

## Supplementary Tables

Peak	Constituents	I.r.i. <sup>a</sup>	Relative abundance (%)																								
			CG					FM					NW					W									
			CA	CI	CO	ME	MO	SA	CA	CI	CO	ME	MO	SA	CA	CI	CO	ME	MO	SA	CA	CI	CO	ME	MO	SA	
1	methanol	353	tr <sup>b</sup>	0.2	- <sup>c</sup>	0.2	-	tr	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
2	ethanol	427	0.2	4.4	2.7	-	2	0.1	17.1	18.9	24.3	21.2	16.6	16.8	20.1	21.3	26.6	23.4	18.2	20.9	20.9	29.3	25.9	25.2	22.2	18.9	
3	butyl methyl ether	604	0.4	3.5	13.8	0.2	1.1	0.2	8.1	9.6	11.4	8.7	9	9.4	10.1	11.2	12.1	10.5	10.1	11.7	13.4	17.4	16.3	15.3	14.4	12	
4	isoamyl alcohol	736	-	tr	0.2	0.2	-	tr	18.5	23.4	23.2	24.9	18.1	22.5	20.6	21.5	22.8	25.4	18.6	21.9	20.7	22.1	22.1	26.1	22.3	25.6	
5	2,3-butanediol	789	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-	tr	-	-	-	-	tr	-	-	-	-	
6	ethyl butyrate	798	-	-	-	tr	-	-	0.1	0.1	0.1	tr	0.2	0.1	0.2	0.1	0.1	tr	0.2	0.1	0.1	0.1	0.1	tr	0.2	0.1	
7	hexanal	802	6.1	-	1.4	7.7	9.3	15	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
8	2-methylethyl butanoate	855	tr	-	-	tr	tr	0.1	tr	-	tr	tr	tr	-	-	0.1	tr	-	-	-	0.1	0.2	0.1	0.2	0.1	0.2	
9	(E)-2-hexenal	856	11.7	1.1	4.5	12.5	tr	13.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
10	(E)-3-hexenol	887	-	-	-	-	6.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
11	1-hexanol	870	12	37.7	24.5	13.4	14.9	4.7	0.1	0.1	0.2	0.2	tr	0.2	0.2	0.1	0.2	0.1	tr	0.2	0.1	0.1	0.2	0.1	tr	0.2	
12	isopentyl acetate	878	-	-	-	-	-	-	4.6	6.1	3	3.1	10.3	9.8	3	2.1	2.5	2	5.1	4.3	3.2	2	2.3	2.2	4.8	4	
13	2-methylbutyl acetate	880	tr	0.5	tr	tr	tr	tr	-	-	-	-	-	-	tr	tr	-	tr	-	-	tr	tr	tr	tr	tr	tr	
14	α-pinene	941	0.2	0.1	0.8	0.3	0.1	0.3	0.2	tr	0.8	-	-	-	-	0.3	-	tr	tr	-	-	-	-	-	-	-	
15	camphene	954	0.7	0.5	0.1	-	0.4	0.9	tr	tr	tr	tr	-	tr	-	0.7	-	0.1	tr	-	tr	-	-	-	-	-	
16	1-heptanol	970	-	0.2	tr	0.2	tr	tr	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
17	sabinene	978	-	-	0.2	2.4	0.1	tr	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
18	β-pinene	982	1.3	0.6	-	-	0.3	1.3	tr	tr	0.1	tr	tr	tr	tr	0.7	-	0.2	tr	-	-	-	-	-	-	-	
19	6-methyl-5-hepten-2-one	985	tr	tr	-	tr	0.2	-	tr	tr	-	tr	tr	tr	tr	tr	-	tr	tr	tr	tr	-	-	-	-	-	
20	hexanoic acid	986	0.1	tr	tr	-	-	-	tr	0.1	0.1	0.1	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	0.1	tr	0.1	
21	myrcene	993	0.3	0.3	0.4	0.2	0.3	tr	tr	-	tr	tr	-	-	tr	0.1	-	tr	tr	tr	-	-	-	-	-	-	
22	3-octanol	995	0.2	0.1	tr	0.1	tr	tr	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
23	ethyl hexanoate	999	-	0.2	tr	tr	0.1	tr	9.2	6.5	7.8	8.1	8.7	7.6	6.2	4.6	5.6	4.2	6.2	5.4	6.8	4.5	6.1	4.1	5.6	6.3	
24	(E)-3-hexenyl acetate	1004	0.3	-	0.3	tr	1	tr	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
25	α-phellandrene	1005	-	0.1	tr	0.2	0.1	tr	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
26	δ-3-carene	1010	0.4	0.2	tr	0.1	0.1	0.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	

