Supplementary Information

Effects of Soil and Vineyard Characteristics on Volatile, Phenolic Composition and Sensory Profile of Cabernet Sauvignon Wines of Campanha Gaúcha

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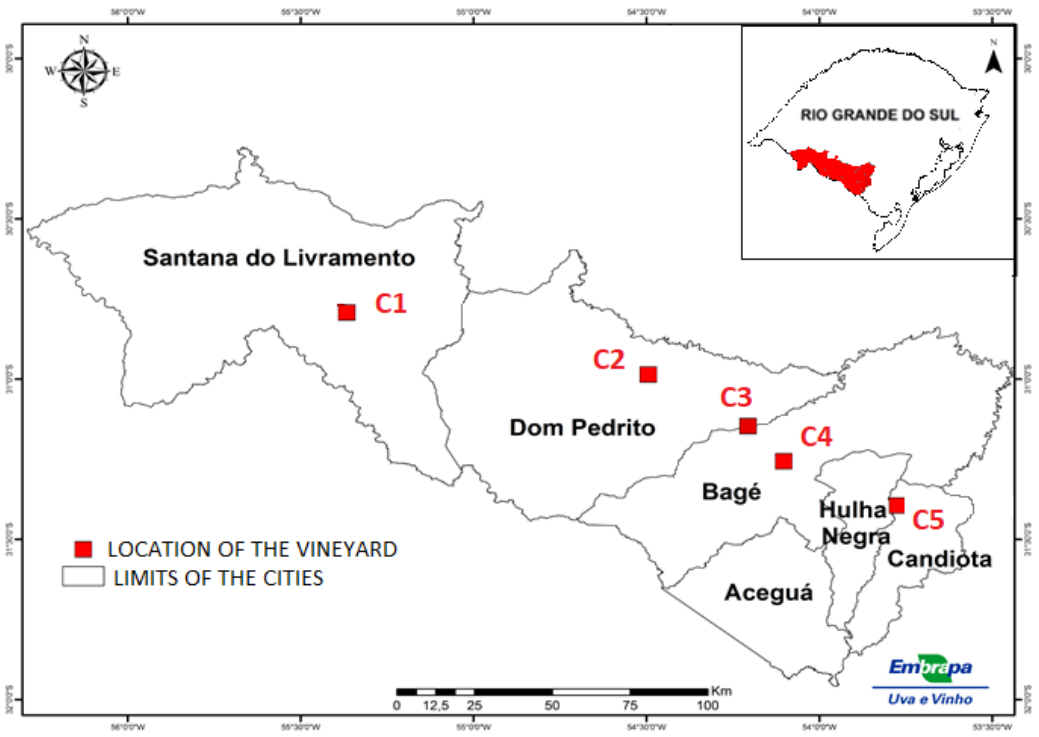

Figure S1. Geographical location of the five vineyards in the Campanha Gaúcha region.

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Table S1. Geographical location, year of vineyard implementation, spacing between the plants and altitude of the five vineyards in the Campanha Gaúcha region

Vineyard	Geographical location[a]	Year of vineyard implementation	Spacing between vines / m	Altitude[b] / m
C1	30°50'0"S, 55°30'0"W	2005	1.0 × 2.8	180
C2	31°00'0"S, 54°30'0"W	2003	1.2 × 3.3	246
C3	31°10'0"S, 54°15'0"W	2004	1.2 × 3.3	337
C4	31°15'0"S, 54°10'0"W	2003	1.0 × 2.5	342
C5	31°25'0"S, 53°50'0"W	2001	1.2 × 3.0	275

[a]S: South, W: West; [b]above sea level.

Table S2. Monthly average of temperature (T), relative humidity (H), solar radiation (R), and precipitation during the cycle of 2013/14 in Campanha Gaúcha, RS, Brazil

Month	T / °C	H / %	R / (MJ m^2 day^{-1})	Precipitation / mm	
				2013/14	Normal (average of 30 years)
August	10.6	74.5	11.5	64.6	109.0
September	14.7	75.7	14.3	129.7	134.0
October	17.0	75.0	20.0	139.1	132.0
November	21.9	73.0	24.2	291.2	96.0
December	24.2	63.8	26.2	14.5	99.0
January	24.2	73.0	22.5	146.2	108.0
February	22.9	78.0	21.1	171.1	114.0
Accumulated				956.4	791.4

