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Identification of Chemical Markers of Commercial Tropical Red Wine Candidates for the São Francisco Valley Geographical Indication

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Abstract

The aim of this study was to identify chemical markers of commercial tropical red wines with the potential to apply for the Geographical Indication-GI São Francisco Valley. Volatile organic compounds of nine different commercial red wines from the São Francisco Valley, located in the Caatinga region of Brazil, that meet the classic oenological parameters for commercialization, were extracted and separated by the HS-SPME/GC–MS technique, and identified. A total of 103 volatile compounds were identified and classified into 13 chemical groups, of which the esters and alcohols were the majority groups. Similarities were found in the composition of 27 compounds identified in all wines; however, the cultivars influenced the distinction of volatiles expressed exclusively in only one type of wine. Among these, 22 compounds were highlighted for having been identified for the first time in wines, such as 3-phenyl-undecane and 4-phenyl-decane. These exclusive compounds are possible markers which confirm the typicality of tropical red wines of this region, and can contribute to the qualitative description and enhancement of regional identity for wines from the São Francisco Valley.

Keywords *Vitis vinifera L.* · Typicality marker · Tropical wine · Volatile compound

Introduction

The aromatic quality of red wines is directly related to their volatile composition, with more than 1000 metabolite compounds among the alcohols, organic acid esters, aldehydes, ethers, ketones, and terpenes. These compounds are present in different concentrations, having been identified in several red wines (Vilanova et al. 2012; Jiang et al. 2013; Sánchez-Palomo et al. 2017; Mota et al. 2020). The different concentrations among the volatiles present in wines contribute to their complexity and molecular diversity due to interactions between the metabolites, providing specific typicalities in function of synergetic and antagonistic effects among them (Bonino et al. 2003).

The complexity of aromas in red wines comes from different sources and are described and characterized by three

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types, namely, the first group originates from the specific grape variety (primary aromas); the second group is formed during winemaking, and may vary according to the types of yeast and elaboration/fermentation protocols (secondary aromas); and the third group is formed during the maturation/aging of wines in oak barrels, as well as during bottle storage (tertiary aromas) (Drappier et al. 2017; Ruiz et al. 2019). These three types of aromas together form what is called the "bouquet" of wines. Complexation/degradation/evolution reactions of volatile compounds may occur during the whole production and aging process of wines in barrels, and the formation of new aromas may also occur. These new volatile compounds are associated with five families of aromatic compounds: furans, lactones, phenolic aldehydes, volatile phenols, and phenyl ketones (Ruiz et al. 2019).

Knowing the identity (origin, formation, and degradation) of the compounds responsible for the aroma and flavor of wines helps to understand the consequences of climate impacts, seasonal conditions, planting decisions, types of grapes, and processing, thus providing improvements in viticulture and winemaking practices (Parker et al. 2017), in addition to assisting in the geographical typification of wines.

It is estimated that 132.16 million liters of fine wines, elaborated with grapes of European varieties (*Vitis vinifera* L.), were consumed in Brazil in 2019, of which 114.175 million liters were imported wines and 17.988 million liters were national wines (Mello and Machado 2020). The Northeast region represented 13.85% of the national wine area, whose viticulture is concentrated in the São Francisco Valley, and has the exceptionality of producing two harvests per year (Mello and Machado 2020).

The São Francisco Valley is the second largest producer of fine wines in the country, and is located in the Northeast of Brazil. The region belongs to the caatinga biome, with a tropical semi-arid climate with high annual average temperatures (26.5 °C), high solar radiation rates (over 3,000 MJ m^{-2} $year^{-1}$), and low rainfall (450–500 mm. $year^{-1}$) (Pereira 2020). Seven wineries have about 700 hectares of vineyards, with an annual production of 7 million liters of fine wines per year, being responsible for 15% of the national production of fine wines, of which 29% are red wines, as well as young and aging wines. They can be marketed about 90 days after harvest or after a period of 4 to 12 months in oak barrels, respectively (Pereira et al. 2018; Pereira 2020). An association of the region's producers/wineries (Vinhovasf) is seeking Geographical Indication (GI) for the still and sparkling wines (*Vitis vinifera* L.) of the São Francisco Valley. This request should occur with the aim of obtaining a quality seal for the products of the region. Therefore, works that enable characterizing and describing the physical–chemical composition of commercial wines are fundamental.

Thus, this study aimed to perform a characterization of the volatile composition of commercial red wines of the VSF in order to contribute to the scientific community, as well as producers in seeking the GI of wines from the region. To our knowledge, this work is innovative and was the first carried out in this sense, even enabling the identification and quantification of volatile compounds, which had not been previously reported that are present in tropical red wines from the Brazilian Northeast.

Material and Methods

Samples and Classical Analyses

This research studied nine commercial red wines from the caatinga biome, whose products will be in the São Francisco Valley Geographical Indication. The wines were stored at a temperature of 16 ± 1 °C until analysis for a period not exceeding 6 months. The characteristics and specificities of each wine are shown in Table 1. The set of samples was

Table 1 Description of the tropical red wine samples from the São Francisco Valley

Wine (Code)	Cultivars	Winery	Vintage	Lot	MT (months)
AB	Alicante Bouschet	9° 24″S; 40° 29′ W	2014	n.d	9
CS	Cabernet Sauvignon	9° 24″S; 40° 29′ W	2015	L1806A15	0
CS/SY	Cabernet Sauvignon/Syrah	9° 24″S; 40° 29′ W	2017	L1832D16	0
PR	Cabernet Sauvignon/Syrah/Alicante Bouschet/ Touriga Nacional/Aragonês	9° 24″S; 40° 29′ W	2013	L17112A08	12
RC	Ruby Cabernet	8°47′S;39° 49′ W	2016	L20/072016	0
RS	Cabernet Sauvignon/Syrah/Alicante Bouschet	9° 24″S; 40° 29′ W	2014	L1833D11	6
SY	Syrah	9° 24″S; 40° 29′ W	2015	L1819D16	0
TN	Touriga Nacional	9° 24″S; 40° 29′ W	2014	L1837E03	9
TP	Tempranillo	9° 24″S; 40° 29′ W	2015	L1820B26	0

MT, maturation time in French oak barrels; *n.d.*, not declared

selected based on the origin of the processed *Vitis vinifera* L. grape. Wines produced by almost all of the grape varieties produced in the region were selected. As they are commercial wines, each one is aged or not at different times, and represent more than 65% of all red wines produced in the region. Some classic enological parameters were determined in order to confirm the quality of commercial wines according to Brazilian and international standards and are shown in Table 2 (OIV 2014). The samples were composed by three bottles (750 mL) from the same batch and the experiments were carried out in triplicate. Red wines were stored at 16° ± 1 °C until the analysis for a period not exceeding 6 months.

Extraction and Chromatographic Analyses to Identify Volatile Compounds in Red Wines

The volatile compounds were extracted by headspace solid-phase microextraction (HS-SPME) adapted from Barros et al. (2012). The fiber used was Polydimethylsiloxane/Divinylbenzene (PDMS/DVB) (Supelco, Bellafonte, PA, USA) and it was conditioned according to the manufacturer's instructions prior to the extraction. First, 30 mL of red wine was transferred to a 100 mL glass vial with a screw cap containing one centre hole of 3 mm radius and a Teflon-lined septum. The volatile compounds were extracted by placing the flask in a 45 °C water bath with internal magnetic stirring. The sample reached equilibrium in 15 min and was then exposed to the fiber for 30 min. Blank analyses were carried out for the dynamic headspace entrainment on the SPME extraction procedure.

A 7890B gas chromatograph (GC) coupled to an Agilent® Technologies 5977B (Little Falls, DE, USA) mass spectrometer (MS) and a Varian® VF-5 MS low bleed/MS fused-silica capillary column (5% phenyl/95% PDMS, 60 m × 0.25 mm I.D. × 0.25 µm film thickness) were used to separate and identify the volatiles collected by SPME. The carrier gas was helium at a 1.2 mL minute $^{-1}$ flow rate. The samples were injected by placing the SPME fiber at the entrance of the GC at 250 °C and splitless injection mode was used with a desorption time of 5 min. The initial oven temperature was 40 °C, which was maintained for 10 min, increased to 250 °C at 7 °C per minute, and then maintained at 250 °C for 5 min. The mass spectrometer was operated in electron impact mode with a source temperature of 250 °C, an ionising voltage of 70 eV, and a scanning range from 35 to 350 m/z at 3.33 scans/s. The transfer line was held at 250 °C. The SPME data were acquired and analyzed using the Mass Hunter software program (Agilent).

The compound identification was based on the comparison of their mass spectra with spectra from previously analyzed authentic compounds, data from the NIST/EPA/NIH Mass Spectral Database (Version 2.2 2014), Mass Spectral Library (Scientific Instrument Services, Ringoes, NJ, USA) or data published elsewhere, and compared to spectra and retention indices of reference compounds. The linear retention index (LRI) was calculated for each volatile compound using the retention times of a homologous series of C8–C20 n-alkanes and by comparing the LRI with those of authentic compounds analyzed under similar conditions to confirm the identification.

