Effect of Simulated Shipping Conditions on Sensory Attributes and Volatile Composition of Commercial White and Red Wines

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Abstract: A major concern when shipping wine is whether the condition in which it is received at its destination is the same as when it left the winery. This study explored the effects of shipping conditions on six varietal wines. Four white wines and four red wines were exposed to four different storage conditions to create 32 treatments. Riesling, Gewürztraminer, Sauvignon blanc, and Chardonnay wines were from one producer and of the same vintage. One Merlot and three Cabernet Sauvignon wines were from different labels by the same producer. Storage conditions included 20°C, 40°C, 20/40°C (reflecting diurnal cycle in temperatures), and a sample that traveled in the trunk of a car for three weeks. The 32 wines were evaluated using sensory descriptive analysis. Trained panelists, 11 for white wine and 13 for red wine, rated the wines on 14 and 23 attributes, respectively. Volatiles were analyzed using a HS-SPME-GC-MS analysis. Both sensory and analytical results showed significant differences among the wines stored at the higher temperatures. Differences were noted for a number of compounds, including higher concentrations of vitispirane 1 and 2, TDN, and *p*-cymene and reductions in several esters and acetates, which are characteristic of aged wines. This is the first study that has assessed sensory changes in wines under conditions that would potentially be experienced by wine in transit.

Key words: wine aroma, sensory descriptive analysis, HS-SPME, GC-MS, storage temperature, PLS

The shelf life of food is defined as the period in which the product will remain safe, is certain to retain desired sensory, chemical, physical, and microbiological characteristics, and complies with any label declaration of nutritional data (IFST 1993). Products with a maximum usable lifetime, such as meats, fruits, vegetables, and dairy, are perishable (Goyal and Giri 2001), and freight and storage conditions are critical in reducing the growth of microorganisms and any chemical (including enzymatic) changes in the food.

Risk-adverse winemaking practices, such as the use of sulfites, lower pH, good winery hygiene, and sterile filtration prior to bottling, limit microbiological growth in packaged wines. Wine therefore exhibits a "random" shelf life, as the chemical changes are as dependent on the initial condition of the product, including packaging, as on the storage and freight conditions of the product. However, the storage and freight conditions of wine prior to consumption may lead to a reduction in wine quality because of unintended physical and chemical changes in the wine.

The Arrhenius equation states that the rate constant of a chemical reaction is exponentially related to the temperature of the system. A summary (Boulton et al. 1996) of research (Ribéreau-Gayon 1933, Ough 1985) has shown that the relative rates of oxygen uptake, browning, and total SO_2 decline in wine would increase 270, 20.7, and 4.8 (red) or 1.7 (white) times faster at 40°C as compared to 10°C. Other research has identified that the low level formation of ethyl carbamate (urethane), primarily from ethanol and urea in wine (Kodama et al. 1994), follows first-order kinetics and is accelerated by storage of wine at high temperatures (Hasnip et al. 2004).

The sensory changes associated with elevated storage temperatures is of major concern to both winemakers and consumers, especially, given that little is known about how temperature fluctuates during shipping or how it affects the sensory attributes of wines sold through retail outlets or directly to consumers. Wine producers typically store wines in cool cellars or air-conditioned facilities, with the exception of Madeira producers who use a baking process known as *estufagem* in the production of their unique

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wines (Campo et al. 2006). Previous work has shown that the temperature variation within a commercial refrigerated shipping container can vary up to 8°C from the set point using an on-off control system and that the sun-exposed roof of a container is usually the warmest area due to a solar effect (Rodríguez-Bermejo et al. 2007). During the summer months in the United States, ambient temperature can fluctuate up to 20°C inside wine shipping containers over a two-week period and up to 13°C on a daily basis (C. Butzke, personal communication, 2009).

Eric Vogt of eProvenance, a company providing wine authentication and monitoring services, monitored the temperature of fine wine sent from France to the United States, United Kingdom, China, Brazil, and Japan. There was a wide range of temperature variation, typically stable during the ocean voyage temperatures but fluctuating widely both before and after the ocean voyage. More than 6% of wines shipped from Europe to the United States experience temperatures above 30°C (E. Vogt, personal communication, 2009). Although this percentage is relatively low, it predominantly reflects the fine wine product category, and thus it is feasible, by including products from the commodity wine category, that the percentage of products subjected to these elevated temperatures could be significantly larger.

Partial least squares (PLS) regression is a powerful multivariate data analysis technique that can be used to relate a number of response (Y) variables to multiple explanatory (X) variables. The method models the underlying factors or linear combinations of independent variables that best describe the dependent variables. That is, PLS analysis can demonstrate the underlying associations between compositional data and sensory attributes. However, an association does not necessarily indicate that the specific compounds are responsible for any one sensory attribute; instead, these compounds should become the focus of future sensory research to confirm their role (Noble and Ebeler 2002). PLS has been extensively used in the grape and wine field (Aznar et al. 2003, Jensen et al. 2008, Lee and Noble 2003, 2006) and recently to compare wine mouthfeel and metabolomic data (Skogerson et al. 2009) and vine vigor status with tannin and sensory data (Cortell et al. 2008).

This study aims to better understand the effect of elevated temperatures, typical of U.S. transcontinental shipping conditions, on wine sensory attributes and volatile composition. The objective of this work was to characterize the relationship between changes in wine volatile composition and sensory attributes associated with wines that experienced elevated storage conditions using PLS regression.

Materials and Methods

Wines and analytical supplies. Four commercially available white wines were purchased from Navarro Vineyards (Philo, CA) and four commercially available red wines were donated by Beringer Vineyards (St. Helena, CA). Details of the wines and the codes that identify them are listed in Table 1. To minimize temperature effects, the wines were obtained from the wineries shortly after bottling and transported directly to Davis during the fall 2008 and stored together at a constant 20°C.

Polydimethylsiloxane (PDMS) solid-phase microextraction (SPME) fibers, 100 µm 23 ga, were purchased from Supelco (Bellefonte, PA). Prior to initial use, all new fibers were conditioned for 30 min at 250°C according to the manufacturer's recommendations. Amber glass, screw-threaded 20-mL headspace vials with magnetic screwcaps and white PTFE/blue silicone (1.3 mm thickness) septa were from Alltech (Alltech Corp, Deerfield, IL). A C8–C20 alkane standard mixture, used for determination of Kovats retention indices (RI), was obtained from Fluka (Sigma-Aldrich, St. Louis, MO).