Table S3. Physico-chemical parameters of must and wines produced during year 2014 with grapes harvested in 2013 from the five different vineyards in Campanha Gaúcha, Brazil showed in Table 1

	C1	C2	C3	C4	C5
	Grape must				
Soluble solids / (°Brix at 20 °C)	19.0	19.0	17.4	18.3	17.8
Density / (g mL^{-1})	1.08	1.08	1.07	1.08	1.07
pH	3.7	3.4	3.4	3.3	3.6
Total acidity / (mEq L^{-1})	78.4	88.9	99.2	101.9	81.1
	Wine				
Density / (g mL^{-1})	0.984	0.984	0.985	0.984	0.984
Alcohol content at 20 °C / (% v/v)	12.1	12.1	11.3	12.0	11.8
pH	4.0	3.7	3.8	3.6	3.9
Total acidity / (mEq L^{-1})	67.1	67.5	78.0	73.2	67.7
Volatile acidity / (mEq L^{-1})	14.2	11.2	17.1	10.8	10.8
Fixed acidity / (mEq L^{-1})	52.9	55.4	59.4	62.1	56.2
Reducing sugars / (g L^{-1})	1.7	1.9	1.5	1.7	1.9
Free SO_2 / (mg L^{-1})	42.8	51.2	46.9	53.1	42.1
Total SO_2 / (mg L^{-1})	92.9	104.4	94.3	79.4	98.4

Table S4. Positively and/or tentatively identified volatile compounds of all Cabernet Sauvignon wines, using HS-SPME-GC × GC-TOFMS with their respective Chemical Abstract Service (CAS) numbers, retention times in the first (^1t_R) and in the second (^2t_R) chromatographic dimensions, experimental retention index (RI_{exp}) and RI reported in scientific literature (RI_{lit}). Chromatographic conditions are described in "Determination of volatile profile" sub-section

No.	Compound[a]	CAS[b]	^1t_R / min	^2t_R / s	RI_{exp}[c]	RI_{lit}[d]	Ref.[e]	Odor[e]
			Acid					
1	acetic acid (Co12)	64-19-7	26.83	1.79	1458	1451	1	pungent, vinegar[2]
2	propanoic acid (Co16)	79-09-4	30.57	1.77	1550	1535	1	
3	2-methyl-propanoic acid	79-31-2	31.73	1.83	1579	1566	1	
4	butanoic acid (Co19)	107-92-6	34.07	1.82	1639	1630	1	rancid[3]
5	isovaleric acid (Co21)	503-74-2	35.58	1.89	1679	1667	4	cheesy, herbaceous[3]
6	2-methyl-butanoic acid (Co21)	116-53-0	35.58	1.90	1679	1686	5	
7	hexanoic acid (Co27)	142-62-1	41.88	1.97	1853	1855	1	
8	2-ethyl-hexanoic acid (Co30)	149-57-5	45.38	2.01	1955	1969	1	
9	heptanoic acid	111-14-8	45.50	1.96	1958	1950	1	
10	2-ethyl-hexenoic acid	13419-69-7	46.08	1.91	1976	1971	6	
11	octanoic acid	124-07-2	49.00	2.10	2067	2069	4	fatty, rancid[7]
12	decanoic acid	334-48-5	55.42	2.16	2280	2269	1	
13	9-decenoic acid	14436-32-9	57.17	2.07	2340	2348	8	
14	benzenecarboxylic acid	65-85-0	59.62	1.79	2424	2423	9	
15	dodecanoic acid	143-07-7	60.32	1.91	2448	2449	5	
			Alcohol					
16	2-methyl-2-propanol	75-65-0	5.13	2.26	905	916	10	
17	ethyl alcohol	64-17-5	5.25	1.98	921	932	11	
18	1-propanol (Co1)	71-23-8	8.87	2.08	1027	1030	4	fruity[3]
19	2-methyl-3-buten-2-ol	115-18-4	8.97	2.19	1032	1036	12	
20	isobutyl alcohol	78-83-1	11.20	2.13	1106	1090	1	oily, bitter, green[2]
21	2-methyl-2-pentanol	590-36-3	11.55	2.45	1114	1112	13	
22	2-propen-1-ol	107-18-6	12.13	1.94	1126	1124	14	
23	2-pentanol	6032-29-7	12.37	2.26	1132	1130	4	
24	1-butanol	71-36-3	13.30	2.17	1153	1149	1	alcoholic[3]
25	3-hexanol (Co3)	623-37-0	15.40	2.51	1200	1192	15	
26	2-methyl-1-butanol (Co4)	137-32-6	15.87	2.35	1210	1204	1	malt, wine, onion[16]
27	3-methyl-1-butanol (Co4)	123-51-3	16.33	2.38	1221	1208	1	solvent[3]
28	2-hexanol	626-93-7	16.57	2.47	1226	1226	4	
29	3-methyl-3-buten-1-ol (Co5)	763-32-6	17.73	2.20	1251	1240	5	
30	1-pentanol (Co5)	71-41-0	17.85	2.28	1254	1256	1	
31	2-heptanol	6033-23-4	20.88	2.63	1321	1318	1	
32	(*Z*)-2-penten-1-ol (Co9)	1576-95-0	21.00	2.18	1324	1317	17	
33	3-methyl-2-buten-1-ol (Co9)	4675-87-0	21.00	2.20	1324	1334	1	
34	3-methyl-1-pentanol	589-35-5	21.23	2.40	1329	1343	1	