Statistical Analysis

Analysis of variance (ANOVA) was used in the classic oenological data associated with the Tukey mean difference test ($p < 0.05$) using the XLSTAT software version 5.03 (Addinsoft, New York, USA, 2014). The results of

Table 2 Classic enological parameters of the commercial red wines studied from the São Francisco Valley

Wine (code)	Density	pH	Alcohol degree (% v/v at 20 °C)	Total acidity (meq L^{-1})	Volatile acidity (meq L^{-1})	Free SO_2 (mg L^{-1})
AB	0.9962 ^{e} ± 0.00	4.08^{c} ± 0.02	13.16 ^{b} ± 0.00	74.23 ^{d} ± 0.00	4.59 $^{b.c}$ ± 0.51	34.88 ^{b} ± 0.00
CS	0.9959 ^{f} ± 0.00	4.16 $^{a.b}$ ± 0.02	12.04 ^{e} ± 0.00	72.00 $^{d.e}$ ± 0.04	2.04 ^{e} ± 0.00	8.96 ^{e} ± 0.00
CS/SY	0.9968 ^{d} ± 0.00	4.16 $^{a.b}$ ± 0.02	12.12 ^{e} ± 0.00	66.74 $^{e.f}$ ± 0.00	3.26 ^{d} ± 0.35	17.78 ^{d} ± 0.00
PR	0.9995 ^{a} ± 0.00	4.08 ^{c} ± 0.00	13.16 ^{b} ± 0.00	86.61 ^{a} ± 0.07	4.65 $^{b.c}$ ± 0.41	15.36^{c} ± 0.00
RC	0.9991 ^{c} ± 0.00	4.13^{b} ± 0.00	13.51 ^{a} ± 0.00	84.91 $^{a.b}$ ± 0.02	4.01 $^{c.d}$ ± 0.41	nd
RS	0.9991 ^{b} ± 0.00	4.08 ^{c} ± 0.00	12.21 ^{d} ± 0.00	80.83 $^{b.c}$ ± 0.04	5.16 ^{b} ± 0.12	34.24 ^{b} ± 0.00
SY	0.9954 h ± 0.00	4.17^{a} ± 0.01	10.61 ^{f} ± 0.00	74.38$^{c.d}$ ± 0.00	4.18 $^{b.c.d}$ ± 0.18	15.04$^{c.d}$ ± 0.03
TN	0.9991 $^{b.c}$ ± 0.00	4.08 ^{c} ± 0.00	13.16 ^{b} ± 0.00	81.85 $^{a.b}$ ± 0.02	6.89 ^{a} ± 0.12	39.04 ^{a} ± 0.01
TP	0.9958 g ± 0.00	4.17^{a} ± 0.01	12.81 ^{c} ± 0.00	66.36 ^{f} ± 0.00	6.52 ^{a} ± 0.54	16.64 ^{c} ± 0.01
Limits[1]			**8.6 to 14**	**40 to 130**	**Max 20**	**Max 300**

[1]Brasil, 2018; *nd*, not detected; *Max*, maximum; *CS*, Cabernet Sauvignon; *CS/SY*, Cabernet Sauvignon/Syrah; *AB*, Alicante Bouschet; *SY*, Syrah; *TP*, Tempranillo; *PR*, Cabernet Sauvignon/Syrah/Alicante Bouschet/Touriga Nacional/Aragonês; *RS*, Cabernet Sauvignon/Syrah/Alicante Bouschet; *TN*, Touriga Nacional; *RC*, Ruby Cabernet; SO_2, total sulfur dioxide. Means followed by the same letter do not differ by the Tukey test ($p < 0.05$)

the volatile compounds were auto-scaled using MATLAB version 7.10.0.499 (The Mathworks, Inc., Natick, MA, R2010a) to perform the comparison of the abundance of the area obtained in each sample, then these treated data were submitted to Pearson's correlation analysis (r), principal component analysis ($p < 0.05$), and hierarchical cluster analysis using XLSTAT software version 5.03 (Addinsoft, New York, USA, 2014).

Results

Classical Analyses

Table 2 presents the results for the classic enological parameters of the commercial tropical wine samples. Significant differences ($p<0.05$) were observed in these parameters, however, all results are consistent with Brazilian and international legislation (OIV 2014; Lima et al. 2015; Padilha et al. 2017; Brasil 2018; Oliveira et al. 2019). It is worth emphasizing that the pH presented very high values, which is justified by the high concentrations of potassium in the soils of the VSF, as well as the high temperatures during the grape ripening, which reduce the organic acids by degradation of malic acid (Lima et al. 2015; Oliveira et al. 2019; Jackson 2020; Pereira 2020).

Determination of Volatile Compounds in Red Wines from the São Francisco Valley

A total of 103 volatile compounds were identified by HS-SPME-CG-MS in the samples of commercial red wines in this study, and the percentage area for each wine is shown in Table 3. The total number of compounds identified in each wine was distinguished according to the varieties used in the elaboration, such as TP (71), SY (69), AB (68), PR (67), RS (60), and CS/SY (50), and similar in the CS, TN, and RC samples (65 compounds). Among the total number of volatile compounds identified in this study, 13 were only identified in one type of red wine, being 1-pentanol and 2,4-dihydroxy-2,5-dimethyl-3(2H)-furanone (RS); hexanoic acid, 2-ethyl-1-hexanol, 4-ethylphenol, 4-ethyl guaiacol, 6-phenyl-dodecane, (Z)-9-tetradecenoic acid, ethyl 9-hexadecenoate, and methyl 11-octadecenoate (RC); ethyl 2,4-hexadienoate (PR), ethyl benzoate and (E)-9-hexadecenoic acid (AB).

The volatile compounds were grouped into 13 chemical classes including esters (36 compounds), alcohols (16), terpenes (11), aromatics (10), acids (9), aldehydes (5), phenols (4), furans (4), hydrocarbons (3), C13-norisoprenoids (2), ketone (1), ether (1), and pyrane (1). A comparison of the sum for the total areas of each chemical group is shown in Fig. 1. With the exception of esters and C13-norisoprenoids, all classes showed significant differences within a class between at least two red wines according to Conover-Iman's non-parametric comparison test ($p < 0.05$).

The esters class was the majority in the number of identified compounds (a total of 36), with 14 being identified in all of the red wines analyzed. The esters class was also the majority in terms of percentage of chromatographic area, as can be seen in Table 3. The CS and SY wines obtained the largest number of compounds (30 and 29, respectively), representing 83.61% and 60.91% of the total chromatographic area, followed by the AB and PR wines (28 compounds each), representing 79.72% and 80.90% of the total area, respectively. The most abundant esters in terms of area percentage were ethyl octanoate (36.65% and 36.09% in AB and CS wines, respectively), diethyl succinate (22.02% in wine from PR), and ethyl decanoate (18.56% in wine from AB). Ethyl 2.4-hexadienoate (4.42% in PR wine), ethyl hexanoate (3.62% in CS wine), ethyl isopentyl succinate (2.74% in RS wine), ethyl 2-methylbutanoate (2. 26% in CS wine), ethyl butanoate (1.89% in AB wine), ethyl glutarate (1.34% in TP wine), ethyl 9-decenoate (1.05% in PR wine), and β-phenethyl acetate (1.01% in CS/SY wine) are also highlighted.

The alcohol class was the second majority in the number of compounds (Table 3) with 16 being identified, of which 6 are present in all nine types of wine, including 3-methyl 1-butanol, 1-hexanol, 3-ethyl-4-methyl-1-pentanol, phenylethyl alcohol, 1-decanol, and hexadecanol. It was also the second major class regarding the area percentage, ranging from 10.72 to 65.97% for wines from the CS/SY and RC cultivars, respectively, which differed significantly among themselves (Fig. 1). Some compounds in this class stood out for area percentage, such as phenylethyl alcohol (64.80% in RC wine), 2.3-butanediol (2.86% in CS wine), 3-methyl 1-butanol (2.66% in TN wine), and 1-hexanol (1.99% in SY wine).

A total of 11 compounds were identified in the terpenes class, with the majority in PR and TP wines with 8 compounds each. No terpenes showed chromatographic area > 1%, and the sum of the total area varied between 0.18 and 1.28% (in CS and PR wines, respectively) (Table 3), differing significantly among themselves (Fig. 1).

A total of 10 compounds were classified in the aromatic group, of which 9 compounds were identified in the RC and TN wines. The total chromatographic area of this class of compounds varied from 0.22 to 1.02% (in RS and NT wines, respectively), differing significantly (Fig. 1).

There were 9 compounds identified for the acids class, with a variation in the total area from 0.62 to 3.52% (Table 3) in the RC and CS/SY wines, respectively, and decanoic acid (representing a chromatographic area of 2.79% in CS/SY wine) and undecanoic acid (1.09% in PR wine) compounds are highlighted.

Table 3 Volatile compounds identified in the red wines of the São Francisco Valley by HS–SPME–GC–MS

Code	Volatile compound	Chemical family	LRI (lit)	LRI (cal)	(%) of total peak area									
					CS	CS/SY	RC	SY	TP	PR	RS	AB	TN	Odor description[1]
99	(E)-9-Hexadecenoic acid	Acid	1942	1939	nd	nd	nd	nd	nd	nd	nd	0.12 ± 0.09	nd	Waxy, creamy, fatty, soapy
91	(Z)-9-Tetradecenoic acid	Acid	1783	1774	nd	nd	0.13 ± 0.05	nd	nd	nd	nd	nd	nd	
54	Decanoic acid	Acid	1373	1378	1.64 ± 0.59	2.79 ± 0.32	0.27 ± 0.06	1.22 ± 0.38	1.62 ± 0.27	1.54 ± 0.61	1.41 ± 0.53	1.43 ± 0.63	1.90 ± 1.05	Rancid, sour, fatty, citrus
75	Dodecanoic acid	Acid	1568	1568	0.11 ± 0.07	0.45 ± 0.09	0.05 ± 0.00	0.22 ± 0.16	0.25 ± 0.08	0.12 ± 0.07	0.11 ± 0.07	nd	0.22 ± 0.11	Coconut, fatty, waxy
13	Hexanoic acid	Acid	990	998	nd	nd	0.06 ± 0.01	nd	nd	nd	nd	nd	nd	Slightly, waxy, fatty
100	n-Hexadecanoic acid	Acid	1968	1960	0.05 ± 0.01	0.28 ± 0.20	0.05 ± 0.03	0.15 ± 0.09	0.04 ± 0.01	0.14 ± 0.17	0.11 ± 0.08	0.12 ± 0.03	0.10 ± 0.13	Waxy, fatty
97	Pentadecanoic acid	Acid	1867	1866	0.02 ± 0.01	nd	0.01 ± 0.01	0.02 ± 0.01	tr	nd	nd	0.06 ± 0.04	nd	
90	Tetradecanoic acid	Acid	1768	1762	0.05 ± 0.03	nd	0.05 ± 0.02	0.08 ± 0.04	0.02 ± 0.01	nd	0.08 ± 0.03	0.20 ± 0.16	0.12 ± 0.11	Waxy, fatty, soapy, coconut
65	Undecanoic acid	Acid	1475	1478	0.42 ± 0.25	nd	nd	nd	0.61 ± 0.10	1.09 ± 0.59	nd	nd	nd	Waxy, creamy, cheese, fatty, coconut
	Total Acids				**2.29**	**3.52**	**0.62**	**1.68**	**2.54**	**2.89**	**1.71**	**1.94**	**2.33**	
40	1-Decanol	Alcohol	1273	1272	0.13 ± 0.04	0.10 ± 0.05	0.04 ± 0.01	0.09 ± 0.00	0.12 ± 0.06	0.13 ± 0.02	0.07 ± 0.02	0.13 ± 0.05	0.14 ± 0.05	Fatty, waxy, floral, orange, sweet, clean, watery
64	1-Dodecanol	Alcohol	1473	1474	0.21 ± 0.15	0.45 ± 0.17	0.13 ± 0.03	nd	0.24 ± 0.15	0.38 ± 0.39	0.19 ± 0.08	0.24 ± 0.17	0.37 ± 0.27	Earthy, soapy, waxy, fatty, honey, coconut
8	1-Hexanol	Alcohol	868	865	0.83 ± 0.26	0.70 ± 0.02	0.27 ± 0.09	1.99 ± 3.00	0.73 ± 0.21	0.46 ± 0.25	0.44 ± 0.16	0.42 ± 0.16	0.71 ± 0.25	Ethereal, fusel, oil, fruity, alcoholic, sweet, green
28	1-Nonanol	Alcohol	1173	1172	0.50 ± 0.12	0.37 ± 0.03	nd	0.22 ± 0.06	0.44 ± 0.10	0.54 ± 0.12	0.34 ± 0.18	0.26 ± 0.12	0.37 ± 0.15	Fresh, clean, fatty, floral, rose, orange, dusty wet, oily
2	1-Pentanol	Alcohol	765	< 800	nd	nd	nd	nd	nd	nd	0.19 ± 0.15	nd	nd	Balsamic, sweet, fusel like
4	2,3-Butanediol	Alcohol	788	< 800	2.86 ± 0.20	nd	nd	nd	nd	nd	2.40 ± 0.27	0.04 ± 0.01	nd	Fruity, creamy, buttery
18	2-Ethyl-1-hexanol	Alcohol	1030	1034	nd	nd	0.17 ± 0.03	nd	nd	nd	nd	nd	nd	Citrus
93	2-Heptadecanol	Alcohol	1802	1799	0.01 ± 0.01	nd	nd	0.01 ± 0.00	0.01 ± 0.00	0.06 ± 0.06	nd	0.02 ± 0.01	nd	
85	2-Hexadecanol	Alcohol	1702	1698	nd	nd	tr	0.01 ± 0.00	0.01 ± 0.00	0.01 ± 0.01	0.01 ± 0.00	0.02 ± 0.01	nd	