27	1-hexyl acetate	1011	tr	2.3	0.8	0.1	0.6	-	0.3	0.1	tr	0.1	0.3	0.5	tr	0.1	tr	tr	tr	0.1	tr	0.1	tr	tr	tr	0.1
28	(E)-2-hexen-1-ol acetate	1013	-	5.3	1.3	-	0.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
29	$\alpha$ -terpinene	1018	0.3	-	tr	0.3	tr	0.1	-	-	-	-	-	-	tr	-	tr	-	-	-	-	-	-	-	-	
30	<i>p</i> -cymene	1027	2.7	2.5	0.1	0.2	1.5	1.1	tr	tr	tr	-	-	-	-	0.8	-	0.6	-	tr	-	-	tr	-	-	-
31	limonene	1032	3.5	3.3	0.3	1.6	2.1	1.9	tr	tr	0.2	-	-	tr	-	1.3	-	0.4	tr	-	tr	tr	tr	tr	tr	tr
32	1,8-cineole	1034	10.5	3.9	8	4.4	6.5	2.3	0.2	0.2	tr	-	-	-	-	-	-	0.3	-	-	-	-	-	-	-	
33	$\gamma$ -terpinene	1062	0.7	1.1	tr	0.3	0.4	0.4	tr	tr	tr	-	-	-	tr	0.3	-	0.1	tr	tr	tr	-	tr	-	tr	-
34	1-octanol	1071	tr	0.2	tr	tr	-	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr
35	terpinolene	1088	-	1	tr	3.9	-	-	tr	tr	tr	tr	-	-	-	0.1	-	tr	tr	tr	tr	0.1	-	-	-	-
36	fenchone	1089	1.7	-	-	-	1.6	0.5	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
37	<i>p</i> -mentha-2,4(8)-diene	1090	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
38	2-nonanone	1093	-	0.2	0.1	-	tr	tr	tr	tr	tr	tr	tr	tr	-	-	tr	-	tr	tr	-	-	tr	-	-	tr
39	ethyl heptanoate	1098	-	tr	-	-	-	-	tr	0.1	tr	tr	tr	tr	-	0.2	0.1	tr	-	tr	tr	0.1	tr	tr	tr	tr
40	<i>n</i> -undecane	1100	0.5	0.7	tr	tr	0.3	0.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
41	isopentyl-2-methyl butanoate	1102	-	-	0.1	tr	-	-	tr	tr	-	-	-	-	-	-	-	-	-	-	tr	-	-	-	-	-
42	nonanal	1103	-	0.4	0.5	1.6	1.2	0.7	-	-	tr	tr	tr	tr	tr	0.1	tr	0.1	tr	tr	0.1	0.1	0.1	tr	tr	tr
43	$\alpha$ -thujone	1106	2	0.4	0.5	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
44	phenylethyl alcohol	1110	tr	-	tr	tr	-	-	2.8	2.3	2.6	3.3	2	2.2	2.6	2.5	2.7	3.9	2.1	2.5	3.4	2.8	2.4	4.5	2.7	3.3
45	<i>endo</i> -fenchol	1113	0.6	0.5	tr	-	0.4	0.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
46	$\beta$ -thujone	1118	0.6	0.3	tr	0.1	0.3	0.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
47	camphor	1143	2.8	1.7	0.4	0.6	2.7	0.8	tr	tr	-	-	-	-	-	tr	-	tr	-	-	-	-	-	-	-	-
48	menthone	1154	1.4	0.3	-	tr	0.2	0.4	-	-	-	-	tr	tr	-	tr	-	tr	tr	-	-	-	-	-	-	-
49	<i>isomenthone</i>	1164	0.4	0.6	-	-	-	0.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
50	<i>trans</i> -pinocamphone	1165	-	-	0.2	-	-	tr	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
51	borneol	1167	-	0.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
52	4-ethyl phenol	1169	0.9	0.2	-	tr	-	-	-	-	-	-	-	tr	-	-	-	-	-	tr	tr	tr	-	tr	tr	-
53	<i>neo</i> -menthol	1170	1.6	-	-	1.1	0.9	0.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
54	octanoic acid	1175	-	-	-	-	-	-	0.2	0.2	0.1	tr	0.1	0.7	tr	tr	tr	tr	tr	tr	0.1	tr	tr	tr	tr	tr
55	1-nonanol	1176	-	1.6	0.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	tr	-	-	-
56	umbellulone	1177	-	-	0.2	0.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
57	4-terpineol	1178	0.3	0.5	tr	0.1	0.2	tr	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
58	butanedioic acid diethyl ester	1179	tr	tr	tr	tr	tr	tr	-	tr	-	-	tr	-	tr	tr	tr	tr	tr	tr	tr	0.2	0.1	0.1	0.2	0.2
59	$\alpha$ -terpineol	1189	0.2	tr	tr	-	-	tr	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
60	methyl salicylate	1192	0.2	tr	tr	0.1	-	tr	tr	tr	tr	tr	tr	tr	-	tr	-	-	tr	-	-	tr	tr	tr	tr	tr