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No.	Compound[a]	CAS[b]	^1t_R / min	^1t_R / s	RI_{exp}[c]	RI_{lit}[d]	Ref.[e]	Odor[e]
			Alcohol					
35	4-methyl-1-pentanol	626-89-1	22.40	2.50	1355	1365	1	
36	1-hexanol	111-27-3	22.28	2.42	1353	1371	1	
37	(*E*)-3-hexen-1-ol (Co10)	928-96-1	22.87	2.39	1366	1366	17	
38	3-ethoxy-1-propanol	111-35-3	23.33	2.39	1376	1364	4	
39	(*Z*)-3-hexen-1-ol	928-96-1	23.80	2.35	1387	1387	4	
40	(*E*)-2-hexen-1-ol	928-95-0	25.20	2.30	1419	1409	17	
41	2-octanol	5978-70-1	25.32	2.80	1422	1418	18	fruity[19]
42	1-octen-3-ol	3391-86-4	26.60	2.61	1453	1456	17	
43	1-heptanol (Co12)	111-70-6	26.83	2.59	1458	1467	1	green[20]
44	6-methyl-5-hepten-2-ol	1569-60-4	27.18	2.69	1467	1468	21	
45	2,6-dimethyl-7-octen-2-ol (Co13)	18479-58-8	27.42	3.04	1472	1474	22	
46	2-ethyl-1-hexanol	104-76-7	28.23	2.71	1492	1491	1	
47	4-hepten-1-ol (Co14)	20851-55-2	28.82	2.48	1506	1502	4	
48	3-ethyl-4-methylpentanol	0-00-0	29.05	2.66	1512	1507	4	
49	2-nonanol	628-99-9	29.40	2.98	1521	1521	4	
50	2,3-butanediol	513-85-9	30.33	2.01	1544	1545	23	fruity[16]
51	1-octanol	111-87-5	31.03	2.70	1562	1558	4	
52	1,3-butanediol	19132-06-0	31.85	1.98	1582	1578	24	
53	(*E*)-2-octen-1-ol	26001-58-1	33.25	2.57	1618	1620	1	
54	2-(2-ethoxyethoxy)-ethanol	111-90-0	33.37	2.51	1621	1619	25	
55	1-nonanol	143-08-8	35.00	2.84	1664	1676	1	
56	(6*Z*)-nonen-1-ol (Co22)	35854-86-5	37.10	2.76	1720	1714	26	melon[20]
57	2-undecanol (Co22)	1653-30-1	37.22	3.30	1723	1724	4	minty, fresh flavors[5]
58	(*E*,*Z*)-3,6-nonadien-1-ol	56805-23-3	38.38	2.66	1755	1762	27	
59	1-decanol	143-08-8	38.85	2.98	1768	1781	1	
60	(*Z*)-4-decen-1-ol (Co24)	57074-37-0	40.02	2.89	1800	1797	28	
61	2-dodecanol	1120-06-5	40.83	3.45	1824	1820	29	
62	benzyl alcohol (Co28)	100-51-6	42.93	2.24	1883	1869	1	
63	phenylethyl alcohol (Co29)	60-12-8	44.22	2.53	1921	1914	4	roses, honey[3]
64	1-dodecanol	112-42-5	45.85	3.27	1969	1977	4	floral[30]
65	1-tetradecanol	112-70-9	52.38	3.53	2178	2175	31	
66	1-hexadecanol	36653-82-4	58.33	3.66	2381	2382	4	

