



ELSEVIER

Contents lists available at ScienceDirect

Data in brief

journal homepage: www.elsevier.com/locate/dib



Data Article

Dataset of concentrations of free terpenes at different phenological stages in *Vitis vinifera* L. Shiraz, Cabernet Sauvignon, Riesling, Chardonnay and Pinot Gris



Jiaqiang Luo ^a, Jessica Brotchie ^a, Meng Pang ^a,
Philip John Marriott ^b, Kate Howell ^a, Pangzhen Zhang ^{a,*}

^a School of Agriculture and Food, Faculty of Veterinary & Agricultural Sciences, The University of Melbourne, Royal Parade, Parkville, Victoria, 3010, Australia

^b School of Chemistry, Monash University Clayton, Victoria, 3800, Australia

ARTICLE INFO

Article history:

Received 2 July 2019

Received in revised form 18 September 2019

Accepted 24 September 2019

Available online 3 October 2019

Keywords:

Shiraz

Cabernet Sauvignon

Riesling

Chardonnay

Pinot Gris

terpene

Evolution

SPME-GC-MS

ABSTRACT

Five *Vitis vinifera* L. cultivars Shiraz, Cabernet Sauvignon, Riesling, Chardonnay and Pinot Gris at different E-L development stages were harvested in two experimental vintages. Temperature and rainfall data of the growing period were obtained from the Australian Government Bureau of Meteorology. Free terpene concentrations of all harvested grape samples were analysed using HS-SPME-GC-MS. One-way ANNOVA was performed to evaluate the significance of changes in terpene concentrations at different maturation stages. More analysis of the data is provided in "Free terpene evolution during the berry maturation of five *Vitis vinifera* L. cultivars" [1].

© 2019 The Author(s). Published by Elsevier Inc. This is an open access article under the CC BY license (<http://creativecommons.org/licenses/by/4.0/>).

DOI of original article: <https://doi.org/10.1016/j.foodchem.2019.125101>.

* Corresponding author.

E-mail address: pangzhen.zhang@unimelb.edu.au (P. Zhang).

<https://doi.org/10.1016/j.dib.2019.104595>

2352-3409/© 2019 The Author(s). Published by Elsevier Inc. This is an open access article under the CC BY license (<http://creativecommons.org/licenses/by/4.0/>).

Specifications Table

Subject area	<i>Phytochemistry, Plant Science</i>
More specific subject area	Aroma chemistry of wine grapes
Type of data	Figure, Table
How data were acquired	Australian Government Bureau of Meteorology and Gas chromatography-mass spectrometry, experimental results
Data format	Raw data (temperature and rainfall) and analysed data (GC-MS)
Experimental factors	Powdered grape samples were extracted with the extraction solution and the solution sampled by headspace solid-phase microextraction.
Experimental features	Samples were collected at fortnight intervals from four weeks post-flowering (wpf) until commercial harvest. HS-SPME-GC-MS was performed to investigate free terpene concentrations of samples of five varieties with different maturity.
Data source location	Mount Langi Ghiran vineyard, Bayindeen, Victoria, Australia (S 37.316071, E143.145032)
Data accessibility	Data is with this article and a supplemental file containing two data files
Related research article	J. Luo, J. Brotchie, M. Pang, P.J. Marriott, K. Howell, P. Zhang, Free terpene evolution during the berry maturation of five <i>Vitis Vinifera</i> L. cultivars, <i>Food Chem.</i> 299 (2019), 125101

Value of the data

- Our previous data [2] showed changes in terpene accumulation during ripening of Shiraz wine grapes. The datasets here provide information about free terpene concentrations at different development stages of *Vitis vinifera* L. cv. Shiraz, Cabernet Sauvignon, Riesling, Chardonnay and Pinot Gris.
- All grape cultivars are located within the same vineyard, which minimizes site variations of environmental and geography factors, which may alter terpene production amongst different cultivars.
- These datasets could provide new insights into the free terpene evolution of five economically important wine grape varieties. Further studies could be conducted to investigate the genetic or metabolic differences among cultivars leading to the variations in terpene production.

1. Data

This present data provide supplementary information to our previous work [1]. Total monoterpene, norisoprenoid and sesquiterpene concentrations at E-L 31, 33, 34, 35 and 38 of each variety in two vintages are plotted in Fig. 1. Temperature and rainfall information of vintages 2016 and 2017 was obtained from the Australian Government Bureau of Meteorology (nearest weather station: Ararat Prison Station, BoM ID: 089085, 15.5 km northwest to the experimental vineyard) and summarized in Table 1. Information of growing degree days (GDD) of each sample collection day is provided in Table 2. Compound identification based on comparison of retention indices and mass spectra are summarized in Table 3 and Table 4, respectively. Concentrations of different classes of free terpenes and total monoterpene and total sesquiterpene in different grape cultivars at different developmental stages are shown in Tables 5–9.

2. Experimental design, materials and methods

Wine grape samples were harvested from a commercial vineyard in the Grampians wine region in Victoria, Australia. In two experimental vintages, vertical shoot positioned (VSP) trellis and drip irrigation systems were applied in the vineyard without significant pest or disease pressure detected. In vintage 2016, sample collection started from 18 December 2015 and continued in two-week intervals until commercial harvest. Matured Chardonnay and Pinot Gris were collected on 13 February 2016, while Shiraz, Cabernet Sauvignon and Riesling were collected on 14 March 2016. In vintage 2017, samples were collected fortnightly from 09 January 2017 due to delayed fruit-setting. The last batches of Riesling, Chardonnay and Pinot Gris were harvested on 20 March 2017 while Shiraz and Cabernet Sauvignon were on 18 April 2017. For each cultivar, grape brunches in triplicate were collected randomly from different positions of randomly selected grapevines ($n > 30$ for each cultivar). Samples were transported to the laboratory on dry ice and stored at -20°C before analysis.

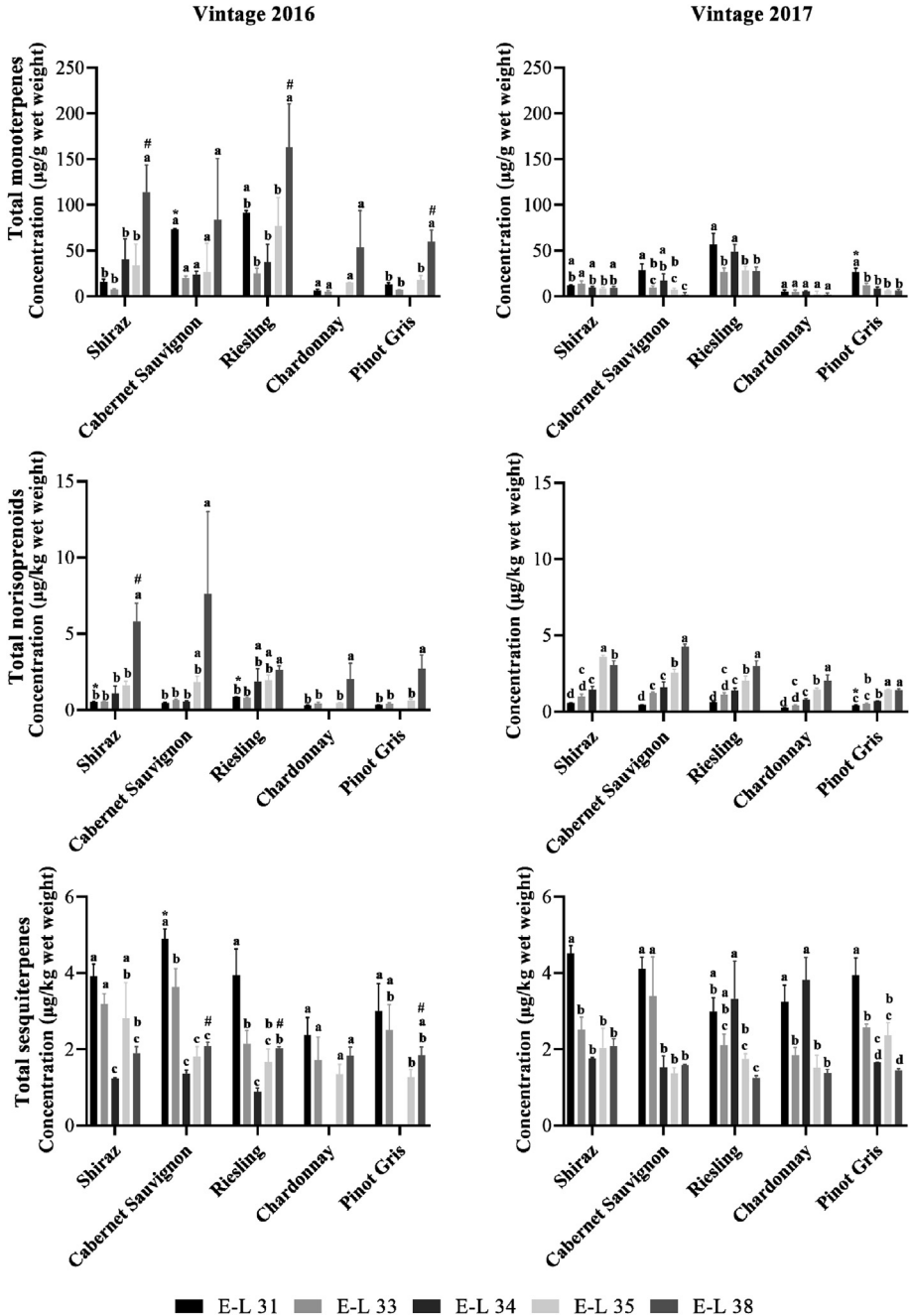


Fig. 1. Total terpene contents of five varieties of wine grapes in two vintages. (a) total monoterpene contents in vintage 2016, (b) total monoterpene contents in vintage 2017, (c) total norisoprenoid contents in vintage 2016, (d) total norisoprenoid contents in vintage 2017, (e) total sesquiterpene contents in vintage 2016, (f) total sesquiterpene contents in vintage 2017. Values labelled with the same lower case letter are not significantly ($p < 0.05$) different within each variety in a vintage. Harvest concentrations of each variety in two vintages labelled with “#” are significantly ($p < 0.05$) different. Concentrations at E-L 31 of each variety in two vintages labelled with “*” are significantly ($p < 0.05$) different. Raw data of the histograms are provided in data file 1.

Table 1
Temperature and rainfall conditions during vintages 2016 and 2017.^a

	January	February	March	April
Vintage 2016				
Mean maximum temperature (°C)	30	28.6	27.4	21.9
Mean minimum temperature (°C)	11.1	13	12.3	8.3
Mean rainfall (mm)	30	50.6	32	33.4
Solar radiation (MJ m ⁻²)	24.1	23.0	16.7	12.8
Vintage 2017				
Mean maximum temperature (°C)	29	27.2	27.7	20.7
Mean minimum temperature (°C)	12.4	10.8	12	8.4
Mean rainfall (mm)	33	18.6	20	70
Solar radiation (MJ m ⁻²)	24.4	21.5	17.3	10.9

^a Data were obtained from the website of the Australian Government Bureau of Meteorology using the Ararat Prison observation station data.

Terpene analysis was conducted on an Agilent 6890 GC coupled with an Agilent 5973 MSD (Agilent Technologies, Santa Clara, CA) and an Agilent PAL multipurpose sampler connected to the GC. The HS-SPME-GC-MS analysis was conducted based on our previous data with some modifications [3].

Briefly, after destemming, grape berries were frozen with liquid nitrogen and then powdered with a stainless steel grinder. Five g of the sample powder was extracted with 30 mL of a pH 3.2 extraction solution, which consisted of 5 g/L polyvinylpyrrolidone (PVPP), 0.5 g/L tartaric acid and 0.5 g/L of sodium sulfite, at room temperature for 24 h with a stirring rate of 100 rpm. A 0.45 µm nylon syringe filter was used to filter the mixture and then 5 mL of the supernatant was mixed with 1 g of sodium chloride and 20 µL of 2 mg/L β-cedrene internal standard in a 20 mL GC vial. The headspace in the GC vial was extracted by using a 65 µm DPMS/DVB SPME fibre (Supelco, Bellefonte, PA) for 60 min with agitation at 45 °C in an agitator mounted on the Agilent PAL multipurpose sampler.

Chromatographic separation was achieved on a J&W DB-5ms capillary column (Agilent Technologies; 30 m × 0.25 mm × 0.25 µm). Purified helium was used as the carrier gas at a constant flow rate of 1.0 mL/min. GC conditions were based on our previous protocol with slight modifications (Zhang et al., 2016). Compounds adsorbed on the SPME fibre were desorbed under pulsed splitless mode and the mass spectrometer was operated in scan/sim mode under positive electron ionization (EI) mode at 70 eV, with a scan range from *m/z* 35 to 280.

As sesquiterpenes exist in trace amounts, simultaneous selected ion monitoring (SIM) mode was used to record common terpene ions: *m/z* 105, 133, 147, 161, and 204 to facilitate locating target compounds. Quantification of terpenes was based on the target ion peak areas.

Table 2
Accumulated growing degree days (GDD)* of sample collection dates. Raw data of the table are provided in data file 2.

Vintage 2016		Vintage 2017	
Date	GDD	Date	GDD
18/12/2015	583.35	9/01/2017	584.25
2/01/2016	757	23/01/2017	726.05
15/01/2019	898.1	10/02/2017	913.8
1/02/2016	1078.1	20/02/2017	983.85
13/02/2016	1208.05	6/03/2017	1128.75
29/02/2016	1356.75	20/03/2017	1273.3
14/03/2016	1531.95	3/04/2007	1369.95
		18/04/2017	1438.05

*GDD of each sample collection date is calculated based on the following equation [5]: GDD =

$$\sum_{1 \text{ Oct}}^{\text{date of sample collection}} \max \left[\left(\frac{T_{\max} + T_{\min}}{2} \right) - 10, 0 \right]$$

Where,

*T*_{max} is the highest temperature of the sample collection day.

*T*_{min} is the lowest temperature of the sample collection day.

Table 3Retention indices relative to *n*-alkanes C7–C30 on a J&W DB-5ms column, reference retention indices, and target ions of identified terpenoids.

	Calculated RI (DB-5)	Terpenoids library RI (DB-1) ^a	NIST library RI (DB-5)	Target ions ^b
<i>Monoterpenoids</i>				
α -Terpinene	1013	1013	1018	121,93,136
Cymene (m- and p-)	1022	1013	1026	119,91,134
1,8-Cineol	1130	1024	1031	81,108,71,154
(E)- β -Ocimene	1044	1041	1026	93,121,79
γ -Terpinene	1055	1051	1060	93,136,121
Terpinolene	1082	1082	1088	136,93,121
p-Cymenene	1086	1075	1080	132,117,91
Linalool	1097	1086	1098	71,93,55,121
Hotrienol	1101	1083	1104	71,82,67
trans-Pinocarveol	1125	1126	1137	55,70,83
Citronellal	1129	1129	1150	69,55,111
Neroloxide	1147	1137	1153	68,83,96
Menthol (+isomenthol)	1172&1175	1172&1176	1174	71,81,95
Terpinen-4-ol	1175	1164	1179	71,93,111,154
α -Terpineol	1192	1176	1189	59,93,121,136
Geraniol	1246	1235	1255	69,41,93,53
Geranylacetone	1442	1430	1452	69,107,93,151
<i>Norisoprenoids</i>				
Theaspirane (Isomer 1)	1292	1299	1298	138,96,82
Theaspirane (Isomer 2)	1310	1313	1298	138,109,82
(E)- β -Damascenone	1372	1363	1385	121,190,69
<i>Sesquiterpenoids</i>				
7-epi- α -Cedrene	1407	1404	1405	119,93,204
Selina-4,11-diene	1467	1475	NA	189,204,81
α -Muurolene	1491	1491	1499	105,161,119,204
δ -Cadinene	1510	1520	1510	161,119,204
Calamenene (cis + trans)	1513	1517	1521	159,202,114
α -Calacorene	1526	1527	1523	157,142,200
ω -Cadinene	1526	1526	1528	119,161,204
γ -Calacorene	1533	1554	1550	157,142,200
Palustrol	1565	1569	1568	111,204,161
1-epi-Cubenol	1620	1623	1625	119,161,204
γ -Eudesmol	1624	1618	1630	189,204,161
Cubenol	1633	1630	1643	161,105,69

^a Only RI values from a DB-1 column are available in the terpenoids library. RI profiles of DB-1 and DB-5 are close as demonstrated in previous data [4].