Experimental design. Twelve bottles of each wine were stored for 21 days under each of four different temperature conditions: (1) constant 20°C to reflect room temperature, (2) constant 40°C to reflect a hot environment, (3) diurnal temperature cycle (20°C/40°C alternating every 12 hr) to simulate transcontinental shipping conditions, and (4) stored in the trunk of a private car to simulate wine shipment with movement. The constant 20°C and 20°C/40°C cycled treatment wines were stored in Percival growth chambers (Boone, IA), chosen because they could be so programmed, while the constant 40°C treatment wines were stored in a Steris Reliance 1044 glassware dryer (Beauport, QC, Canada). The wines stored in the car trunk were driven around Davis, California, from 11 to 31 Dec 2008.

Temperature monitoring. Ambient temperature was monitored using Tinytag data loggers, model TG-3080, with a 10K NTC Thermistor sensor (Omni Instruments, Arroyo Grande, CA) able to record temperatures from -40°C to 85°C ± 1°C within the temperature range studied with a total reading capacity of 8,000. The loggers were set to start recording ambient temperature in synchronized time every 10 min over the three-week period at which point the logged information was downloaded with Tinytag Explorer Software (SWD-0040) using an ACS-3030 USB inductive pad.

Sensory analysis. White wines were evaluated by a trained panel of 11 volunteers (five men and six women) and the red wines were evaluated by a second trained panel of 13 volunteers (six men and seven women). All panelists were between the ages of 21 and 35, had previous wine-tasting experience, and were selected based on interest and availability. During initial sessions, panelists developed their own descriptive terminology through consensus to describe and differentiate the wines. Panelists were

Table 1 Details of wines used in this study.

Code	Variety	Vintage	Alcohol (%)
W1	Riesling	2006	13.1
W2	Gewürztraminer	2006	13.5
W3	Sauvignon blanc	2006	13.3
W4	Chardonnay	2006	13.4
R1	Merlot	2005	13.9
R2	Cabernet Sauvignon	2006	13.3
R3	Cabernet Sauvignon	2006	13.7
R4	Cabernet Sauvignon	2005	13.6

trained with the reference standards over eight subsequent training sessions to align panelist terminology. These reference standards (Table 2, Table 3) were presented in black wineglasses.

Quantitative descriptive analysis. Panelists in the red and white wine groups were asked to evaluate each of the 16 wine treatments in triplicate over the course of six sessions, equating to 8 wines per session presented in a randomized block design. Before each formal evaluation session, the established reference standards were assessed to refresh each panelist's memory. All wine samples were presented in ISO wineglasses (ISO 3591:1977), covered with plastic lids, labeled with a unique three-digit codes, under red lighting (to mask differences in color), in separate booths equipped with a computer screen and mouse for data collection. Ambient temperature was 20°C. Wines were assessed monadically and panelists were asked to rate attributes using a continuous unstructured scale (10 cm). A 30-second rest was included between each sample during which the panelist was asked to refresh his or her palate with water and an unsalted water cracker. FIZZ software (ver. 2.31G; Biosystèmes, Couternon, France) was used for data acquisition and for generating a randomized presentation order using a modified Williams Latin Square design.

GC-MS instrumentation. All experimentation was conducted using a Gerstel MPS2 autosampler with agitator (Baltimore, MD) coupled to an Agilent 6890N gas chromatograph with an Agilent 5975 inert mass selective detector (Little Falls, DE). The GC oven was equipped with a 30 m DB-WAX capillary column (0.25 mm i.d. and 0.25 µm film thickness) (J&W Scientific, Folsom, CA) with a 0.75 mm i.d. SPME inlet liner (Supelco, Bellefonte, PA).

Chromatographic conditions. The injector was held at 250°C in the splitless mode with a purge-off time of 1 min, a 50 $mL.min^{-1}$ split vent flow at 1 min, and a 20 $mL.min^{-1}$

Table 2 Composition of sensory reference standards used to define aroma and taste attributes for white wine study.

Attribute/descriptor	Composition[a]
Aroma	
Apple/pear	⅛ x medium Granny Smith apple, chopped
	⅛ x medium Bosc pear, chopped
Burnt rubber	1 x rubber band lit on fire and immediately extinguished and placed in wine
Canned vegetable	¼ x tsp canned corn juice (Del Monte)
	¼ x tsp asparagus juice (Raleys)
Cardboard	4 x 1 inch squares of corrugated cardboard
Citrus	⅛ x medium grapefruit with skin
	⅛ x medium lemon with skin
Diesel	2007 Werner Riesling Kabinett[b]
Floral	1 x lemon blossom torn in pieces (no wine)
Herbaceous	1 x leaf of agapanthus (Lily of the Nile), ripped
	2 x fresh French green beans, chopped
Tropical fruit	2 x 1 inch cubes fresh pineapple
	⅙ x fresh mango
	¼ x fresh apricot
	¼ x tsp dried sweetened coconut
Oak/fresh wood	3 x 1 cm cubes oak chips, soaked overnight and removed
Oxidized	Domecq Manzanilla Sherry
Taste	
Bitter	800 mg caffeine in 500 mL water
Sour	200 mg citric acid in 500 mL water
Sweet	20 g sucrose in 500 mL water

[a]All standards prepared in 60 mL Franzia White Chablis unless otherwise noted.
[b]Presented during training only.

Table 3 Composition of sensory reference standards used to define aroma and taste attributes for red wine study.

Attribute/descriptor	Composition[a]
Aroma	
Candy	8 x Jelly Belly beans, squashed
Canned veggie	1 x tsp canned corn juice (Del Monte)
	1 x tsp asparagus juice (Raleys)
	1 x tsp green bean juice (Del Monte)
	1 x tsp olive juice
Cardboard	5 x 1 inch squares corrugated cardboard
Citrus/orange peel	1 x tsp orange marmalade
	2 x 1 cm squares orange peel
Dark fruit	10 x frozen blackberries (Best Yet)
	20 x blueberries (Cascadian Organic)
Dried fruit	2 x dried figs (Sunmaid)
	3 x prunes (Sunmaid)
	20 x raisins (Sunmaid)
Fresh vegetable	2 x fresh green beans, chopped
	0.5 oz fresh green bell pepper
Herbal	¼ x tsp oregano (McCormick)
	¼ x tsp basil (McCormick)
Jam fruit	2 x tsp blueberry jam (Smuckers)
	2 x tsp blackberry jam (Smuckers)
	2 x tsp raspberry jam (Smuckers)
Leather	6 x 1 inch leather shoe laces (Kiwi Outdoor)
Menthol	4 x drops Nature's Alchemy Eucalyptus 100% pure essential oil in 200 mL water, 10 mL solution in 40 mL wine
Oak/fresh wood	3 x 1 cm cubes oak chips, soaked overnight and removed
Oxidized	20 mL Domecq Manzanilla Sherry
Pungent	30 mL Popov tsp Vodka plus acetone (nail polish remover)
Red berries	2 x strawberries (California grown, purchased fresh and frozen)
	8 x frozen raspberries (Best Yet)
Spicy	¼ x tsp freshly ground black pepper
Toast	¼ x tsp coffee in 300 mL red base wine with ⅛ x tsp liquid smoke
Tobacco	1 x cigarette (Camel Lights)
	⅛ x teaspoon pencil shavings
Vanilla/caramel/cocoa	¼ tsp vanilla-caramel Coffee-mate nondairy creamer
	¼ tsp Natural cocoa powder (Scharffen Berger)
	1 x piece milk chocolate (Euphoria Chocolate Company)
Taste	
Sweet	20 g sucrose in 500 mL water
Sour	200 mg citric acid in 500 mL water
Bitter	800 mg caffeine in 500 mL water
Astringent	312 mg alum in 500 mL water

