, four judges who had previous experience with GC-O were used. Assessors were seated in front of the sniffing port and asked to smell the effluent of the column. An "olfactometer button" (Gerstel, Germany) was depressed when an aroma was detected. The initiation and termination of aroma detection was recorded by an HP Pascal workstation. Judges also gave verbal descriptions of perceived odors that the experimenter recorded. Each fraction of the four wines (CAL, CDB-C, DEL, and JL) which had been shown to have the largest differences in aroma by sensory descriptive analysis (*17*) was evaluated once by GC-O by each of the four judges. For the remaining eight wines (identified in **Table 1**), two judges evaluated each fraction once. Peaks were identified as odor-active using a modified definition of the detection frequency method (*20*). A peak was reported as OA, if it was detected by two or more judges in the same wine.

Identification. Odor-active compounds screened by GC-O were tentatively identified by comparison of the Kovats retention index (KI) (*21*) and the MS fragmentation pattern with those of reference compounds or with mass spectra in the Wiley 275 library and previously reported Kovats retention indices. The Kovats retention indices (KI) of unknown compounds were determined by injection of the sample

with a homologous series of alkanes (C_6-C_{28}). GC/MS conditions were the same as described above.

Quantification. The relative concentrations of the odor-active volatiles in all 19 wines were determined by GC-MS (TIC) by comparison with concentrations of internal standards, assuming a response factor of 1. Methyl octanoate, 2-methyl-1-pentanol, and 3-methyl-3-hydroxy-2-butanone were used as the internal standards for fractions 1, 2, and 3, respectively.

Statistical Analysis. Analyses of variance were run on the GC data using PROC GLM on Statistical Analysis Systems (SAS) for Windows, version 6.12 (Cary, NC). Principal component analysis (PCA) was performed on the mean ratings for eight sensory attributes using the covariance matrix with no rotation on SAS. The sensory data set included eight aroma descriptors, which were peach/apricot, citrus, floral, caramel, butter, vanilla, spice and oak. The GC data set included 74 OA volatiles. Of the 81 OA compounds quantified, five compounds (ethyl acetate, 1,1-diethoxy ethane, ethyl propionate, ethyl isobutyrate, and 2-pentanone) were eliminated from the instrumental data set because they could not be quantified in many of the wines, as were β-damascenone and unknown KI = 2157, which could not be quantified in any wine.

PLS is a "soft modeling" method, which extracts linear combinations of variables from one data set (OA volatiles) that best predict variation in another data set (sensory ratings). To explore the relationship between this sensory profile data and the OA volatiles for these 19 wines, partial least squares regression analysis (PLS) was conducted using the UNSCRAMBLER ver.7.6 (CAMO A/S, Trondheim, Norway). A second PLS was run excluding all OA compounds for which less than 50% variance was explained. The 16 odor-active compounds selected for the resulting PLS model are identified in **Table 2**. In all PLS analyses, the odor-active volatiles were standardized (mean/standard deviation), while the aroma intensity ratings were assigned a weighting of 1 (unstandardized). In both PLS models, the GC data were treated as the independent variables (*X* matrix), with the sensory data used as the dependent variables (*Y* matrix).

RESULTS AND DISCUSSION

GC-O. Eighty-one odor-active peaks were detected by two or more judges in at least one fraction of one of the four wines evaluated by GC-O by four judges. With the exception of 1-butanol and two unknown compounds (KI = 1762 and 2371), the same OA peaks were also detected in one or more of the other eight wines, in which no additional OA compounds were found. In **Table 2**, the KI, tentative identification, fraction in which the compound was detected and aroma descriptions by GC-O are shown for the OA compounds. In addition, for the four wines for which GC-O was performed by four judges, the number of times each peak was detected is reported.

With the exception of huge peaks such as fusel alcohols and organic acids, which eluted in two fractions, the internal standards and each volatile were detected in only one fraction. Although many of the tentatively identified OA compounds have not been reported in Chardonnays, all have been previously reported in grapes or wines of other varieties of *Vitis vinifera* (see **Table 2**) or studies of oak flavor (*22*).

As shown in the PCA of the sensory data (**Figure 1**), the wines were primarily separated by intensity of "oak" terms (oak, caramel, butter, vanilla, and spice) versus "fruit" descriptors (peach/apricot, citrus, and apple) and floral. For example, wines CAL and DEL are high in the fruity and floral notes and low in oak terms, whereas the converse is true for wines JL and CDC. The detection frequencies of the odorants were inspected to see if there was any correspondence to these sensory notes (**Table 2**). Wines with higher intensity of oaky and spicy notes, such as wines JL and CDB-C, had fairly high detection frequencies for "oaky/spicy" compounds, most of which arise from oak-aging, such as (*trans*) oak lactone, eugenol, 4-vinyl guaiacol, vanillin, and furfural. Similarly, linalool and α-terpineol had high detection frequencies in the wines high in fruitiness and floral notes, such as CAL and DEL. Other volatiles such as the fruity esters produced during fermentation did not show appreciable differences in detection frequencies among the wines. Perhaps this is because the esters are ubiquitously present at concentrations well above threshold levels.