^b The first of the target ions was used as quantifier and others were qualifiers.

A mixed alkane standard (C7–C30) was used to determine the retention index (RI; *I*) for each peak. Terpene identification was carried out by matching the mass spectrum and *I* value in the terpenoids library using MassFinder 4 software (Hochmuth Scientific Consulting, Hamburg, Germany). Although *I* values in the terpenoids library are based on a J&W DB1 column while in this present data a DB-5 column was used, these two nonpolar columns have very close *I* profiles as shown in previous data [4]. Therefore, *I* values from the terpenoids library are reliable in facilitating the tentative identification in the present data. Peak integration was then conducted with the Agilent ChemStation software based on the responses of target ions. Calculated and reference RI are summarized in Table 3. Mass spectra of semi-quantified terpenes are provided in Table 4. Quantification of each terpene was performed against calibration curves constructed by a series of standards including, α -terpineol, linalool, geraniol, geranylacetone. α -Terpinene, cymene (m- and p-), 1,8-cineol, (E)- β -ocimene, γ -terpinene, terpinolene, p-cymenene and hotrienol were semi-quantified using a linalool standard. All sesquiterpenoids and norisoprenoids were semi-quantified with the internal standard β -cedrene and expressed as equivalent concentrations.

Significant ($p < 0.05$) differences in terpene concentrations at different development stages of each grape cultivar were analysed by one-way ANOVA using SPSS 24 (SPSS Inc., Chicago, IL).

Table 4

Comparisons between reference terpenoid mass spectra from the terpenoids library (upper frame) and for an experimental peak in a representative sample (lower frame).

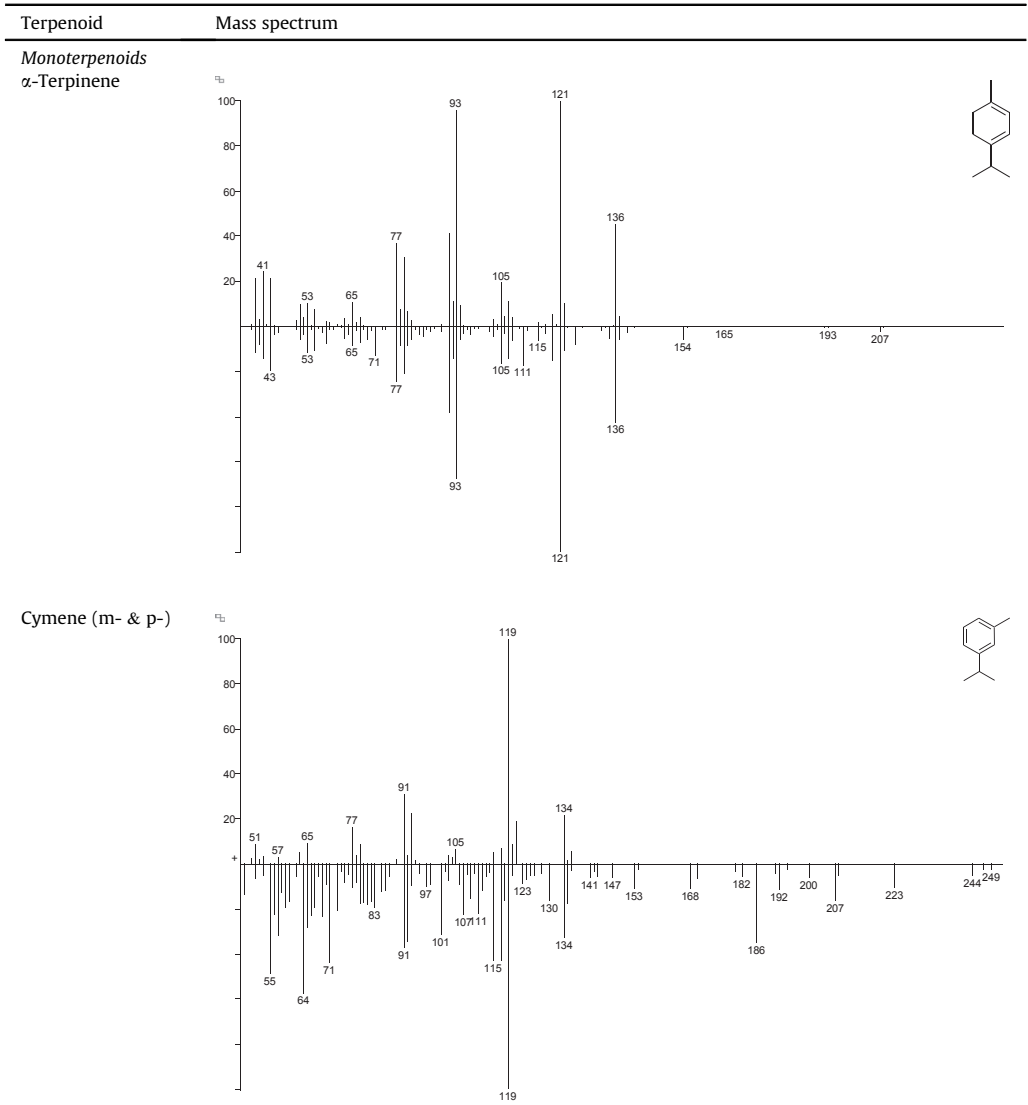
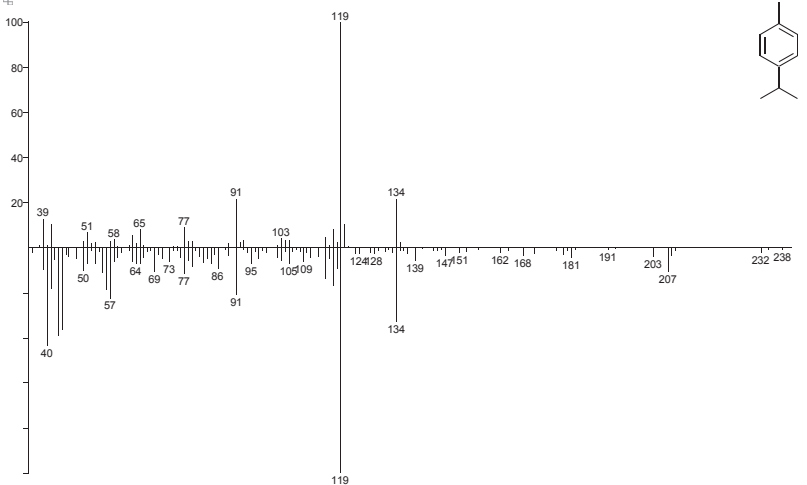
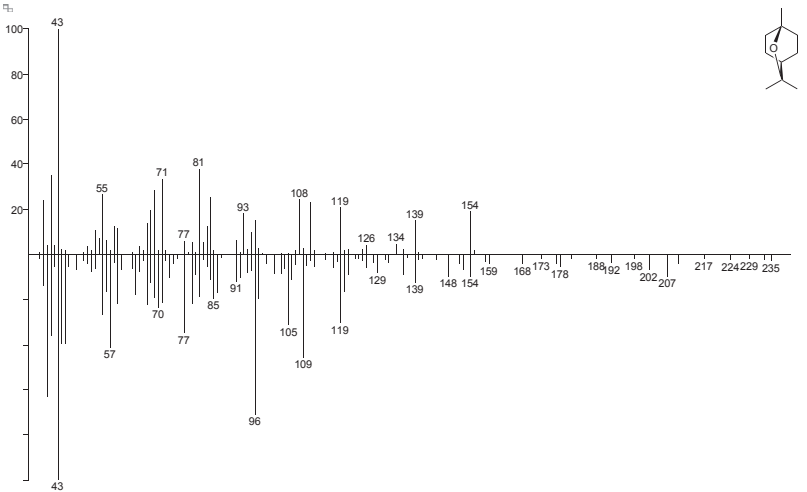


Table 4 (continued)

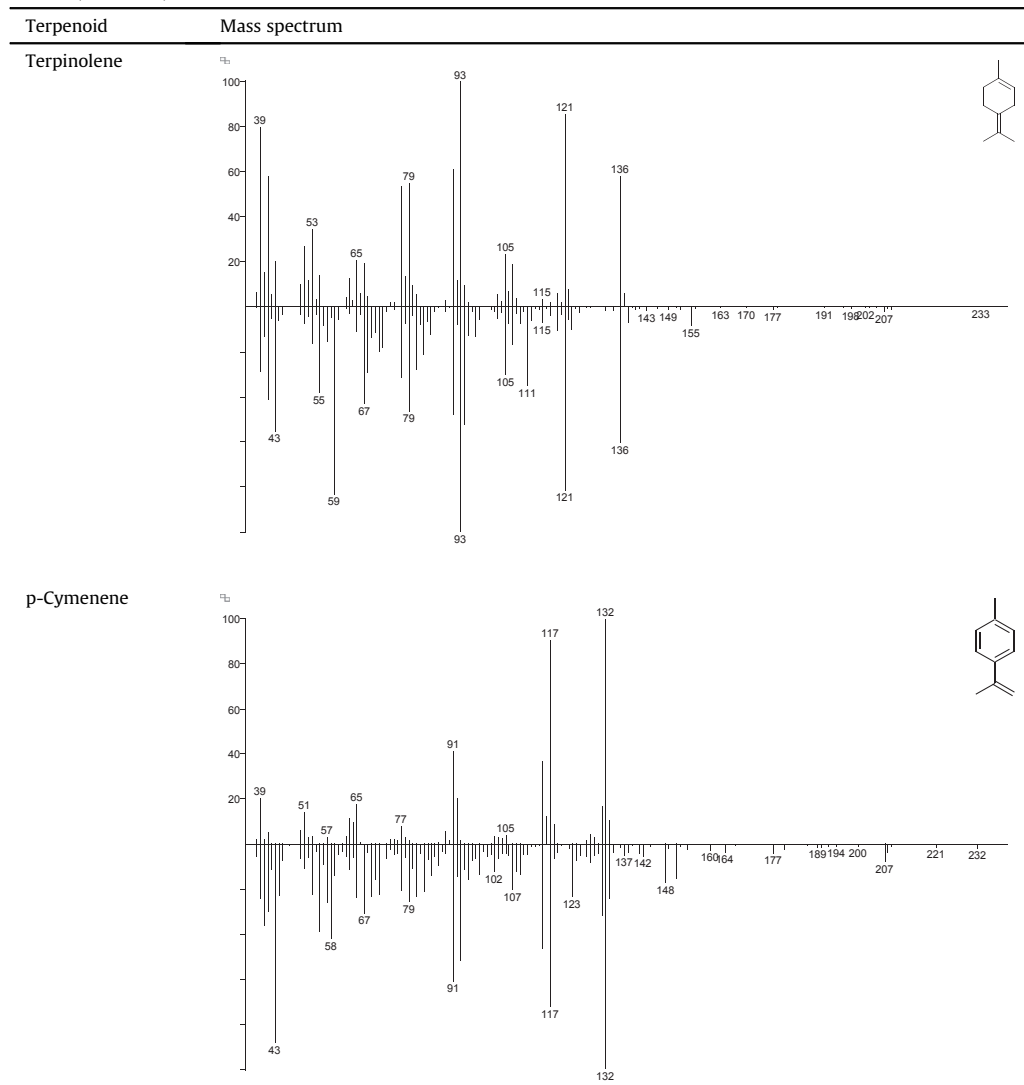
Terpenoid	Mass spectrum
	 <p>Mass spectrum showing relative intensity (%) versus m/z. The base peak is at m/z 119. Other significant peaks are labeled at m/z 39, 40, 50, 51, 57, 58, 64, 65, 69, 73, 77, 86, 91, 95, 103, 109, 124, 128, 134, 139, 147, 151, 162, 168, 181, 191, 203, 207, 232, and 238.</p>
1,8-Cineol	 <p>Mass spectrum showing relative intensity (%) versus m/z. The base peak is at m/z 43. Other significant peaks are labeled at m/z 55, 57, 70, 71, 77, 81, 85, 91, 93, 96, 105, 108, 109, 119, 126, 129, 134, 139, 148, 154, 159, 168, 173, 178, 188, 192, 198, 202, 207, 217, 224, 229, and 235.</p>

(continued on next page)

Table 4 (continued)

Terpenoid	Mass spectrum
(<i>E</i>)- β -Ocimene	<p>Mass spectrum of (<i>E</i>)-β-Ocimene. The x-axis represents the mass-to-charge ratio (m/z) from 41 to 235, and the y-axis represents relative intensity from 0 to 100. The base peak is at m/z 93. Other significant peaks are labeled at m/z 39, 41, 53, 55, 67, 70, 79, 105, 111, 121, 127, 131, 136, 151, 156, 169, 177, 191, 207, 213, 223, 227, and 235. The chemical structure of (<i>E</i>)-β-Ocimene is shown to the right.</p>
γ -Terpinene	<p>Mass spectrum of γ-Terpinene. The x-axis represents the mass-to-charge ratio (m/z) from 41 to 207, and the y-axis represents relative intensity from 0 to 100. The base peak is at m/z 93. Other significant peaks are labeled at m/z 41, 43, 53, 55, 65, 70, 77, 82, 97, 105, 115, 121, 129, 136, and 207. The chemical structure of γ-Terpinene is shown to the right.</p>

Table 4 (continued)



(continued on next page)