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No.	Compound[a]	CAS[b]	^1t_R / min	^2t_R / s	RI_{exp}[c]	RI_{lit}[d]	Ref.[e]	Odor[e]
			Aldehyde					
67	2-propenal	107-02-8	3.85	2.02	894	876	32	
68	3-methyl-butanal	590-86-3	4.90	2.74	913	900	33	
69	2-butenal (Co1)	123-73-9	8.63	2.63	1027	1037	34	fruity[3]
70	3-methyl-2-butenal (Co3)	107-86-8	15.40	2.97	1200	1202	35	
71	octanal (Co8)	124-13-0	19.37	4.26	1280	1282	17	green, orange, juicy[3]
72	nonanal	124-19-6	24.03	4.45	1393	1388	4	
73	decanal	112-31-2	28.47	4.62	1498	1494	1	
74	benzaldehyde (Co15)	100-52-7	29.52	2.97	1524	1513	4	almond[7]
75	2-methyl-benzaldehyde	529-20-4	33.48	3.20	1625	1621	36	
76	benzene acetaldehyde	122-78-1	34.42	2.97	1649	1631	4	
77	4-ethyl-benzaldehyde	4748-78-1	37.80	3.42	1739	1730	37	
78	3-(2,6,6-trimethyl-1-cyclohexen-1-yl)-2-propenal	4951-40-0	44.92	3.58	1942	1952	38	
			Ester					
79	methyl acetate	79-20-9	3.50	2.09	840	827	39	
80	ethyl acetate	141-78-6	4.20	2.47	905	887	17	
81	ethyl propanoate	105-37-3	6.07	3.31	955	953	40	sweet, fruity[3]
82	ethyl 2-methyl-propanoate	97-62-1	6.42	3.41	960	968	40	
83	propyl acetate	109-60-4	6.53	3.00	966	972	39	
84	ethyl 2-propenoate	140-88-5	7.12	2.86	971	980	41	
85	2-methylpropyl acetate	110-19-0	7.70	3.39	1002	1011	23	
86	ethyl butanoate	105-54-4	8.52	3.74	1021	1023	4	fruity[3]
87	ethyl 2-methyl-butanoate	7452-79-1	9.10	4.20	1033	1036	4	
88	ethyl isovalerate	108-64-5	9.68	4.08	1037	1053	4	fruity[3]
89	3-methylbutyl formate	110-45-2	9.80	3.15	1039	1042	4	
90	isoamyl acetate	123-92-2	11.78	4.12	1119	1124	17	fruity, banana[3]
91	methyl hexanoate (Co2)	106-70-7	14.70	4.16	1185	1183	4	
92	3-methylbutyl 2-methyl-propanoate	2050-01-3	14.93	5.43	1191	1187	42	
93	ethyl hexanoate	123-66-0	16.92	4.81	1234	1238	1	fruity[3]
94	3-methylbutyl butanoate (Co6)	2445-69-4	18.32	5.28	1265	1259	4	
95	hexyl acetate	142-92-7	18.67	4.40	1273	1276	17	
96	ethyl 2-oxo-propanoate (Co7)	617-35-6	18.90	2.68	1277	1268	34	
97	(*Z*)-ethyl 3-hexenoate	64187-83-3	20.07	4.14	1303	1291	4	
98	ethyl heptanoate	106-30-9	21.47	4.96	1335	1336	1	

