SUPPLEMENTARY DATA
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SUPPLEMENTARY DATA

Table S1. Concentration of free and potential monoterpenes and norisoprenoids, and flavonol glycosides in must for the three grapevine age groups (n = 4) from 2015 to 2017. The last two columns display the *p*-values for the Kruskal–Wallis tests (α = 0.05) for age group and year with Dunn's post hoc comparisons.

Year	2015			2016			2017				
Age group	**1971**	**1995**	**2012**	**1971**	**1995**	**2012**	**1971**	**1995**	**2012**	**Age group**	**Year**
Free monoterpenes and norisoprenoids (µg L^{-1})											
linalool	5.8 ± 0.6	6.1 ± 0.7	8.9 ± 1.5	12.9 ± 1.3	14.1 ± 2.5	15.6 ± 3.5	11.9 ± 1.4	11.3 ± 1.6	11.8 ± 2.1	0.501	<0.001^{a,b,b}
Potentially volatile monoterpenes and norisoprenoids (µg L^{-1})											
α-terpineol	244.0 ± 11.9	242.3 ± 15.8	330.5 ± 25.6	407.1 ± 7.3	400.6 ± 11.3	586 ± 67.7	372.8 ± 26.4	389.5 ± 31.8	516.8 ± 71.7	0.021	<0.001^{a,b,b}
nerol oxide	43.9 ± 3.8	49.6 ± 3.1	69 ± 6.4	48.1 ± 3.4	59.3 ± 5.6	69.1 ± 4.4	47.5 ± 2.9	53.8 ± 3.3	61.2 ± 6.1	<0.001^{a,ab,b}	0.363
cis-linalool oxide	24.2 ± 1.7	26.4 ± 1.8	34.1 ± 1.8	24.5 ± 1.1	29.3 ± 1.4	30.5 ± 1.0	23.6 ± 1.1	24.7 ± 1.4	24.9 ± 1.8	<0.001^{a,ab,b}	0.011
trans-linalool oxide	18.7 ± 0.9	21.0 ± 1.4	25.1 ± 1.2	19.4 ± 1.1	23.2 ± 1.6	23.9 ± 1.0	19.2 ± 0.9	20.2 ± 0.8	20.8 ± 1.2	<0.001^{a,ab,b}	0140
vitispirane	34.6 ± 7.8	39.6 ± 3.8	83 ± 12.4	49.4 ± 6.6	63.9 ± 11.9	106.5 ± 18.2	52.2 ± 4.7	74.4 ± 14	121.5 ± 44.7	<0.001^{a,a,b}	0.025
TDN	3.3 ± 0.6	4.6 ± 0.5	8.8 ± 1.2	6.8 ± 1.6	12 ± 2.9	17.9 ± 4.2	6.3 ± 0.8	9.3 ± 1.8	13.9 ± 3.2	<0.001^{a,ab,b}	0.001^{a,b,b}
Flavonol glycosides (mg L^{-1})											
quercetin-3-galactoside	0.04 ± 0.01	0.05 ± 0.01	0.03 ± 0.01	0.16 ± 0.04	0.12 ± 0.00	0.09 ± 0.02	0.27 ± 0.09	0.22 ± 0.02	0.28 ± 0.04	0.905	<0.001^{a,ab,b}
quercetin-3-glucuronide	0.18 ± 0.05	0.21 ± 0.08	0.19 ± 0.05	0.33 ± 0.04	0.36 ± 0.03	0.30 ± 0.06	0.50 ± 0.17	0.38 ± 0.18	0.58 ± 0.07	0.959	<0.001^{a,ab,b}
quercetin-3-glucoside	0.24 ± 0.06	0.33 ± 0.10	0.32 ± 0.05	0.31 ± 0.03	0.40 ± 0.07	0.47 ± 0.07	0.33 ± 0.11	0.34 ± 0.05	0.46 ± 0.07	0.007	0.027

Fractions of monoterpenes and norisoprenoids that were below the detection limit across all samples were excluded from the table. Initially planted grapevines: Old in 1971; Mature in 1995; Young in 2012.

Table S2. Eigenvalues from the PCA in Figure 1.

	Dim 1	Dim 2	Dim 3	Dim 4	Dim 5	Dim 6	Dim 7	Dim 8	Dim 9	Dim 10
Eigenvalue	5.61	2.05	1.04	0.72	0.30	0.11	0.07	0.06	0.03	0.01
Variance (%)	56.12	20.51	10.36	7.22	3.02	1.15	0.69	0.60	0.25	0.10
Cumulative (%)	56.12	76.63	86.99	94.20	97.22	98.36	99.05	99.65	99.90	100.00

Table S3. Eigenvectors from the PCA in Figure 1, shown up to dimension 3.

	Dim 1	Dim 2	Dim 3
Free linalool	0.861	-0.011	-0.308
Bound cis-linalool oxide	0.817	-0.360	-0.040
Bound nerol oxide	0.942	-0.152	0.168
Bound trans-linalool oxide	0.886	-0.223	-0.128
Bound vitispirane	0.798	0.174	0.383
Bound α-terpineol	0.923	0.126	-0.055
Bound TDN	0.888	-0.084	0.336
Quercetin-3-galactoside	0.407	0.774	-0.399
Quercetin-3-glucuronide	0.258	0.911	-0.162
Quercetin-3-glucoside	-0.144	0.604	0.668

Table S4. PLS-DA parameters of sensitivity, specificity, and accuracy for young, mature and old grapevines in 2015, 2016, and 2017.

PLS-DA parameter	Young	Mature	Old
2015			
Sensitivity	1.00	0.25	0.50
Specificity	1.00	0.75	0.63
Accuracy	1.00	0.50	0.56
2016			
Sensitivity	0.75	0.75	0.75
Specificity	1.00	0.75	0.88
Accuracy	0.88	0.87	0.81
2017			
Sensitivity	1.00	0.50	0.25
Specificity	0.88	0.75	0.75
Accuracy	0.94	0.63	0.5

Initially planted grapevines: Old in 1971; Mature in 1995; Young in 2012.

Table S5. VIP scores and loading directions for the top five important variables (VIP > 1) on components 1 and 2 of the PLS-DA in 2015, 2016, and 2017.

Year	Component 1	Component 2
2015	**[−] TDN (1.31)** **[−] Vitispirane (1.30)** [−] Nerol oxide (1.18) [−] *cis*-linalool oxide (1.12) **[−] α-Terpineol (1.08)**	[+] TDN (1.20) [+] Vitispirane (1.14) [+] quer-3-glc (1.07) [+] α-Terpineol (1.05) [+] Nerol oxide (1.05)
2016	[+] Quer-3-gal (1.30) **[−] Vitispirane (1.29)** **[−] TDN (1.27)** [−] Nerol oxide (1.23) **[−] α-Terpineol (1.08)**	[+] *cis*-linalool oxide (1.33) [+] *trans*-linalool oxide (1.25) [−] α-Terpineol (1.25) [+] Querc-3-glucuronide (1.14)
2017	**[−] TDN (1.60)** **[−] Vitispirane (1.51)** [+] Linalool (1.10) [−] Querc-3-glc (1.06) **[−] α-Terpineol (1.03)**	[+] TDN (1.46) [+] Vitispirane (1.33)

The sign in square brackets represents the direction of the loading. The number in round brackets is the VIP score of the variable for the relevant component.