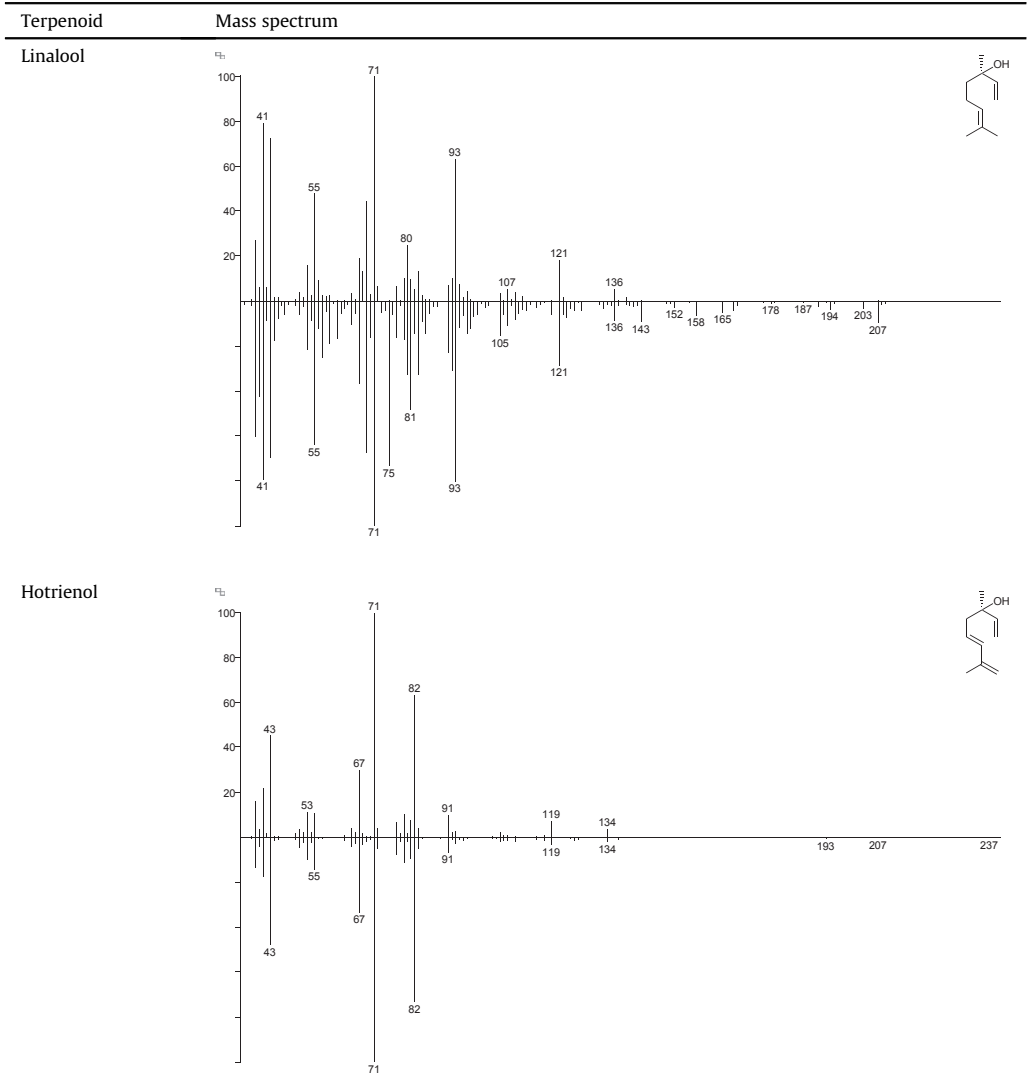

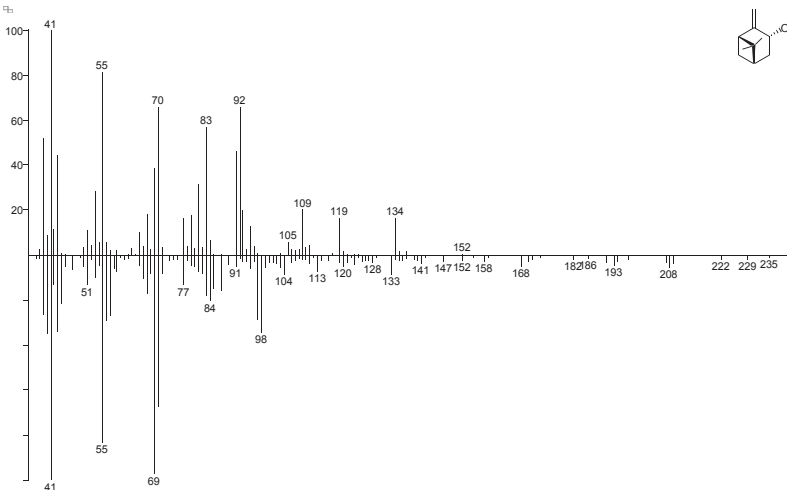
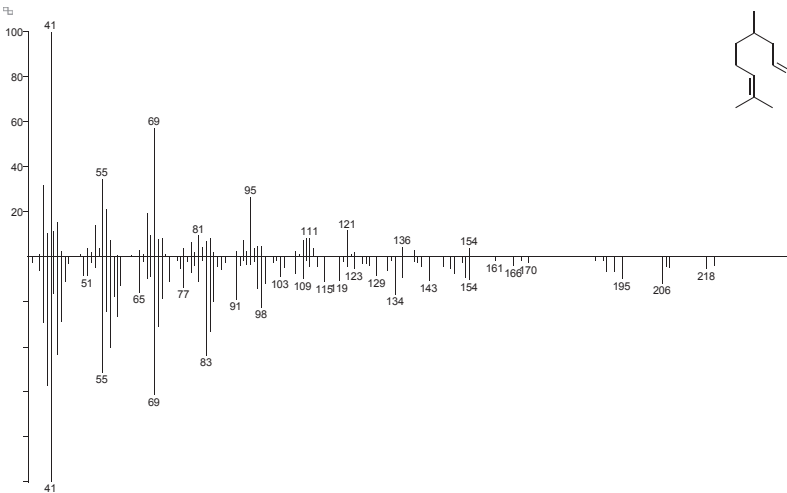
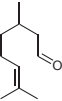
Table 4 (continued)

Table 4 (continued)

Terpenoid	Mass spectrum	
trans-Pinocarveol		
Citronellal		

(continued on next page)

Table 4 (continued)

Terpenoid

Mass spectrum

Neroloxide

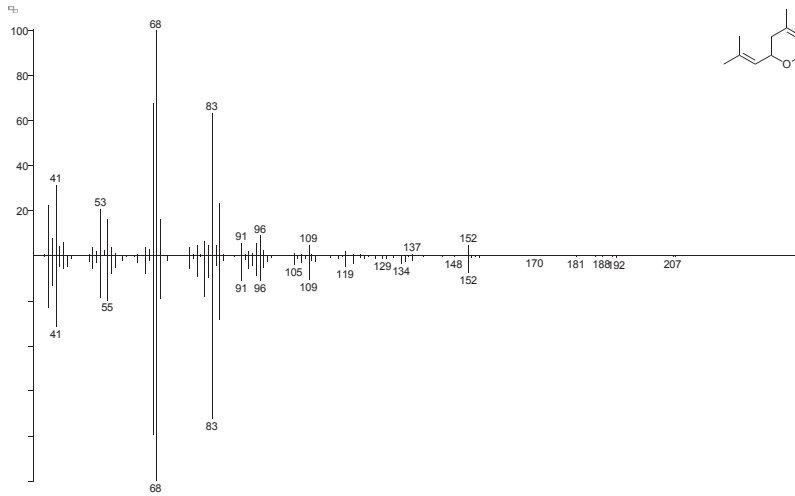
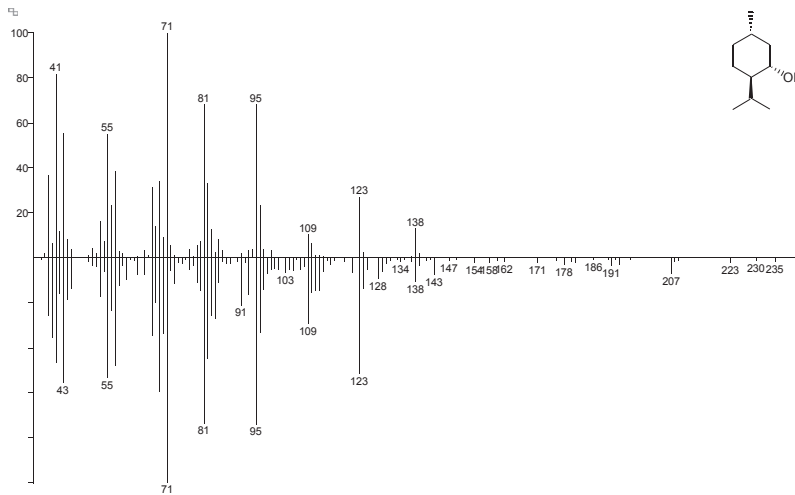
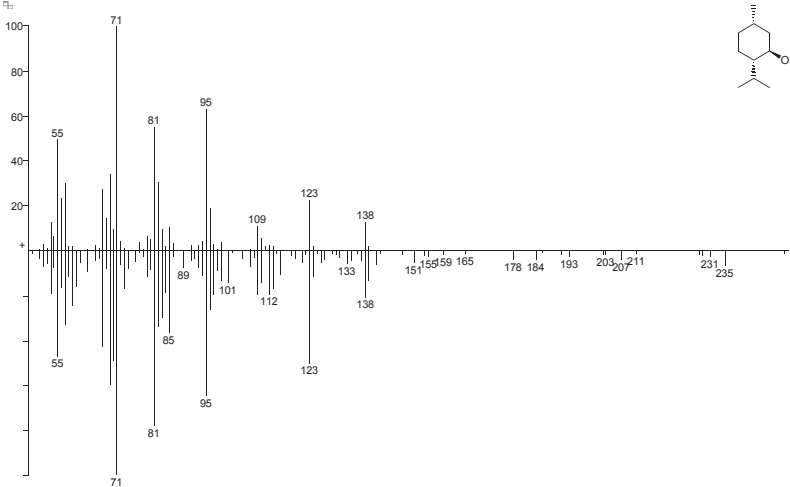

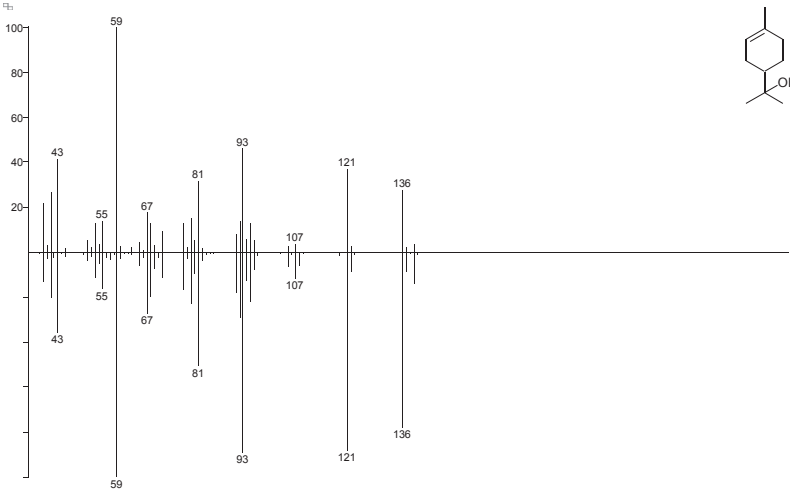
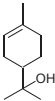
Menthol
(+isomenthol)

Table 4 (continued)

Terpenoid	Mass spectrum	
 <p>Mass spectrum showing relative intensity (%) versus m/z for a bicyclic terpenoid with a hydroxyl group. The base peak is at m/z 71. Other significant peaks are labeled at m/z 55, 81, 95, 109, 123, and 138.</p>	 <p>Chemical structure of a bicyclic terpenoid with a hydroxyl group.</p>	
α -Terpineol	 <p>Mass spectrum showing relative intensity (%) versus m/z for α-Terpineol. The base peak is at m/z 59. Other significant peaks are labeled at m/z 43, 67, 81, 93, 107, 121, and 136.</p>	 <p>Chemical structure of α-Terpineol.</p>

(continued on next page)

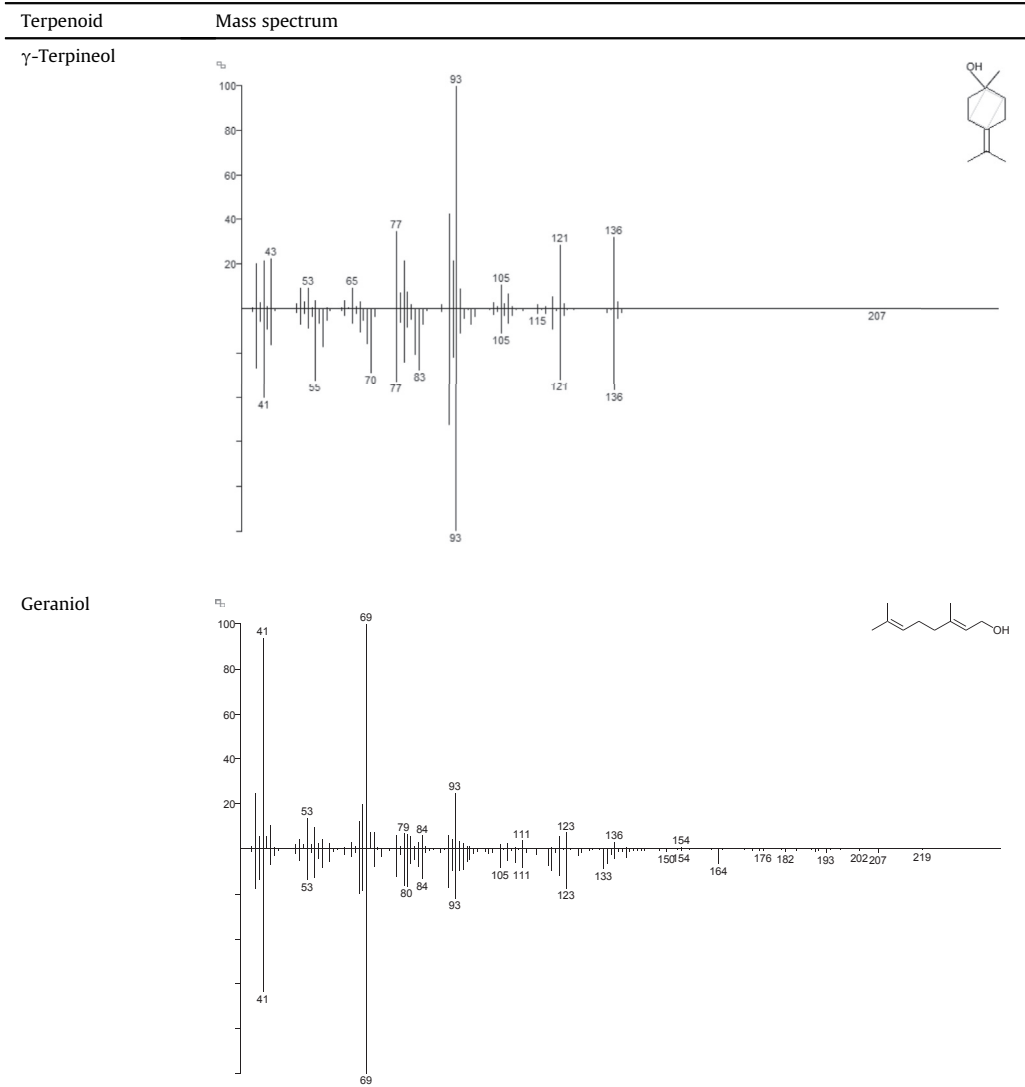
Table 4 (continued)

Table 4 (continued)

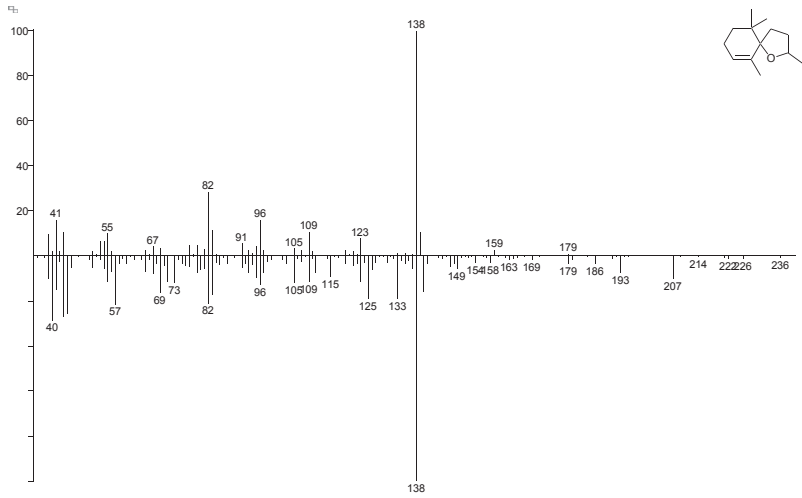
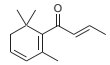
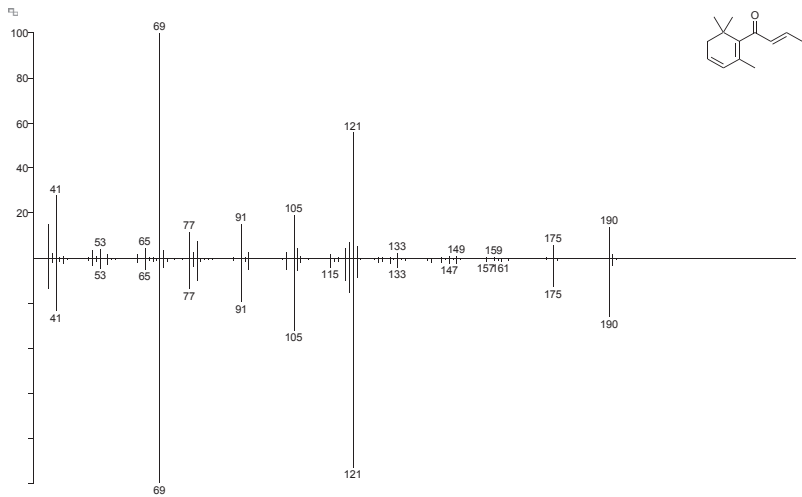
Terpenoid	Mass spectrum	Chemical structure
Geranylacetone	<p>Mass spectrum of Geranylacetone. The x-axis represents the mass-to-charge ratio (m/z) from 43 to 236, and the y-axis represents relative intensity from 0 to 100%. The base peak is at m/z 43. Other labeled peaks include m/z 53, 63, 69, 77, 81, 83, 93, 107, 109, 115, 120, 121, 125, 131, 136, 143, 147, 151, 157, 161, 170, 176, 177, 184, 194, 204, 209, 220, 224, and 236.</p>	<p>Chemical structure of Geranylacetone: <chem>CC(=O)C=CC=CC</chem></p>
Norisoprenoids Theaspirane (Isomer 1)	<p>Mass spectrum of Theaspirane (Isomer 1). The x-axis represents the mass-to-charge ratio (m/z) from 41 to 233, and the y-axis represents relative intensity from 0 to 100%. The base peak is at m/z 138. Other labeled peaks include m/z 41, 55, 67, 71, 77, 82, 82, 91, 96, 96, 105, 105, 109, 109, 123, 123, 129, 138, 147, 155, 159, 162, 171, 179, 179, 189, 197, 206, 215, 228, and 233.</p>	<p>Chemical structure of Theaspirane (Isomer 1): <chem>CC1=C(C)C2C(C1)OC2</chem></p>

