SUPPLEMENTARY DATA
Davide Slaghenaufi, Enrico Peruch, Marco De Cosmi, Léa Nouvelet and Maurizio Ugliano (2021).
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S.1. Supplementary material. Retention indices, quantification ions of studied compounds.

	LRI[1]	Identification[2]	Quantitation ion m/z	Qualifier ions m/z	LOD (µg/L)	LOQ (µg/L)
1-Butanol	1159	RS	56	55	0.02	0.06
1-Pentanol	1256	RS	55	56, 57, 70	0.04	0.11
Isoamyl alcohol	1220	RS	57	55, 56, 70	0.02	0.06
Phenylethyl Alcohols	1920	RS	91	65, 92, 122	1.95	5.84
Methionol	1715	RS	106	88, 73	1.71	5.13
1-Hexanol	1316	RS	56	55, 69	0.76	2.27
trans-3-Hexen-1-ol	1379	RS	67	55, 69, 82	0.4	1.21
cis-3-Hexen-1-ol	1391	RS	68	55, 69, 83	1.23	3.68
cis-2-Hexen-1-ol	1415	RS	67	82, 57	0.4	1.2
trans-2-Hexen-1-ol	1404	RS	67	82, 71, 57	0.3	0.9
Isoamyl acetate	1125	RS	70	55, 60, 87	0.03	0.1
n-Hexyl acetate	1271	RS	56	55, 61, 84	0.03	0.1
Ethyl 3-methyl butanoate	1069	RS	88	57, 60, 85	0.3	0.9
Ethyl butanoate	1032	RS	71	88	0.01	0.04
Ethyl hexanoate	1240	RS	88	60, 99	5.82	17.47
Ethyl octanoate	1430	RS	88	57, 100, 127	0.54	1.63
Ethyl decanoate	1640	RS	88	71, 101, 155	0.16	0.49
Ethyl lactate	1340	RS	75	88, 90	2.1	6.3
3-Methylbutanoic acid	1667	RS	60	87	0.17	0.52
Hexanoic acid	1839	RS	60	73, 87	0.15	0.46
Octanoic acid	2071	RS	60	73, 101, 115	0	0.01
cis-Linalool oxide	1437	RS	59	111, 94	0.02	0.07
trans-Linalool oxide	1469	RS	59	111, 94	0.02	0.07
Linalool	1547	RS	71	121, 93	0.08	0.25
Geraniol	1860	RS	93	123, 121, 105	0.06	0.2
β-Citronellol	1771	RS	69	82, 81, 67	0.07	0.21
α-Terpineol	1701	RS	136	121, 93, 59	0.23	0.7
Terpinen-4-ol	1614	RS	71	111, 93, 86	0.02	0.05
8-Hydroxylinalool	2301	LRI MS	71	137, 119, 67	-	-

Nerol	1812	RS	93	121, 84, 69	0.04	0.12
β-Damascenone	1825	RS	69	190, 121, 105	0.01	0.03
α-Ionone	1853	RS	121	136, 192	0.02	0.06
α-Ionol	1925	RS	95	123, 138	0.04	0.12
3-Oxo-α-ionol	2555	LRI MS	108	152	-	-
3-Hydroxy-β-damascone	2535	LRI MS	69,00	175, 193, 208	-	-
3-Hydroxy-7,8-dihydro-α-ionol	2778	LRI MS	208	193, 175	-	-
Benzaldehyde	1538	RS	106,00	51, 77, 105	0,05	0,14
Benzyl Alcohols	1874	RS	106	105, 77, 51	0.03	0.1
Vanillin	2572	RS	151	81, 152, 109	0.01	0.02
Vanillyl alcohol	2762	RS	154,00	65, 93, 137	0,40	1,20
4-Ethylguaiacol	1988	RS	137	122, 152	0.03	0.09
4-Vinyl guaiacol	2212	RS	150	107, 135	0.07	0.21
Ethyl vanillate	2665	RS	151	168, 196	2.36	7.09
Methyl vanillate	2630	RS	151	123, 182	0.97	2.91
2,6-Dimethoxyphenol	2270	RS	154	95, 111, 139	0.01	0.03

[1] Linear Retention Index (LRI) were determined on DB-WAX polar column, as described by van Den Dool and Kratz (1963).

[2] RS identified using reference standard; LRI MS tentatively identified by comparing the Linear Retention Index and mass spectra with those of literature.

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S.2. Supplementary material. Data minimum (Min), maximum (Max) Mean, standard deviation (SD), significance (P-value).