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No.	Compound[a]	CAS[b]	^1t_R / min	^2t_R / s	RI_{exp}[c]	RI_{lit}[d]	Ref.[e]	Odor[e]
			Ester					
99	ethyl 2-hexenoate	27829-72-7	21.93	4.40	1346	1329	38	
100	ethyl 2-hydroxy-propanoate	687-47-8	22.05	2.39	1347	1334	1	
101	methyl octanoate	111-11-5	23.92	4.65	1390	1378	4	
102	ethyl 2-hydroxy-3-methyl-butanoate	07-06-41	25.55	2.74	1428	1422	4	
103	ethyl octanoate (Co11)	106-32-1	25.90	5.28	1437	1424	34	fruity[16]
104	isopentyl hexanoate (Co12)	2198-61-0	26.83	5.74	1460	1452	4	sweet fruity[23]
105	ethyl 7-octenoate	35194-38-8	28.00	4.55	1487	1478	40	
106	ethyl 2-hydroxy-butanoate (Co15)	5405-41-4	29.52	2.42	1524	1518	4	fruity, floral[19]
107	ethyl nonanoate	123-29-5	30.10	5.28	1539	1526	4	
108	ethyl 2-hydroxy-4-methyl-pentanoate (Co16)	10348-47-7	30.45	2.79	1547	1547	1	
109	isobutyl caprylate (Co17)	03-06-61	30.68	5.84	1554	1550	4	
110	isoamyl lactate	19329-89-6	31.50	2.74	1574	1570	4	
111	methyl decanoate	110-42-9	32.43	4.95	1598	1593	1	
112	ethyl decanoate (Co19)	110-38-3	34.18	5.48	1644	1638	1	fruity, grape,[7] sweet[43]
113	3-methylbutyl octanoate	2035-99-6	34.88	5.96	1662	1658	4	
114	ethyl benzoate (Co20)	93-89-0	35.23	3.59	1670	1664	1	
115	diethyl butanedioate (Co21)	123-25-1	35.70	3.35	1682	1690	1	faint, pleasant[3]
116	ethyl 9-decenoate	67233-91-4	36.17	4.84	1695	1711	4	
117	phenylmethyl acetate	140-11-4	37.68	3.24	1736	1726	4	
118	methyl 2-hydroxy-benzoate	119-36-8	39.20	3.26	1778	1775	1	
119	diethyl pentanedioate	818-38-2	39.50	3.48	1788	1780	4	
120	ethyl benzeneacetate (Co23)	101-97-3	39.67	3.55	1791	1783	4	
121	2-phenylethyl formate (Co23)	104-62-1	39.67	3.08	1791	1784	44	
122	ethyl isobutyl succinate (Co24)	123-25-1	40.02	3.71	1801	1791	38	
123	methyl dodecanoate (Co25)	111-82-0	40.13	5.22	1805	1793	1	
124	ethyl 2-hydroxy-benzoate	118-61-6	40.48	3.53	1814	1798	4	
125	2-phenylethyl acetate (Co26)	103-45-7	40.72	3.50	1821	1829	1	floral, rose, sweet, honey, fruity[3]
126	ethyl dodecanoate	106-33-2	41.65	5.62	1848	1835	1	
127	3-methylbutyl pentadecanoate	2306-91-4	42.23	6.15	1865	1859	4	
128	2-phenylethyl 2-methyl-propanoate (Co28)	103-48-0	42.93	4.08	1884	1877	45	
129	ethyl tetradecanoate	124-06-1	48.42	5.85	2050	2065	1	

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No.	Compound[a]	CAS[b]	^1t_R / min	^2t_R / s	RI_{exp}[c]	RI_{lit}[d]	Ref.[e]	Odor[e]
			Ester					
130	ethyl 3-phenyl-2-propenoate	103-36-6	51.10	3.44	2135	2149	46	
131	methyl hexadecanoate	1731-84-6	53.55	5.65	2218	2213	4	
132	ethyl hexadecanoate	628-97-7	54.72	6.00	2258	2246	1	
133	ethyl hydrogen succinate	1070-34-4	58.57	1.88	2388	2395	6	
			Furan					
134	2-methyl-furan	534-22-5	4.43	2.34	880	863	34	
135	2,5-dimethyl-furan	625-86-5	6.59	2.91	930	949	34	
136	2-pentyl-furan	3777-69-3	16.68	4.50	1229	1231	17	
137	furfural (Co13)	98-01-1	27.30	2.39	1469	1462	4	
138	ethyl 2-furoate (Co18)	614-99-3	33.72	2.92	1631	1618	1	balsamic[20]
139	2-furanmethanol (Co20)	98-00-0	35.23	2.02	1670	1661	4	
140	5-ethoxydihydro-2(3*H*)-furanone	932-85-4	37.45	2.84	1729	1728	47	
			Ketone					
141	diacetyl [2,3-butanedione]	431-03-8	6.65	2.29	980	977	17	buttery[3]
142	2,3-pentanedione	600-14-6	9.45	2.64	1048	1055	34	
143	(*E*)-3-penten-2-one	3102-33-8	12.25	2.88	1129	1126	17	
144	cyclopentanone	120-92-3	14.58	3.36	1182	1192	29	
145	acetoin [3-hydroxy-2-butanone] (Co8)	513-86-0	19.37	2.18	1287	1304	1	creamy, fatty[3]
146	2-methyl-2-cyclopenten-1-one (Co10)	1120-73-6	22.87	3.33	1366	1357	34	
147	2,5-hexanedione (Co14)	110-13-4	28.82	2.78	1506	1505	48	
148	3-methyl-2-cyclopenten-1-one	2758-18-1	29.17	3.11	1515	1513	49	
149	3-methyl-2-cyclohexen-1-one	1193-18-6	32.08	3.75	1589	1595	17	
150	acetophenone	98-86-2	34.53	3.11	1652	1649	1	
151	4-methyl-acetophenone	122-00-9	39.08	3.33	1775	1778	50	
152	3-ethyl-2-hydroxy-2-cyclopenten-1-one	21835-01-8	44.33	4.18	1925	1924	51	
			Lactone					
153	isocaprolactone	3123-97-5	32.20	2.88	1595	1615	52	
154	γ-butyrolactone (Co18)	96-48-0	33.72	2.61	1633	1635	5	caramel, sweet[16]
155	δ-valerolactone	542-28-9	40.25	2.84	1805	1785	35	coconut,[53] cheese[54]
156	γ-octalactone (Co29)	104-50-7	44.22	3.30	1918	1911	22	
157	tetrahydro-6-propyl-2*H*-pyran-2-one	698-76-0	45.73	3.32	1966	1947	39	coconut[16]
158	dihydro-5-pentyl-2(3*H*)-furanone	104-61-0	47.83	3.30	2030	2010	39	
159	pantolactone	5405-40-3	48.07	2.09	2037	2033	55	