(continued on next page)

Table 4 (continued)

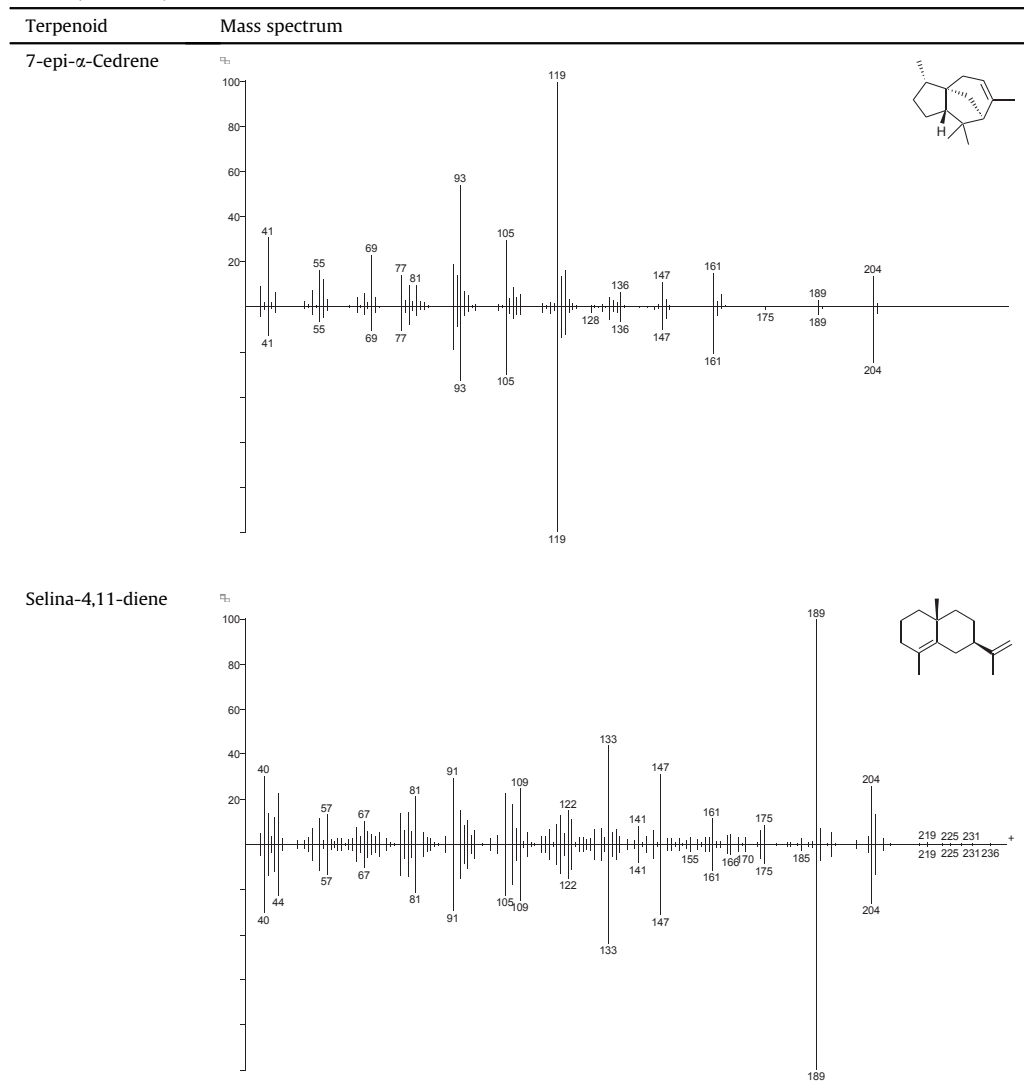
Terpenoid

Mass spectrum

Theaspirane
(Isomer 2)*(E)*- β -Damascenone

Sesquiterpenoids

Table 4 (continued)



(continued on next page)

Table 4 (continued)

Terpenoid

Mass spectrum

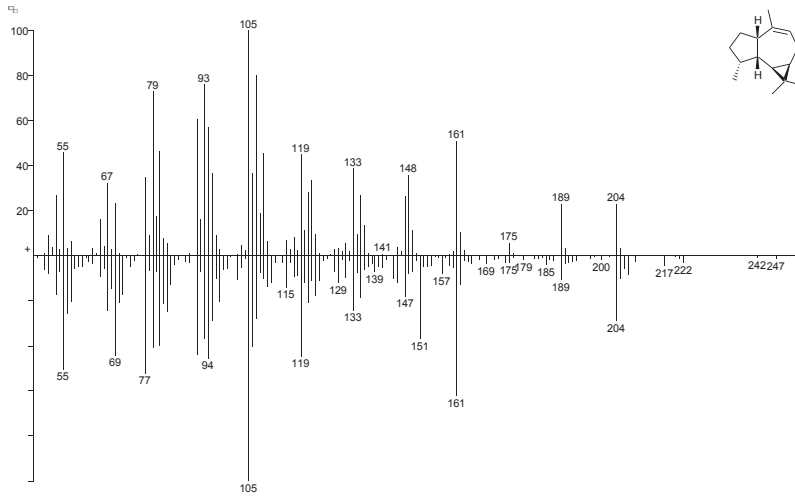
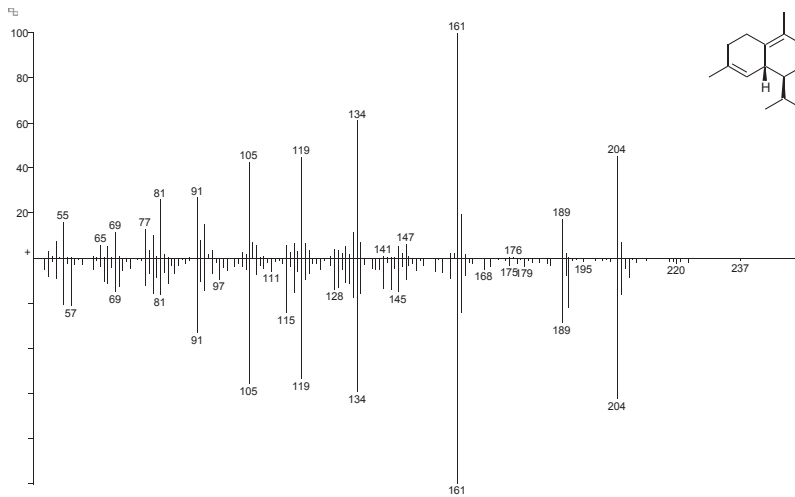
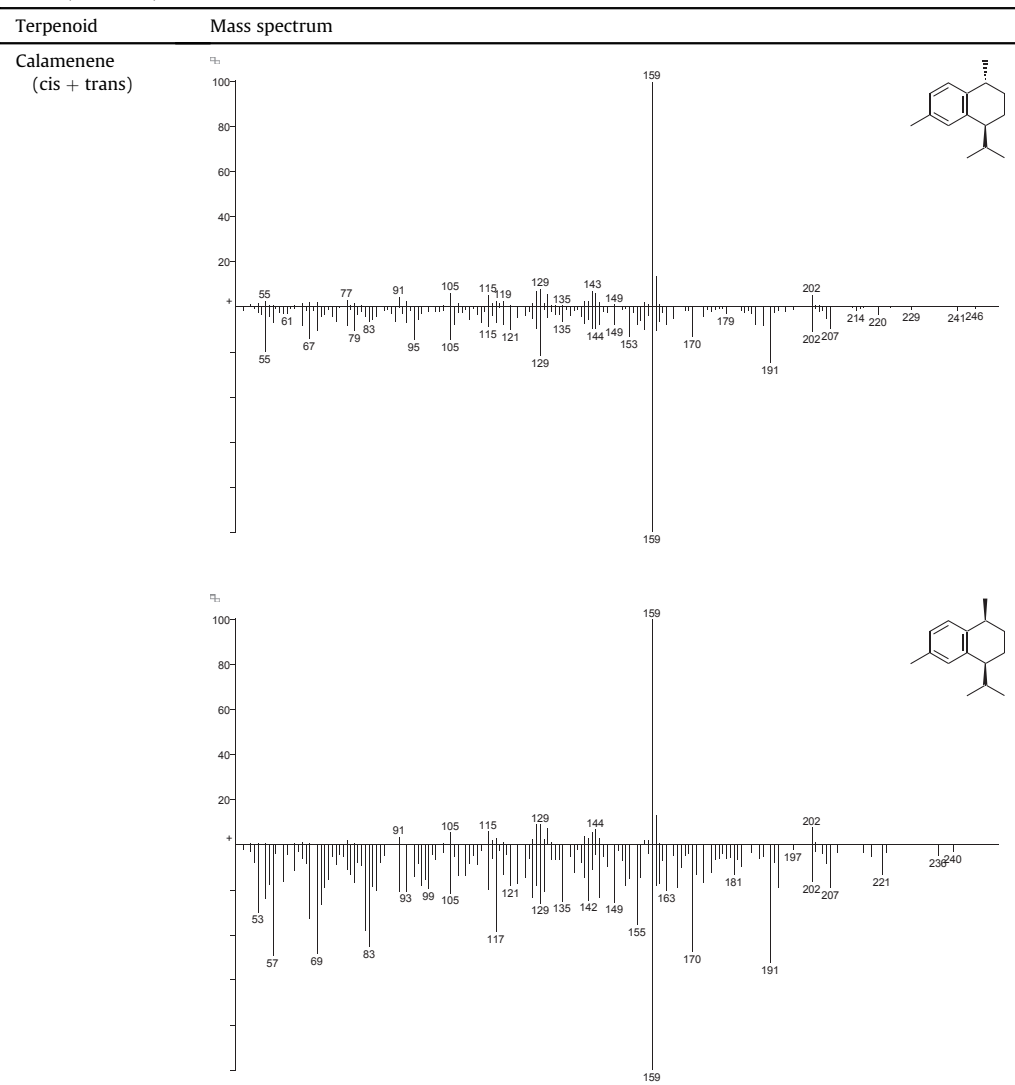
 α -Muurolene δ -Cadinene

Table 4 (continued)



(continued on next page)

Table 4 (continued)

Terpenoid

Mass spectrum

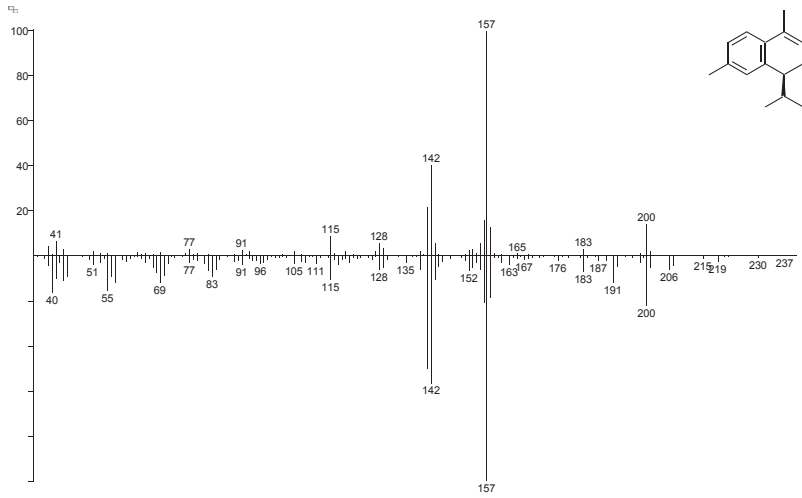
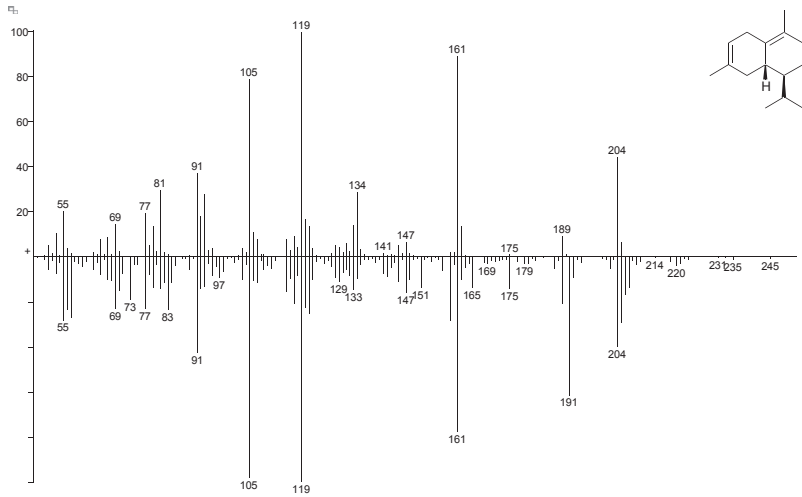
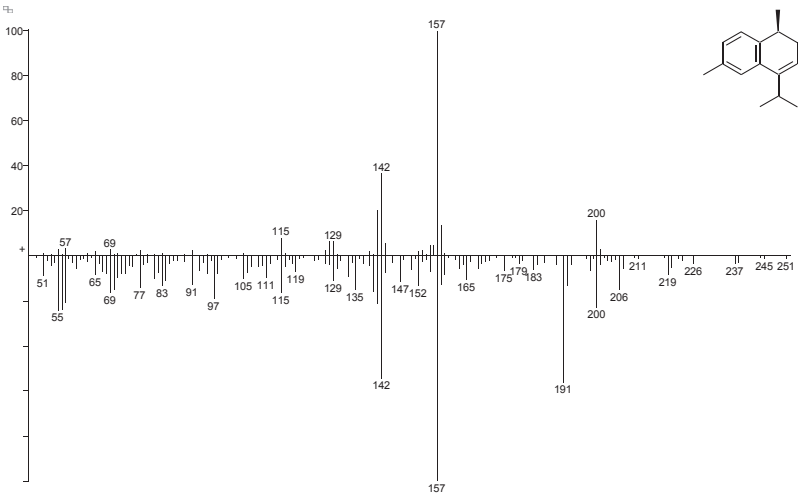
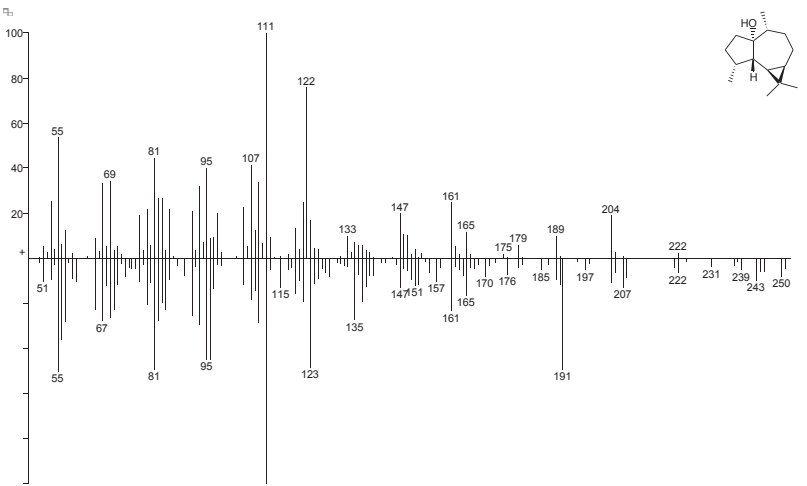
 α -Calacorene ω -Cadinene

Table 4 (continued)

Terpenoid	Mass spectrum
γ -Calacorene	 <p>Mass spectrum of γ-Calacorene. The x-axis represents the mass-to-charge ratio (m/z) from 51 to 251, and the y-axis represents relative intensity from 0 to 100%. The base peak is at m/z 157. Other prominent peaks are at m/z 142, 200, 191, 115, 129, 57, 69, 55, 147, 152, 165, 175, 179, 183, 206, 211, 219, 226, 237, 245, and 251. The chemical structure of γ-Calacorene is shown to the right.</p>
Palustrol	 <p>Mass spectrum of Palustrol. The x-axis represents the mass-to-charge ratio (m/z) from 51 to 250, and the y-axis represents relative intensity from 0 to 100%. The base peak is at m/z 111. Other prominent peaks are at m/z 122, 55, 81, 95, 107, 133, 147, 161, 165, 175, 179, 189, 204, 191, 115, 147, 151, 165, 170, 176, 185, 197, 207, 222, 231, 239, 243, and 250. The chemical structure of Palustrol is shown to the right.</p>

(continued on next page)

Table 4 (continued)