Variable	Minimum	Maximum	Mean	SD	P value[a]	Significant
trans-2-Hexenol	0,000	4,790	1,383	1,745	0,000151	Yes
Methionol	78,000	250,000	170,820	54,874	< 0,0001	Yes
cis-2-Hexenol	4,940	21,050	10,194	3,695	< 0,0001	Yes
Methyl vanillate	3,620	62,620	16,059	14,505	< 0,0001	Yes
Ethyl vanillate	25,210	114,650	63,030	22,587	< 0,0001	Yes
1-Butanol	32,212	157,374	89,895	39,570	< 0,0001	Yes
Isoamyl alcohol	30109,100	44782,780	37622,402	3579,355	< 0,0001	Yes
1-Hexanol	769,833	2160,780	1512,601	412,340	< 0,0001	Yes
trans-3-Hexenol	12,920	112,883	47,954	28,150	< 0,0001	Yes
cis-3-Hexenol	3,371	225,798	72,865	79,208	< 0,0001	Yes
Benzyl alcohol	17,208	793,815	178,257	198,389	< 0,0001	Yes
2-Phenylethyl alcohol	19012,870	30766,550	23820,115	2838,831	0,0110399	Yes
Vanillyl alcohol	0,197	15,652	3,015	3,558	< 0,0001	Yes
Ethyl butanoate	53,213	161,738	98,360	29,509	< 0,0001	Yes
Ethyl 3-methyl butanoate	5,800	33,040	18,331	7,221	0,0393583	Yes
Isoamyl acetate	719,680	2314,964	1156,194	405,250	0,0002394	Yes
Ethyl hexanoate	51,840	177,446	122,482	41,002	0,0001779	Yes
n-Hexyl acetate	0,139	4,959	0,798	1,129	0,13741	No
Ethyl lactate	397,067	1398,087	832,419	278,071	0,0003094	Yes
Ethyl octanoate	31,410	133,004	82,172	29,167	0,0019291	Yes
Ethyl decanoate	14,760	185,994	33,932	31,090	0,6409289	No
cis-Linalool oxide	0,081	4,010	1,554	0,950	< 0,0001	Yes
trans-Linalool oxide	-0,030	1,792	0,440	0,550	< 0,0001	Yes
Linalool	2,148	26,849	12,736	6,922	< 0,0001	Yes
Terpinen-4-ol	0,100	2,580	0,930	0,662	< 0,0001	Yes
α-Terpineol	1,030	8,812	3,656	2,224	< 0,0001	Yes
β- Citronellol	4,560	21,765	13,641	5,176	< 0,0001	Yes

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Nerol	2,378	7,603	4,985	1,548	0,0006082	Yes
Geraniol	2,121	9,087	6,231	1,915	< 0,0001	Yes
8-Hydroxylinalool	0,001	0,498	0,047	0,095	0,394855	No
Benzaldehyde	0,000	1,519	0,563	0,384	0,018015	Yes
Vanillin	3,420	43,813	18,227	11,617	0,004148	Yes
3-Methylbutanoic acid	0,168	43,560	15,555	11,448	< 0,0001	Yes
Hexanoic acid	1116,950	1901,336	1374,424	168,692	0,0908963	No
Octanoic acid	1050,552	1766,930	1385,815	175,031	0,0016244	Yes
β-Damascenone	681,637	1452,550	1136,653	221,813	0,0002536	Yes
α-Ionol	0,497	4,499	2,689	1,129	< 0,0001	Yes
α-Ionone	0,008	0,871	0,289	0,268	0,0003777	Yes
β-Ionone	0,028	7,631	1,821	2,092	0,1630861	No
3-Hydroxy-β-damascone	-0,035	0,380	0,118	0,128	0,1357862	No
3-Oxo-α-ionol	0,001	0,463	0,077	0,092	0,0981213	No
3-Hydroxy-7,8-dehydro-α-ionol	0,113	1,760	0,451	0,311	0,4073038	No
4-Ethylguaiacol	0,000	0,191	0,032	0,043	0,0593306	No
4-Vinilguaiacol	-0,055	0,190	0,036	0,050	0,3540429	No
2,6-Dimethoxyphenol	7,548	45,445	20,137	9,343	0,0005698	Yes
Malvidin-3-glucoside	0,073	6,870	2,104	2,023	0,000361	Yes
Delphinidin	20,225	656,661	299,343	180,806	< 0,0001	Yes
Peonidin	2,837	586,797	92,193	150,914	< 0,0001	Yes
Quercetin-3-glucoside	0,000	14,862	1,829	3,798	< 0,0001	Yes
Myricetin	0,000	55,870	14,464	15,299	< 0,0001	Yes
Kaempferol	0,000	19,744	4,821	5,235	< 0,0001	Yes
Catechin	0,000	16,490	1,700	4,145	< 0,0001	Yes
Epicatechin	8,236	73,119	33,329	13,535	< 0,0001	Yes
Epicatechin gallate	0,000	12,584	5,857	3,069	< 0,0001	Yes
Caffeic acid	0,000	19,636	6,907	6,261	0,037297	Yes
Coumaric acid	0,458	13,018	3,850	3,142	< 0,0001	Yes
Feluric acid	0,000	4,448	0,864	1,280	< 0,0001	Yes
Gallic acid	0,000	15,947	5,136	5,929	< 0,0001	Yes