Table S4. Positively and/or tentatively identified volatile compounds of all Cabernet Sauvignon wines, using HS-SPME-GC × GC-TOFMS with their respective Chemical Abstract Service (CAS) numbers, retention times in the first (^1t_R) and in the second (^2t_R) chromatographic dimensions, experimental retention index (RI_{exp}) and RI reported in scientific literature (RI_{lit}). Chromatographic conditions are described in "Determination of volatile profile" sub-section (cont.)

No.	Compound[a]	CAS[b]	^1t_R / min	^2t_R / s	RI_{exp}[c]	RI_{lit}[d]	Ref.[e]	Odor[e]
			Phenol					
160	phenol	108-95-2	47.37	1.93	2015	2015	56	
161	4-ethyl-2-methoxy-phenol	2785-89-9	47.95	2.68	2034	2033	1	
162	4-methyl-phenol	108-39-4	49.82	2.01	2092	2094	57	
163	3-methyl-phenol	108-39-4	50.05	2.00	2100	2102	56	
164	4-ethyl-phenol	123-07-9	52.62	2.07	2184	2190	4	
165	2-(1,1-dimethylethyl)-4-methyl-phenol	2409-55-4	54.37	2.35	2244	2235	58	
166	2,4-bis(1,1-dimethylethyl)-phenol	96-76-4	56.70	2.60	2324	2321	57	
			Terpene					
167	thujene	02-05-67	7.93	5.46	1012	1020	59	
168	myrcene	123-35-3	13.25	5.34	1154	1165	17	
169	limonene (Co2)	5989-54-8	14.70	6.04	1186	1198	17	
170	eucalyptol	470-82-6	15.17	6.49	1196	1209	17	
171	β-ocimene	3338-55-4	17.50	5.15	1247	1238	12	
172	*p*-cymene (Co6)	527-84-4	18.32	5.09	1265	1266	45	
173	α-terpinolene (Co7)	586-62-9	18.78	6.02	1276	1280	12	
174	*p*-cymenene (Co11)	1195-32-0	25.90	4.22	1437	1433	12	
175	linalool (Co17)	78-70-6	30.68	2.95	1553	1555	1	citrus, pine,[16] solvent, hydrocarbon, coffee[60]
176	4-terpinenol	562-74-3	32.67	3.67	1604	1602	1	
177	hotrienol	29957-43-5	33.13	2.82	1615	1611	61	
178	menthol (Co19)	490-99-3	34.18	3.21	1643	1637	39	
179	*p*-ment-6-en-2-one	499-71-8	35.47	4.34	1677	1669	62	peppermint[16]
180	isopiperitone (Co22)	89-81-6	37.22	4.10	1723	1730	63	
181	carvone	99-49-0	37.57	3.90	1733	1748	40	mint[64]
182	linalool oxide	14049-11-7	37.87	2.91	1740	1720	65	
183	1,2-dihydro-1,1,6-trimethyl-naphthalene (TDN)	30364-38-6	37.92	4.96	1743	1751	66	
184	citronellol	1117-61-9	38.97	2.85	1771	1778	1	petrolly kerosene-like aroma[3]
185	nerol (Co25)	106-25-2	40.13	2.83	1804	1798	1	
186	sabinol	09-02-10	40.37	2.92	1810	1800	67	