Terpenoid	Mass spectrum
1- <i>epi</i> -Cubenol	<p>Chemical structure of 1-<i>epi</i>-Cubenol: <chem>CC1=C(C)C2=C(C1)C=C(C2)O</chem></p>
γ -Eudesmol	<p>Chemical structure of γ-Eudesmol: <chem>CC1=C(C)C2=C(C1)C=C(C2)O</chem></p>

Table 4 (continued)

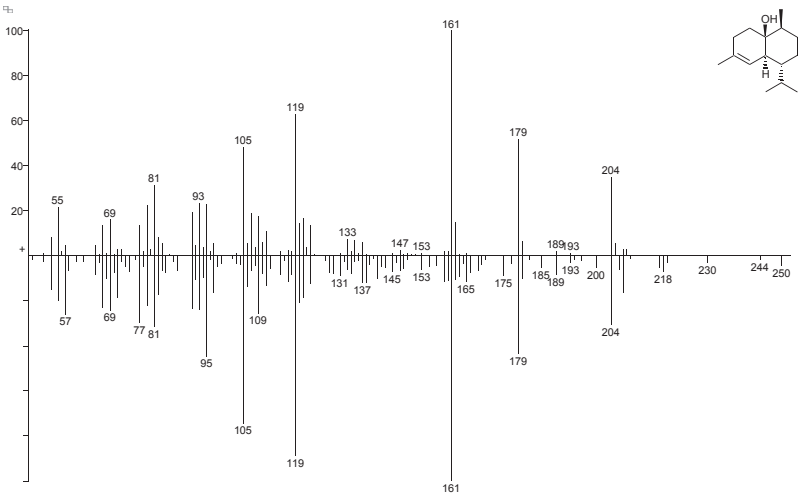
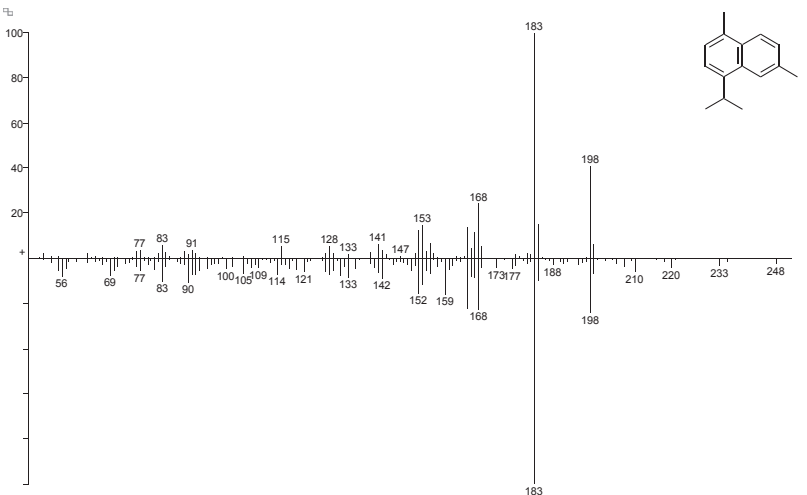
Terpenoid	Mass spectrum
Cubenol	 <p>Chemical structure of Cubenol: <chem>CC1=C(C)C2=C(C1)C(O)C=C2</chem></p>
Cadalene	 <p>Chemical structure of Cadalene: <chem>CC1=C(C)C=C2C=C(C)C=C12</chem></p>

Table 5
Terpene concentrations at different developmental stages of Shiraz in the two experimental vintages.

Vintage 2016	wpf4	wpf6	wpf8	wpf10	wpf12	wpf14	wpf16
Monoterpenoids							
α -Terpinene	<0.01	<0.01	<0.01	0.31 ± 0.08	<0.01	<0.01	<0.01
Cymene (m- and p-)	<0.01	<0.01	<0.01	0.62 ± 0.31a	0.65 ± 0.19a	0.5 ± 0.15a	1.17 ± 0.56a
1,8-Cineol	ND	ND	ND	ND	ND	ND	ND
(E)- β -Ocimene	<0.01	ND	ND	ND	ND	ND	ND
γ -Terpinene	ND	ND	ND	ND	ND	ND	ND
Terpinolene	<0.01	<0.01	<0.01	0.25 ± 0.13	<0.01	<0.01	<0.01
p-Cymenene	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	0.22 ± 0.16
Linalool	2.25 ± 0.2bc	0.78 ± 0.16c	2.59 ± 2.73abc	0.8 ± 0.56c	10.68 ± 3.42ab	6.63 ± 4.32abc	12.06 ± 6.9a
Hotrienol	<0.01	<0.01	0.89 ± 0.94b	0.11 ± 0.06b	4.19 ± 0.87a	1.41 ± 0.12b	0.49 ± 0.41b
trans-Pinocarveol	<0.01	<0.01	0.94 ± 0.46c	7.17 ± 0.79bc	11.7 ± 1.13ab	9.06 ± 5.92bc	20.08±2a
Citronellal	0.17 ± 0.08c	<0.01	1.5 ± 0.56c	12.27 ± 1.42bc	19.05 ± 1.72ab	15.56 ± 9.55b	31.52 ± 3.72a
Neroloxide	<0.01	<0.01	<0.01	<0.01	0.46 ± 0.29	<0.01	<0.01
Menthol (+isomenthol)	<0.01	<0.01	<0.01	3.57 ± 0.5b	5.35 ± 0.54ab	3.78 ± 2.88b	9.09 ± 1.03a
Terpinen-4-ol	<0.01	<0.01	<0.01	0.07 ± 0.06b	<0.01	<0.01	0.38 ± 0.27a
α -Terpineol	2.2 ± 0.06bc	0.48 ± 0.1c	1.87 ± 1.2bc	2.35 ± 0.02bc	4.38 ± 0.52ab	3.22 ± 2.38abc	6.43 ± 1.32a
Geraniol	1.44 ± 0.26bc	1.44 ± 0.07bc	2.62 ± 1.52abc	1.06 ± 0.17c	6.17 ± 1.59a	5.25 ± 2.26a	4.99 ± 1.3ab
Geranylacetone	9.35 ± 2.98a	4.66 ± 0.86a	31.31 ± 14.36a	14.2 ± 7.37a	24.02 ± 6.86a	21.46 ± 16.1a	27.49 ± 14.32a
Total	15.48 ± 3.45c	7.46 ± 0.88c	40.15 ± 22.56bc	33.92 ± 23.52bc	86.63 ± 10.44ab	66.23 ± 44.01abc	113.8 ± 30.13a
Norisoprenoids							
Theaspirane (Isomer 1)	0.18 ± 0.01ab	0.12 ± 0.01ab	0.25 ± 0.16ab	0.05±0b	0.36 ± 0.06a	0.15 ± 0.09ab	0.2 ± 0.18ab
Theaspirane (Isomer 2)	0.12±0ab	0.1 ± 0.01ab	0.18 ± 0.1a	0.04±0b	0.18 ± 0.02a	0.08 ± 0.05ab	0.09 ± 0.05ab
(E)- β -Damascenone	0.24±0c	0.34 ± 0.03c	0.65 ± 0.26c	1.53 ± 0.28bc	4.59 ± 0.35a	3.84 ± 1.95ab	5.5 ± 0.97a
Total	0.54 ± 0.01c	0.56 ± 0.03c	1.08 ± 0.51c	1.61 ± 0.28bc	5.13 ± 0.39a	4.08 ± 2.08ab	5.79 ± 1.2a
Sesquiterpenoids							
7-epi- α -Cedrene	1.71 ± 0.3ab	2.24 ± 0.23a	0.72 ± 0.02d	1.57 ± 0.48bc	0.96 ± 0.02cd	1 ± 0.03cd	1 ± 0.06cd
Selina-4,11-diene	0.12 ± 0.01a	0.05±0b	0.03 ± 0.01c	0.02±0c	ND	ND	ND
α -Muurolene	0.13 ± 0.01a	0.14±0a	0.05 ± 0.01b	0.06 ± 0.03b	ND	ND	ND
δ -Cadinene	ND	ND	ND	0.12 ± 0.1a	0.11 ± 0.03a	0.17 ± 0.07a	0.18 ± 0.04a
Calamenene (cis + trans)	0.29 ± 0.01a	0.12 ± 0.01b	0.07 ± 0.01b	0.15 ± 0.07b	0.1 ± 0.03b	0.07 ± 0.02b	0.1 ± 0.02b
α -Calacorene	0.08 ± 0.02a	0.03±0ab	0.02 ± 0.01b	0.06 ± 0.04ab	0.04 ± 0.02ab	0.03 ± 0.02ab	0.05 ± 0.02ab
ω -Cadinene	0.21 ± 0.02a	0.08 ± 0.01b	0.04 ± 0.01b	0.07 ± 0.02b	0.04 ± 0.02b	0.06 ± 0.02b	0.07 ± 0.02b
γ -Calacorene	0.76 ± 0.01a	0.33 ± 0.03bc	0.13 ± 0.05d	0.37 ± 0.14b	0.15 ± 0.03cd	0.16 ± 0.07cd	0.21 ± 0.04bcd
Palustrol	0.13 ± 0.02a	0.01±0b	0.02 ± 0.01b	0.03 ± 0.02b	0.03 ± 0.01b	0.06 ± 0.03b	ND
1-epi-Cubenol	0.16 ± 0.01a	0.03 ± 0b	0.04 ± 0.01b	0.09 ± 0.06ab	0.1 ± 0ab	0.1 ± 0.02ab	0.14 ± 0.07a
γ -Eudesmol	0.13 ± 0.01a	0.03 ± 0b	0.02 ± 0b	0.1 ± 0.07ab	ND	ND	ND
Cubenol	0.08 ± 0.01a	0.03 ± 0.01a	0.03 ± 0.01a	0.07 ± 0.05a	0.05 ± 0.02a	0.07 ± 0.02a	0.09 ± 0.06a
Cadalene	0.13 ± 0.01a	0.11 ± 0.01a	0.05 ± 0.02c	0.09 ± 0.02ab	0.03 ± 0.01c	0.04 ± 0.02c	0.05 ± 0.02bc
Total	3.92 ± 0.31a	3.19 ± 0.27a	1.23 ± 0.03c	2.81 ± 0.94ab	1.61 ± 0.09c	1.78 ± 0.14bc	1.89 ± 0.18bc

Vintage 2017

<i>Monoterpenoids</i>								
α -Terpinene	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
Cymene (m- and p-)	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
1,8-Cineol	ND	ND	ND	ND	ND	ND	ND	ND
(E)- β -Ocimene	0.14 \pm 0.09	<0.01	ND	ND	ND	<0.01	<0.01	<0.01
γ -Terpinene	ND	ND	ND	ND	ND	ND	ND	ND
Terpinolene	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
p-Cymenene	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
Linalool	1.03 \pm 0.31bcd	1.6 \pm 0.56ab	0.57 \pm 0.12cd	0.39 \pm 0.13d	0.94 \pm 0.13bcd	1.14 \pm 0.16bc	1.18 \pm 0.21abc	1.89 \pm 0.11a
Hotrienol	1.11 \pm 0.87b	5.63 \pm 1.64a	5.46 \pm 1.45a	3.37 \pm 1.76ab	2.47 \pm 0.74ab	0.99 \pm 0.24b	0.19 \pm 0.02b	0.27 \pm 0.18b
trans-Pinocarveol	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
Citronellal	<0.01	<0.01	<0.01	<0.01	<0.01	0.22 \pm 0.1a	0.08 \pm 0.04b	0.26 \pm 0.14a
Neroloxide	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
Menthol (+isomenthol)	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
Terpinen-4-ol	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
α -Terpineol	<0.01	0.44 \pm 0.2ab	0.23 \pm 0.02b	<0.01	0.37 \pm 0.17ab	0.53 \pm 0.33ab	0.57 \pm 0.11ab	0.77 \pm 0.13a
Geraniol	1.36 \pm 0.18d	1.18 \pm 0.29d	0.9 \pm 0.2d	1.14 \pm 0.04d	1.39 \pm 0.18d	1.96 \pm 0.19c	3.72 \pm 0.19a	2.62 \pm 0.14b
Geranylacetone	8.54 \pm 0.75a	8.54 \pm 0.22a	6.64 \pm 2.76ab	4.85 \pm 1.04ab	2.98 \pm 1.73b	3.17 \pm 1.78b	5.18 \pm 2.44ab	3.32 \pm 1.67b
Total	12.21 \pm 0.43abc	17.62 \pm 2.82a	13.98 \pm 3.16ab	9.76 \pm 1.25bc	8.15 \pm 1.78bc	7.94 \pm 2.19c	10.86 \pm 2.15bc	9.05 \pm 1.92bc
<i>Norisoprenoids</i>								
Theaspirane (Isomer 1)	0.15 \pm 0a	0.16 \pm 0.03a	0.11 \pm 0.02b	0.08 \pm 0.01bc	0.06 \pm 0cd	0.05 \pm 0cd	0.04 \pm 0d	0.04 \pm 0d
Theaspirane (Isomer 2)	0.14 \pm 0.01a	0.13 \pm 0.02a	0.08 \pm 0.01b	0.07 \pm 0bc	0.05 \pm 0cd	0.04 \pm 0d	0.03 \pm 0d	0.03 \pm 0d
(E)- β -Damascenone	0.3 \pm 0.02f	0.49 \pm 0.11ef	0.82 \pm 0.13de	1.29 \pm 0.21d	3.49 \pm 0.1a	2.77 \pm 0.05b	1.95 \pm 0.24c	2.97 \pm 0.29b
Total	0.58 \pm 0.01e	0.78 \pm 0.16e	1.01 \pm 0.15de	1.44 \pm 0.22d	3.6 \pm 0.1a	2.85 \pm 0.05b	2.02 \pm 0.24c	3.03 \pm 0.3b
<i>Sesquiterpenoids</i>								
7-epi- α -Cedrene	3.18 \pm 0.25a	3.63 \pm 1a	1.52 \pm 0.25b	1.11 \pm 0.06b	1.45 \pm 0.47b	1.3 \pm 0.15b	1.1 \pm 0.12b	1.11 \pm 0.19b
Selina-4,11-diene	0.09 \pm 0.01a	0.08 \pm 0.03ab	0.05 \pm 0.01bc	0.03 \pm 0cd	0.03 \pm 0.01cd	0.02 \pm 0.01cd	0.01 \pm 0cd	0.01 \pm 0d
α -Muurolene	0.05 \pm 0.01bc	0.16 \pm 0.04a	0.16 \pm 0.03a	0.09 \pm 0.02bc	0.1 \pm 0.01b	0.06 \pm 0.01bc	0.04 \pm 0.01c	0.04 \pm 0.01c
δ -Cadinene	ND	ND	ND	ND	ND	ND	ND	ND
Calamenene (cis + trans)	0.15 \pm 0.02ab	0.2 \pm 0.05a	0.15 \pm 0.01ab	0.08 \pm 0.02c	0.08 \pm 0.02c	0.06 \pm 0.03c	0.06 \pm 0.01c	0.1 \pm 0.01bc
α -Calacorene	0.06 \pm 0.01a	0.05 \pm 0.01ab	0.03 \pm 0bc	0.02 \pm 0c	ND	ND	ND	ND
ω -Cadinene	0.18 \pm 0.02a	0.12 \pm 0.02b	0.04 \pm 0c	0.04 \pm 0.01c	0.03 \pm 0c	0.03 \pm 0c	0.03 \pm 0c	0.03 \pm 0.01c
γ -Calacorene	0.42 \pm 0.03abc	0.56 \pm 0.14a	0.34 \pm 0.03bcd	0.22 \pm 0.01de	0.2 \pm 0.02de	0.18 \pm 0.01e	0.28 \pm 0.03cde	0.48 \pm 0.05ab
Palustrol	0.14 \pm 0.03a	0.04 \pm 0b	0.01 \pm 0b	0.01 \pm 0b	0.01 \pm 0b	ND	ND	ND
1-epi-Cubenol	0.09 \pm 0.02a	0.06 \pm 0.02b	0.04 \pm 0bc	0.02 \pm 0c	0.02 \pm 0c	0.03 \pm 0c	0.02 \pm 0c	0.02 \pm 0.01c
γ -Eudesmol	0.02 \pm 0bc	0.04 \pm 0.01a	0.03 \pm 0ab	0.02 \pm 0bc	0.02 \pm 0bc	0.02 \pm 0bc	0.01 \pm 0c	0.02 \pm 0.01bc
Cubenol	0.07 \pm 0.01a	0.05 \pm 0.02a	0.03 \pm 0b	0.02 \pm 0b	0.02 \pm 0.01b	0.03 \pm 0b	0.02 \pm 0.01b	0.02 \pm 0b
Cadalene	0.06 \pm 0e	0.17 \pm 0.03b	0.12 \pm 0.01c	0.08 \pm 0.01cde	0.08 \pm 0.01cde	0.08 \pm 0de	0.1 \pm 0.01cd	0.23 \pm 0.02a
Total	4.51 \pm 0.2a	5.15 \pm 1.35a	2.51 \pm 0.34b	1.75 \pm 0.03b	2.04 \pm 0.52b	1.81 \pm 0.13b	1.68 \pm 0.11b	2.08 \pm 0.19b

Notes: Linalool, α -terpineol, geraniol and geranylacetone were quantified using their pure standard compounds. α -terpinene, cymene (m- and p-), 1,8-cineol, (E)- β -ocimene, γ -terpinene, terpinolene, p-cymenene and hotrienol were semi-quantified using a linalool standard. All monoterpenes are expressed at $\mu\text{g/g}$ grape sample. All sesquiterpenoids and norisoprenoids were semi-quantified with the internal standard β -cedrene and expressed as equivalent concentrations of the internal standard at $\mu\text{g/kg}$ grape sample. ND: not detected. Values labelled with the same lower case letter in the same row are not significantly ($p < 0.05$) different. Raw data of the table are provide in data file 1.