Total Polyphenols	0,000	19,202	5,186	4,173	< 0,0001	Yes
Tannins	615,331	3503,000	1517,048	746,519	< 0,0001	Yes
Anthocyanins	288,321	2212,475	1022,766	602,949	< 0,0001	Yes
Fruity	4,199	263,250	69,428	73,922	< 0,0001	Yes
Vinous	43,542	112,325	69,734	19,602	0,0006185	Yes
Floral	85,739	177,881	118,207	22,560	0,0007383	Yes
Spicy	0,366	2,588	1,427	0,616	< 0,0001	Yes
Green	0,097	0,954	0,454	0,228	< 0,0001	Yes
Ripe fruit	1,294	2,286	1,682	0,238	< 0,0001	Yes
trans-2-Hexenol	10,485	97,895	58,281	23,841	< 0,0001	Yes

[a] Values are statistically significant at $p < 0.05$

S.3. Supplementary material. Terpenes Pearson correlation matrix.

Variables	Nerol	8-Hydroxylinalool	α-Terpineol	Linalool	Geraniol	β-Citronellol	*cis*-Linalool oxide	Terpinen-4-ol	*trans*-Linalool oxide
Nerol	**1**	0,224	0,092	0,125	0,334	0,298	0,028	0,238	0,090
8-Hydroxylinalool	0,224	**1**	**0,598**	**0,501**	0,281	0,234	-0,026	0,028	0,026
α-Terpineol	0,092	**0,598**	**1**	**0,945**	**0,585**	**0,487**	-0,295	-0,224	-0,137
Linalool	0,125	**0,501**	**0,945**	**1**	**0,723**	**0,661**	**-0,423**	-0,327	-0,254
Geraniol	0,334	0,281	**0,585**	**0,723**	**1**	**0,828**	-0,313	0,128	-0,157
β-Citronellol	0,298	0,234	**0,487**	**0,661**	**0,828**	**1**	-0,316	0,030	-0,209
cis-Linalool oxide	0,028	-0,026	-0,295	**-0,423**	-0,313	-0,316	**1**	**0,430**	0,276
Terpinen-4-ol	0,238	0,028	-0,224	-0,327	0,128	0,030	**0,430**	**1**	**0,609**
trans-Linalool oxide	0,090	0,026	-0,137	-0,254	-0,157	-0,209	0,276	**0,609**	**1**

Values in bold are different from 0 with a significance level α=0,05

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S.4. Supplementary material. Odorant series, odor threshold and OAV for studied wines. Aromatic series: a) fruity, b) vinous, c) floral, d) spicy, e) green, f) ripe fruit.