Each of the eight identified compounds, previously reported by Moio et al. (*7*) as contributing to the distinctiveness of Burgundian Chardonnay were found in all wines in the present study. In contrast, only two of the four compounds claimed by Le Fur et al. (*9*) to be potent odorants in French Chardonnays were detected in these 19 wines (guaiacol (2-methoxy phenol) and ethyl cinnamate). Four norisoprenoids (vitispirane, β-damascenone, 3-oxo-α-ionol, and TDN (1,1,6-trimethyl-1,2-dihydronaphthalene)) have been suggested to be important to the aroma of Chardonnay (*6*, *10*, *23*). In the present study, only β-damascenone and 3-oxo-α-ionol were found. β-Damascenone elicited a strong honey/cooked apple note in six wines, but was not detected by GC/O in the other six. Upon elution of 3-oxo-α-ionol, a low intensity of spiciness was detected in wines JL and CDB-C but not detected by GC/O in the fruity CAL and DEL wines. However, both compounds were detected by GC-MS in all wines.

Composition of OA Compounds. The mean concentrations of 79 OA compounds are given in **Table 3** for the 19 wines. Of 81 OA compounds, two compounds (β-damascenone and unknown KI = 2157) could not quantified because of weak chromatographic signals. Over 80% of the total volatile material was contributed by seven compounds: isoamyl alcohol, 2,3-butanediol, diethyl malate, acetic acid, hexanoic acid, octanoic acid, and 2-phenylethanol. Except for three compounds (2,3-butanediol, diethyl malate, and acetic acid), the concentration of these compounds did not vary much across wines. Thus these compounds are speculated to contribute to the background or base flavor of these wines rather than to differentiate among the wines.

To simplify inspection of **Table 3**, compounds are grouped by their aromas as described by GC−O. The wines are arranged from left to right to reflect the progression in aroma character from very oaky (low fruity) to very fruity (low oaky) wines. The individual concentrations of the oak-associated OA compounds roughly correspond to intensity of oaky aromas of these wines. Guaiacol, the oak lactone isomers, 4-ethyl guaiacol, eugenol, and vanillin, which mainly come from oak barrel contact, were found in higher concentrations in oaky/spicy wines than those in fruity and floral wines. JL, which was the most intense in oak, vanilla, and spice aromas by descriptive analysis, had the highest concentrations of furfural, guaiacol, 4-ethyl phenol, 4-ethyl guaiacol, (*cis*) oak-lactone, eugenol, and vanillin. In examining the pattern of distribution of the "floral" compounds, concentrations of three compounds (linalool, α-terpeneol and a "minty" unknown (KI = 1688)) correlated significantly with the intensity of the floral aroma (r = 0.80, 0.69, 0.75 respectively). DEL wine had the highest concentration of these three "floral" compounds, while they were far lower in the oaky/spicy wines (JL, CDB-C, VMEres, TES) than in other floral and fruity wines (CAL, SH, FET, VME). The higher concentrations of these terpenes in DEL reflect its varietal composition. DEL had 2% (v/v) Muscat Canelli and 1% White Riesling, whereas the other 18 wines were 100% Chardonnay. Unlike the floral compounds, the sums of the concentrations of the fruity odor compounds were similar across all 19 wines, even though there were large variations in fruitiness.

Table 2. Odor-Active Compounds Found in Californian Chardonnay Wines. Frequency of Detection in GC–O Analyses and Odor Description by Four Judges