Table 6
Terpene concentrations at different developmental stages of Cabernet Sauvignon in the two experimental vintages.

Vintage 2016	wpf4	wpf6	wpf8	wpf10	wpf12	wpf14	wpf16
Monoterpenoids							
α -Terpinene	9.17 ± 0.13a	1.02 ± 0.19b	0.2 ± 0.09b	<0.01	0.45 ± 0.2b	0.44 ± 0.04b	1.28 ± 1.67b
Cymene (m- and p-)	2.94 ± 0.03a	0.42 ± 0.12a	<0.01	<0.01	1.04 ± 0.3a	0.95 ± 0.14a	1.8 ± 2.52a
1,8-Cineol	9.12 ± 0.77a	2.28 ± 0.24b	0.55 ± 0.15c	<0.01	ND	ND	ND
(E)- β -Ocimene	ND	ND	ND	ND	ND	ND	ND
γ -Terpinene	20.99 ± 0.68a	5.14 ± 0.37b	ND	ND	ND	ND	ND
Terpinolene	5.64 ± 0.09a	0.87 ± 0.01b	0.1 ± 0.05c	<0.01	0.29 ± 0.2c	<0.01	<0.01
p-Cymenene	0.13 ± 0.05a	<0.01	<0.01	<0.01	0.12 ± 0.06a	<0.01	<0.01
Linalool	0.55 ± 0.16a	<0.01	<0.01	0.83 ± 1.01a	4 ± 0.77a	1.73 ± 1.36a	4.72 ± 4.83a
Hotrienol	<0.01	<0.01	<0.01	0.3 ± 0.18a	0.32 ± 0.36a	<0.01	<0.01
trans-Pinocarveol	0.2 ± 0.1b	<0.01	<0.01	<0.01	15.83±3a	6.25 ± 3.73ab	14.3 ± 8.1a
Citronellal	0.37 ± 0.16b	<0.01	<0.01	<0.01	26.19 ± 4.58a	10.6 ± 5.39ab	24.63 ± 12.89a
Neroloxide	<0.01	<0.01	<0.01	<0.01	ND	ND	ND
Menthol (+isomenthol)	<0.01	<0.01	<0.01	<0.01	10.64 ± 1.99a	3.87 ± 2.07a	9.51 ± 6.13a
Terpinen-4-ol	5.66 ± 0.88a	0.18 ± 0.09b	<0.01	<0.01	0.36 ± 0.24b	<0.01	<0.01
α -Terpineol	6.98 ± 0.87a	1.77 ± 0.19ab	0.69 ± 0.23b	<0.01	4.91 ± 0.77ab	3.04 ± 0.09ab	4.58 ± 4.56ab
Geraniol	1.04 ± 0.14a	0.98 ± 0.03a	0.91 ± 0.15a	1.07 ± 0.19a	1.63 ± 0.13a	1.63 ± 0.72a	1.43 ± 0.36a
Geranylacetone	10.46 ± 1.67a	7.42 ± 2.03a	20.88 ± 4.22a	10.79 ± 6.77a	27.24 ± 6.74a	19.31 ± 15.08a	19.54 ± 23.15a
Total	73.19±1a	20.09 ± 2.08a	23.37 ± 4.33a	26.46 ± 31.28a	92.98 ± 17.43a	46.51 ± 30.96a	83.36 ± 67.39a
Norisoprenoids							
Theaspirane (Isomer 1)	0.05 ± 0a	0.05 ± 0a	0.04 ± 0.01a	0.07 ± 0.01a	0.06 ± 0.02a	0.05 ± 0.03a	ND
Theaspirane (Isomer 2)	0.04 ± 0.01a	0.05 ± 0.01a	0.04 ± 0.01a	0.05 ± 0a	0.06 ± 0.01a	ND	ND
(E)- β -Damascenone	0.37 ± 0.03b	0.55 ± 0.06b	0.47 ± 0.04b	1.72 ± 0.41ab	5.84 ± 0.82ab	4.95 ± 2.44ab	7.6 ± 5.42a
Total	0.47 ± 0.04b	0.65 ± 0.05b	0.56 ± 0.06b	1.83 ± 0.39ab	5.96 ± 0.83ab	5 ± 2.46ab	7.6 ± 5.42a
Sesquiterpenoids							
7-epi- α -Cedrene	2.13 ± 0.03a	2.53 ± 0.46a	0.82 ± 0.05b	1.13 ± 0.19b	0.94 ± 0.03b	1.05 ± 0.1b	1.08 ± 0.06b
Selina-4,11-diene	0.08 ± 0.01a	0.02 ± 0b	0.02 ± 0b	0.02 ± 0.01b	ND	ND	ND
α -Muurolene	0.07 ± 0.01a	0.07 ± 0.01a	0.04 ± 0.01a	0.07 ± 0.04a	ND	ND	ND
δ -Cadinene	ND	ND	ND	ND	0.12 ± 0.01a	0.15 ± 0.05a	0.19 ± 0.03a
Calamenene (cis + trans)	0.46 ± 0.04a	0.17 ± 0.01b	0.08±0c	0.09 ± 0.01c	0.1 ± 0.02bc	0.07 ± 0.01c	0.1 ± 0.05bc
α -Calacorene	0.12 ± 0.03a	0.04 ± 0.01b	0.02±0b	0.03 ± 0.02b	0.04±0b	0.04 ± 0.01b	0.06 ± 0.02b
ω -Cadinene	0.24 ± 0.01a	0.08 ± 0.01b	0.03±0c	0.05 ± 0.01bc	0.07 ± 0.01bc	0.05 ± 0.01bc	0.06 ± 0.04bc
γ -Calacorene	1.18 ± 0.1a	0.45 ± 0.04b	0.23 ± 0.06c	0.21 ± 0.04c	0.22 ± 0.01c	0.21 ± 0.06c	0.24 ± 0.08c
Palustrol	0.2 ± 0.03a	0.02 ± 0b	ND	ND	0.07 ± 0.01b	0.05 ± 0.02b	0.06±0b
1-epi-Cubenol	0.15 ± 0.01ab	0.04 ± 0.01bc	0.03 ± 0d	0.06 ± 0.07bcd	0.17 ± 0.03a	0.12 ± 0.05abc	0.15 ± 0.02ab
γ -Eudesmol	0.07 ± 0.01a	0.03 ± 0b	0.01 ± 0c	0.02 ± 0.01bc	ND	ND	ND
Cubenol	0.07 ± 0.01abc	0.03 ± 0bc	0.02 ± 0c	0.04 ± 0.04abc	0.11 ± 0.02a	0.09 ± 0.03ab	0.08 ± 0.03abc
Cadalene	0.12 ± 0a	0.13 ± 0.02a	0.06 ± 0b	0.08 ± 0.01b	0.05 ± 0b	0.05 ± 0.01b	0.06 ± 0.02b
Total	4.89 ± 0.26a	3.62 ± 0.49b	1.36 ± 0.1d	1.8 ± 0.27cd	1.87 ± 0.09cd	1.89 ± 0.14cd	2.07 ± 0.11c

Vintage 2017	2	7	12	17	22	27	32	37
	wpf4	wpf6	wpf8	wpf10	wpf12	wpf14	wpf16	wpf18
<i>Monoterpenoids</i>								
α -Terpinene	3.12 ± 0.95a	2.51 ± 0.29a	0.81 ± 0.32b	0.95 ± 0.06b	<0.01	<0.01	<0.01	<0.01
Cymene (m- and p-)	0.85 ± 0.4ab	1.25 ± 0.22a	0.39 ± 0.17b	0.62 ± 0.25ab	<0.01	<0.01	<0.01	<0.01
1,8-Cineol	8.83 ± 2.08a	6.28 ± 1.07a	1.64 ± 0.44b	2.19 ± 1.67b	<0.01	ND	ND	ND
(E)- β -Ocimene	<0.01	ND	ND	ND	ND	ND	ND	ND
γ -Terpinene	7.39 ± 1.87a	8.91 ± 1.15a	ND	ND	ND	ND	ND	ND
Terpinolene	1.68 ± 0.38a	1.45 ± 0.25a	0.31 ± 0.12b	0.42 ± 0.16b	<0.01	<0.01	<0.01	<0.01
p-Cymenene	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
Linalool	0.45 ± 0.18a	0.25 ± 0.21a	<0.01	0.74 ± 0.66a	0.29 ± 0.17a	0.12 ± 0.1a	0.12 ± 0.09a	0.11 ± 0.03a
Hotrienol	0.21 ± 0.17a	0.81 ± 0.32a	0.22 ± 0.08a	0.91 ± 0.46a	<0.01	<0.01	<0.01	<0.01
trans-Pinocarveol	<0.01	<0.01	<0.01	0.23 ± 0.08	<0.01	<0.01	<0.01	<0.01
Citronellal	<0.01	<0.01	<0.01	0.4 ± 0.47a	0.16 ± 0.1a	0.21 ± 0.17a	0.09 ± 0.03a	0.21 ± 0.07a
Neroloxide	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	ND	ND
Menthol (+isomenthol)	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
Terpinen-4-ol	0.96 ± 0.34a	0.72 ± 0.34a	<0.01	<0.01	<0.01	<0.01	<0.01	<0.01
α -Terpineol	0.73 ± 0.09ab	1.46 ± 0.33a	0.41 ± 0.05b	1.33 ± 0.49a	0.06 ± 0.04b	0.32 ± 0.39b	0.4 ± 0.14b	0.18 ± 0.1b
Geraniol	0.71 ± 0.03d	0.73 ± 0.06d	0.62 ± 0.05d	0.72 ± 0.07d	1.73 ± 0.08a	1.07 ± 0.19c	1.39 ± 0.12b	1.25 ± 0.13bc
Geranylacetone	3.83 ± 1.39ab	5.77 ± 2.07ab	5.57 ± 1.03ab	8.76 ± 4.31a	4.85 ± 1.89ab	1.21 ± 2.12b	0.95 ± 1.68b	0.39 ± 2.05b
Total	28.76 ± 6.78ab	30.23 ± 4.51a	9.91 ± 1.58cd	17.01 ± 7.63bc	7.02 ± 2.02cd	2.88 ± 2.42d	2.79 ± 1.77d	2.07 ± 2.15d
<i>Norisoprenoids</i>								
Theaspirane (Isomer 1)	0.03 ± 0.01bc	0.06 ± 0.01a	0.05 ± 0.01ab	0.05 ± 0.02a	0.03±0bc	0.02±0c	0.01 ± 0.01c	0.01 ± 0c
Theaspirane (Isomer 2)	0.03 ± 0ab	0.05 ± 0.02a	0.03 ± 0ab	0.05 ± 0.02a	0.03 ± 0ab	0.02 ± 0.01b	0.02 ± 0.01b	0.01 ± 0b
(E)- β -Damascenone	0.37 ± 0.02e	0.91 ± 0.09de	1.13 ± 0.06de	1.47 ± 0.36d	2.46 ± 0.27c	3.51 ± 0.35ab	3.07 ± 0.54bc	4.23 ± 0.18a
Total	0.44 ± 0.02e	1.02 ± 0.11de	1.21 ± 0.07de	1.57 ± 0.39d	2.51 ± 0.27c	3.55 ± 0.36ab	3.1 ± 0.54bc	4.26 ± 0.18a
<i>Sesquiterpenoids</i>								
7-epi- α -Cedrene	2.74 ± 0.25ab	3.5 ± 1.77a	2.42 ± 0.87ab	1.12 ± 0.19b	1.06 ± 0.14b	1.57 ± 0.16ab	1.04 ± 0.05b	1.27 ± 0.02b
Selina-4,11-diene	0.05 ± 0.01a	0.04 ± 0.01ab	0.03 ± 0b	ND	ND	ND	ND	ND
α -Muurolene	0.03 ± 0.01b	0.06±0b	0.05 ± 0.01ab	ND	ND	ND	ND	ND
δ -Cadinene	ND	ND	ND	ND	ND	ND	ND	ND
Calamenene (cis + trans)	0.17 ± 0.04ab	0.24 ± 0.03a	0.16 ± 0.04b	0.11 ± 0.01bc	0.05±0c	0.08 ± 0.01c	0.05 ± 0.01c	0.06 ± 0.01c
α -Calacorene	0.07 ± 0.02a	0.07 ± 0.01a	0.03 ± 0.01b	ND	ND	ND	ND	ND
ω -Cadinene	0.19 ± 0.03a	0.11 ± 0.02b	0.05 ± 0.01c	ND	ND	ND	ND	ND
γ -Calacorene	0.5 ± 0.06b	0.78 ± 0.05a	0.46 ± 0.06b	0.18 ± 0.09c	0.19 ± 0.01c	0.24 ± 0.03c	0.18 ± 0.02c	0.2 ± 0.01c
Palustrol	0.16 ± 0.03a	0.04 ± 0.01b	0.01±0c	ND	ND	ND	ND	ND
1-epi-Cubenol	0.07 ± 0.02a	0.06 ± 0.01a	0.02 ± 0.01b	0.02 ± 0b	0.02 ± 0b	0.02 ± 0b	0.01 ± 0b	ND
γ -Eudesmol	0.01 ± 0b	0.02 ± 0a	0.02 ± 0.01a	0.01±0ab	ND	ND	ND	ND
Cubenol	0.06 ± 0.02a	0.04 ± 0.01ab	0.02 ± 0.01b	0.02±0b	ND	ND	ND	ND
Cadalene	0.04 ± 0.01c	0.18 ± 0.02a	0.11 ± 0.02b	0.05 ± 0.03c	0.04 ± 0c	0.07 ± 0c	0.05 ± 0c	0.06 ± 0.01c
Total	4.11 ± 0.31ab	5.14 ± 1.91a	3.39 ± 1.03abc	1.52 ± 0.31c	1.37 ± 0.14c	1.98 ± 0.16bc	1.33 ± 0.07c	1.59 ± 0.01c

Notes: Linalool, α -terpineol, geraniol and geranylacetone were quantified using their pure standard compounds. α -terpinene, cymene (m- and p-), 1,8-cineol, (E)- β -ocimene, γ -terpinene, terpinolene, p-cymenene and hotrienol were semi-quantified using a linalool standard. All monoterpenes are expressed at $\mu\text{g/g}$ grape sample. All sesquiterpenoids and norisoprenoids were semi-quantified with the internal standard β -cedrene and expressed as equivalent concentrations of the internal standard at $\mu\text{g/kg}$ grape sample. ND: not detected. Values labelled with the same lower case letter in the same row are not significantly ($p < 0.05$) different. Raw data of the table are provide in data file 1.

Table 7

Terpene concentrations at different developmental stages of Riesling in the two experimental vintages.