[a]All standards prepared in 60 mL Franzia Vitners Select Cabernet Sauvignon unless otherwise noted.

gas saver flow at 5 min. Ultra-high-purity helium (Praxair, Danbury, CT) was used as the carrier gas at a constant flow rate of 1.2 mL.min^{-1}. The temperature program was 40°C for 1 min, 5°C.min^{-1} to 185°C, then 40°C.min^{-1} to 240°C, held for 3.62 min, with a total run time of 35 min. The transfer line and ion source were maintained at 240 and 230°C, respectively. The detector collected masses between 40 and 240 amu with a scan rate of 6.61 scans.sec^{-1}. All samples were analyzed in triplicate, and the sample sequence order was randomized within replicate blocks using a random number generator (http://www.random.org).

HS-SPME extraction conditions. Samples were incubated at 30°C with agitation at 500 rpm for 5 min and allowed to rest for an additional 5 min before extraction. The headspace was sampled for 15 min with the vial at ambient temperature (25°C ± 2°C). The PDMS fiber was desorbed in the inlet at 250°C for 1 min. The fiber was then reconditioned in the inlet for a further 4 min to prevent analyte carryover between samples.

GC-MS data analysis software. GC-MS interrogation and spectral deconvolution was conducted using AMDIS ver. 2.65 (Build 116.66) (National Institute of Standards and Technology, Gaithersburg, MD) (Stein 1999) using a component width of 32 scans, two adjacent peak subtraction, high sensitivity, resolution, and shape requirements. Compound mass spectral data were compared against the NIST 2005 Mass Spectral Library, and calculated retention indices were compared to published retention indices (Stein 2010) for identity confirmation. Peak area integration of unique masses was conducted using MSD Chemstation (G1701-90057; Agilent).

Statistical analysis. All statistical analyses were conducted using JMP (ver. 8.0.2; SAS Institute Inc., Cary, NC). A four-way analysis of variance (ANOVA) was conducted using the restricted maximum likelihood (REML) method to test the effects of treatment, wine, judge, replicate and all two-way interactions for each sensory attribute using a pseudo-mixed model with the judge by treatment and judge by wine interactions as denominators. A two-way ANOVA was used to analyze effects of treatment and wine and their two-way interaction for all volatile compounds measured. Where treatment had a significant effect for both the analytical and sensory results, partial least squares (PLS) regression analysis was used to combine the normalized mean values for significant volatile components (X-variables) and sensory attributes (Y-variables). Mean values were normalized against the maximum value for any one treatment by wine combination so that each variable had an equivalent influence on the PLS model. Cross-validation was used to determine the lowest number of extracted factors required to minimize the root mean square error of prediction (RMSEP). The PLS output scores and loadings were normalized and plotted, for the significant factors, using JMP. The variable influence on projection (VIP) values and regression coefficients were used to determine which predictive (X) variables were important in modeling the response (Y) variables. VIP values provide weighted sums of squares of the PLS weights calculated from the Y-variance of each PLS component (Wold et al. 2001). The regression coefficients for each X-attribute were assessed in relation to the Y-attributes through two-way hierarchical cluster analysis using a minimal variance algorithm (Ward 1963). The cluster membership was then analyzed using a one-way ANOVA to determine whether X-attribute clusters responded differently for each Y-attribute. Where treatment did not have a significant effect for both the analytical and sensory results, principal component analysis (PCA) was used to explore the interrelationships between the attributes and the samples.

Results

Temperature results. The 20°C treatment had a relatively constant temperature with a mean of 20.8 (± 0.4)°C over the 21-day period. The 40°C treatment had an ~24-hr timelag before reaching the intended 40°C temperature (Figure 1). This resulted in the 40°C treatment wines experiencing a mean temperature of 35.0 (± 7.2)°C over the 21-day period. The 20°C/40°C cycled treatment also experienced a timelag oscillating between ~26 and ~35°C over a 24-hr period, with ~2 hr at the ~35°C temperature each cycle. This resulted in a mean temperature of 28.7 (± 4.3)°C over the 21-day period. The wine stored in the car trunk had the lowest temperatures of all treatments, with a mean of 14.3 (± 3.4)°C over the 21-day period.

Analysis of white wine. The four-way ANOVA, using a pseudo-mixed model, showed that the apple, canned vegetable, citrus, diesel, floral, oxidized, rubber, and tropical fruit sensory attributes were significantly different across the treatments in the white wine study (Table 4). A two-way ANOVA of the 48 identified volatile compounds showed that 26 compounds were significantly different due to treatment (Table 5).