Table 3 (continued)

Code	Volatile compound	Chemical family	LRI (lit)	LRI (cal)	(%) of total peak area									
					CS	CS/SY	RC	SY	TP	PR	RS	AB	TN	Odor description[1]
49	2-Undecanol	Alcohol	1308	1304	0.08 ± 0.04	nd	0.04 ± 0.01	0.23 ± 0.32	0.06 ± 0.02	0.05 ± 0.01	nd	0.04 ± 0.01	nd	Waxy, fatty, clean, oily, fresh, fishy, nut
17	3-Ethyl-4-methyl-1-pentanol	Alcohol	1023	1023	0.06 ± 0.03	0.04 ± 0.01	0.07 ± 0.01	0.08 ± 0.11	0.02 ± 0.01	0.04 ± 0.04	0.01 ± 0.01	0.04 ± 0.01	0.02 ± 0.01	
1	3-Methyl 1-butanol	Alcohol	736	< 800	1.74 ± 1.49	1.00 ± 0.27	0.27 ± 0.04	1.79 ± 0.75	2.24 ± 0.55	2.17 ± 0.57	2.60 ± 2.01	0.31 ± 0.50	2.66 ± 2.36	Fusel, oil, alcoholic, whiskey, fruity, banana
11	3-Methyl 2-hexanol	Alcohol	909	879	nd	0.06 ± 0.01	0.15 ± 0.06	0.04 ± 0.02	nd	nd	nd	nd	nd	
98	Hexadecanol	Alcohol	1884	1880	0.02 ± 0.01	0.05 ± 0.01	0.01 ± 0.01	0.04 ± 0.01	0.03 ± 0.00	0.03 ± 0.01	0.02 ± 0.00	0.06 ± 0.04	0.03 ± 0.02	Waxy, clean, greasy, floral,
21	Octanol	Alcohol	1075	1075	0.24 ± 0.15	0.16 ± 0.03	nd	0.20 ± 0.24	0.10 ± 0.06	0.46 ± 0.65	0.40 ± 0.41	0.13 ± 0.03	0.18 ± 0.11	Waxy, green, orange, aldehydic, rose, mushroom
23	Phenylethyl alcohol	Alcohol	1116	1110	4.04 ± 1.44	44.23 ± 3.41	64.80 ± 5.96	29.71 ± 3.77	21.26 ± 7.26	8.60 ± 10.96	21.34 ± 3.60	14.76 ± 7.49	20.37 ± 10.23	Floral, rose, dried, rose flower, rose water
	Total alcohols				**10.72**	**47.15**	**65.96**	**34.41**	**25.27**	**12.94**	**28.00**	**16.47**	**24.84**	
63	(E)-2-Dodecenal	Aldehyde	1468	1465	0.12 ± 0.09	nd	nd	0.19 ± 0.18	0.08 ± 0.00	nd	nd	nd	nd	Citrus, metallic, mandarin, orange, waxy aldehydic
96	10-Octadecenal	Aldehyde	1863	1860	0.02 ± 0.01	nd	nd	0.04 ± 0.02	0.01 ± 0.00	0.03 ± 0.02	nd	nd	0.05 ± 0.06	
31	Decanal	Aldehyde	1205	1204	0.10 ± 0.11	0.08 ± 0.03	nd	0.14 ± 0.12	nd	nd	0.85 ± 1.39	0.03 ± 0.01	0.04 ± 0.01	Sweet, waxy, orange peel, floral
58	Dodecanal	Aldehyde	1409	1409	0.12 ± 0.19	0.19 ± 0.10	0.05 ± 0.04	0.05 ± 0.06	0.12 ± 0.09	0.14 ± 0.18	0.05 ± 0.06	0.04 ± 0.03	0.27 ± 0.32	Soapy, waxy, aldehydic, citrus, green, floral
38	Geranial	Aldehyde	1268	1267	0.10 ± 0.04	nd	0.07 ± 0.04	nd	0.18 ± 0.09	nd	nd	nd	nd	Citrus, lemon
	Total aldehydes				**0.46**	**0.27**	**0.13**	**0.42**	**0.40**	**0.17**	**0.90**	**0.07**	**0.36**	
86	2-Phenyl-undecane	Aromatic	1708	1703	nd	0.02 ± 0.00	0.01 ± 0.00	nd	0.01 ± 0.00	tr	0.01 ± 0.00	0.01 ± 0.01	0.02 ± 0.02	
82	3-Phenyl-undecane	Aromatic	1667	1668	nd	0.17 ± 0.03	0.06 ± 0.02	nd	0.15 ± 0.14	0.11 ± 0.07	nd	0.07 ± 0.02	0.34 ± 0.24	
74	4-Phenyl-decane	Aromatic	1546	1550	nd	0.06 ± 0.01	0.01 ± 0.00	nd	nd	0.03 ± 0.02	0.02 ± 0.01	0.03 ± 0.00	0.11 ± 0.04	
89	4-Phenyl-dodecane	Aromatic	1742	1749	0.02 ± 0.01	0.01 ± 0.00	0.01 ± 0.00	0.02 ± 0.01	0.03 ± 0.01	0.01 ± 0.01	0.02 ± 0.01	0.03 ± 0.02	0.03 ± 0.02	

Table 3 (continued)

Code	Volatile compound	Chemical family	LRI (lit)	LRI (cal)	(%) of total peak area									
					CS	CS/SY	RC	SY	TP	PR	RS	AB	TN	Odor description[1]
95	4-Phenyl-tridecane	Aromatic	1840	1839	0.02 ± 0.01	nd	nd	nd	0.02 ± 0.00	nd	nd	nd	0.07 ± 0.09	
71	5-Phenyl-decane	Aromatic	1535	1542	nd	0.08 ± 0.00	0.02 ± 0.02	0.04 ± 0.06	0.09 ± 0.09	0.04 ± 0.03	0.01 ± 0.01	0.04 ± 0.03	0.14 ± 0.12	
88	5-Phenyl-dodecane	Aromatic	1730	1737	0.04 ± 0.02	0.05 ± 0.01	0.01 ± 0.00	0.02 ± 0.01	0.05 ± 0.01	0.08 ± 0.10	0.04 ± 0.03	0.01 ± 0.01	0.04 ± 0.04	
80	5-Phenyl-undecane	Aromatic	1632	1638	0.09 ± 0.06	0.15 ± 0.02	0.04 ± 0.02	0.09 ± 0.11	0.11 ± 0.09	0.09 ± 0.06	0.06 ± 0.02	0.09 ± 0.05	0.18 ± 0.12	
87	6-Phenyl-dodecane	Aromatic	1726	1731	nd	nd	0.03 ± 0.01	nd	nd	nd	nd	nd	nd	
79	6-Phenyl-undecane	Aromatic	1628	1634	0.04 ± 0.04	0.06 ± 0.02	0.01 ± 0.01	0.02 ± 0.00	0.05 ± 0.03	0.05 ± 0.04	0.02 ± 0.01	0.03 ± 0.03	0.08 ± 0.08	
	Total aromatic				**0.21**	**0.61**	**0.22**	**0.19**	**0.51**	**0.43**	**0.17**	**0.31**	**1.02**	
52	1,2-Dihydro-1,5,8-trimethyl-naphthalene	C13-norisoprenoid	1354	1351	0.15 ± 0.03	nd	0.07 ± 0.02	0.17 ± 0.07	0.19 ± 0.05	0.20 ± 0.06	0.12 ± 0.07	0.17 ± 0.08	0.03 ± 0.01	Licorice
83	4-Isopropyl-1,6-dimethyl-naphthalene	C13-norisoprenoid	1674	1679	0.11 ± 0.04	0.23 ± 0.15	0.06 ± 0.01	0.08 ± 0.04	0.13 ± 0.07	0.11 ± 0.01	0.07 ± 0.03	0.04 ± 0.01	0.13 ± 0.04	
	Total C13-norisoprenoids				**0.25**	**0.23**	**0.13**	**0.25**	**0.31**	**0.32**	**0.19**	**0.22**	**0.16**	
84	2-Ethylhexyl octanoate	ester	1688	1693	0.02 ± 0.01	nd	nd	0.07 ± 0.03	0.03 ± 0.00	0.05 ± 0.04	0.03 ± 0.02	0.07 ± 0.03	nd	
10	2-Methylbutyl acetate	Ester	880	878	0.16 ± 0.15	nd	nd	0.43 ± 0.08	0.07 ± 0.03	0.11 ± 0.03	0.07 ± 0.01	0.18 ± 0.07	0.08 ± 0.08	Fruit, sweet banana, juicy fruit, fruity
61	2-Methylbutyl octanoate	Ester	1449	1450	0.03 ± 0.01	nd	0.02 ± 0.02	0.04 ± 0.03	0.10 ± 0.07	0.01 ± 0.01	0.05 ± 0.04	nd	0.02 ± 0.02	
60	3-Methylbutyl octanoate	Ester	1446	1447	0.12 ± 0.06	0.19 ± 0.03	0.13 ± 0.06	0.17 ± 0.10	0.24 ± 0.05	0.12 ± 0.05	0.11 ± 0.08	0.17 ± 0.10	0.17 ± 0.07	Sweet, oily, fruity, green, soapy, pineapple coconut
44	Bornyl acetate	Ester	1285	1286	nd	nd	nd	nd	nd	0.02 ± 0.00	nd	nd	0.01 ± 0.00	Woody, pine, herbal, cedar, spice
59	Ethyl isopentyl succinate	Ester	1432	1431	0.74 ± 0.20	0.83 ± 0.22	0.69 ± 0.03	0.63 ± 0.46	0.55 ± 0.13	0.83 ± 0.25	2.74 ± 3.77	0.54 ± 0.17	0.73 ± 0.25	
29	Diethyl succinate	Ester	1182	1182	20.88 ± 8.45	15.44 ± 0.60	9.43 ± 1.11	9.30 ± 2.28	13.43 ± 4.80	22.02 ± 7.73	17.83 ± 6.83	14.68 ± 5.15	19.92 ± 7.45	Mild, fruity, cooked, apple
22	Ethyl 2,4-hexadienoate	Ester	1097	1103	nd	nd	nd	nd	nd	4.42 ± 3.06	nd	nd	nd	Warm, fruity, anise, licorice, ether
6	Ethyl 2-methylbutanoate	Ester	849	842	2.26 ± 0.75	nd	0.27 ± 0.39	nd	nd	nd	2.17 ± 1.06	0.02 ± 0.01	0.03 ± 0.00	Fruity, estry, and berry