Vintage 2016	wpf4	wpf6	wpf8	wpf10	wpf12	wpf14
<i>Monoterpenoids</i>						
α -Terpinene	9.87 ± 0.24a	1.82 ± 0.47b	1.43±1b	0.59 ± 0.17b	0.61 ± 0.31b	0.53 ± 0.4b
Cymene (m- and p-)	6.03 ± 0.12a	0.86 ± 0.48b	1.95 ± 1.45b	0.45 ± 0.36b	0.96 ± 0.61b	0.11 ± 0.13b
1,8-Cineol	0.64 ± 0.27	<0.01	<0.01	ND	ND	ND
(<i>E</i>)- β -Ocimene	<0.01	<0.01	ND	ND	1.51 ± 0.58b	4.6 ± 2.07a
γ -Terpinene	26.79 ± 1.35a	7.33 ± 0.85b	ND	ND	ND	ND
Terpinolene	10.38 ± 0.1a	2.9 ± 0.71c	2.19 ± 1.18c	0.79 ± 0.23c	2.96 ± 0.64bc	6.31 ± 2.59b
p-Cymenene	0.73 ± 0.08a	<0.01	0.43 ± 0.01b	<0.01	<0.01	<0.01
Linalool	3.8 ± 0.38c	1.17 ± 0.24c	2.87 ± 2.06c	6.03 ± 2.53c	29.19 ± 8.44b	58.55 ± 15.31a
Hotrienol	1.33 ± 0.33c	0.8 ± 0.54c	1.85 ± 1.3c	9.97 ± 5.1bc	20.38 ± 1.81ab	35.5 ± 12.34a
trans-Pinocarveol	0.23 ± 0.02a	0.16±0a	0.56 ± 0.38a	10.07 ± 6.5a	3.42 ± 1.31a	1.91 ± 0.31a
Citronellal	0.59 ± 0.51b	0.73 ± 0.06b	1.41 ± 0.56b	16.11 ± 8.58a	6.15 ± 1.56ab	4.17 ± 0.31ab
Neroloxide	<0.01	<0.01	<0.01	1.12 ± 0.74b	5.61 ± 1.16ab	7.87 ± 3.25a
Menthol	<0.01	<0.01	0.09 ± 0.07b	5.89 ± 4.11a	2.01 ± 0.8ab	1.12 ± 0.21ab
(+isomenthol)						
Terpinen-4-ol	6.99 ± 0.03a	0.82 ± 0.29b	1.18 ± 0.5b	<0.01	<0.01	<0.01
α -Terpineol	17.14 ± 0.3ab	5.43 ± 0.82c	5.96 ± 2.94bc	4.89 ± 3.26c	11.21 ± 2.4abc	21.76 ± 8.74a
Geraniol	1.53 ± 0.05bc	0.97 ± 0.06c	1.46 ± 0.38bc	2.93 ± 0.56bc	4.18 ± 0.59b	10.32 ± 2.38a
Geranylacetone	5.12 ± 0.33b	2.29 ± 1.7b	17.39 ± 7.18a	17.66 ± 3.36a	8.87 ± 4.96ab	10.13 ± 0.35ab
Total	91.11 ± 2.81abc	24.99 ± 5.83c	37.59 ± 19.56bc	76.78 ± 31.27bc	97.27 ± 21.98ab	162.83 ± 47.65a
<i>Norisoprenoids</i>						
Theaspirane (Isomer 1)	0.32 ± 0.02ab	0.21 ± 0.02b	0.58 ± 0.29a	0.2 ± 0.01b	0.17 ± 0.07b	0.07 ± 0.02b
Theaspirane (Isomer 2)	0.22 ± 0.02b	0.16 ± 0.04b	0.52 ± 0.25a	0.21 ± 0.02b	0.14 ± 0.05b	0.06 ± 0.01b
(<i>E</i>)- β -Damascenone	0.32 ± 0.01d	0.43 ± 0.02d	0.77 ± 0.29cd	1.53 ± 0.37bc	2.88 ± 0.65a	2.46 ± 0.26ab
Total	0.86 ± 0.03b	0.81 ± 0.04b	1.87 ± 0.83ab	1.93 ± 0.38ab	3.18 ± 0.76a	2.6 ± 0.28a
<i>Sesquiterpenoids</i>						
7-epi- α -Cedrene	2.72 ± 0.73a	1.6 ± 0.34b	0.71 ± 0.06b	0.89 ± 0.12b	1 ± 0.01b	1.15 ± 0.02b
Selina-4,11-diene	0.03±0a	0.01 ± 0b	ND	ND	ND	ND
α -Murolene	0.07 ± 0.01b	0.11 ± 0.01a	0.05 ± 0.02bc	ND	0.04 ± 0.01bc	0.03±0c
δ -Cadinene	ND	ND	ND	0.11 ± 0.06ab	0.07 ± 0.01b	0.21 ± 0.04a
Calamenene (cis + trans)	0.18 ± 0.02a	0.08 ± 0.01b	ND	0.06 ± 0.01b	0.06 ± 0.01b	0.07 ± 0.01b
α -Calacorene	0.06 ± 0.01a	0.02±0b	ND	0.06 ± 0.02a	0.04±0ab	0.06 ± 0.01a
ω -Cadinene	0.04 ± 0.01a	ND	ND	0.05 ± 0.01a	0.04 ± 0.01a	0.05 ± 0a
γ -Calacorene	0.46 ± 0.03a	0.18 ± 0.01bc	0.06 ± 0.01bc	0.2 ± 0.1b	0.13 ± 0.01c	0.22 ± 0.01b
Palustrol	0.09 ± 0.01a	0.01 ± 0c	ND	0.04 ± 0.01b	0.03 ± 0bc	0.02 ± 0.01bc
1-epi-Cubenol	0.06 ± 0.01b	0.02±0c	0.02±0c	0.13 ± 0.02a	0.09±0b	0.09 ± 0.02b
γ -Eudesmol	0.06 ± 0.01a	0.02 ± 0b	ND	ND	ND	ND
Cubenol	0.05 ± 0.01bc	0.03 ± 0c	0.02 ± 0.01c	0.09 ± 0.03a	0.06 ± 0ab	0.08 ± 0.01ab
Cadalene	0.1 ± 0.02a	0.08 ± 0.01ab	0.02 ± 0c	0.04 ± 0.02c	0.05 ± 0.01bc	0.06 ± 0.02bc
Total	3.94 ± 0.69a	2.15 ± 0.34b	0.89 ± 0.1c	1.67 ± 0.34bc	1.61 ± 0.04bc	2.03 ± 0.04b
Vintage 2017	wpf4	wpf6	wpf8	wpf10	wpf12	
<i>Monoterpenoids</i>						
α -Terpinene	7.38 ± 1.85a	2.27 ± 0.63ab	3.5 ± 0.74b	1.63 ± 0.27ab	0.5 ± 0.25c	
Cymene (m- and p-)	2.63 ± 0.84a	0.7 ± 0.08c	2 ± 0.52ab	0.87 ± 0.27bc	0.21 ± 0.07c	
1,8-Cineol	1.03 ± 0.59	<0.01	ND	ND	ND	
(<i>E</i>)- β -Ocimene	0.35 ± 0.08	<0.01	ND	ND	<0.01	
γ -Terpinene	15.88 ± 3.79a	5.61 ± 1.04b	11.34 ± 2.05ab	ND	ND	
Terpinolene	6.84 ± 1.53a	2.24 ± 0.43bc	3.64 ± 0.81b	1.79 ± 0.32bc	1.03 ± 0.38c	
p-Cymenene	0.18 ± 0.01	<0.01	<0.01	<0.01	<0.01	

Table 7 (continued)

Vintage 2017	wpf4	wpf6	wpf8	wpf10	wpf12
Linalool	3.54 ± 1.1a	1.34 ± 0.1b	1.4 ± 0.15b	1.21 ± 0.23b	4.24 ± 0.78a
Hotrienol	5.49 ± 1.29b	5.88 ± 0.95b	14.82 ± 2.09a	14.3 ± 2.2a	12.51 ± 2.08a
trans-Pinocarveol	ND	<0.01	<0.01	<0.01	<0.01
Citronellal	ND	<0.01	<0.01	<0.01	<0.01
Neroloxide	0.25 ± 0.06c	<0.01	2.46 ± 0.56a	1.55 ± 0.45ab	0.9 ± 0.32bc
Menthol (+isomenthol)	ND	<0.01	<0.01	<0.01	<0.01
Terpinen-4-ol	3.15 ± 0.9a	0.26 ± 0.33b	1.17 ± 0.38b	0.25 ± 0.23b	<0.01
α-Terpineol	6.62 ± 1.29a	2.08 ± 0.49c	4.59 ± 1.1ab	3.33 ± 0.47bc	2.54 ± 0.35bc
Geraniol	1.11 ± 0.02b	0.89 ± 0.18b	0.94 ± 0.04b	1.21 ± 0.28b	3.58 ± 0.39a
Geranylacetone	2.4 ± 0.92b	5.18 ± 0.88a	3 ± 0.39ab	2.2 ± 0.77b	1.9 ± 1.1b
Total	56.58 ± 12.51a	26.61 ± 4.41b	48.86 ± 8.06a	28.35 ± 4.53b	27.44 ± 4.74b
<i>Norisoprenoids</i>					
Theaspirane (Isomer 1)	0.16 ± 0.03ab	0.19±0a	0.21 ± 0.04a	0.15 ± 0.02ab	0.11 ± 0.01b
Theaspirane (Isomer 2)	0.17 ± 0.02bc	0.25 ± 0.03a	0.19 ± 0.03ab	0.13 ± 0.03bc	0.11 ± 0.01c
(E)-β-Damascenone	0.27 ± 0.03d	0.66 ± 0.12cd	0.99 ± 0.12c	1.74 ± 0.27b	2.74 ± 0.34a
Total	0.59 ± 0.07d	1.1 ± 0.15cd	1.38 ± 0.16c	2.03 ± 0.32b	2.97 ± 0.36a
<i>Sesquiterpenoids</i>					
7-epi-α-Cedrene	2.22 ± 0.33ab	1.46 ± 0.19b	2.72 ± 0.92a	1.28 ± 0.13b	1.04 ± 0.06b
Selina-4,11-diene	0.04 ± 0.01a	0.02 ± 0b	ND	ND	ND
α-Muurolene	0.03±0b	0.07 ± 0.01bc	0.13 ± 0.03a	0.08 ± 0.01b	ND
δ-Cadinene	ND	ND	ND	ND	ND
Calamenene (cis + trans)	0.09 ± 0.01a	0.07 ± 0.02a	0.09 ± 0a	0.06 ± 0.01a	0.03±0b
α-Calacorene	0.04 ± 0.01a	0.02 ± 0b	ND	ND	ND
ω-Cadinene	0.05 ± 0a	0.03 ± 0b	0.03 ± 0.01b	ND	ND
γ-Calacorene	0.25 ± 0a	0.24 ± 0.06a	0.21 ± 0.03a	0.2 ± 0.01a	0.11 ± 0.02b
Palustrol	0.12 ± 0.02a	0.02 ± 0.01b	ND	ND	ND
1-epi-Cubanol	0.05 ± 0.01a	0.03 ± 0.01ab	0.03 ± 0.01b	0.02 ± 0b	0.02 ± 0b
γ-Eudesmol	0.02 ± 0a	0.01 ± 0b	0.02 ± 0a	0.01 ± 0b	ND
Cubanol	0.05 ± 0.01a	0.04 ± 0.01a	0.03 ± 0ab	0.02 ± 0.01b	0.01±0b
Cadalene	0.04 ± 0.01b	0.08 ± 0.02a	0.08 ± 0.01a	0.07 ± 0.01a	0.04±0b
Total	2.99 ± 0.36ab	2.1 ± 0.3abc	3.32 ± 0.99a	1.75 ± 0.14bc	1.25 ± 0.07c

Notes: Linalool, α-terpineol, geraniol and geranylacetone were quantified using their pure standard compounds. α-terpinene, cymene (m- and p-), 1,8-cineol, (E)-β-ocimene, γ-terpinene, terpinolene, p-cymenene and hotrienol were semi-quantified using a linalool standard. All monoterpenes are expressed at μg/g grape sample. All sesquiterpenoids and norisoprenoids were semi-quantified with the internal standard β-cedrene and expressed as equivalent concentrations of the internal standard at μg/kg grape sample. ND: not detected. Values labelled with the same lower case letter in the same row are not significantly ($p < 0.05$) different. Raw data of the table are provide in data file 1.

Table 8

Terpene concentrations at different developmental stages of Chardonnay in the two experimental vintages.

Vintage 2016	wpf4	wpf6	wpf8	wpf10	
<i>Monoterpenoids</i>					
α -Terpinene	ND	ND	ND	ND	
Cymene (m- and p-)	<0.01	<0.01	<0.01	<0.01	
1,8-Cineol	ND	ND	ND	ND	
(E)- β -Ocimene	ND	ND	ND	ND	
γ -Terpinene	ND	ND	ND	ND	
Terpinolene	<0.01	<0.01	<0.01	<0.01	
p-Cymenene	<0.01	<0.01	<0.01	<0.01	
Linalool	<0.01	0.64 \pm 0.6a	<0.01	5.29 \pm 5a	
Hotrienol	ND	ND	ND	ND	
trans-Pinocarveol	<0.01	<0.01	<0.01	7.59 \pm 5.79	
Citronellal	<0.01	0.63 \pm 0.47b	<0.01	13.18 \pm 9.92a	
Neroloxide	ND	ND	ND	ND	
Menthol (+isomenthol)	<0.01	<0.01	<0.01	4.64 \pm 3.72	
Terpinen-4-ol	ND	ND	ND	ND	
α -Terpineol	0.08 \pm 0.05a	0.2 \pm 0.24a	<0.01	2.4 \pm 2.83a	
Geraniol	0.88 \pm 0.09a	0.83 \pm 0.07a	0.92 \pm 0.16a	2.22 \pm 1.46a	
Geranylacetone	5.33 \pm 1.42a	3.02 \pm 0.13a	13.69 \pm 0.82a	18.12 \pm 12.05a	
Total	6.3 \pm 1.46a	4.92 \pm 1.36a	14.62 \pm 0.98a	53.56 \pm 40.31a	
<i>Norisoprenoids</i>					
Theaspirane (Isomer 1)	0.05 \pm 0.01a	0.08 \pm 0.04a	0.03 \pm 0.01a	ND	
Theaspirane (Isomer 2)	0.05 \pm 0.01a	0.05 \pm 0.02a	0.03 \pm 0.01a	ND	
(E)- β -Damascenone	0.2 \pm 0.04b	0.3 \pm 0.03b	0.39 \pm 0.04b	2.02 \pm 1.04a	
Total	0.3 \pm 0.05b	0.43 \pm 0.08b	0.45 \pm 0.04b	2.02 \pm 1.04a	
<i>Sesquiterpenoids</i>					
7-epi- α -Cedrene	1.62 \pm 0.44a	1.2 \pm 0.58a	0.92 \pm 0.2a	1.01 \pm 0.02a	
Selina-4,11-diene	0.05 \pm 0.02a	ND	0.03 \pm 0a	ND	
α -Muurolene	ND	ND	ND	ND	
δ -Cadinene	ND	ND	ND	0.13 \pm 0.05	
Calamenene (cis + trans)	0.04 \pm 0.02b	0.08 \pm 0.01a	0.06 \pm 0.01ab	0.07 \pm 0.01a	
α -Calacorene	0.03 \pm 0ab	0.02 \pm 0b	ND	0.05 \pm 0.02a	
ω -Cadinene	0.09 \pm 0.02a	0.05 \pm 0.01b	0.04 \pm 0.01b	0.05 \pm 0.01b	
γ -Calacorene	0.31 \pm 0.02a	0.18 \pm 0.05a	0.17 \pm 0.05a	0.24 \pm 0.1a	
Palustrol	0.01 \pm 0.01b	ND	ND	0.04 \pm 0.01a	
1-epi-Cubenol	0.06 \pm 0b	0.04 \pm 0.01b	0.03 \pm 0b	0.1 \pm 0.02a	
γ -Eudesmol	0.04 \pm 0.01a	0.03 \pm 0.01a	0.03 \pm 0.01a	ND	
Cubenol	0.02 \pm 0b	0.02 \pm 0b	0.02 \pm 0b	0.07 \pm 0.02a	
Cadalene	0.09 \pm 0.01a	0.1 \pm 0.03a	0.07 \pm 0.01a	0.06 \pm 0.03a	
Total	2.36 \pm 0.47a	1.71 \pm 0.61a	1.34 \pm 0.27a	1.83 \pm 0.23a	
Vintage 2017	4	9	14	19	24
	wpf4	wpf6	wpf8	wpf10	wpf12
<i>Monoterpenoids</i>					
α -Terpinene	ND	ND	ND	ND	ND
Cymene (m- and p-)	<0.01	<0.01	<0.01	<0.01	<0.01
1,8-Cineol	ND	ND	ND	ND	ND
(E)- β -Ocimene	ND	ND	ND	ND	ND
γ -Terpinene	ND	ND	ND	ND	ND
Terpinolene	<0.01	<0.01	<0.01	<0.01	<0.01
p-Cymenene	<0.01	<0.01	<0.01	<0.01	<0.01
Linalool	<0.01	<0.01	0.09 \pm 0.03a	0.2 \pm 0.22a	0.37 \pm 0.02a
Hotrienol	ND	ND	ND	ND	ND
trans-Pinocarveol	<0.01	<0.01	<0.01	<0.01	<0.01