PLS analysis with cross-validation, using all significant volatile components to predict the significant sensory attributes, determined that the PLS model with the lowest root mean square error of prediction (RMSEP = 0.791) used four latent vectors. However, the fourth latent vector provided little additional information compared with the first three

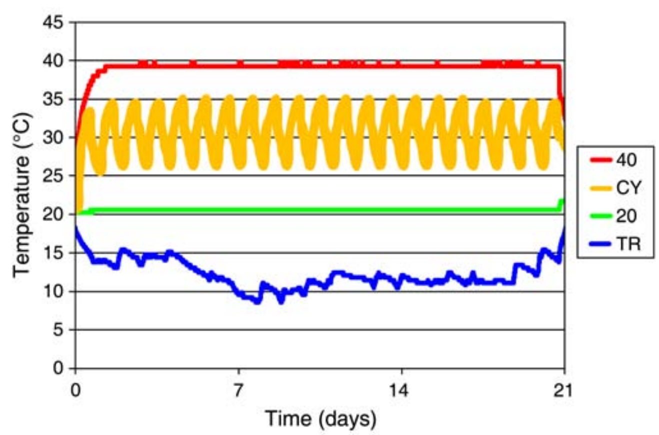

Figure 1 Ambient temperature monitored using Tinytag data loggers for each temperature treatment. Treatments: car trunk (TR), constant 20°C (20), cycled 20°C/40°C (CY), and constant 40°C (40).

latent vectors (RMSEP = 0.881); therefore, only the first three latent vectors are presented. Linalool, propyl octanoate, nerol oxide, hexyl acetate, *p*-cymene, and 2-phenylethyl acetate were considered important variables in defining the final PLS model with variable influence on projection (VIP) values above the 75% quartile (Table 6).

The PLS model differentiated among the wines in the first two latent vectors, grouping similar wines by variety, and accounting for 55.3% and 49.8% of the variance for the X and Y variables, respectively (Figure 2). The third latent vector accounted for an additional 20.3% and 12.4% of the variance for the X and Y variables, respectively, differentiating products primarily by heat treatment. Wines in either the constant 20°C or car trunk treatment tended to group in the first, second, and third vectors compared with similar wines in the 20°C/40°C cycled treatment or the constant 40°C treatment (Figure 3).

The tropical fruit and apple sensory attributes were negatively correlated with the rubber and diesel sensory attributes (Figure 2). The opposition of these sensory attributes characterized the first latent vector, which accounted for the greatest percentage of variance for the sensory attributes in the PLS model.

The tropical fruit sensory attribute was positively correlated with compounds in clusters 1 and 4 and negatively correlated with compounds in cluster 8. Hexyl acetate had the strongest positive correlation with the tropical fruit sensory attribute, and linalool, propyl octanoate, and isoamyl acetate had the next strongest association (Table 6). The apple sensory attribute was not well described by any one cluster of compounds; however, it was positively correlated with ethyl decanoate and negatively correlated with ethyl 2-furoate.

Compounds in cluster 2, including the norisoprenoids 1,1,6-trimethyl-l,2-dihydronaphthalene (TDN), vitispirane 1 and 2, and β-damascenone, were strongly correlated with the diesel sensory attribute (Table 6). The rubber sensory attribute was negatively correlated with 2-phenylethyl acetate, propyl octanoate, and hexyl acetate and positively correlated with ethyl 2-furoate and vitispirane 2. However, there was no specific compound cluster that correlated well with the rubber attribute.

The second latent vector was characterized by the separation of the citrus and floral from the canned vegetable and oxidized sensory attributes. The citrus and floral attributes were associated with the aromatic white wine varieties Riesling (W1) and Gewürztraminer (W2). The canned vegetable and oxidized sensory attributes were associated with the Sauvignon blanc (W3) and Chardonnay (W4) wines (Figure 2).

Linalool and propyl octanoate, compounds in cluster 4, were important in defining the second latent vector, strongly positively correlated with the citrus and floral sensory attributes, and strongly negatively correlated with the canned vegetable and oxidized sensory attributes (Table 6). The citrus attribute was positively correlated with the X-attributes from clusters 3, 4, and 6, while the floral attribute was positively correlated with compounds from clusters 1, 3, and 4. The canned vegetable attribute was negatively correlated to compounds in clusters 3, 4, and 6. Compounds in cluster 4 were also negatively correlated with the oxidized attribute.

Analysis of red wine. In the red wine study, 30 of the 47 volatile compounds changed with respect to temperature treatment (Table 5). However, only two sensory attributes, dry fruit and canned vegetable, were significantly different due to the temperature treatment, with both attributes higher for wines in the 40°C treatment (Table 4). Consequently, only the volatile compounds that were significantly different due to treatment were included in the principal component analysis (PCA).

The first two principal components accounted for 38.5% and 30.8% of the variance in the first and second dimension, respectively (Figure 4). Wines tended to separate due to heat treatment mostly in the first dimension. As with the white wine study, wines in the constant 20°C or car trunk treatment tended to group and were clearly different to wines in the 20°C/40°C cycled or the constant 40°C treatment. There was little separation of the wines, with Merlot (R1) and Cabernet (R2) wines separated from Cabernet (R3) and Cabernet (R4) wines in the second dimension.

Wines that experienced heat were positively correlated with TDN, vitispirane 1 and 2, dehydroxylinalool oxide A, and *p*-cymene and negatively correlated with methyl decanoate, ethyl decanoate, ethyl dodecanoate, isoamyl octanoate and decanoate, propyl octanoate, and linalool.

The separation of the wines in the second dimension was driven by one of the Cabernet (R2) wines, which had significantly higher concentrations of hexyl acetate and lower levels of diethyl succinate and terpinolene than the other wines (data not presented). Both Merlot (R1) and Cabernet (R2) wines were lower in α-terpinene and *p*-cymene and higher in ethyl 9-decanoate than Cabernet (R3) and Cabernet (R4) wines.

Table 4 Sensory attributes found to be significant due to treatment for white and red wine products. Values represent least square means (LSM) (± SE) for four-way ANOVA. A pseudo-mixed model using the judge x treatment and judge x wine interactions as denominators was used in all cases.

	Treatment[a]			
Attribute	**TR**	**20**	**CY**	**40**
White wine				
Apple	3.1 ± 0.2	3.1 ± 0.2	3.1 ± 0.2	2.5 ± 0.2
Canned vegetable	1.3 ± 0.2	1.1 ± 0.2	1.2 ± 0.2	2.1 ± 0.2
Citrus	2.4 ± 0.2	2.6 ± 0.2	2.6 ± 0.2	2.0 ± 0.2
Diesel	1.0 ± 0.2	1.1 ± 0.2	1.3 ± 0.2	1.6 ± 0.2
Floral	3.2 ± 0.2	2.8 ± 0.2	2.8 ± 0.2	2.2 ± 0.2
Oxidized	0.9 ± 0.1	0.7 ± 0.1	0.8 ± 0.1	1.0 ± 0.1
Rubber	1.0 ± 0.2	1.0 ± 0.2	1.2 ± 0.2	2.0 ± 0.2
Tropical fruit	2.8 ± 0.2	2.5 ± 0.2	2.6 ± 0.2	2.1 ± 0.2
Red wine				
Canned vegetable	0.9 ± 0.1	0.8 ± 0.1	0.8 ± 0.1	1.2 ± 0.1
Dry fruit	2.2 ± 0.1	2.2 ± 0.1	2.0 ± 0.1	2.6 ± 0.1

[a]TR: car trunk; 20: constant 20°C; CY: cycled 20°C/40°C; 40: constant 40°C.