Compounds	Odor threshold (µg/L) [1]	Aromatic series	Corvina 7	Corvina 48	Corvina 446	Corvinone 2	Corvinone 3	Corvinone 4	Corvinone 6	Molinara	Rondinella	Oseleta	Rabosso	Croatina	Sangiovese	Cabernet Sauvignon
1-Butanol	150000 [2]	b	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0	0	0	0	0	0.001	0
Isoamyl alcohol	30000 [1]	bd	1.409	1.241	1.226	1.298	1.33	1.249	1.286	1.281	1.06	1.119	1.219	1.287	1.477	1.076
1-Hexanol	8000 [1]	e	0.219	0.19	0.185	0.255	0.268	0.202	0.171	0.099	0.121	0.249	0.159	0.161	0.237	0.133
trans-3-Hexenol	1000 [5]	e	0.019	0.016	0.018	0.065	0.067	0.052	0.059	0.026	0.013	0.108	0.027	0.07	0.076	0.054
cis-3-Hexenol	400 [1]	e	0.538	0.523	0.493	0.086	0.077	0.041	0.033	0.009	0.367	0.054	0.15	0.04	0.084	0.057
cis-2-Hexenol	400 [4]	e	0.019	0.013	0.016	0.029	0.028	0.024	0.027	0.023	0.019	0.051	0.019	0.032	0.026	0.032
Ethyl butanoate	20 [1]	ab	5.085	4.04	4.124	4.897	7.55	4.579	4.918	3.42	3.115	2.695	4.935	7.815	6.225	5.45
Ethyl 3-methyl butanoate	3 [1]	ab	8.407	5.717	6.790	10.093	6.433	2.123	6.523	5.667	3.967	4.267	6.500	5.200	10.700	3.200
Isoamyl acetate	30 [1]	ab	43.967	29.87	36.744	34.633	59.552	30.748	46.667	36.167	24.933	30.133	32.333	31.9	74.467	27.433
Ethyl hexanoate	14 [1]	ab	12.643	9.514	9.211	10.693	11.659	6.596	12.329	9.336	8.457	4.029	4.757	8.5	11.021	3.736
n-Hexyl acetate	1500 [2]	ab	0.001	0	0	0	0	0	0	0	0.001	0	0	0	0	0
Ethyl lactate	154000 [2]	ab	0.007	0.005	0.007	0.008	0.006	0.004	0.006	0.005	0.004	0.003	0.006	0.004	0.008	0.003
Ethyl octanoate	5 [1]	ab	25.2	19.72	15.158	21.174	16.926	13.11	26.26	19.2	18.08	6.7	9.12	16.46	15.4	7.6
Ethyl decanoate	200 [1]	ab	0.575	0.163	0.16	0.182	0.11	0.15	0.223	0.135	0.14	0.075	0.083	0.166	0.139	0.076
Linalool	15 [2]	c	1.729	1.212	1.573	0.952	1.277	0.813	0.94	0.84	0.647	0.433	0.467	0.36	0.507	0.147
Terpinen-4-ol	100 [8]	c	0.009	0.005	0.01	0.002	0.003	0.005	0.005	0.017	0.017	0.024	0.001	0.009	0.01	0.014
α-Terpineol	250 [3]	c	0.034	0.019	0.033	0.012	0.018	0.012	0.016	0.015	0.008	0.007	0.009	0.006	0.012	0.004
β-Citronellol	40 [2]	c	0.426	0.472	0.395	0.423	0.462	0.36	0.226	0.518	0.475	0.273	0.168	0.25	0.21	0.12
Nerol	400 [4]	c	0.015	0.017	0.009	0.012	0.014	0.009	0.012	0.016	0.009	0.016	0.006	0.019	0.014	0.009
Geraniol	30 [1]	c	0.283	0.285	0.237	0.216	0.255	0.189	0.213	0.223	0.283	0.217	0.083	0.137	0.183	0.1
3-Methylbutanoic acid	33 [1]	b	45.182	38.909	39.927	47.242	34.939	36.212	41.515	44.212	40.909	46.727	36.758	43.455	50.091	36.97
Hexanoic acid	420 [1]	b	3.517	3.321	3.435	3.555	4.2	3.131	3.467	3.31	2.914	3.229	2.619	2.907	3.769	2.819
Octanoic acid	500 [1]	b	2.888	2.104	2.63	2.226	2.398	2.116	2.846	2.71	2.386	1.386	1.95	2.036	2.562	1.586
β-Damascenone	0,05 [1]	f	67.2	55.2	52.2	86	78.8	66.8	84.6	64	46	12	22	32	34	52
α-Ionone	0,1 [1]	f	6.1	2.8	4.5	5.5	1.3	6.3	0.1	0	6	2	1	2	3	0
β-Ionone	0,09 [1]	f	2.667	3.444	0.778	3.111	3.889	0.111	0.333	0	0	0	0	2.222	2.222	0
Vanillin	60 [2]	d	0.222	0.266	0.21	0.421	0.461	0.277	0.417	0.285	0.692	0.01	0.003	0.163	0.2	0.005
Vanillyl alcohol	5000 [6]	d	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Methyl vanillate	3000 [2]	d	0.003	0.003	0.003	0.005	0.004	0.005	0.004	0.001	0.001	0.02	0.01	0.005	0.007	0.003
Ethyl vanillate	990 [2]	d	0.063	0.079	0.06	0.082	0.065	0.087	0.06	0.026	0.078	0.114	0.039	0.049	0.039	0.05
Benzaldehyde	2000 [7]	d	0.021	0.007	0.021	0.009	0.007	0.007	0.013	0.009	0.005	0.011	0.004	0.008	0.004	0.002
Benzyl alcohol	200000 [7]	d	0.001	0.001	0.001	0	0	0	0	0	0.001	0.004	0	0	0.001	0.001
4-Ethylguaiacol	33 [1]	d	0.001	0.002	0	0.004	0.001	0.001	0	0	0	0	0	0	0	0.003
4-Vinylguaiacol	380 [6]	d	0.088	0.11	0.088	0.248	0.133	0.143	0.131	0.074	0.131	0.157	0.044	0.062	0.106	0.052
2,6-Dimethoxy-phenol	570 [7]	d	0.001	0	0.001	0.003	0	0	0.001	0	0.002	0.003	0	0	0.002	0.002

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