			detection frequency[c]					
KI[a]	F[b]	odorants	JL	CDB–C	CAL	DEL	odor description[d]	ref[e]
885	III	ethyl acetate[f]	2	2	2	2	sweet, fruity	c–e
900	III	1,1-diethoxy ethane[g]	4	4	2	1	buttery, creamy	c–e
950	I	ethyl propionate[f]	1	1	1	0	juicy fruit	c–e
955	I	ethyl isobutyrate[f]	1	2	1	2	fruity	c–f
960	I	2-pentanone[g]	0	3	2	1	fruity	d,e
1028	I	ethyl butanoate[f]	4	3	4	4	fruity, banana	b–f
1038	III	1-propanol[g]	2	2	0	2	musty	c,d,e
1053	I	ethyl 3-methyl butanoate[f]	3	4	3	4	fruity, apple	b–f
1085	II, III	2-methyl-1-propanol[g]	3	2	2	2	glue, alcohol	c–f
1116	II	2-pentanol[g]	1	1	2	0	green-fruit, sweet	d,e
1118	I	isoamyl acetate[f,i]	2	2	3	4	banana	b–f
1138	III	1-butanol[g]	1	1	0	0	medicinal	c,d,e
1206	II, III	2/3 methylbutanol[g]	4	4	4	4	balsamic, alcohol	b–f
1229	I	ethyl hexanoate[f]	4	3	4	4	fruity-juicy	a–f
1272	III	acetoin[g]	4	4	4	2	butterscotch	c,d,e
1276	I	unknown[i]	3	1	3	3	plastic	
1354	II	1-hexanol[g]	3	2	1	2	green grass	a,c,d–f
1379	II	(trans) 3-hexen-1-ol[g]	2	0	1	1	green	a,c,d,e
1427	I	ethyl octanoate[f]	1	0	0	1	sweet, soapy, fresh	a,c,d–f
1434	III	acetic acid[g]	4	4	4	4	vinegar	d,e,f
1458	II	furfural[g]	3	4	3	3	woody, almond	c,d,e
1487	II	2-ethyl-1-hexanol[g]	2	0	0	2	mild green, alcohol	c,d
1500	II	2-acetyl furan[f,i]	2	1	0	0	sweet caramel	c,d
1523	II	propanoic acid[g]	0	0	1	3	soy	d,e
1542	III	2,3-butanediol (d,l)[g]	0	2	2	0	butter, creamy	d
1544	II	linalool[g,i]	2	1	1	4	floral	a–f
1557	III	2-methyl propanoic acid[g]	1	2	2	0	sweaty	d,e
1587	III	unknown	0	0	2	1	glue, alcohol, thinner	
1614	II, III	butanoic acid[g]	4	4	4	4	sweaty	a, d–f
1630	I	ethyl decanoate[g]	2	0	1	1	fruity	a,c,d,e
1635	III	butyrolactone[g]	3	4	2	2	sweet, musty	a,c,d,e
1651	III	unknown	2	0	2	2	perfumy rose	
1652	I	unknown	3	0	0	0	fruity	
1660	II, III	2/3 methyl butanoic acid + furfuryl alcohol[g,i]	4	3	4	4	stinky socks, sweaty	c–f
1687	II	α-terpineol[g]	0	0	0	2	minty	a,c,d
1688	III	unknown[i]	0	0	2	1	minty	
1700	I	unknown	0	0	2	2	bread, smokey	
1714	III	3-methylthio-1-propanol[g]	4	3	4	3	potato	b,d–f
1722	II	unknown	0	0	1	1	chemical, green	
1730	II	pentanoic acid[g]	2	2	2	2	sweaty	a,d
1740	III	unknown	2	0	1	0	musty	
1762	I	unknown	0	0	0	3	honey	
1809	I	2-phenylethyl acetate[f,i]	4	4	4	4	honey, apple	c–f
1810	III	unknown	3	4	4	4	cooked sugar, honey	
1813	II	β-damascenone[g]	1	0	4	4	honey, cooked apple	a,c–f
1840	II	hexanoic acid[g]	4	4	4	4	sweaty	a,d–f
1853	II	2-methoxy phenol[f,i]	4	1	2	3	smoky, spicy	b–f
1886	III	(*cis*) oak-lactone[f,i]	2	1	0	0	spicy	b,-e
1910	II, III	2-phenyl alcohol[g]	4	4	3	4	floral	a–f
1957	III	(trans) oak-lactone[f,i]	3	3	3	3	spicy	c–e
1962	II	(*trans*) 2-hexenoic acid[g]	0	0	1	2	fatty, musty	g
1972	II	unknown	0	0	2	0	spicy, brown	
1973	I	unknown[i]	0	0	3	1	bandaid, caramel	
2024	II	4-ethyl guiacol[f, i]	3	1	2	2	spicy, smokey	e
2033	III	pantolactone[g]	4	4	4	4	cotton candy	d,e
2053	III	diethyl malate[g]	2	3	4	2	brown sugar	d
2058	II	octanoic acid[g]	2	4	3	3	cheese	a,d,f
2079	III	γ–nonalactone[g,i]	2	3	3	0	sweet, creamy	a,d,e
2100	II	unknown	0	0	0	2	cottoncandy	
2101	III	homofuraneol[g]	0	0	3	3	cotton candy, jam	f
2130	III	unknown	2	2	3	0	sweet, creamy	
2139	I	ethyl cinnamate[g]	1	1	1	3	raisin	b–f
2156	III	unknown	4	2	1	3	cooked sugar, apple sauce	
2157	II	unknown	0	0	4	3	cooked sugar, spicy	
2164	II	eugenol[f,i]	4	4	3	3	clove	a,b,d–f
2171	III	diethyl-2-hydroxy- pentanedioate[h]	3	2	3	0	cotton candy	d
2195	II	4-ethyl phenol[g]	2	0	1	2	medicinal, phenolic	b,d,e
2200	III	4-vinyl-2-methoxy-phenol[g]	4	4	3	4	smokey, nutty	a,b,d–f
2220	III	unknown [i]	0	2	0	3	smokey, woody	
2234	II	unknown	0	0	2	1	spicy	
2241	III	4-ethoxycarbonyl-γ-butanolactone[h]	2	2	2	3	smokey, toasted	d,e
2272	II	decanoic acid[g]	0	4	4	2	dusty	a,d,e

Table 2. (Continued)

KI[a]	F[b]	odorants	detection frequency[c] JL	CDB–C	CAL	DEL	odor description[d]	ref[e]
2273	III	2,6-dimethoxyphenol[g]	4	3	3	0	nutty, smokey	h
2358	III	diethyl tartarate[g]	4	3	1	2	earthy, musty	a,d
2371	II	unknown	0	0	0	2	mushroom	
2400	III	unknown	2	2	3	2	thinner	
2481	III	unknown	2	0	2	2	mothball	
2512	III	5-hydroxymethyl-2-furfural[g]	2	0	0	0	cardboard, paper	d,e
2561	III	vanilin[f,i]	4	4	3	4	vanilla	a,b,d–f
2640	III	acetovanillone[g]	2	2	0	0	spicy, sweet	a,d,e
2650	III	3-oxo-α-ionol[h]	3	2	0	0	spicy	a

[a] Kovats indices of unknown compounds on DB–WAX column. [b] Fraction in which most of compound appeared after column chromatography. [c] Detection frequency of term used over 4 GC/O runs. [d] Odor description usually reported by at least 2 judges. [e] Volatiles reported previously in wines or grapes. Letter corresponds to numbered reference. a,(*10*); b, (*7*); c, (*23*); d, (*2*); e, (*5*); f, (*19*); g, (*25*); h, (*26*). [f] Identified by comparison with MS spectra and KI of authentic references. [g] Identified by comparison with published MS spectra and KI. [h] Identified by comparison with MS spectra in Wiley 275 library. [i] Odor-active compounds used in second PLS model.