Discussion

White wines. The white wines showed significant differences due to variety and heat treatment. The sensory attributes that showed significance across the wines included canned vegetable, citrus, diesel, floral, oxidized, rubber, and tropical fruit. The constant 40°C heat treatment had a greater impact on the aroma and volatile composition of the wines compared with the 20°C/40°C cycled treatment and also compared with the constant 20°C and car trunk treatments, which were not significantly different (Figure 3). The two heated treatments tended toward the diesel, oxidized, and rubber aroma attributes and away from the

Table 5 Treatment significance values for two-way ANOVA for white and red wines. Values marked in bold italics are significant at $p \leq 0.05$.

CAS	Compound	Unique ion[a]	RT (min)	RI[b] (calc)	RI[c] (lit)	White	Red
105-54-4	Ethyl butanoate	71	4.143	1029	1031	0.993	0.222
71-23-8	1-Propanol	59	4.244	1035	1030	0.950	0.745
7452-79-1	Ethyl 2-methylbutyrate	102	4.426	1046	1036	***<0.001***	***<0.001***
108-64-5	Ethyl 3-methylbutyrate	88	4.693	1062	1053	***0.002***	***<0.001***
78-83-1	Isobutanol	43	5.329	1100	1097	0.876	0.644
7392-19-0	Dehydroxylinalool oxide A	139	5.420	1104	1096	<0.001	<0.001
123-92-2	Isoamyl acetate	43	5.737	1118	1117	***<0.001***	0.427
99-86-5	α-Terpinene	121	6.888	1170	1175	0.237	***<0.001***
106-70-7	Methyl hexanoate	74	7.188	1184	1190	0.268	0.674
123-51-3	Isoamyl alcohol	55	7.859	1213	1215	0.584	0.185
123-66-0	Ethyl hexanoate	88	8.362	1233	1230	0.750	***0.007***
99-87-6	*p*-Cymene	119	9.125	1264	1253	***<0.001***	***<0.001***
142-92-7	Hexyl acetate	43	9.301	1271	1269	***<0.001***	***0.002***
586-62-9	Terpinolene	121	9.460	1278	1276	0.363	***<0.001***
97-64-3	Ethyl lactate	45	11.083	1342	1342	0.311	***<0.001***
876-17-5	(*Z*)-Rose oxide[d]	139	11.287	1350	1338	0.183	ND
111-27-3	1-Hexanol	56	11.451	1357	1354	0.761	0.682
111-11-5	Methyl octanoate	74	12.249	1389	1387	***0.045***	***<0.001***
106-32-1	Ethyl octanoate	88	13.493	1439	1438	***0.012***	***<0.001***
64-19-7	Acetic acid	45	13.811	1452	1449	0.075	0.742
2198-61-0	Isoamyl hexanoate	70	13.986	1459	1464	0.019	<0.001
1786-08-9	Nerol oxide	68	14.228	1468	1473	***<0.001***	***0.016***
624-13-5	Propyl octanoate	145	15.477	1520	1514	***<0.001***	***<0.001***
65416-59-3	Vitispirane 1	192	15.549	1523	1526	***<0.001***	***<0.001***
65416-59-3	Vitispirane 2	192	15.595	1525	1529	***<0.001***	***<0.001***
123-29-5	Ethyl nonanoate	88	15.879	1530	1528	0.005	<0.001
78-70-6	Linalool	71	16.204	1550	1554	***<0.001***	***<0.001***
111-87-5	1-Octanol	56	16.488	1562	1561	0.428	0.715
110-42-9	Methyl decanoate	74	17.266	1595	1590	***<0.001***	***<0.001***
614-99-3	Ethyl 2-furoate	95	17.808	1618	1621	***<0.001***	***<0.001***
110-38-3	Ethyl decanoate	88	18.334	1641	1647	<0.001	<0.001
2035-99-6	Isoamyl octanoate	70	18.729	1658	1652	***<0.001***	***<0.001***
123-25-1	Diethyl succinate	101	19.118	1675	1677	***<0.001***	***<0.001***
67233-91-4	Ethyl 9-decenoate	88	19.454	1690	1689	***<0.001***	***<0.001***
98-55-5	α-Terpineol	59	19.610	1697	1687	0.529	0.061
30364-38-6	TDN	157	20.472	1736	1731	<0.001	<0.001
101-97-3	Ethyl phenylacetate	91	21.445	1781	1783	0.804	***<0.001***
103-45-7	2-Phenylethyl acetate	104	22.072	1810	1809	***<0.001***	0.787
23726-93-4	β-Damascenone	69	22.191	1816	1813	***0.046***	0.564
106-33-2	Ethyl dodecanoate	88	22.764	1843	1840	***<0.001***	***<0.001***
142-62-1	Hexanoic acid	60	22.919	1851	1840	0.430	0.178
2306-91-4	Isoamyl decanoate	70	23.141	1861	1859	***<0.001***	***<0.001***
100-51-6	Benzyl alcohol	71	23.396	1873	1869	0.055	***0.004***
55013-32-6	(*Z*)-Oak-lactone	99	23.497	1878	1886	0.301	0.516
60-12-8	Phenylethyl alcohol	91	24.097	1907	1910	0.574	0.145
39638-67-0	(*E*)-Oak-lactone	99	24.900	1948	1957	0.456	0.192
2785-89-9	4-Ethylguaiacol[e]	137	26.401	2020	2024	ND	***0.050***
124-07-2	Octanoic acid	60	27.180	2062	2060	0.507	0.090

[a]Unique ion (*m/z*): used for peak area determination.
[b]RI: retention indices calculated from C8–C20 n-alkanes.
[c]RI: retention indices reported in the literature for polyethylene glycol capillary GC columns (Stein 2010).
[d]Compound only detected in white wines.
[e]Compound only detected in red wines.

citrus, floral, and tropical fruit aromas. These observations are consistent with previous research that has shown elevated storage temperatures decrease the floral character and enhance characters such as honey, butter/vanilla, oak, tea/tobacco, rubber, and smoky in white wines, which are typical of aged wines (De La Presa-Owens and Noble 1997, Francis et al. 1994).