61	ethyl octanoate	1196	-	-	tr	-	-	-	15.9	15	12.5	14.2	17.1	15.1	23.6	19.3	17.5	17.84	25.4	20.9	20.9	13.8	16.3	13.3	17.9	16.8
62	methyl chavicol	1197	1.5	1	-	-	0.6	0.5	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
63	<i>n</i> -dodecane	1200	-	-	0.2	0.5	-	tr	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
64	decanal	1204	2.1	0.4	0.8	3	3.7	1.1	tr	tr	tr	-	tr	tr	tr	-	-	tr	tr	tr	tr	tr	tr	tr	tr	tr
65	octanol acetate	1214	0.3	0.1	-	-	tr	0.2	tr	tr	tr	tr	tr	tr	-	-	-	-	tr	-	-	-	-	-	-	
66	citronellol	1230	0.1	-	-	-	-	-	tr	tr	tr	tr	tr	tr	tr	-	-	-	-	-	tr	-	tr	tr	-	tr
67	thymol methyl ether	1235	-	0.1	-	tr	0.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
68	pulegone	1237	0.4	tr	-	-	0.2	0.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
69	carvone	1244	0.3	0.2	-	-	0.1	0.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
70	isopentyl hexanoate	1255	0.6	0.5	-	-	-	-	0.2	tr	tr	0.2	0.1	0.1	tr	tr	tr	tr	0.1	0.1	tr	tr	tr	tr	tr	tr
71	2-phenyl ethyl acetate	1258	tr	-	-	-	-	tr	0.3	0.1	0.1	0.1	0.2	0.2	tr	0.3	tr	tr	tr	tr	tr	tr	tr	0.1	tr	0.1
72	linalool acetate	1259	0.8	0.2	-	0.1	0.3	0.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
73	<i>trans</i> -sabinene hydrate acetate	1260	-	-	-	-	tr	tr	-	-	-	-	-	-	tr	-	tr	-	-	tr	tr	tr	tr	tr	tr	0.1
74	4-ethyl-2-methoxyphenol	1273	-	0.1	-	-	-	tr	-	-	-	-	-	-	-	-	-	-	-	-	-	-	tr	-	-	
75	<i>neo</i> -menthyl acetate	1274	0.1	0.1	-	0.2	0.3	tr	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
76	isobornyl acetate	1285	7.7	3.1	0.3	0.3	5	3.4	tr	tr	tr	-	-	-	tr	tr	tr	0.2	tr	tr	tr	-	0.1	-	-	tr
77	<i>trans</i> -sabinyl acetate	1291	-	-	-	tr	-	tr	-	-	-	-	-	-	-	-	-	-	-	tr	tr	-	-	-	-	-
78	2-undecanone	1294	-	-	0.1	-	-	-	tr	tr	tr	tr	tr	0.1	-	-	tr	tr	tr	tr	-	-	tr	-	-	tr
79	menthyl acetate	1297	1.3	0.3	-	0.4	0.7	0.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
80	ethyl nonanoate	1320	0.2	0.2	0.3	2.5	-	tr	0.2	0.3	0.3	0.3	0.3	0.3	0.2	tr	0.5	tr	tr	tr	0.2	0.3	0.1	0.7	0.4	0.5
81	<i>n</i> -tridecane	1300	0.4	0.6	0.5	0.3	0.3	0.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
82	undecanal	1306	0.2	0.1	0.1	0.3	0.4	0.1	tr	tr	tr	-	-	tr	-	-	-	-	-	tr	-	tr	tr	tr	tr	tr
83	dihydrocarveol acetate	1307	-	0.2	-	tr	-	tr	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
84	<i>n</i> -nonanol acetate	1312	-	1	tr	1.2	-	tr	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
85	dihydro citronellol acetate	1319	-	0.2	0.2	-	-	tr	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
86	methyl decanoate	1327	tr	0.2	0.4	-	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr
87	<i>neo-iso</i> -verbanol acetate	1328	0.3	0.2	0.1	-	tr	tr	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
88	$\alpha$ -terpinyl acetate	1352	0.8	0.3	tr	-	0.4	0.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
89	citronellyl acetate	1357	tr	tr	0.1	tr	-	tr	tr	tr	tr	tr	tr	tr	-	-	-	-	-	-	tr	tr	tr	tr	-	tr
90	cyclosativene	1368	0.4	0.2	1.2	0.8	tr	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
91	$\alpha$ -copaene	1376	0.3	0.4	tr	tr	0.4	0.1	tr	tr	tr	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
92	$\beta$ -bourbonene	1384	-	-	1.5	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	
93	( <i>E</i> )- $\beta$ -damascenone	1386	0.1	0.1	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	tr	-	-	tr	tr	tr	tr	tr	tr	tr	tr	tr