Table 3 (continued)

Code	Volatile compound	Chemical family	LRI (lit)	LRI (cal)	(%) of total peak area									
					CS	CS/SY	RC	SY	TP	PR	RS	AB	TN	Odor description[1]
35	Ethyl 2-phenylacetate	Ester	1246	1244	0.36 ± 0.45	1.97 ± 0.12	0.18 ± 0.06	1.49 ± 1.11	1.09 ± 0.86	0.31 ± 0.30	nd	0.15 ± 0.06	0.36 ± 0.22	Sweet, floral, honey, rose, balsamic, cocoa
56	Ethyl 9-decenoate	Ester	1387	1389	0.40 ± 0.01	0.78 ± 0.17	0.15 ± 0.03	0.25 ± 0.09	0.46 ± 0.13	1.05 ± 0.10	0.36 ± 0.12	0.43 ± 0.22	0.56 ± 0.03	Fruity, fatty
101	Ethyl 9-hexadecenoate	Ester	1977	1974	nd	nd	0.19 ± 0.11	nd	nd	nd	nd	nd	nd	
27	Ethyl benzoate	Ester	1171	1168	nd	nd	nd	nd	nd	nd	nd	0.29 ± 0.25	nd	Fruity, dry, musty, sweet, wintergreen
5	Ethyl butanoate	Ester	802	801	nd	nd	nd	1.14 ± 0.73	nd	nd	nd	1.89 ± 1.05	0.95 ± 1.34	Fruity, juicy, fruit, pineapple, cognac
57	Ethyl decanoate	Ester	1396	1398	14.85 ± 2.81	7.80 ± 0.61	6.51 ± 3.12	16.02 ± 5.87	16.62 ± 4.80	16.80 ± 5.37	11.71 ± 6.97	18.56 ± 8.20	16.13 ± 6.47	Sweet, waxy, fruity, apple, grape, oily brandy
77	Ethyl dodecanoate	Ester	1595	1596	0.46 ± 0.14	0.29 ± 0.04	0.40 ± 0.19	0.53 ± 0.14	0.53 ± 0.19	0.56 ± 0.16	0.42 ± 0.22	0.58 ± 0.29	0.55 ± 0.21	Mango, sweet, waxy, floral, soapy, clean
43	Ethyl glutarate	Ester	1283	1280	1.20 ± 0.12	nd	0.04 ± 0.05	0.97 ± 0.29	1.34 ± 0.35	0.02 ± 0.01	0.01 ± 0.01	nd	0.01 ± 0.01	
102	Ethyl hexadecanoate	Ester	1993	1994	0.04 ± 0.02	0.10 ± 0.01	0.88 ± 0.76	0.10 ± 0.02	0.13 ± 0.00	0.13 ± 0.05	0.11 ± 0.02	0.16 ± 0.10	0.13 ± 0.06	Mild, waxy, fruity, creamy, milky, balsam
15	Ethyl hexanoate	Ester	1000	1003	3.62 ± 0.91	1.40 ± 0.17	0.81 ± 0.38	1.61 ± 0.65	1.98 ± 0.24	2.78 ± 0.76	2.68 ± 0.55	2.76 ± 0.96	2.22 ± 0.44	Sweet, fruity, pineapple, waxy, green banana
7	Ethyl isovalerate	Ester	854	847	0.10 ± 0.03	nd	0.63 ± 0.75	0.01 ± 0.00	nd	nd	0.61 ± 0.48	0.07 ± 0.04	0.08 ± 0.05	Sweet, diffusive, estry, fruity, sharp, pineapple, apple, green
47	Ethyl nonanoate	Ester	1296	1297	0.17 ± 0.03	0.14 ± 0.03	0.07 ± 0.04	0.21 ± 0.05	0.18 ± 0.07	0.21 ± 0.08	0.08 ± 0.02	0.28 ± 0.08	0.15 ± 0.09	Fruity, rose, waxy, rum, wine natural tropical
30	Ethyl octanoate	Ester	1196	1198	36.09 ± 6.14	14.95 ± 0.24	7.72 ± 4.17	26.61 ± 7.47	30.12 ± 9.10	29.07 ± 11.13	25.98 ± 9.54	36.65 ± 7.63	25.27 ± 10.31	Fruity, wine, waxy, sweet, apricot, banana brandy, pear
39	Ethyl salicylate	Ester	1270	1268	0.03 ± 0.01	nd	tr	0.11 ± 0.06	nd	0.03 ± 0.01	nd	0.11 ± 0.03	nd	
92	Ethyl tetradecanoate	Ester	1794	1794	0.03 ± 0.01	0.01 ± 0.00	0.57 ± 0.24	0.02 ± 0.00	0.02 ± 0.00	0.02 ± 0.01	0.04 ± 0.03	0.04 ± 0.01	0.03 ± 0.02	Sweet, waxy, violet, orris

Table 3 (continued)

Code	Volatile compound	Chemical family	LRI (lit)	LRI (cal)	(%) of total peak area									
					CS	CS/SY	RC	SY	TP	PR	RS	AB	TN	Odor description[1]
78	Geranyl isovalerate	Ester	1606	1599	0.06 ± 0.04	0.09 ± 0.00	nd	0.04 ± 0.01	0.07 ± 0.02	0.05 ± 0.03	0.04 ± 0.01	0.05 ± 0.02	0.09 ± 0.04	Sweet, fruity, green, oily, herbal, fruity
16	Hexyl acetate	Ester	1011	1018	0.02 ± 0.00	0.02 ± 0.00	nd	0.01 ± 0.01	0.04 ± 0.03	0.04 ± 0.04	0.02 ± 0.01	nd	nd	Fruity, green, apple, banana, sweet
9	Isoamyl acetate	Ester	876	875	0.85 ± 0.17	0.68 ± 0.14	0.46 ± 0.06	nd	0.51 ± 0.06	0.70 ± 0.09	0.62 ± 0.09	0.70 ± 0.13	0.58 ± 0.16	Sweet, fruity, banana, solvent
81	Isoamyl decanoate	Ester	1646	1650	0.10 ± 0.03	0.50 ± 0.16	0.24 ± 0.17	0.16 ± 0.06	0.31 ± 0.17	0.44 ± 0.37	nd	0.29 ± 0.11	0.23 ± 0.19	Waxy, banana, fruity, sweet, cognac, green
36	Isoamyl hexanoate	Ester	1252	1250	0.03 ± 0.01	0.76 ± 0.75	0.02 ± 0.02	0.05 ± 0.01	0.05 ± 0.03	0.08 ± 0.07	0.03 ± 0.03	0.05 ± 0.03	0.04 ± 0.03	Fruity, banana, apple, pineapple, green
45	Isobornyl acetate	Ester	1286	1289	0.04 ± 0.00	0.09 ± 0.02	0.02 ± 0.01	0.07 ± 0.02	0.08 ± 0.03	0.06 ± 0.02	nd	0.07 ± 0.02	0.07 ± 0.03	Balsam, camphor, herbal, woody, sweet
51	Isobutyl octanoate	Ester	1348	1345	0.03 ± 0.02	nd	0.01 ± 0.00	0.03 ± 0.02	0.05 ± 0.02	nd	0.03 ± 0.02	0.05 ± 0.01	nd	Fruity, green, oily, floral
48	Isomenthol acetate	Ester	1305	1302	0.09 ± 0.07	nd	nd	0.10 ± 0.02	0.19 ± 0.22	0.13 ± 0.08	nd	0.06 ± 0.02	nd	
103	Methyl 11-octadecenoate	Ester	2115	2123	nd	nd	0.05 ± 0.03	nd	nd	nd	nd	nd	nd	
50	Methyl decanoate	Ester	1325	1326	0.03 ± 0.01	nd	nd	0.03 ± 0.01	0.05 ± 0.01	0.06 ± 0.03	0.04 ± 0.02	0.03 ± 0.02	0.06 ± 0.02	Oily, wine, fruity, floral
46	Propyl octanoate	Ester	1290	1293	0.04 ± 0.02	nd	0.02 ± 0.01	0.04 ± 0.01	0.06 ± 0.01	nd	nd	nd	0.08 ± 0.05	Coconut, caco, gin
37	β-Phenethyl acetate	Ester	1258	1256	0.75 ± 0.18	1.01 ± 0.08	0.90 ± 0.01	0.66 ± 0.26	0.73 ± 0.22	0.80 ± 0.19	0.56 ± 0.16	0.81 ± 0.39	0.78 ± 0.25	Floral, rose, sweet, honey, fruity tropical
	Total esters				**83.61**	**47.03**	**30.42**	**60.91**	**69.02**	**80.90**	**66.34**	**79.72**	**69.33**	
3	2-Ethyl-1-butanol, methyl ether	Ether	778	< 800	2.06 ± 1.50	nd	nd	0.62 ± 0.64	nd	nd	1.59 ± 2.64	0.08 ± 0.03	nd	
	Total ether				**2.06**	**0.00**	**0.00**	**0.62**	**0.00**	**0.00**	**1.59**	**0.08**	**0.00**	
32	2,3-Dihydrobenzofuran	Furan	1224	1220	nd	0.21 ± 0.12	0.05 ± 0.02	0.10 ± 0.08	0.05 ± 0.03	0.13 ± 0.12	0.16 ± 0.12	0.11 ± 0.13	0.06 ± 0.06	
12	2,4-Dihydroxy-2,5-dimethyl-3(2H)-furanone	Furan	989	995	nd	nd	nd	nd	nd	nd	0.02 ± 0.01	nd	nd	Fruity, green, earthy, beany, vegetable metallic
14	2-Pentyl Furan	Furan	993	999	nd	0.04 ± 0.02	nd	0.02 ± 0.01	nd	nd	nd	nd	nd	Sweet, citrus, herbal, green, celery, spicy minty, woody