Linalool played an important role in defining both aromatic varieties, Riesling (R1) and Gewürztraminer (R2) wines. Monoterpenes are important to the aroma of white wines made from Muscat varieties and aromatic non-Muscat varieties (Mateo and Jimeńez 2000, Rapp 1998, Ribéreau-Gayon et al. 1975), with well-documented correlations between floral sensory attributes and high levels of linalool (Campo et al. 2005, De La Presa-Owens and Noble 1997, Lee and Noble 2003, 2006). Linalool was closely associated with the Gewürztraminer wines, whereas TDN, vitispirane 1 and 2, and *p*-cymene were closely associated with the Riesling wines. TDN and vitispirane are typically found in Riesling wines that have been bottle aged (Simpson 1979) and or heated (Simpson 1978).

The Sauvignon blanc wines (W3) were characterized by higher concentrations of diethyl succinate (Figure 2), which has been shown to increase with wine age in Airen white wines (Gonzalez-Viñas et al. 1996) and Spanish cava (Francioli et al. 2003, Riu-Aumatell et al. 2006). However, other research has indicated that this increase in white wines

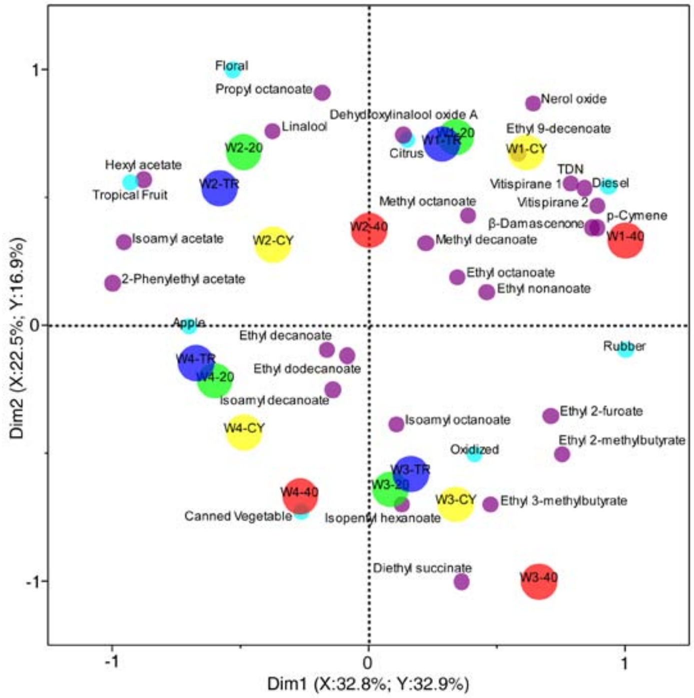

Figure 2 Partial least squares analysis of white wine products. Purple circles represent volatile composition loadings (X matrix), light blue circles represent sensory attribute loadings (Y matrix), and large circles represent sample scores for factor 1 (Dim1) and factor 2 (Dim2). Sample codes listed in Table 1. Treatments: car trunk (TR), constant 20°C (20), cycled 20°C /40°C (CY), and constant 40°C (40).

Table 6 Regression coefficients of centered and scaled X-variables for each Y-variable from the four-component PLS model of the white wines. X-variables are ordered by descending variable influence on projection (VIP) value. Compound cluster membership determined using hierarchal cluster analysis.

X-variable	VIP	Cluster	Apple	Canned veg	Citrus	Diesel	Floral	Oxidized	Rubber	Tropical fruit
Linalool	1.810	4	-0.02	-0.24	0.27	-0.02	0.26	-0.14	-0.06	0.11
Propyl octanoate	1.550	4	0.07	-0.20	0.19	-0.01	0.18	-0.10	-0.10	0.11
Nerol oxide	1.290	3	-0.07	-0.14	0.15	0.09	0.11	-0.05	0.05	0.00
Hexyl acetate	1.286	1	0.06	-0.05	0.06	-0.05	0.13	-0.08	-0.10	0.12
p-Cymene	1.269	3	-0.08	-0.14	0.15	0.08	0.07	-0.03	0.07	-0.04
2-Phenylethyl acetate	1.209	1	0.09	0.03	-0.02	-0.07	0.05	-0.04	-0.10	0.10
Isoamyl acetate	1.166	1	0.05	0.00	0.01	-0.06	0.09	-0.06	-0.09	0.11
Ethyl succinate	1.144	5	-0.03	0.08	-0.09	-0.02	-0.14	0.08	0.05	-0.10
Dehydroxylinalool oxide A	1.126	3	-0.06	-0.14	0.16	0.04	0.15	-0.08	0.02	0.04
Ethyl dodecanoate	1.123	6	0.07	-0.16	0.14	-0.06	0.07	-0.04	-0.08	0.03
Vitispirane 2	1.115	2	-0.07	-0.03	0.02	0.11	-0.01	0.02	0.09	-0.06
Ethyl 2-furoate	1.092	8	-0.11	-0.04	0.05	0.05	-0.02	0.02	0.10	-0.09
Isoamyl decanoate	1.088	6	0.07	-0.14	0.13	-0.07	0.06	-0.04	-0.09	0.03
Vitispirane 1	1.053	2	-0.06	-0.03	0.02	0.11	0.00	0.01	0.08	-0.05
β-Damascenone	1.006	2	-0.03	-0.01	-0.01	0.09	-0.05	0.04	0.07	-0.06
TDN	1.002	2	-0.05	-0.02	0.01	0.11	-0.01	0.02	0.08	-0.04
Ethyl 2-methylbutyrate	0.978	8	-0.06	-0.05	0.05	0.03	-0.04	0.03	0.07	-0.09
Isoamyl octanoate	0.916	6	0.05	-0.12	0.11	-0.05	0.03	-0.02	-0.06	0.00
Ethyl decanoate	0.878	6	0.10	-0.07	0.05	-0.05	0.01	-0.01	-0.09	0.03
Ethyl 3-methylbutyrate	0.830	8	-0.05	-0.05	0.05	-0.01	-0.03	0.02	0.05	-0.07
Methyl octanoate	0.794	5	0.03	0.08	-0.11	0.06	-0.08	0.05	0.02	-0.02
Methyl decanoate	0.776	5	0.06	0.08	-0.12	0.04	-0.09	0.05	0.00	-0.01
Ethyl nonanoate	0.767	7	0.02	-0.10	0.08	0.02	0.02	0.00	-0.01	-0.02
Ethyl 9-decenoate	0.761	2	0.00	-0.03	0.01	0.08	0.00	0.01	0.03	-0.01
Isopentyl hexanoate	0.629	7	0.00	-0.05	0.05	-0.04	-0.02	0.01	-0.01	-0.04
Ethyl octanoate	0.619	7	0.05	-0.05	0.03	0.02	-0.01	0.01	-0.03	0.00

does not occur at cooled storage temperatures of 0 to 5°C over a 12-month period (Marais and Pool 1980, Pérez-Coello et al. 2003). For all white wines, diethyl succinate was higher in the 40°C treatment; however, the Sauvignon blanc wines had substantially higher initial concentrations compared to the other varieties.