Table 8 (continued)

Vintage 2017	4	9	14	19	24
	wpf4	wpf6	wpf8	wpf10	wpf12
Citronellal	<0.01	<0.01	0.13 ± 0.08	<0.01	<0.01
Neroloxide	ND	ND	ND	ND	ND
Menthol (+isomenthol)	<0.01	<0.01	<0.01	<0.01	<0.01
Terpinen-4-ol	ND	ND	ND	ND	ND
α -Terpineol	<0.01	<0.01	<0.01	0.34 ± 0.29	<0.01
Geraniol	0.64 ± 0.04b	0.63 ± 0.07b	0.65 ± 0.01b	0.79 ± 0.09b	0.98 ± 0.05a
Geranylacetone	4.5 ± 2.16a	3.83 ± 2.8a	4.77 ± 0.68a	1.08 ± 3.29a	0.64 ± 1.67a
Total	5.14 ± 2.15a	4.47 ± 2.77a	5.61 ± 0.59a	2.23 ± 3.48a	2.01 ± 1.68a
<i>Norisoprenoids</i>					
Theaspirane (Isomer 1)	0.05 ± 0.01a	0.04 ± 0.01a	0.03 ± 0ab	0.03 ± 0b	ND
Theaspirane (Isomer 2)	0.05 ± 0.01a	0.04 ± 0.01a	ND	ND	ND
(E)- β -Damascenone	0.19 ± 0.01d	0.33 ± 0.03cd	0.77 ± 0.05c	1.41 ± 0.11b	2.03 ± 0.4a
Total	0.28 ± 0.02d	0.41 ± 0.05cd	0.8 ± 0.05c	1.43 ± 0.11b	2.03 ± 0.4a
<i>Sesquiterpenoids</i>					
7-epi- α -Cedrene	2.15 ± 0.4b	1.37 ± 0.17bc	3.31 ± 0.58a	1.17 ± 0.26c	1.15 ± 0.1c
Selina-4,11-diene	0.07 ± 0.02a	0.04±0b	0.03 ± 0.01b	0.02 ± 0.01b	ND
α -Muurolene	ND	ND	ND	ND	ND
δ -Cadinene	ND	ND	ND	ND	ND
Calamenene (cis + trans)	0.12 ± 0.02a	0.04 ± 0.01c	0.08 ± 0.01b	0.06 ± 0.01bc	0.03 ± 0.01c
α -Calacorene	0.03 ± 0.01	ND	ND	ND	ND
ω -Cadinene	0.1±0a	0.04±0b	0.04 ± 0.01b	ND	ND
γ -Calacorene	0.47 ± 0.05a	0.22 ± 0.02bc	0.22 ± 0.02b	0.16 ± 0.07bc	0.12 ± 0.01c
Palustrol	0.05 ± 0.01	ND	ND	ND	ND
1-epi-Cubanol	0.08 ± 0.01a	0.03 ± 0.01b	0.02 ± 0c	0.02 ± 0c	0.01 ± 0c
γ -Eudesmol	0.04 ± 0.01a	0.02 ± 0b	0.03 ± 0.01bc	0.03 ± 0.01bc	0.02 ± 0.01b
Cubanol	0.04 ± 0.01a	0.01 ± 0b	ND	ND	ND
Cadalene	0.09 ± 0a	0.06 ± 0.01abc	0.08 ± 0.01ab	0.05 ± 0.02c	0.04 ± 0c
Total	3.24 ± 0.45a	1.85 ± 0.2b	3.81 ± 0.59a	1.51 ± 0.34b	1.38 ± 0.1b

Notes: Linalool, α -terpineol, geraniol and geranylacetone were quantified using their pure standard compounds. α -terpinene, cymene (m- and p-), 1,8-cineol, (E)- β -ocimene, γ -terpinene, terpinolene, p-cymenene and hotrienol were semi-quantified using a linalool standard. All monoterpenes are expressed at $\mu\text{g/g}$ grape sample. All sesquiterpenoids and norisoprenoids were semi-quantified with the internal standard β -cedrene and expressed as equivalent concentrations of the internal standard at $\mu\text{g/kg}$ grape sample. ND: not detected. Values labelled with the same lower case letter in the same row are not significantly ($p < 0.05$) different. Raw data of the table are provide in data file 1.

Table 9

Terpene concentrations at different developmental stages of Pinot Gris in the two experimental vintages.

Vintage 2016	45	50	55	60	
	wpf4	wpf6	wpf8	wpf10	
<i>Monoterpenoids</i>					
α -Terpinene	0.45 ± 0.19a	0.28 ± 0.19a	0.13 ± 0.12a	<0.01	
Cymene (m- and p-)	<0.01	<0.01	0.15 ± 0.02a	0.39 ± 0.48a	
1,8-Cineol	ND	ND	ND	ND	
(E)- β -Ocimene	<0.01	ND	ND	ND	
γ -Terpinene	2.6 ± 0.68	ND	ND	ND	
Terpinolene	0.29 ± 0.2a	0.22 ± 0.11a	0.06 ± 0.07a	<0.01	
p-Cymenene	<0.01	<0.01	<0.01	<0.01	
Linalool	0.2 ± 0.14b	0.23 ± 0.17b	0.5 ± 0.28b	3.96 ± 1.69a	
Hotrienol	<0.01	<0.01	<0.01	<0.01	
trans-Pinocarveol	<0.01	<0.01	<0.01	9.27 ± 1.11	
Citronellal	<0.01	0.45 ± 0.34b	0.7 ± 0.45b	16.45 ± 2.36a	
Neroloxide	<0.01	ND	ND	ND	
Menthol (+isomenthol)	<0.01	<0.01	<0.01	5.42 ± 0.91	
Terpinen-4-ol	<0.01	<0.01	<0.01	<0.01	
α -Terpineol	1.16 ± 0.44a	1.36 ± 0.16a	1.11 ± 0.77a	2.14 ± 0.23a	
Geraniol	0.98 ± 0.22b	0.85 ± 0.11b	0.95 ± 0.14b	3.2 ± 1.27a	
Geranylacetone	7.41 ± 1.67bc	3.3 ± 1.26c	14.81 ± 3.83ab	18.99 ± 4.58a	
Total	13.09 ± 2.05b	6.74 ± 0.74b	18.05 ± 4.72b	59.9 ± 12.76a	
<i>Norisoprenoids</i>					
Theaspirane (Isomer 1)	0.06 ± 0.01a	0.06 ± 0.02ab	0.03 ± 0.01b	ND	
Theaspirane (Isomer 2)	0.07 ± 0.01a	0.04 ± 0.02ab	0.03 ± 0.01b	ND	
(E)- β -Damascenone	0.19 ± 0.03b	0.31 ± 0.04b	0.56 ± 0.1b	2.69 ± 0.9a	
Total	0.33 ± 0.02b	0.41 ± 0.07b	0.62 ± 0.12b	2.69 ± 0.9a	
<i>Sesquiterpenoids</i>					
7-epi- α -Cedrene	2.04 ± 0.69a	1.61 ± 0.57ab	0.82 ± 0.15b	0.97 ± 0.06ab	
Selina-4,11-diene	0.07 ± 0.01a	0.03 ± 0.01b	0.02 ± 0.01b	ND	
α -Muuroolene	0.09 ± 0.01b	0.17 ± 0.05a	0.08 ± 0.02b	0.04 ± 0.02b	
δ -Cadinene	ND	ND	ND	0.12 ± 0.03	
Calamenene (cis + trans)	0.11 ± 0.01a	0.11 ± 0a	0.08±0b	0.08±0b	
α -Calacorene	0.05 ± 0a	0.03 ± 0a	ND	0.06 ± 0.02a	
ω -Cadinene	0.07 ± 0a	0.03 ± 0c	ND	0.05 ± 0.01b	
γ -Calacorene	0.31 ± 0a	0.3 ± 0.09a	0.14 ± 0.05a	0.2 ± 0.08a	
Palustrol	0.04 ± 0.01a	ND	ND	0.04±0a	
1-epi-Cubenol	0.06 ± 0.01b	0.03 ± 0.01c	0.02 ± 0.01c	0.13 ± 0.02a	
γ -Eudesmol	0.04 ± 0.01a	0.04±0a	0.02 ± 0.01a	ND	
Cubenol	0.05±0b	0.04 ± 0.01bc	0.02 ± 0.01c	0.09 ± 0.01a	
Cadalene	0.08 ± 0.01ab	0.11 ± 0.02a	0.06±0b	0.06 ± 0.03b	
Total	3.01 ± 0.71a	2.5 ± 0.68ab	1.26 ± 0.21b	1.84 ± 0.22ab	
Vintage 2017	5	10	15	20	25
	wpf4	wpf6	wpf8	wpf10	wpf12
<i>Monoterpenoids</i>					
α -Terpinene	3.5 ± 0.55a	0.99 ± 0.29b	<0.01	<0.01	0.06 ± 0.03c
Cymene (m- and p-)	0.74 ± 0.21	<0.01	<0.01	<0.01	<0.01
1,8-Cineol	ND	ND	ND	ND	ND
(E)- β -Ocimene	<0.01	ND	ND	ND	ND
γ -Terpinene	8.98 ± 1.01a	3.95 ± 0.86b	ND	ND	ND
Terpinolene	2.29 ± 0.47a	0.53 ± 0.23b	<0.01	<0.01	0.07 ± 0.04c
p-Cymenene	<0.01	<0.01	<0.01	<0.01	<0.01
Linalool	1.1 ± 0.25a	0.41 ± 0.12b	0.05 ± 0.02b	1.54 ± 0.32a	1.37 ± 0.05a
Hotrienol	0.57 ± 0.14a	0.2 ± 0.11b	<0.01	<0.01	0.1 ± 0.14b
trans-Pinocarveol	<0.01	<0.01	<0.01	<0.01	<0.01
Citronellal	<0.01	<0.01	0.16 ± 0.12a	<0.01	0.18 ± 0.05a
Neroloxide	<0.01	<0.01	<0.01	ND	ND
Menthol (+isomenthol)	<0.01	<0.01	<0.01	<0.01	<0.01
Terpinen-4-ol	1.18 ± 0.45	<0.01	<0.01	<0.01	<0.01
α -Terpineol	2.76 ± 0.64a	0.68 ± 0.21b	<0.01	1.31 ± 0.15b	0.86 ± 0.28b
Geraniol	0.82 ± 0.0c4	0.78 ± 0.07c	0.86 ± 0.14c	1.58 ± 0.19b	2.24 ± 0.19a

Table 9 (continued)

Vintage 2017	5	10	15	20	25
	wpf4	wpf6	wpf8	wpf10	wpf12
Geranylacetone	4.46 ± 0.92bc	4.57±1b	7.49 ± 1.4a	2.02 ± 0.49bc	1.64 ± 1.33c
Total	26.43 ± 4.27a	12.22 ± 2.16b	8.51 ± 1.55b	6.66 ± 0.46b	6.49 ± 1.18b
<i>Norisoprenoids</i>					
Theaspirane (Isomer 1)	0.07 ± 0.01a	0.05 ± 0.02ab	0.04±0b	0.03 ± 0.01b	ND
Theaspirane (Isomer 2)	0.06 ± 0.01a	0.06 ± 0.01ab	0.04±0bc	0.03±0c	ND
(<i>E</i>)-β-Damascenone	0.28 ± 0.02c	0.42 ± 0.03c	0.6 ± 0.04b	1.38 ± 0.06a	1.4 ± 0.11a
Total	0.41 ± 0.04c	0.52 ± 0.03bc	0.68 ± 0.04b	1.43 ± 0.07a	1.4 ± 0.11a
<i>Sesquiterpenoids</i>					
7-epi-α-Cedrene	3.16 ± 0.53a	1.78 ± 0.14b	1.16 ± 0.01b	1.7 ± 0.3b	1.17 ± 0.02b
Selina-4,11-diene	0.07 ± 0.01a	0.05 ± 0.02ab	0.02 ± 0.01b	0.03 ± 0.02b	ND
α-Murolene	0.04 ± 0.01b	0.08 ± 0.02a	0.06 ± 0.01ab	0.09 ± 0.02a	ND
δ-Cadinene	ND	ND	ND	ND	ND
Calamenene (cis + trans)	0.1 ± 0.01a	0.11 ± 0.02a	0.06 ± 0b	0.1 ± 0.01a	0.05 ± 0.01b
α-Calacorene	0.03±0a	0.03±0a	0.02 ± 0b	0.02 ± 0b	ND
ω-Cadinene	0.06 ± 0.01a	0.03 ± 0.01b	0.02±0c	ND	ND
γ-Calacorene	0.25 ± 0.03a	0.27 ± 0.03a	0.19 ± 0.01bc	0.24 ± 0.01ab	0.16 ± 0.02c
Palustrol	0.07 ± 0.01a	0.03±0b	ND	ND	ND
1-epi-Cubanol	0.05 ± 0.01a	0.03 ± 0.01ab	0.02 ± 0b	0.02 ± 0b	0.02 ± 0.01b
γ-Eudesmol	0.03 ± 0.01a	0.02 ± 0ab	0.01±0b	0.03 ± 0a	ND
Cubanol	0.04±0a	0.04 ± 0.02a	0.02±0a	0.03 ± 0a	ND
Cadalene	0.03 ± 0.01d	0.09 ± 0.01a	0.07 ± 0.01bc	0.09 ± 0.01ab	0.05 ± 0.01cd
Total	3.93 ± 0.47a	2.57 ± 0.1b	1.65 ± 0.01cd	2.36 ± 0.35bc	1.45 ± 0.04d

Notes: Linalool, α-terpineol, geraniol and geranylacetone were quantified using their pure standard compounds. α-terpinene, cymene (m- and p-), 1,8-cineol, (*E*)-β-ocimene, γ-terpinene, terpinolene, p-cymenene and hotrienol were semi-quantified using a linalool standard. All monoterpenes are expressed at μg/g grape sample. All sesquiterpenoids and norisoprenoids were semi-quantified with the internal standard β-cedrene and expressed as equivalent concentrations of the internal standard at μg/kg grape sample. ND: not detected. Values labelled with the same lower case letter in the same row are not significantly ($p < 0.05$) different. Raw data of the table are provide in data file 1.

Acknowledgements

This project is sponsored by the School of Agriculture and Food, Faculty of Veterinary and Agricultural Sciences, the University of Melbourne, and Veski through the Veski Sustainable Agricultural Fellow program awarded to Dr Pangzhen Zhang. We thank the support of the Mount Langi Ghiran during this data and for donating grape samples. The authors thank Mr Damien Sheehan, Mr Ben Haines and Ms Jess Robertson for their expert technical assistance. The authors are also grateful to students Jocelyn How, Qianyun Lei, Yit Tao Loo, Fangping Luo, Meiyin Lin, Junda Liu, Yijia Xu, Yi Ding and Qianhui Yao of the Wine and Viticulture Research Group at the University of Melbourne for assistance in sample collection and processing.

Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.dib.2019.104595>.

References

- [1] J. Luo, J. Brotchie, M. Pang, P.J. Marriott, K. Howell, P. Zhang, Free terpene evolution during the berry maturation of five *Vitis Vinifera* L. cultivars, *Food Chem.* 299 (2019) 125101.
- [2] P. Zhang, S. Fuentes, T. Siebert, M. Krstic, M. Herderich, E.W.R. Barlow, Comparison data of common and abundant terpenes at different grape development stages in Shiraz wine grapes, *Data Brief* 8 (2016) 1127–1136.

- [3] P. Zhang, S. Fuentes, T. Siebert, M. Krstic, M. Herderich, E.W.R. Barlow, Terpene evolution during the development of *Vitis vinifera* L. cv. Shiraz grapes, *Food Chem.* 204 (2016) 463–474.
- [4] K.L. Goodner, Practical retention index models of OV-101, DB-5, and DB-Wax for flavor and fragrance compounds, *LWT* 41 (2008) 951–958.
- [5] C. Jarvis, E.W.R. Barlow, R. Darbyshire, I. Goodwin, Relationship between viticultural climatic indices and grape maturity in Australia, *Int. J. Biometeorol.* 61 (2017) 1849–1862.