Table 3 (continued)

Code	Volatile compound	Chemical family	LRI (lit)	LRI (cal)	(%) of total peak area									
					CS	CS/SY	RC	SY	TP	PR	RS	AB	TN	Odor description[1]
34	5-Hydroxymethylfurfural	Furan	1233	1230	nd	nd	nd	nd	0.38 ± 0.49	0.03 ± 0.01	nd	nd	0.11 ± 0.08	Fatty, buttery, musty, waxy, caramellic
	Total furans				**0.00**	**0.25**	**0.05**	**0.11**	**0.43**	**0.16**	**0.18**	**0.11**	**0.16**	
72	2,6,10-Trimethyltetradecane	Hydrocarbon	1541	1545	nd	0.04 ± 0.00	nd	0.02 ± 0.01	0.02 ± 0.00	nd	nd	0.01 ± 0.01	0.03 ± 0.02	
41	2,6,11-Trimethyldodecane	Hydrocarbon	1275	1275	nd	nd	nd	nd	nd	nd	nd	0.03 ± 0.02	0.07 ± 0.05	
66	3-Butyl-1,2,4-cyclopentanetrione	hydrocarbon	1486	1485	0.19 ± 0.05	0.26 ± 0.06	0.19 ± 0.02	0.12 ± 0.02	0.14 ± 0.01	0.67 ± 0.11	0.11 ± 0.01	nd	nd	
	Total hydrocarbon				**0.19**	**0.30**	**0.19**	**0.14**	**0.17**	**0.67**	**0.11**	**0.05**	**0.09**	
94	2-Hexadecan-2-one	Ketone	1806	1808	0.02 ± 0.01	nd	nd	0.01 ± 0.01	0.04 ± 0.01	nd	nd	nd	0.11 ± 0.06	Fruity
	Total ketones				**0.02**	**0.00**	**0.00**	**0.01**	**0.04**	**0.00**	**0.00**	**0.00**	**0.11**	
69	2,4-Di-tert-butylphenol	Phenol	1519	1514	nd	nd	nd	0.07 ± 0.01	0.07 ± 0.01	0.04 ± 0.03	0.07 ± 0.01	0.06 ± 0.02	0.11 ± 0.03	Phenolic
42	4-Ethyl guaiacol	Phenol	1282	1279	nd	nd	1.10 ± 0.24	nd	nd	nd	nd	nd	nd	Spicy and clove-like with medicinal, woody, and sweet vanilla nuances
26	4-Ethylphenol	Phenol	1169	1167	nd	nd	0.36 ± 0.30	nd	nd	nd	nd	nd	nd	Smoke, phenolic
53	Eugenol	Phenol	1357	1357	nd	nd	0.01 ± 0.00	nd	nd	0.07 ± 0.01	nd	nd	nd	Sweet, spicy, clove like, woody,
	Total phenols				**0.00**	**0.00**	**1.47**	**0.07**	**0.07**	**0.11**	**0.07**	**0.06**	**0.11**	
24	Hydroxydihydromaltol	Pyran	1151	1147	nd	0.20 ± 0.00	nd	0.05 ± 0.04	0.57 ± 0.45	0.13 ± 0.07	0.29 ± 0.14	0.08 ± 0.01	0.26 ± 0.16	Creamy, sweet, fruity peach,
	Total pyran				**0.00**	**0.20**	**0.00**	**0.05**	**0.57**	**0.13**	**0.29**	**0.08**	**0.26**	
70	(E)-Calamenene	Terpene	1529	1527	nd	nd	nd	0.03 ± 0.01	0.04 ± 0.00	0.13 ± 0.12	0.03 ± 0.00	0.03 ± 0.01	0.05 ± 0.01	Clove-like, herbaceous
33	Citronellol	Terpene	1228	1228	nd	0.09 ± 0.06	0.01 ± 0.00	nd	0.02 ± 0.01	nd	0.03 ± 0.02	0.03 ± 0.01	nd	Floral, rosy, sweet, citrus
55	Damascenone	Terpene	1386	1385	0.02 ± 0.01	nd	0.02 ± 0.00	nd	0.01 ± 0.01	nd	nd	nd	nd	Woody, sweet, fruity, earthy with green floral nuances
76	Germacrene B	Terpene	1591	1588	nd	nd	nd	0.02 ± 0.00	nd	0.03 ± 0.01	0.05 ± 0.03	nd	nd	Woody, earthy, spicy
62	Humulene	Terpene	1453	1453	0.04 ± 0.02	0.08 ± 0.01	nd	0.03 ± 0.00	0.06 ± 0.01	0.09 ± 0.07	nd	0.04 ± 0.01	0.09 ± 0.05	Woody

Table 3 (continued)

Code	Volatile compound	Chemical family	LRI (lit)	LRI (cal)	(%) of total peak area									
					CS	CS/SY	RC	SY	TP	PR	RS	AB	TN	Odor description[1]
20	Linalool oxide	Terpene	1074	1071	nd	0.24 ± 0.02	nd	0.35 ± 0.18	0.21 ± 0.07	0.35 ± 0.09	nd	0.49 ± 0.30	0.42 ± 0.15	Woody, floral, cooling, terpy and slightly green
25	Nerol oxide	Terpene	1153	1154	nd	nd	nd	nd	nd	0.33 ± 0.55	nd	nd	0.12 ± 0.09	Green, vegetative and floral
73	α-Calacorene	Terpene	1542	1548	0.07 ± 0.01	nd	0.02 ± 0.01	0.08 ± 0.02	0.15 ± 0.03	0.13 ± 0.05	0.07 ± 0.04	0.10 ± 0.05	0.09 ± 0.06	Woody
68	α-Farnesene	Terpene	1508	1513	nd	nd	0.01 ± 0.00	0.04 ± 0.01	0.04 ± 0.01	0.11 ± 0.06	nd	0.05 ± 0.01	nd	Citrus, herbal, lavender, bergamot
67	α-Muurolene	Terpene	1499	1501	nd	nd	nd	0.57 ± 0.31	0.16 ± 0.09	0.12 ± 0.09	0.12 ± 0.07	0.17 ± 0.05	0.32 ± 0.30	
19	γ-Terpinene	Terpene	1060	1063	0.05 ± 0.02	0.03 ± 0.02	0.71 ± 0.15	nd	nd	nd	0.14 ± 0.05	nd	0.13 ± 0.02	Oily, woody, terpene, lemon/lime tropical herbal
	Total terpenes				**0.18**	**0.44**	**0.77**	**1.12**	**0.69**	**1.28**	**0.45**	**0.91**	**1.23**	

[1]Aroma description obtained from an online database available at Pherobase (2020); *LRI lit.*, linear retention index of literature; *LRI cal.*, linear retention index calculated; *nd*, not detected; *tr*, trace; *CS*, Cabernet Sauvignon; *CS/SY*, Cabernet Sauvignon/Syrah; *AB*, Alicante Bouschet; *SY*, Syrah; *TP*, Tempranillo; *PR*, Cabernet Sauvignon/Syrah/Alicante Bouschet/Touriga Nacional/Aragonês; *RS*, Cabernet Sauvignon/Syrah/Alicante Bouschet; *TN*, Touriga Nacional; *RC*, Ruby Cabernet