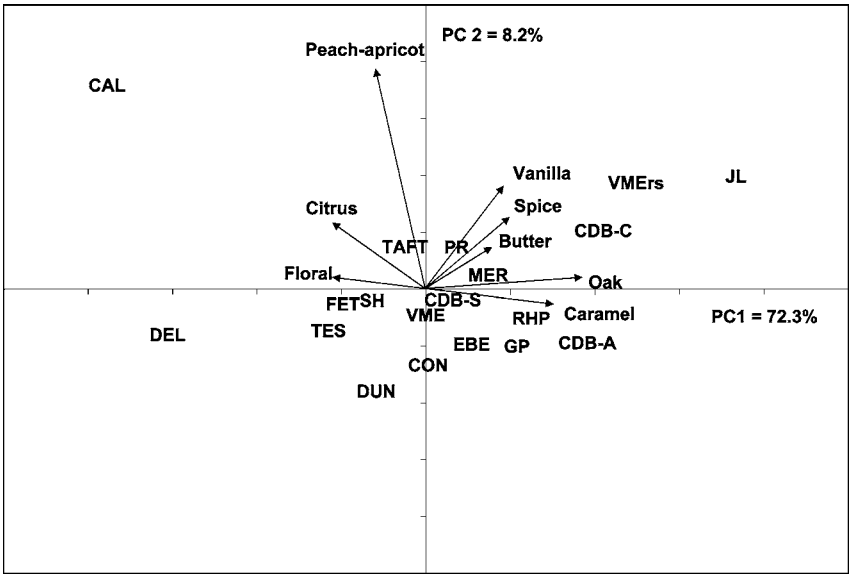

Figure 1. Principal Component Analysis of 19 wines from descriptive analysis using 8 aroma terms (*17*). Attribute loadings are shown as vectors; wine scores are shown as capital letters. Wine codes are defined in **Table 1**.

Relating Instrumental and Sensory Data. The PLS model using 74 GC peaks yielded a one-dimensional model which explained 67% of variance in the sensory data and 17% of the GC data in the first dimension. In **Figure 2**, the correlation loadings for the sensory terms (in capitals) and the OA compounds are shown with the wine scores. Similar to the pattern seen in the PCA (**Figure 1**), there is a distinct separation between fruity/floral and oak related terms and between fruity wines (CAL, DEL) and oaky wines (JL, CDB-C, VMEres, CDB-A, TES) along the first dimension. Similarly, the first dimension contrasts compounds with fruity/floral aromas versus those that have oaky notes. Linalool and unknown 1688 (which had a minty odor), were associated with the "floral" sensory attribute. Fruity esters such as isoamyl acetate and 2-phenylethyl acetate were located close to the "peach" and "citrus" attributes. Similarly, oaky odor compounds (4-ethyl guaiacol, eugenol, 2-acetyl furan, (*cis*) oak-lactone, 2-methoxy phenol, and vanillin were associated with "oak" and "spice" sensory attributes. (*trans*) Oak-lactone and γ-nonalactone were more closely associated with the "vanilla" and "butter" terms.

The center ellipsoid in **Figure 2** indicates 50% explained variation. This means that all the GC peaks located inside this circle were poorly modeled and mathematically do not explain variation in the sensory data. The PLS was rerun after eliminating these peaks to more clearly see the relationships between OA compounds that had a strong predictive relationship to the sensory terms. The PLS model using 16 OA peaks (**Figure 3**) explained 64% variance in the sensory data and 47% for the GC variables. All 16 of the OA variables were significantly modeled in this PLS, as determined by the uncertainty test (*24*). As with the PLS model using 74 OA peaks, compounds with oaky/spicy notes are located close to the oaky sensory terms, while those with fruity or floral notes are located closely to citrus and peach and floral, respectively, indicating their strong correlations. For example, vanillin is significantly correlated with "oak", "vanilla" and "spice", respectively, $r = 0.85$, 0.84, and 0.78 ($p < 0.001$).

Although the PLS model shows a strong relationship between these 16 OA volatiles and the sensory profile data, it does not establish a causal relationship. Only by sensory evaluation of wines or systems spiked with selected compounds can it be determined if OA compounds contribute significantly to the characteristic aromas of Chardonnay wines.