[illegible]



160	ethyl hexadecanoate	1993	-	-	-	-	-	-	tr	0.1	tr	tr	tr	tr	-	-	-	-	-	-	tr	tr	tr	tr	tr	tr
161	<i>epi</i> -13-manoyl oxide	2017	-	0.5	0.2	0.5	0.2	-	tr	tr	tr	tr	-	tr	-	-	-	-	-	-	-	-	tr	-	-	-
Monoterpene hydrocarbons			10.1	9.7	1.9	9.5	5.4	6.2	0.2	-	1.1	-	-	-	-	4.3	-	1.4	-	-	-	0.1	-	-	-	-
Oxygenated monoterpenes			32.6	13	10	8.4	19.9	9.2	0.2	0.2	-	-	-	-	-	-	-	0.5	-	-	-	-	0.1	-	-	0.1
Sesquiterpene hydrocarbons			10.1	8.5	21.6	8.1	6	2.4	-	0.1	-	-	-	-	-	0.2	0.1	-	-	-	-	-	-	-	-	-
Oxygenated sesquiterpenes			0.2	-	0.9	2.7	0.7	4.9	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Oxygenated diterpenes			-	0.5	0.2	0.5	0.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Apocarotenoids			0.8	0.1	0.6	6.3	4.4	11.4	-	-	0.1	0.3	0.1	0.1	-	-	-	-	-	-	0.1	-	-	-	-	-
Phenylpropanoids			1.5	1	-	-	0.6	0.5	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Non-terpene acids			0.1	-	-	5.2	-	-	0.2	0.3	0.2	0.1	0.1	0.7	-	-	-	-	-	-	0.1	-	-	0.1	-	0.1
Non-terpene alcohols/phenols			13.3	44.7	27.6	14.1	23.1	4.8	38.5	44.7	50.3	49.6	36.7	41.7	43.5	45.4	52.3	52.8	38.9	45.5	45.1	54.3	50.6	55.9	47.2	48
Non-terpene aldehydes			20.1	2	7.3	25.1	14.6	30.5	-	-	-	-	-	-	-	0.1	-	0.1	-	-	0.1	0.1	0.1	-	-	-
Non-terpene esters			3.3	10.6	3.3	7.2	3.5	4.1	50.4	43.5	34.9	29.3	53	46.5	45	37.8	34.3	33.3	49.8	41.6	39.4	27.3	31.8	27.5	37	37.5
Non-terpene ethers			0.4	3.5	13.8	0.2	1.1	0.2	8.1	9.6	11.4	8.7	9	9.4	10.1	11.2	12.1	10.5	10.1	11.7	13.4	17.4	16.3	15.3	14.4	12
Non-terpene hydrocarbons			1.3	2.3	1.9	3.8	2.1	1.5	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Non-terpene ketones			-	0.2	0.2	-	0.2	-	-	-	-	-	-	0.1	-	-	-	-	-	-	-	-	-	-	-	-
Total identified			93.8	96.1	89.3	91.1	81.8	75.7	97.6	98.4	98	88	98.9	98.5	98.6	99	98.8	98.6	98.8	98.8	98.2	99.2	98.9	98.8	98.6	97.7

<sup>a</sup> Linear retention indices on a DB-5 column; <sup>b</sup> Traces, <0.1%; <sup>c</sup> Not detected. Abbreviations: CG=crushed and destemmed grapes; FM=fermented must with marcs; NW: new wine, 2 months old; W=wine, 7 months old; CA=Canaiolo; CI=Ciliegiolo; CO=Colorino; ME=Merlot; MO=Montepulciano; SA=Sangiovese.

**Figure S1.** Principal component analysis (PCA) loadings plot.