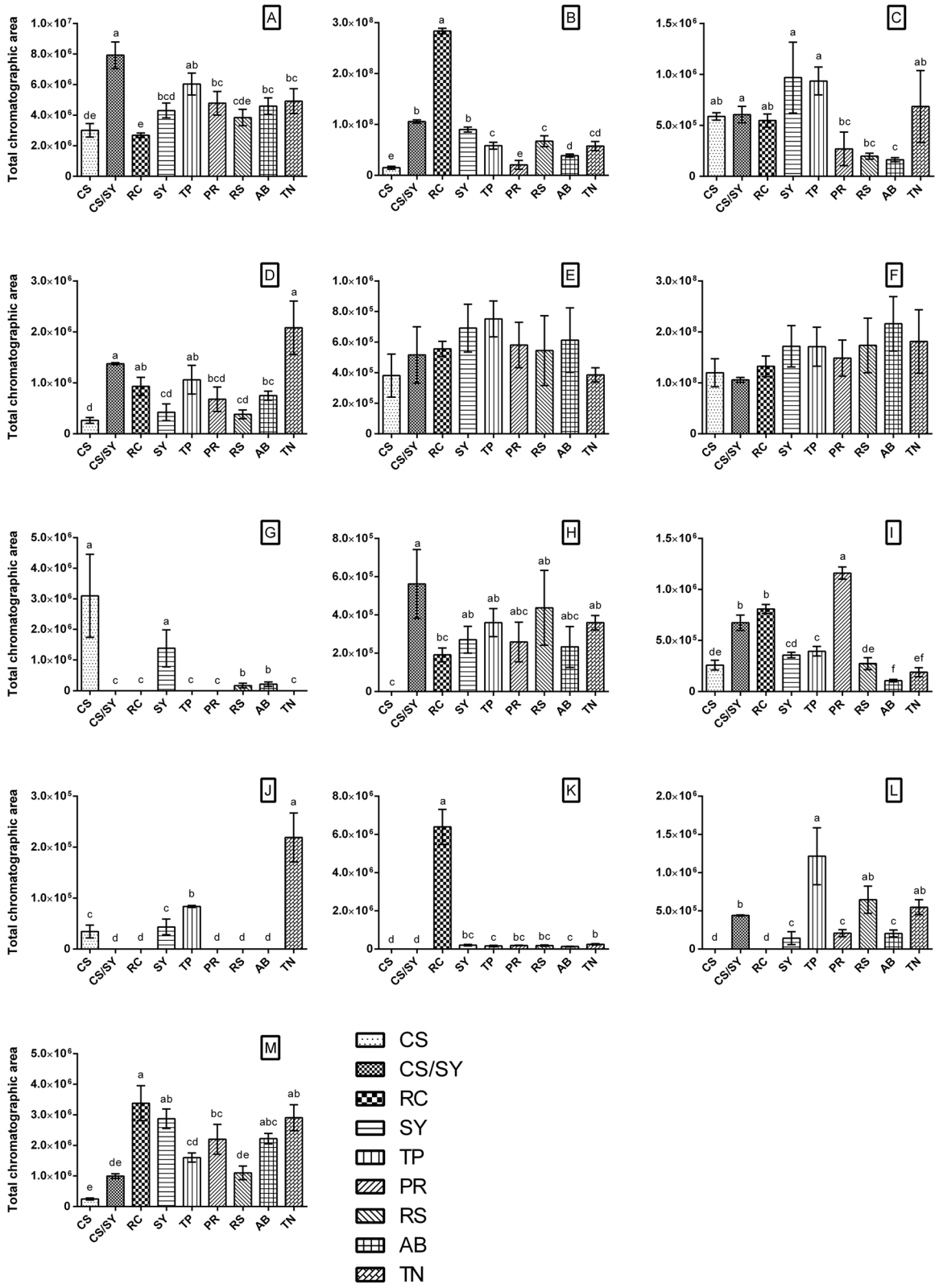

Fig. 1 Total area values of the chemical group **A** acids; **B** alcohols; **C** aldehydes; **D** aromatics; **E** C13-norisiprenoids; **F** esters; **G** ethers; **H** furans; **I** hydrocarbon; **J** ketones; **K** phenols; **L** pyrans; **M** terpenes, identified in red wines. Footnote: a,b,c Different letters in the same bar chart indicate significant difference by the Conover-Iman test ($p < 0.05$). CS: Cabernet Sauvignon; CS/SY: Cabernet Sauvignon/Syrah; AB: Alicante Bouschet; SY: Syrah; TP: Tempranillo; PR: Cabernet Sauvignon/Syrah/Alicante Bouschet/Touriga Nacional/Aragonês; RS: Cabernet Sauvignon/Syrah/Alicante Bouschet; TN: Touriga Nacional; RC: Ruby Cabernet

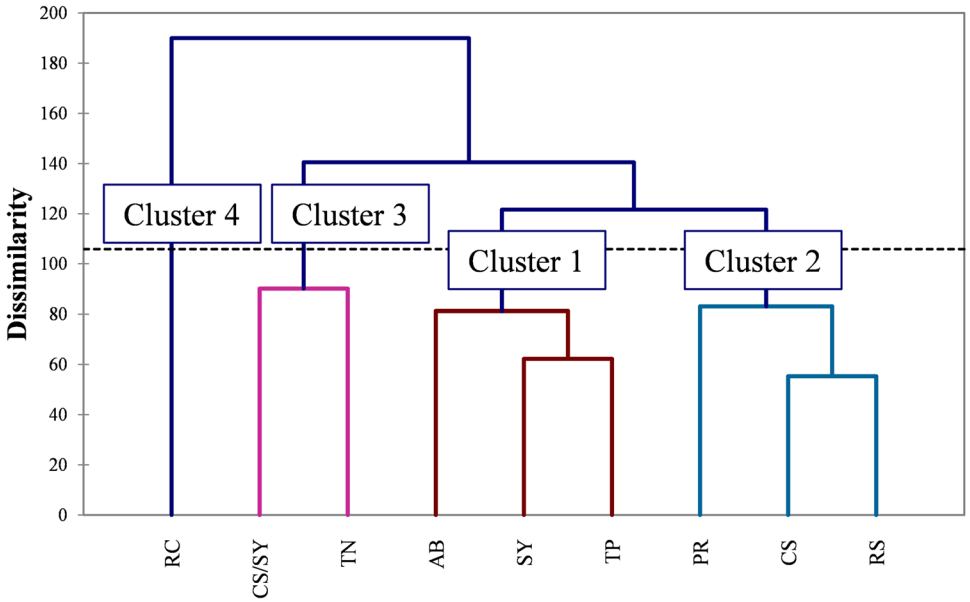

Fig. 2 Dendrogram formed from the volatile compounds of nine wines obtained by the Ward method and Euclidean distance. Footnote: CS: Cabernet Sauvignon; CS/SY: Cabernet Sauvignon/Syrah; AB: Alicante Bouschet; SY: Syrah; TP: Tempranillo; PR: Cabernet Sauvignon/Syrah/Alicante Bouschet/Touriga Nacional/Aragonês; RS: Cabernet Sauvignon/Syrah/Alicante Bouschet; TN: Touriga Nacional; RC: Ruby Cabernet;

The minority of compounds in terms of quantity, aldehydes obtained a maximum of 5 metabolites in CS wine, and the total area percentage varied from 0.07 to 0.90% in wines from AB and RS, respectively. There were 4 compounds identified within the phenols, 3 of which were detected in CR wine, with a total chromatographic area variation of 0.06 to 1.47% in wines from AB and CR, respectively. Furthermore, 4 compounds were identified among the furans, of which the majority of the wines detected 2 compounds, and presented a total area variation of 0.05 to 0.43% in the RC and TP wines, respectively.

Other identified minority compounds were classified as C13-norisoprenoid (2 compounds), and the others with one compound each, such as ketone, ether, and pyrane groups, representing total chromatographic areas of 0.32%, 0.11%, and 0.57%, respectively. Only the C13-norisoprenoid did not differ significantly from the classes of minority compounds mentioned above (Fig. 1).

Clustering, Principal Component Analysis, and Pearson Correlation

A cluster hierarchical analysis was performed using the volatile compound data of the nine commercial red wines analyzed (Table 3). A graphical representation is presented in the form of a dendrogram, whose separation criterion was the Euclidean distance (%) (Fig. 2). It is possible to clearly observe the formation of four groups, and cluster 4 is formed by a single wine (RC), having been isolated compared to the others. Cluster 1 is formed by the AB, SY, and TP wines, while cluster 2 is formed by the PR, CS, and RS wines, and cluster 3 is formed by the CS/SY and TN wines.

Principal component analysis (PCA) was performed with the area data of the auto-scaled volatile compounds of the nine red wines in this study, and differentiated by colors according to chemical class in Fig. 3. The first principal component (PC1) explained 24.71% of the total variation between the samples, and together with the second component (PC2, which explained 18.84%), explained 43.55% of the variability between the volatiles. Figure 3 (PC1 × PC2) separates and groups the wines in a similar way as Fig. 2 (dendrogram). Therefore, it is possible to more clearly observe the greater contribution of the ester, terpene, and alcohol classes in the profile of wines from cluster 1; the alcohol, ether, and acid classes in cluster 2; the aromatics class in the profile of wines from cluster 3; and some specific compounds in the cluster 4.

The red wines with similar volatile profiles were positioned in different regions in the PCA, with the compounds with significant factor loads and ≥ 0.7 being considered for discussion. Therefore, it was verified that only the RC wine was allocated in the positive axis of the PC1, separating this wine from the others. In addition, PC2 separated the TN and CS/SY wines (cluster 3) from the others, being located on the positive axis of PC2.

The volatile compounds which most contributed to the characterization of RC wine were ethyl isovalerate, 3-methyl-2-hexanol, hexanoic acid, 2-ethyl-1-hexanol, γ-terpinene, phenylethyl alcohol, 4-ethylphenol, β-phenethyl acetate, 4-ethyl guaiacol, damascenone, 6-phenyl-dodecane, (Z)-9-tetradecenoic acid, ethyl tetradecanoate, ethyl 9-hexadecenoate, ethyl hexadecanoate, and methyl 11-octadecenoate. Moreover, the compounds associated with TP (cluster 1) and PR (cluster 2) wines were 1-nonanol, 1-decanol, and methyl decanoate.

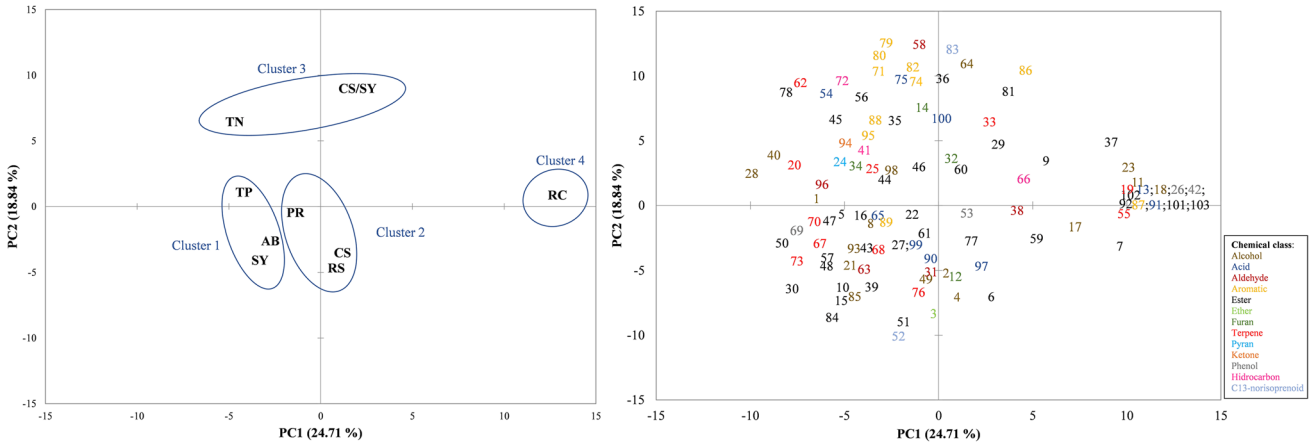

Fig. 3 PCA projection of volatile compound data of red wines obtained using the HS-SPME-GC–MS method. Footnote: See Table 2 for wine codes. CS: Cabernet Sauvignon; CS/SY: Cabernet Sauvignon/Syrah; AB: Alicante Bouschet; SY: Syrah; TP: Tempranillo; PR: Cabernet Sauvignon/Syrah/Alicante Bouschet/Touriga Nacional/Aragonês; RS: Cabernet Sauvignon/Syrah/Alicante Bouschet; TN: Touriga Nacional; RC: Ruby Cabernet

The CS/SY and TN wines (cluster 3) were characterized by the volatile compounds isoamyl hexanoate, dodecanal, humulene, 1-dodecanol, 5-phenyl-decane, 2,6,10-trimethyltetradecane, 4-phenyl-decane, dodecanoic acid, 6-phenyl-undecane, 5-phenyl-undecane, 3-phenyl-undecane, 4-isopropyl-1,6-dimethyl-naphthalene, and 2-phenyl-undecane. Furthermore, the wines from AB and SY (cluster 1), RS and CS (cluster 2) obtained a greater contribution from the 1,2-dihydro-1,5,8-trimethyl-naphthalene compound.