CONCLUSION

OA compounds were detected by GC−O of volatile fractions isolated from 12 wines. The same compounds were found in

Table 3. Mean Concentrations (mg/L) of Odor-active Compounds in 19 Wines ($n = 2$)

KI[a]	code[b]	JL	VMEres	CDB-A	CDB-C	TES	PR	EBE	MER	GP	CDB-S	RHP	DUN	CON	VME	TAFT	FET	SH	DEL	CAL
										Fruity										
885	etac	1.913	2.888		6.805	3.107			1.505			1.461		2.540	2.396	2.033		7.916	6.805	7.226
950	etprop		0.066			0.053			0.120			0.083		0.081		0.100				0.055
955	etibut		0.067			0.060			0.027			0.036		0.063		0.028				0.031
960	2pentone	1.312	0.180		1.609	0.136			0.492			0.440		0.179	0.691	0.415		0.316	0.566	0.501
1028	etbut	1.040	0.657	0.726	1.086	0.695	0.879	0.664	0.823	1.136	0.445	0.743	1.081	0.734	0.715	0.918	0.563	1.360	0.906	0.844
1053	etipent	0.041	0.059	0.011	0.051	0.056	0.009	0.008	0.083	0.007	0.015	0.092	0.004	0.049	0.028	0.057	0.006	0.038	0.029	0.042
1116	2pentol	0.380	0.033	0.132	0.676	0.043	0.189	0.097	0.107	0.196	0.119	0.044	0.129	0.084	0.313	0.199	0.207	0.089	0.088	0.140
1118	isoamac	0.349	0.246	0.307	0.417	0.246	0.129	0.220	0.476	0.159	0.237	0.715	0.247	0.442	0.491	0.530	0.307	0.690	0.522	0.519
1229	ethex	0.600	0.835	1.243	1.341	0.755	0.794	0.774	0.787	0.795	0.983	0.952	0.664	0.864	0.779	1.178	0.822	0.693	0.722	0.843
1427	etoct	0.808	1.482	1.761	1.877	1.212	1.477	1.249	1.285	1.455	1.785	1.387	1.109	1.486	1.322	1.939	1.388	1.162	1.098	1.284
1630	etdec	0.128	0.224	0.221	0.218	0.182	0.257	0.198	0.205	0.195	0.293	0.209	0.143	0.284	0.224	0.297	0.180	0.268	0.177	0.191
1652	unk1652	0.399	1.318	0.291	0.070	0.379	0.271	0.826	0.143	0.118	0.272	0.551	0.058	0.263	0.310	0.177	0.083	0.008	0.028	0.010
1809	phenylac	0.056	0.091	0.073	0.049	0.047	0.034	0.066	0.068	0.041	0.084	0.090	0.036	0.128	0.081	0.099	0.077	0.121	0.068	0.079
2139	etcinna	0.006	0.007	0.002	0.006	0.007	0.002	0.001	0.005	0.004	0.002	0.004	0.003	0.006	0.012	0.011	0.002	0.033	0.004	0.003
										Floral										
1544	linalool	0.031	0.019	0.033	0.040	0.027	0.014	0.028	0.037	0.024	0.054	0.021	0.029	0.070	0.088	0.056	0.043	0.109	0.142	0.050
1651	unk1651	0.058	0.111	0.078	0.016	0.096	0.104	0.098	0.091	0.085	0.046	0.048	0.120	0.125	0.057	0.063	0.059	0.039	0.043	0.045
1687	aterpnol	0.034	0.021	0.106	0.109	0.043	0.051	0.078	0.026	0.053	0.107	0.016	0.044	0.058	0.075	0.066	0.086	0.044	0.181	0.111
1688	unk1688	0.018	0.018	0.060	0.000	0.019	0.022	0.028	0.024	0.068	0.035	0.018	0.032	0.022	0.024	0.018	0.054	0.052	0.110	0.071
1910	phenylol	116.85	92.78	90.04	30.88	62.15	66.73	74.90	144.28	47.99	54.38	27.03	103.76	48.86	101.92	60.20	88.09	39.90	52.49	153.84
										Butter, creamy										
900	diethox	0.479	0.893		0.214	0.732			0.998			0.514		0.743	1.395	0.923		0.533	0.649	1.303
1272	acetoin	1.675	3.234	4.808	1.237	0.743	2.651	1.048	1.298	2.334	4.572	0.430	0.698	1.917	2.020	2.601	0.966	2.464	0.247	3.245
1542	btudiol	1.196	28.467	33.690	1.075	33.712	53.677	89.854	39.568	38.408	27.807	25.474	41.842	41.456	20.245	16.980	48.756	0.304	17.302	29.095