The Chardonnay (W4) wines were positively correlated with the canned vegetable sensory attribute and negatively correlated with compounds that were significantly different due to temperature treatment, including linalool, TDN, and vitispirane 1 and 2. The Chardonnay wines were the only white wines to spend time in new oak barrels and underwent partial malolactic fermentation. These wines were significantly higher in ethyl lactate, produced through malolactic fermentation (Boido et al. 2009), and both (*E*)- and (*Z*)-oak lactones, found in wines fermented in oak (Ibern-Gómez et al. 2001) (data not presented). It is possible that the canned vegetable sensory attribute was associated with the oxidative formation of methional (Silva Ferreira and Guedes De Pinho 2004), which can produce a cooked vegetable character in white wines (Escudero et al. 2000). However, the analytical conditions used within this study may not have been sufficiently sensitive to detect this trace compound.

In the current study, the samples that were exposed to heat tended to have higher concentrations of TDN and vitispirane 1 and 2 and lower concentrations of isoamyl acetate, hexyl acetate, and 2-phenylethyl acetate, in agreement with previous research on wines stored at elevated temperatures (Leino et al. 1993, Marais and Pool 1980, Ramey and Ough 1980). In a study on the influence of storage temperature on the volatile compounds of young white wines, there was a decrease in ethyl esters and acetates during uncontrolled storage conditions and times (1, 2, 3, and 4 years and recently bottled wines) (Pérez-Coello et al. 2003). Wines that were stored chilled (0 and 10°C) underwent fewer chemical alterations, thus retaining their youthful wine aromas, as found in other research (Marais and Pool 1980).

It is likely that variety, wine style, initial bottled wine quality, and the stage of bottle maturation will determine the degree that elevated temperatures impact wine sensory characteristics. In a previous study, noticeable changes in

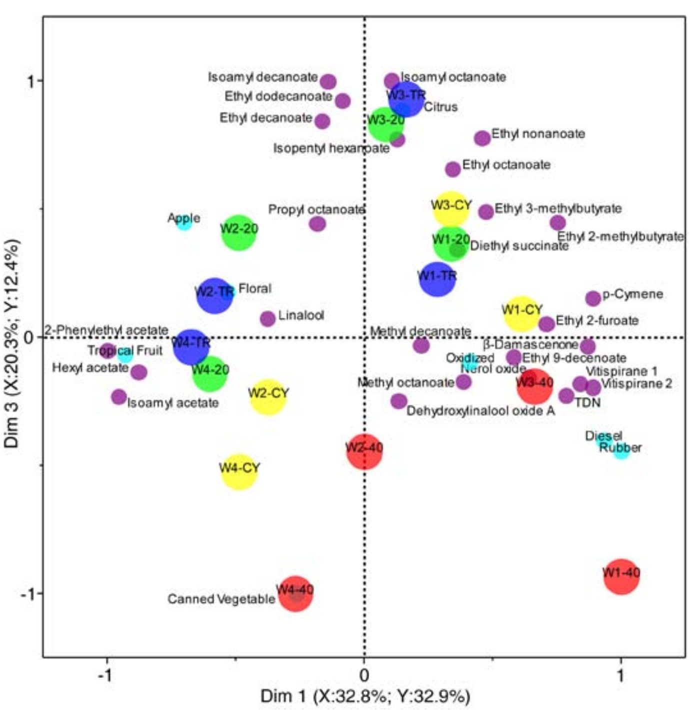

Figure 3 Partial least squares analysis of white wine products. Purple circles represent volatile composition loadings (X matrix), light blue circles represent sensory attribute loadings (Y matrix), and large circles represent sample scores for factor 1 (Dim1) and factor 3 (Dim3). Sample codes listed in Table 1. Treatments: car trunk (TR), constant 20°C (20), cycled 20°C /40°C (CY), and constant 40°C (40).

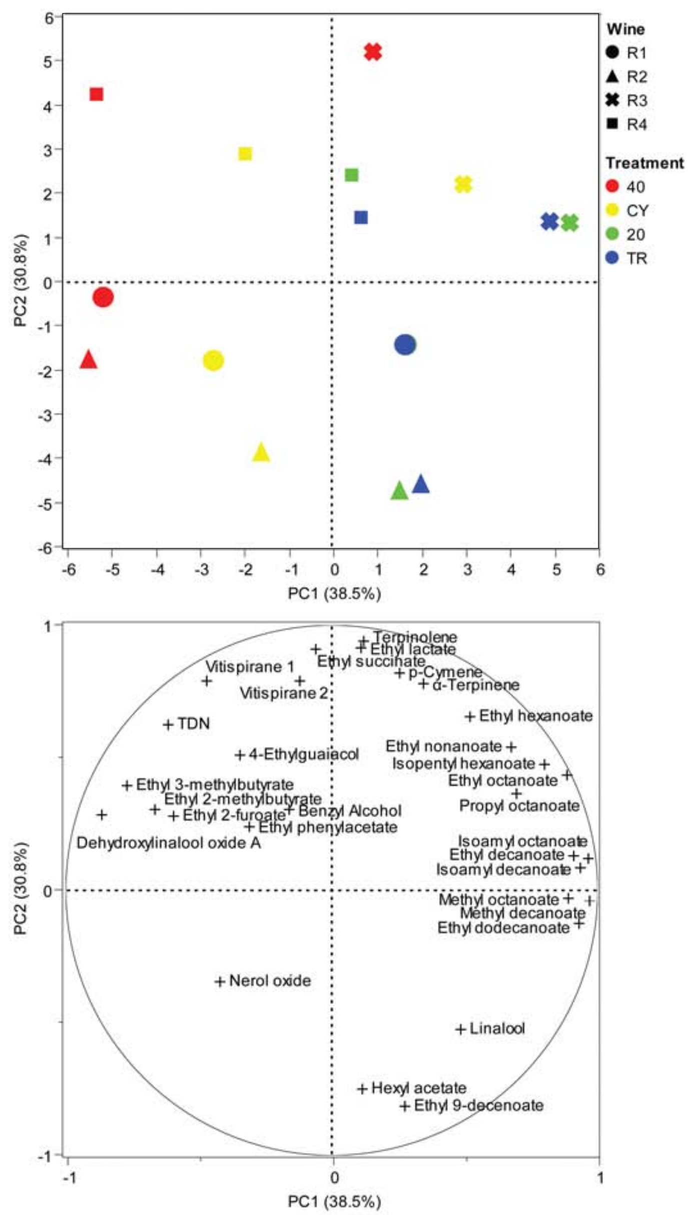

Figure 4 Principal component analysis of red wine products. Sample codes listed in Table 1. Treatments: car trunk (TR), constant 20°C (20), cycled 20°C /40°C (CY), and constant 40°C (40).