A Pearson's correlation analysis (r) was subsequently performed on the 20 volatile compounds with percentage of area $\geq 1\%$, in order to identify the correlation between the volatile compounds detected in red wines (Table 4). Positive and significant correlations ($p < 0.05$) were observed in the esters class, whose ethyl octanoate correlated with three esters, namely, ethyl hexanoate ($r = 0.82$), ethyl butanoate ($r = 0.70$), and ethyl decanoate ($r = 0.90$). Furthermore, ethyl decanoate correlated positively with ethyl butanoate ($r = 0.81$) and ethyl isopentyl succinate correlated with ethyl 2-methylbutanoate ($r = 0.69$).

Positive correlations were also observed between ethyl 2-methylbutanoate and 2,3-butanediol esters and alcohols ($r = 0.98$); between β-phenethyl acetate and phenylethyl alcohol ($r = 0.96$); and between ethyl 2,4-hexadienoate and undecanoic acid ($r = 0.70$). Other compounds also had positive correlations, such as 4-ethyl guaiacol with phenylethyl alcohol ($r = 0.94$), and β-phenethyl acetate ($r = 0.90$); 2-ethyl-1-butanol, methyl ether with 2,3-butanediol ($r = 0.85$), and ethyl 2-methylbutanoate ($r = 0.79$). A negative and significant correlation ($p < 0.05$) was only obtained by ethyl glutarate and diethyl succinate ($r = -0.80$) in the other compounds.

Discussion

The volatile profile of nine commercial tropical red wines, which may in the future obtain the Geographical Indication São Francisco Valley, was analyzed herein for the first time. Unfortunately, there are no studies of these wines to compare the results obtained. The objective was to identify the volatile compounds that could typify the red wines and be used as chemical markers. The study presented two important aspects. Firstly, commercial red wines, already validated in terms of quality and acceptability by consumers, were chosen to be studied. The second aspect is that the wines were indicated by the wineries' oenologists/owners based on the potential for obtaining the GI.

Classical Analyses

All the results of the classical analyses performed (Table 2) are in accordance with the Brazilian and international wine laws (OIV 2014; Brasil 2018). The samples presented similarities and differences ($p<0.05$) regarding the different parameters. The alcohol content was similar to the values reported by Oliveira et al. (2019) and Garaguso and Nardini (2015) in red wines from VSF and Italy, respectively. The registered variations are possible due to the winemaking processes used and climate variations (Sánchez-Palomo et al. 2017).

The pH values obtained exceeded the ideal recommended range for red wines, between 3.4 and 3.8, due to high temperatures during maturation and high potassium concentration in the soils of the region (Rankine 1999; Jackson 2020).

Agronomic management is among the alternatives for reducing pH to maintain the balanced concentration of acids in ripe berries (increased productivity), as well as the use of correctives to reduce the concentration of potassium in the soil, and acidification during winemaking with tartaric or lactic acids (Ribéreau-Gayon et al. 2006; Lima et al. 2015; Jackson 2020).

The density of the wines in this study shows that the samples were dry wines, being similar to those obtained in other studies (Ivanova-Petropulos et al. 2015; Lima et al. 2015; Oliveira et al. 2019). The results of total titratable acidity, volatile acidity, and free sulfur dioxide were varied when compared to other studies, mainly depending on the oenological potential of the grapes at harvest (climate), as well as the elaboration protocols (Lombardi et al. 2017; Sánchez-Palomo et al. 2017; Oliveira et al. 2019; Valentin et al. 2020). However, all parameters are in accordance with Brazilian and international legislation (OIV 2014; Brasil 2018). Total acidity contributes to microbial/biological stabilization and the freshness taste of wines (Ribéreau-Gayon et al. 2006; Ivanova-Petropulos et al. 2015).

Volatile Profile of Wines and Varietal Effect

Red wines were characterized by a total of 103 volatile compounds belonging to different chemical classes. Some compounds were highlighted by their abundance of chromatographic area, such as ethyl octanoate, diethyl succinate, ethyl decanoate, ethyl 2,4-hexadienoate, ethyl hexanoate, ethyl isopentyl succinate, ethyl 2-methylbutanoate, ethyl butanoate, ethyl glutarate, ethyl 9-decenoate, and β-phenethyl acetate; phenylethyl alcohol, 2,3-butanediol, 3-methyl 1-butanol,1-hexanol, and decanoic and undecanoic acids.

The esters are highlighted in quantity and number among the classes. These compounds are produced during the alcoholic fermentation and Acyl-CoA, and contribute with floral and fruity notes in wines (Ilc et al. 2016; Mota et al. 2020). The esters stood out in the CS wine profile, a French cultivar introduced in Brazil in 1921 (Orlando et al. 2008), with ethyl octanoate (36.09%), followed by diethyl succinate (20.88%), ethyl decanoate (14.85%), and ethyl hexanoate (3.62%). They were also the majority in the PR wine profile, but with lower area percentages, except in the diethyl succinate (22.02%) and ethyl decanoate (16.80%) compounds. Diethyl succinate has been identified in previous studies as a marker for aged wines (Voce et al. 2019), including being identified after 30 and 42 months of bottling, being a marker linked to aging in the winter wines from Syrah (Mota et al. 2020). However, this compound was also reported in a study with young and experimental wines from different cultivars, such as Cabernet Sauvignon, Pinot Noir, Syrah, and Merlot from Italy (Englezos et al. 2018), as well as in study with Malbec wines from different harvests (Sánchez-Palomo et al. 2017).

The class of alcohols, from which the most compounds are derived from the alcoholic fermentation by yeasts, is responsible for about 50% of the aromatic constituents of wines (excluding ethanol) (Jackson 2020). The RC wine was highlighted in this class of compounds with a total area percentage of 65.96%, of which 64.80% was represented by the phenylethyl alcohol compound. The second major wine in the alcohol class was the CS/SY blend, with 47.15% of the total area percentage, of which 44.23% were represented by the phenylethyl alcohol compound. This compound is considered the most important phenolic superior alcohol and can give rose flavor (Pherobase 2020; Jackson 2020). In a study of CS and Syrah wines from Greece, phenylethyl alcohol and 3-methyl 1-butanol compounds were prominent from CS, while 1-hexanol compound was the most present in wines from CS and SY (Karabagias et al. 2020). In the current study, 1-hexanol was also the majority in SY, considered the main red grape grown in the São Francisco Valley (Oliveira et al. 2019), contributing with fruity notes.

Terpenes were one of the minor classes of compounds, but no less important. This is because these compounds have a very low olfactory threshold, allowing the perception in low concentrations (Condurso et al. 2016). The 11 terpenes identified in the wines suggest a contribution to floral, sweet, fruity, citrus, and woody aromas. Among the analyzed wines, AB presented 8 terpenes identified, more than TN wines (6 terpenes), which has been considered in previous studies as rich in terpenic compounds when compared with more than 75 different varietals (Pinho et al. 2007; Petronilho et al. 2020). In the sensorial profile of Touriga Nacional wines from VSF, they were described by floral aromas on the first harvest of the year (July), and fruity and spicy aromas on the second harvest (Oliveira et al. 2018). Thus, we suggest that the 6 terpenes identified in the TN wines, such as linalool oxide, nerol oxide, humulene, α-muurolene, (E)-calamenene, and α-calacorene, were the potential compounds responsible for these aromatic descriptors.

Discrimination and Similarities of Wines

Several controlled or unknown factors can influence the similarities and differences of wines from different grape varieties. It is possible to observe that the combination of cultivar, viticultural management, and winemaking techniques could influence the volatile composition of wines. All the red wines were made in the same winery, with the exception of the RC. It is worth mentioning that some of the young wines presented similar volatile characteristics to wines aged in oak barrels, and did not differ in the formation of clusters 1, 2, and 3 (Fig. 2). This result can be explained by possible blends between wines from the winery.

A large study conducted by Valentin et al. (2020), with 83 red wines from four South American countries, indicated that the chemical and volatile characteristics of two Brazilian red wines from Merlot were allocated to the same cluster of 18 wines of Carmenere from Chile, for unknown reasons. However, the wines in this study presented similar geographical location, which may have been influenced the similarity between wines of different varieties, blends, vintages, and age. The RC wine was an exception, because it presented greater dissimilarity compared to the others. This differentiation can be attributed to the distinction of the vine management, as well as with possible specific enological protocols (Jackson 2020).

One of the most common enological practices in the winemaking process is the blend of wines. This can be carried out by blending musts from different grape varieties, or even by blending monovarietal wines prepared differently in the cellar to obtain commercial wines (Alañón et al. 2015). The monovarietal CS and SY wines studied and the wine from the blending of their musts (CS/SY) were differentiated by clusters, and this can be attributed to enological practice.

The graphical representation by PCA (Fig. 3) confirmed the results of the cluster hierarchical analysis. The wines located in the first two PCs were discriminated mainly by the main volatile markers, according to different vintages and cultivars. Chemometric studies carried out by Valentin et al. (2020) indicated that wine discrimination, considering the volatile composition, may present a low variance percentage. In the present study, PC1 × PC2 explained 43.55% of the total variability; however, they are important markers describing the typicality of the wines.

Some esters identified in the wine profiles presented positive and significant correlations ($p < 0.05$) between them, and characterized wines from different clusters. The ethyl octanoate and ethyl hexanoate, ethyl butanoate, and ethyl decanoate compounds; and the ethyl decanoate and ethyl butanoate volatile compounds characterized wines from cluster 1. The ethyl isopentyl succinate ester compound correlated with ethyl 2-methylbutanoate, characterized wines from cluster 2.