2079	nonlactn	0.614	0.309	0.205	0.423	0.655	0.529	0.263	0.437	0.325	0.225	0.307	0.211	0.389	0.175	0.269	0.495	0.351	0.084	0.227
2130	unk2130	0.407	1.194	1.207	0.366	1.230	2.835	1.689	1.171	1.251	1.146	0.752	0.491	1.794	0.483	1.032	1.426		0.213	0.456
										Oak-related										
1458	furfural	21.19	1.65	0.55	4.05	0.95	0.67	0.42	0.52	1.41	0.57	1.82	0.36	0.54	0.92	0.89	0.33	0.23	0.18	0.24
1853	metxphenl	0.284	0.105	0.067	0.134	0.254	0.037	0.041	0.151	0.086	0.038	0.110	0.040	0.060	0.091	0.051	0.023	0.021	0.049	0.025
1886	oaklactnc	0.382	0.208	0.194	0.346	0.080	0.232	0.166	0.171	0.106	0.087	0.065	0.059	0.062	0.084	0.078	0.067	0.037	0.053	0.033
1957	oaklactnt	0.996	0.960	1.355	0.329	0.834	0.783	0.502	0.472	0.985	0.724	0.796	0.727	0.605	0.492	0.343	0.472	0.198	0.149	0.173
1972	unk1972	0.000	0.019	0.015	0.000	0.046	0.012	0.010	0.043	0.013	0.011	0.013	0.011	0.016	0.011	0.011	0.012	0.094	0.037	4.043
2024	etguiacl	0.050	0.021	0.008	0.015	0.014	0.007	0.005	0.019	0.009	0.004	0.004	0.003	0.004	0.006	0.007	0.003	0.000	0.003	0.000
2164	eugenol	0.362	0.157	0.249	0.327	0.102	0.099	0.081	0.114	0.110	0.174	0.101	0.078	0.073	0.089	0.076	0.031	0.019	0.059	0.021
2195	4etphenl	0.129	0.008	0.000	0.089	0.039	0.005	0.009	0.020	0.003	0.000	0.012	0.006	0.011	0.005	0.035	0.006		0.020	0.014
2200	viguiacl	0.380	1.730	1.415	1.024	3.259	0.560	0.667	1.105	0.853	1.860	3.456	0.981	2.612	1.259	1.590	0.896	1.342	1.493	1.356
2220	unk2220	0.108	0.171	0.317	0.140	0.521	0.279	0.100	0.102	0.224	0.286	0.055	0.165	0.088	0.127	0.079	0.141	0.050	0.091	0.078
2234	unk2234	0.042	0.057	0.127	0.044	0.139	0.041	0.027	0.059	0.058	0.123	0.065	0.041	0.090	0.077	0.065	0.054	0.082	0.078	0.081
2241	4ecbulac	1.522	5.220	6.106	1.653	6.081	3.512	3.968	4.270	6.526	5.846	3.872	5.250	5.696	2.770	2.434	4.480	2.041	2.456	1.417
2273	syringol	0.244	0.537	0.512	0.086	0.684	0.439	0.416	0.454	0.499	0.685	0.699	0.314	0.628	0.376	0.510	0.378	0.155	0.231	0.066
2561	vanilin	1.223	0.983	1.172	0.345	0.787	0.760	0.610	0.634	0.572	0.613	0.745	0.239	0.288	0.496	0.378	0.390	0.254	0.166	0.107
2640	acvaniln	0.391	0.876	1.068	0.262	1.056	0.971	0.897	0.853	1.386	1.155	0.523	1.594	0.849	0.554	0.516	0.979	0.253	0.352	0.233
2650	oxoionl	0.301	2.674	1.721	0.551	1.428	0.451	0.922	0.997	0.787	1.426	0.987	0.885	2.282	0.426	0.540	0.662	0.625	0.866	0.478
										Burnt sugar, caramel										
1500	2acfyran	0.313	0.123	0.214	0.221	0.073	0.117	0.120	0.070	0.069	0.110	0.079	0.069	0.042	0.084	0.086	0.049		0.044	0.030
1762	unk1762	0.010	0.009	0.003	0.010	0.005	0.001	0.001	0.004	0.003	0.001	0.004	0.002	0.006	0.006	0.003	0.002	0.037	0.009	0.006
1810	unk1810	2.723	6.885	5.190	1.592	7.242	4.107	6.078	5.263	6.691	5.345	8.175	9.052	8.199	6.067	4.523	5.693	4.721	4.803	3.554
1973	unk1973	0.000	0.006	0.002	0.007	0.006	0.000	0.002	0.003	0.003	0.001	0.003	0.003	0.005	0.004	0.004	0.001	0.028	0.009	0.019
2033	panlactn	0.191	0.691	0.767	0.163	0.702	0.518	0.531	0.407	0.532	0.860	0.497	0.535	0.582	0.511	0.306	0.626	0.153	0.364	0.413