wine aroma of oaked and unoaked Chardonnays occurred between five and nine days of storage at elevated temperatures, respectively (De La Presa-Owens and Noble 1997). In contrast, in Chenin blanc, Riesling, and Colombard bottled under screwcap, the young wine bouquet remained unchanged over a 12-month period at storage temperatures of 0 and 10°C (Marais and Pool 1980). In addition, there was a dramatic loss of young wine bouquet and the development of a maturation bouquet over the same period when the wines were stored at 20 and 30°C. Samples of Colombard stored for two years at 0°C showed no deterioration of young wine bouquet, and the 10°C storage temperature decreased only slightly.

A loss of fruity and floral aromas in young white wine during storage is associated with the hydrolytic loss of acetates and esters (Marais and Pool 1980, Pérez-Coello et al. 2003, Ramey and Ough 1980). The enhancement of aged characters has been correlated with the oxidative formation of methional and phenylacetaldehyde (Silva Ferreira and Guedes De Pinho 2004) and increases in TDN and vitispirane (Simpson 1979) due to acid hydrolysis of aroma precursors (Francis et al. 1994, Versini et al. 2001).

These studies and the results of the current study emphasize the importance of storage temperature for the maintenance of fresh aromas. From the current study, it is difficult to determine the minimum length of time that is required to cause the observed changes in the white wine sensory attributes. However, this study clearly reinforces the need for cooled storage conditions for white wine in transit and in storage.

Red wines. Little research has been conducted to assess the sensory changes in red wines stored at different temperatures. In the current study only the dry fruit and canned vegetable sensory attributes were significantly different due to treatment, indicating that the red wines were relatively unchanged due to the treatments imposed. However, that may not be the case for all red wines.

Changes in red wine volatile composition were similar to changes in the white wines assessed in that the constant 20°C and trunk treatment wines were not greatly modified while the constant 40°C treatment was clearly changed. The constant 40°C treatment wines were characterized by lower concentrations of linalool, ethyl octanoate, nonanoate, decanoate, and dodecanoate, methyl octanoate and decanoate, isoamyl octanoate and decanoate, isopentyl hexanoate, and ethyl 9-decanoate and by higher concentrations of ethyl 2-furoate, ethyl phenylacetate, dehydroxylinalool oxide A, *p*-cymene, TDN, and vitispirane 1 and 2. Thus, there were substantial changes to the volatile composition of the wines.

Previous research has examined the effects of temperature on a red blend of Zinfandel, Petite Syrah, and Gamay at 28, 32, 38, 43, and 47°C over three weeks with high and low levels of SO_2 (Ough 1985). The concentration of isoamyl acetate decreased with increasing temperature; ethyl hexanoate, octanoate, and decanoate showed no clear relationship to the temperature treatment; and the level of SO_2 had no obvious effect over the period (Ough 1985).

Increases in TDN and vitispiranes in wines can be attributed to hydrolysis of multiple glycosylated precursors under acidic conditions, which can be accelerated by elevated temperatures (Francis et al. 1994, Versini et al. 2001, Winterhalter 1991, Winterhalter et al. 1990). Temperature and pH are particularly important to the formation of both TDN and vitispiranes (Silva Ferreira and Guedes De Pinho 2004). In addition, *p*-cymene can be produced through heated acid hydrolysis of aroma precursor fractions from grapes (Schneider et al. 2001, Williams et al. 1982).

The loss of linalool due to increased storage temperature is undesirable in citrus juices (Perez-Cacho and Rouseff 2008) and has been attributed to the coinciding increase in α-terpineol (Pérez-López et al. 2006). The loss of linalool and increase in α-terpineol has also been observed in heated black currant juice (Varming et al. 2004). It is suggested that the transformation of linalool to α-terpineol occurs through the protonation of linalool's hydroxyl group (Haleva-Toledo et al. 1999). It was previously observed that the degradation of linalool, and formation of linalool oxides, was significantly greater at 45°C when compared to 15°C (Silva Ferreira et al. 2002). In the current study, dehydroxylinalool oxide A and linalool were negatively correlated, with dehydroxylinalool oxide A positively correlated with the constant 40°C treatment. The lack of a significant increase in α-terpineol suggests that, in wine, linalool predominantly forms linalool oxides because of elevated temperature storage.

The major observation in the red wine study was a clear separation of the constant 40°C heat treatment wines from the other three treatments due to changes in volatile composition. However, a change in volatile composition was not coupled to differences in the majority of the sensory descriptors used in this study. As the study was conducted with only a few commercial wines, the sensory results may not reflect potential changes in other red wines. This hypothesis is supported by the observation of substantial changes to the volatile composition of the wines under the treatment conditions. These compositional changes may have more significant sensory consequences for other red wines. Further research is warranted to more clearly understand the influence of temperature on red wine aroma and composition.

Conclusion

The objective of this study was to explore the sensory repercussions of adverse temperature conditions on white and red wines. The wines were exposed to simulated shipping conditions and then evaluated using sensory descriptive analysis. There was a significant impact of the constant 40°C heat treatment on the aromatic properties of the wines. The 40°C treatment produced the most significant differences among the white wines by increasing diesel, oxidized, and rubber aromas and decreasing citrus, floral, and tropical fruit aromas. The magnitude of the effect was significant, although less pronounced, in the red wines, with increased dried fruit and canned vegetable aromas.

PLS analysis of the white wines identified compounds that may be useful markers, including vitispirane 1 and 2, TDN, *p*-cymene, and a number of esters and acetates, for monitoring wine product development on-shelf or for confirming that wines have not experienced any adverse conditions during shipping. Volatile analysis showed a number of compounds were affected by the temperature treatments. However, an untargeted analytical method was used to measure volatiles, and thus it is possible that other compounds could be altered due to elevated temperatures. Future research should document the changes in other varietal wines under varied temperature conditions to better understand the changes in wine due to transport and storage.

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