Other positive and significant correlations were presented by compounds of different classes, which characterized the wines of cluster 2, including the ethyl 2-methylbutanoate and 2,3-butanediol; ethyl 2,4-hexadienoate and undecanoic acid; 2-ethyl-1-butanol, methyl ether with 2,3-butanediol and ethyl 2-methylbutanoate. The positive correlation ($p < 0.05$) between β-phenethyl acetate and phenylethyl alcohol, and 4-ethyl guaiacol, phenylethyl alcohol and β-phenethyl acetate, characterized the wines belonging to the cluster 4.

The only negative and significant correlation ($p < 0.05$) was obtained between ethyl glutarate and diethyl succinate compounds, which characterized the wines of clusters 2 and 3, respectively. This suggests that higher amounts of ethyl glutarate in wines from cluster 2, lower content of diethyl succinate in wines from cluster 3, and vice-versa. It is common that positive correlations are found between some compounds in wines and their precursors, as showed in previous study, between ethyl octanoate and octanoic acid compounds; and between ethyl hexanoate and hexanoic acid (Caliari et al. 2014).

Establishment of Potential Origin Markers

The wine composition is associated with several factors, such as their geographical origin (climate and soil), the grapevine management, as well as the winemaking process in enology. However, the description of its typicality, as well as its traceability is a great challenge from the legal and economic points of view to guarantee authenticity (Alañón et al. 2015). In this scenario, the description of the volatile composition of commercial products can provide the "fingerprint" of the wines and assist in their classification and traceability according to their terroir, geographical origin, variety, and age/stability, with possible aging in barrels.

The volatile profile of the nine commercial wines analyzed in this study presented three particularities: (i) compounds identified exclusively in only one kind of wine; (ii) compounds identified in different area abundances in all wines; and (iii) new volatile compounds, which were identified and reported for the first time in red wines. Thus, the results obtained in this study allow us to identify and suggest potential volatile compound markers of the studied wines according to the different varieties, as well as according to the elaboration protocols.

The volatile compounds exclusively identified in the RC wine were (Z)-9-tetradecenoic and hexanoic acids, 2-ethyl-1-hexanol alcohol, 6-phenyl-dodecane aromatic compound, ethyl 9-hexadecenoate, methyl 11-octadecenoate esters, 4-ethyl guaiacol, and 4-ethyl phenol as phenols. These two volatile phenol compounds can be markers of wine contamination by the *Brettanomyces*/*Dekkera* yeasts, with the increase of volatile acidity (Jackson 2020). The distinction of this wine may have been due not only to the variety but also to winemaking protocols. A previous study with Ruby Cabernet wines in Brazil showed the presence of vegetable, salt, and oak aromatic descriptors (Miele and Rizzon 2011). However, the volatile compounds identified in the RC wines of the present study suggest some descriptors, such as fatty, waxy, citrus, spicy, woody, sweet vanilla, smoky, and phenols (Table 3).

It is interesting to highlight that the unique presence of (E)-9-hexadecenoic acid and ethyl benzoate compounds in AB wine, as well as 1-pentanol and 2,4-dihydroxy-2,5-dimethyl-3(2H)-furanone compounds in RS wine. The furanone compound originates from aging in oak barrels (Jackson

Table 4 Results of Pearson's correlation analysis (*r*) between volatile compounds from São Francisco Valley red wines with a chromatographic area (≥ 1%)

Code*	Volatile compounds	54	65	1	4	8	23	5	6	15	22	29	30	35	37	43	56	57	59	3	42
54	Decanoic acid	**1**																			
65	Undecanoic acid	−0.1378	**1**																		
1	3-Methyl 1-Butanol	0.2106	0.2286	**1**																	
4	2,3-Butanediol	−0.2139	−0.1664	0.1485	**1**																
8	1-Hexanol	0.1718	−0.2411	0.3242	−0.2780	**1**															
23	Phenylethyl alcohol	−0.2994	−0.3790	−0.3718	−0.2727	0.0532	**1**														
5	Ethyl butanoate	0.1247	−0.4359	0.0044	−0.3522	0.3548	−0.1982	**1**													
6	Ethyl 2-methylbutanoate	−0.2896	−0.2199	0.1201	**0.9817**	−0.3021	−0.1016	−0.3923	**1**												
15	Ethyl hexanoate	−0.1298	−0.1000	0.1413	0.4155	−0.2605	−0.5490	0.5166	0.3665	**1**											
22	Ethyl 2,4-hexadienoate	−0.1873	**0.7019**	0.0580	−0.1874	−0.3167	−0.2731	−0.2450	−0.2073	−0.0135	**1**										
29	Diethyl succinate	−0.0021	−0.1909	0.1105	0.0046	−0.5903	0.2659	0.0381	0.1065	0.2170	0.1265	**1**									
30	Ethyl octanoate	0.0252	0.0005	0.2621	0.0349	0.2001	−0.5380	**0.7023**	−0.0349	**0.8180**	−0.1373	−0.1330	**1**								
35	Ethyl 2-phenylacetate	0.6564	−0.0199	0.0994	−0.4585	0.6456	0.1040	−0.0695	−0.4947	−0.6569	−0.2521	−0.5060	−0.2190	**1**							
37	β-Phenethyl acetate	−0.1962	−0.3464	−0.4692	−0.4565	−0.0461	**0.9575**	−0.0612	−0.2957	−0.4945	−0.2240	0.3526	−0.4622	0.1021	**1**						
43	Ethyl glutarate	−0.0696	0.3426	0.3032	−0.0772	0.6277	−0.1742	−0.0660	−0.1407	−0.2118	−0.2399	**−0.7991**	0.2426	0.4782	-0.2764	**1**					
56	Ethyl 9-decenoate	0.5961	0.3636	0.2237	−0.3492	−0.2678	−0.2980	−0.0896	−0.3864	−0.1146	0.6151	0.3864	−0.1751	0.1852	−0.1564	−0.4404	**1**				
57	Ethyl decanoate	−0.0660	−0.0662	0.2786	−0.2840	0.3367	−0.2203	**0.8071**	−0.2976	0.6206	−0.1316	0.0140	**0.8965**	−0.1512	−0.1259	0.2124	−0.1675	**1**			
59	Ethyl isopentyl succinate	−0.1453	−0.3872	0.1576	0.5605	−0.2006	0.4060	−0.3092	**0.6887**	0.1488	−0.1770	0.5087	−0.1614	−0.3131	0.2619	−0.4105	−0.1309	−0.1611	**1**		
3	2-Ethyl-1-butanol, methyl ether	−0.2999	−0.1932	0.0494	**0.8543**	0.0758	−0.3276	−0.1873	**0.7917**	0.2746	−0.2441	−0.4172	0.0646	−0.2660	−0.5336	0.2326	−0.5613	−0.2322	0.1984	**1**	
42	4-Ethyl guaiacol	−0.5713	−0.2224	−0.4471	−0.1874	−0.1610	**0.9357**	−0.2450	−0.0194	−0.4234	−0.1250	0.3106	−0.5113	−0.1839	**0.8988**	−0.2088	−0.3767	−0.2195	0.3487	−0.2441	**1**

*See Table 2 for wine codes. Values in bold are different from 0 with significant correlations at 5% probability of error ($p < 0.05$). *CS*, Cabernet Sauvignon; *CS/SY*, Cabernet Sauvignon/Syrah; *AB*, Alicante Bouschet; *SY*, Syrah; *TP*, Tempranillo; *PR*, Cabernet Sauvignon/Syrah/Alicante Bouschet/Touriga Nacional/Aragonês; *RS*, Cabernet Sauvignon/Syrah/Alicante Bouschet; *TN*, Touriga Nacional; *RC*, Ruby Cabernet

2020). Both wines were produced in the same winery and aged in French oak barrels for 9 and 6 months, respectively.

The compounds with the highest area representation that characterized all nine wine samples were 3-methylbutyl octanoate, ethyl isopentyl succinate, diethyl succinate, ethyl 9-decenoate, ethyl decanoate, ethyl dodecanoate, ethyl hexadecanoate, ethyl hexanoate, ethyl nonanoate, ethyl octanoate, ethyl tetradecanoate, isoamyl hexanoate, and β-phenethyl acetate. Regardless of the vintage, cultivar, viticultural practices or winemaking, this set of compounds are possible markers of wines from the São Francisco Valley, belonging to the group of esters whose terroir is unique in the world, producing the tropical wines in Brazil (Pereira 2020).

Some alcohols were also identified in all nine wines, such as 1-decanol, 1-hexanol, 3-ethyl-4-methyl-1-pentanol, 3-methyl 1-butanol, hexadecanol, and phenylethyl alcohol. In addition, other compounds of the acid, aromatic, and C13-norisoprenoid classes were identified. Decanoic acid and n-hexadecanoic acid were prominent in the acid class, while the 4-phenyl-dodecane, 5-phenyl-dodecane, 5-phenyl-undecane, and 6-phenyl-undecane compounds from the aromatics class were common in all wines. These compounds need to be highlighted because they are new, being cited and reported for the first time in red wines. The two compounds identified in the C13-norisoprenoid class were present in all nine wines studied, whose 1,2-dihydro-1,5,8-trimethyl-naphthalene was also identified for the first time in red wines.

Another 17 compounds were identified for the first time in red wines (totaling 22 compounds, with the compounds: (Z)-9-tetradecenoic acid, 2-heptadecanol, 10-octadecenal, 3-phenyl-undecane, 4-phenyl-decane, 4-phenyl-tridecane, 2-phenyl-undecane, 5-phenyl-decane, 6-phenyl-dodecane, 2-hexadecan-2-one, 2-ethylhexyl octanoate, geranyl isovalerate, isomenthol acetate, 2,6,11-trimethyldodecane, 3-butyl-1,2,4-cyclopentanetrione, 2-ethyl-1-butanol methyl ether, and germacrene B. These compounds can contribute with olfactory descriptors as licorice, sweet, fruity, oily, herbal, woody, earth, and spicy notes (Table 2). From these, 45% belong to the aromatic class whose presence has already been identified in honey and fruit (Grygorieva et al. 2017; Tang et al. 2017; El-hefny et al. 2018).

Conclusions

For the first time, volatile commercial tropical red wines originating from the San Francisco Valley were identified. Similarities and differences were detected between the volatile profile of these wines, being influenced by characteristics such as vintage, variety, and winery (enological practices). Some volatile compounds previously identified and described by the literature, and some exclusive compounds for the first time identified in these wines, were considered potential markers. These compounds can be useful to describe the quality and typicality of the products, and also may contribute to the traceability and authenticity of wines from this region.

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Data Availability The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

Declarations

Informed Consent Informed consent is not applicable.

Conflict of Interest The authors declare no competing interests.

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