Table 3. (Continued)

KI[a]	code[b]	JL	VMEres	CDB-A	CDB-C	TES	PR	EBE	MER	GP	CDB-S	RHP	DUN	CON	VME	TAFT	FET	SH	DEL	CAL
										Burnt sugar, caramel (Continued)									
2053	dietmal	18.25	33.02	43.34	4.99	52.07	36.40	92.74	11.22	14.37	47.98	27.84	20.73	26.72	14.57	9.54	55.93	10.03	8.82	18.18
2100	unk2100	0.251	0.386	0.089	0.446	0.174	0.124	0.192	0.072	0.055	0.043	0.141	0.014	0.028	0.104	0.049	0.024	0.113	0.078	0.070
2101	homofura	0.159	0.206	0.126	0.092	0.374	0.345	0.298	0.250	0.225	0.182	0.293	0.195	0.283	0.139	0.206	0.269	0.111	0.136	0.242
2156	unk2156	0.074	0.058	0.067	0.072		0.031	0.039	0.052	0.059	0.078	0.024	0.041	0.140	0.136	0.062	0.059		0.142	0.091
2171	det2pen	2.933	7.871	10.914	3.670	8.989	6.066	6.410	6.884	10.462	9.965	4.806	7.772	6.348	4.333	3.952	6.344	3.197	2.524	2.155
										Alcohol										
1354	1hexol	5.022	2.182	3.598	1.985	2.601	2.740	1.747	2.051	4.090	3.777	2.715	4.912	2.298	2.881	1.899	3.532	2.750	3.051	2.325
1379	3hexenol	0.218	0.117	0.114	0.203	0.137	0.118	0.063	0.190	0.118	0.104	0.082	0.137	0.073	0.123	0.152	0.107	0.111	0.114	0.062
1487	2ethexol	0.108	0.094	0.116	0.200	0.183	0.125	0.152	0.248	0.148	0.167	0.143	0.153	0.120	0.131	0.263	0.143	68.33	0.122	0.107
1722	unk1722	0.032	0.047	0.022	0.046	0.042	0.007	0.015	0.049	0.006	0.018	0.043	0.013	0.012	0.055	0.007	0.017	0.035	0.026	0.019
1038	1pronol	0.197	0.144	0.092	0.306	0.139	0.039	0.096	0.693	0.051	0.072	0.109	0.066	0.115	0.199	0.194	0.071	0.613	0.364	0.219
1085	2me1prop	3.057	0.410	0.312	2.330	0.450	0.211	0.245	0.504	0.287	0.295	0.692	0.299	0.645	0.823	0.295	0.204	1.017	1.198	0.642
1138	1butol	0.430	0.064	0.103	0.460	0.089	0.180	0.099	0.179	0.103	0.090	0.087	0.114	0.121	0.346	0.176	0.094	0.095	0.276	0.327
1206	isopenol	57.44	36.51	113.48	61.26	42.04	103.55	81.03	48.80	112.11	108.71	44.25	101.33	56.29	69.09	52.38	92.90	41.47	65.10	63.56
1714	methiopro	0.459	2.024	2.054	0.410	3.027	1.719	2.017	2.210	3.579	2.491	1.180	3.428	3.710	1.488	0.983	2.369	1.273	1.327	1.489
										Acids										
1434	Hac	11.29	11.93	25.19	6.46	8.31	46.60	45.75	12.09	31.42	21.05	7.87	35.35	7.96	9.96	7.19	23.33	10.30	8.78	10.00
1523	propic	0.614	0.606	0.253	0.680	0.571	0.469	0.928	0.749	0.381	0.063	1.800	0.559	0.424	0.474	0.485	0.160	1.780	0.399	0.279
1557	mepropic	0.578	0.929	0.891	0.451	0.688	0.932	0.795	0.878	1.064	0.818	0.648	1.008	1.290	0.824	0.594	0.774	0.615	0.373	0.278
1614	butic	1.505	1.652	4.703	1.972	1.626	2.005	2.193	1.381	3.841	4.553	1.934	3.631	1.866	1.535	1.603	4.111	2.330	1.769	1.824
1660	me+fur	4.038	2.734	3.085	1.912	2.507	3.575	3.098	3.897	3.071	3.297	2.098	3.025	1.645	5.028	1.474	1.785	1.522	2.270	1.270
1730	pentic	0.036	0.066	0.032	0.021	0.065	0.016	0.023	0.071	0.023	0.023	0.035	0.032	0.020	0.047	0.015	0.029	0.535	0.036	0.020
1840	hexic	6.666	7.788	18.762	17.107	7.488	11.581	10.245	7.006	12.991	16.699	7.368	10.319	7.566	7.314	8.669	13.828	8.473	6.199	7.375
1962	hexeic	0.000	0.166	0.126	0.000	0.230	0.080	0.088	0.150	0.109	0.139	0.169	0.109	0.049	0.127	0.150	0.152	0.000	0.130	0.079
2058	octic	11.82	14.45	30.13	50.56	13.46	19.07	16.37	12.98	22.11	31.51	12.80	15.23	14.35	13.73	16.83	21.62	11.32	10.15	12.52
2272	decic	3.670	5.453	7.139	14.149	4.397	5.304	4.557	5.263	5.774	9.036	4.329	3.344	5.188	4.561	5.658	5.154	4.064	0.549	3.533
										Miscellaneous										
1276	unk1276	0.143	0.197	0.080	0.109	0.164	0.181	0.107	0.156	0.106	0.068	0.048	0.080	0.028	0.138	0.039	0.042	0.107	0.028	0.017
1587	unk1587	0.127	0.209	0.081	0.129	0.153	0.038	0.045	0.245	0.060	0.050	0.122	0.072	0.229	0.257	0.147	0.074	0.166	0.207	0.284
1635	bulactn	1.660	5.180	2.238	1.089	5.395	2.760	3.959	3.762	3.034	2.492	3.080	4.573	4.648	3.843	2.350	2.776	1.708	2.597	2.327
1700	unk1700	0.003	0.031	0.010	0.007	0.028	0.009	0.009	0.015	0.016	0.010	0.008	0.012	0.032	0.014	0.018	0.005		0.010	0.002
1740	unk1740	0.390	0.796	1.738	0.339	1.117	0.352	1.840	2.303	0.966	1.646	1.532	1.176	1.161	1.453	1.311	1.786	1.379	1.445	0.902
2358	diettar	0.338	3.454	5.204	1.122	3.335	8.937	4.921	0.968	7.792	4.428	1.313	1.708	2.119	1.499	1.221	3.449	0.619	0.304	0.691
2371	unk2371	0.285	0.024	0.069	0.445	0.037	0.012	0.016	0.032	0.027	0.043	0.031	0.010	0.037	0.021	0.028	0.022	0.163	0.094	0.091
2400	unk2400	69.99	172.04	449.92	70.32	218.87	297.26	248.39	168.83	444.40	516.11	102.94	378.69	215.43	155.31	115.28	271.91	57.33	82.60	86.53
2481	unk2481	0.265	0.226	0.488	0.283	1.506	0.654	1.090	1.341	2.137	0.559	0.116	0.541	0.261	0.174	0.537	0.832	0.364	0.315	0.205
2512	hmf	0.175	0.115	0.198	0.036	0.110	0.085	0.085	0.245	0.219	0.177	0.082	0.000	0.016	0.060	0.053	0.120	0.114	0.044	0.058

[a] Kovatis indices of unknown compounds on DB-WAX column. [b] See Table 2 for full name of compound.