Table S4. Positively and/or tentatively identified volatile compounds of all Cabernet Sauvignon wines, using HS-SPME-GC × GC-TOFMS with their respective Chemical Abstract Service (CAS) numbers, retention times in the first (^1t_R) and in the second (^2t_R) chromatographic dimensions, experimental retention index (RI_{exp}) and RI reported in scientific literature (RI_{lit}). Chromatographic conditions are described in "Determination of volatile profile" sub-section (cont.)

No.	Compound[a]	CAS[b]	^1t_R / min	^2t_R / s	RI_{exp}[c]	RI_{lit}[d]	Ref.[e]	Odor[e]
187	β-damascenone (Co26)	23726-93-4	40.72	4.47	1821	1831	1	
188	geraniol (Co27)	624-15-7	41.88	2.80	1854	1853	17	sweet, fruity,[16] rose-like[3]
189	geranyl acetone (Co27)	3879-26-3	42.00	4.39	1858	1856	1	
			Terpene					
190	nerolidol	142-50-7	48.30	3.69	2045	2039	68	
191	thymol	499-75-2	53.78	2.29	2224	2205	69	
			Sulfur compound					
192	methyl thiolacetate	1534-08-3	8.98	2.88	1034	1050	70	
193	dihydro-2-methyl-3(2*H*)-thiophenone	13679-85-1	29.75	3.25	1530	1518	4	
194	2-(methylthio)-ethanol	5271-38-5	29.87	2.22	1532	1516	45	
195	ethyl 3-(methylthio)propanoate	13327-56-5	31.38	3.50	1571	1560	4	
196	3-(methylthio)-1-propanol (Co22)	505-10-2	37.22	2.31	1723	1721	4	
197	benzothiazole (Co30)	95-16-9	45.38	3.19	1956	1956	1	boiled cabbage[3]

[a]Co-elutions were numbered from Co1 to Co30 and these numbers are written between parentheses after the compound's name. Whenever compounds are followed by the same number, they co-eluted in ^{1}D; [b]CAS: Chemical Abstract Service; [c]RI_{exp}: experimental retention index (RI) calculated using *n*-alkanes (C9-C24) with a DB-Wax (100% polyethyleneglycol) × DB-17 ms ([50%-phenyl]-methylpolysiloxane) column set; [d]RI_{lit}: literature RI on a DB-WAX column or equivalent stationary phase in 1D-GC; [e]reference.

Table S5. Mean score of descriptive attributes for appearance, aroma and taste and mouth sensations evaluated by the sensory trained panel for each wine (12 judges, 3 repetitions *per* sample): C1, C2, C3, C4, and C5. Experimental procedure of descriptive analysis (DA) is mentioned in "Characterization of the wines sensory profile using sensory descriptive analysis" sub-section