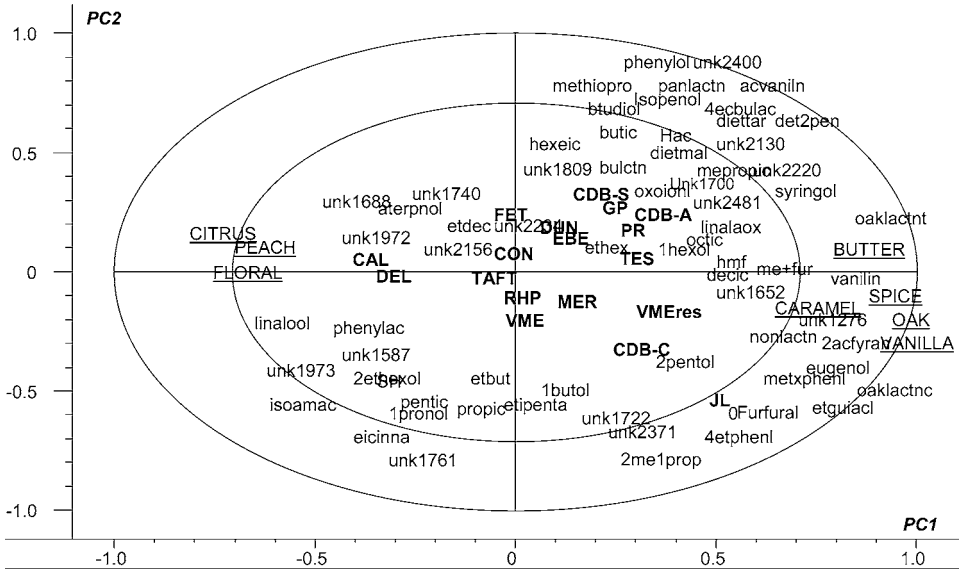

Figure 2. Correlation loadings from PLS of 74 GC variables (small letters) and 8 sensory variables (capital letters). Bold capital letters are wine scores. Explained variance for *X* (GC data) is 7 and 23% for PC1 and PC2, respectively, and for *Y* (Sensory data) is 64 and 4%, respectively. Codes for wines and OA compounds are defined in **Table 1** and **Table 3**, respectively.

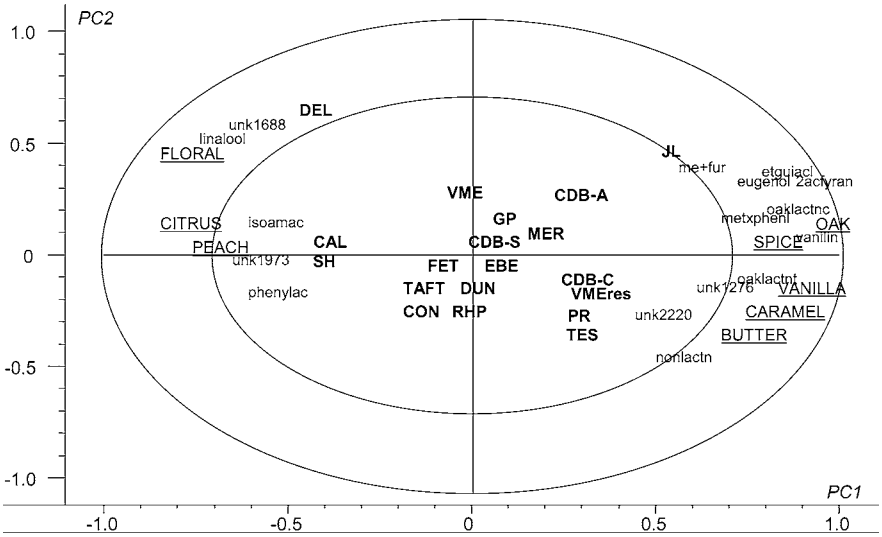

Figure 3. Correlation loadings from PLS of 16 GC variables (small letters) and 8 sensory variables (capital letters). Bold capital letters are wine scores. Explained variance for *X* (GC data) is 47 and 8% for PC1 and PC2, respectively, and for *Y* (Sensory data) is 64 and 6%, respectively. Codes for wines and OA compounds are defined in **Table 1** and **Table 3**, respectively.

all nineteen wines by GC-MS. PLS regression analysis yielded a configuration similar to that found by PCA of the sensory descriptive analysis data for the same wines. The largest difference among the wines was a contrast between wines high in intensity of floral and fruity notes (and high in concentrations of compounds with floral aromas, such as linalool and α-terpineol) and wines high in oaky and spicy notes (and high in concentration of oak lactones, vanillin, 2-methoxy phenol, and eugenol). However, sensory evaluation of these OA compounds must be made to confirm that they contribute to the aroma of Chardonnay wines and determine which are most important in producing the characteristic flavor of these wines.

ABBREVIATIONS USED

PCA, principal component analysis; PLS, partial least-squares regression; GC, gas chromatography; GC-O, gas chromatography-olfactometry; GC-MS, gas chromatography-mass spectrometry; OA, odor-active

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