Attribute	C1	C2	C3	C4	C5
Aroma					
Aromatic intensity	5.8 ± 0.1a	5.3 ± 0.4ab	3.8 ± 0.5d	5.7 ± 0.5a	4.5 ± 0.3cd
Aroma of red fruits	5.3 ± 0.1a	4.8 ± 0.2a	2.9 ± 0.2b	5.0 ± 0.3a	3.4 ± 0.3b
Aroma of dry fruits	3.2 ± 0.2a	2.8 ± 0.2ab	2.7 ± 0.1ab	2.8 ± 0.1ab	2.4 ± 0.4b
Alcoholic aroma	4.2 ± 0.4a	3.8 ± 0.5ab	3.0 ± 0.2c	4.2 ± 0.4a	3.5 ± 0.3bc
Spices aroma	2.4 ± 0.1a	2.3 ± 0.2ab	1.8 ± 0.3b	2.2 ± 0.1ab	2.3 ± 0.3ab
Herbaceous aroma	1.9 ± 0.5b	2.2 ± 0.4ab	2.7 ± 0.4a	1.9 ± 0.2b	2.4 ± 0.1ab
Undesirable aroma	0.2 ± 0.1a	0.3 ± 0.1a	0.5 ± 0.1a	0.3 ± 0.1a	0.5 ± 0.1a
Vegetal aroma	2.2 ± 0.2a	2.3 ± 0.3a	2.4 ± 0.2a	2.2 ± 0.3a	2.5 ± 0.1a
Appearance					
Color intensity	6.9 ± 0.3a	5.0 ± 0.3c	2.1 ± 0.1e	5.7 ± 0.3b	3.3 ± 0.2d
Red-purple tonality	7.0 ± 0.2a	5.3 ± 0.3bc	2.2 ± 0.1e	5.8 ± 0.1b	3.3 ± 0.2d
Taste and mouth sensation					
Gustatory persistence	5.5 ± 0.4a	4.7 ± 0.4b	3.2 ± 0.2c	5.3 ± 0.1ab	3.5 ± 0.3c
Body	5.4 ± 0.2a	4.4 ± 0.5bc	2.8 ± 0.3e	4.8 ± 0.3ab	3.4 ± 0.4de
Smell and taste harmony	5.3 ± 0.1a	4.9 ± 0.3a	3.9 ± 0.4b	4.9 ± 0.2a	4.0 ± 0.3b
Astringency	3.8 ± 0.2a	3.3 ± 0.1ab	2.5 ± 0.3b	3.9 ± 0.4a	3.2 ± 0.4ab
Bitterness	2.7 ± 0.3a	2.4 ± 0.4ab	1.9 ± 0.2b	2.8 ± 0.5a	2.6 ± 0.5ab
Sourness	4.4 ± 0.4ab	4.5 ± 0.3ab	4.1 ± 0.4b	4.8 ± 0.2a	4.0 ± 0.4b
Sweetness	1.6 ± 0.2a	1.7 ± 0.3a	1.8 ± 0.1a	1.4 ± 0.3a	1.4 ± 0.4a

In the same line means showing common letter are not significantly different (p = 5%) according to ANOVA and Tukey's test.

Table S6. Aroma compounds of the 26 odoriferous regions found in C1 Cabernet Sauvignon wine using only one-dimensional gas chromatography with different detectors: olfactometry, mass spectrometric and flame ionization. Experimental procedure is mentioned in "Determination of volatile profile" sub-section

r[a]	Compound (No.)[b]	RI_{OSME}[c]	RI_{FID}[c]	I[d]	OSME area ± SD[e] / %
A	ethyl propanoate (No. 81)	969	965	5.1	3.4 ± 0.3
B	diacetyl [2,3-butanedione] (No. 141)	981	980	4.6	4.4 ± 0.5
C	ethyl butanoate (No. 86)	1037	1020	4.0	1.9 ± 0.2
D	1-propanol (No. 18, Co1)	1054	1041	4.9	3.5 ± 0.4
E	ethyl isovalerate (No. 88)	1068	1066	4.9	3.0 ± 0.4
F	isobutyl alcohol (No. 20)	1098	1099	4.8	3.1 ± 0.3
G	isoamyl acetate (No. 90)	1124	1122	4.5	2.7 ± 0.3
H	1-butanol (No. 24)	1187	1175	3.7	2.5 ± 0.2
I	isoamyl alcohol (3-methyl-1-butanol, No. 27, Co4)	1209	1215	5.9	6.6 ± 0.8
J	ethyl hexanoate (No. 93)	1236	1235	5.6	4.3 ± 0.5
K	acetoin [3-hydroxy-2-butanone] (No. 145, Co8)	1299	1281	2.3	2.1 ± 0.2
L	ethyl octanoate (No. 102, Co11)	1435	1437	3.5	2.7 ± 0.3
M	acetic acid (No. 1, Co12)	1461	1454	6.9	8.5 ± 0.7
N	benzaldehyde (No. 74, Co15)	1526	1523	2.6	1.2 ± 0.3
O	2,3-butanediol (No. 50)	1538	1542	4.0	1.9 ± 0.2
P	1-octanol (No. 41)	1573	1579	3.7	2.2 ± 0.2
Q	γ-butyrolactone (No. 154, Co18)	1635	1629	5.5	4.0 ± 0.4
R	ethyl decanoate (No. 112, Co19)	1651	1641	4.1	2.9 ± 0.3
S	diethyl butanedioate (No. 115, Co21)	1682	1684	6.9	9.1 ± 1.2
T	3-(methylthio)-1-propanol (No. 196, Co22)	1729	1714	5.4	4.9 ± 0.6
U	1,2-dihydro-1,1,6-trimethyl-naphthalene (TDN) (No. 183)	1741	1739	4.6	2.8 ± 0.3
V	diethyl pentanedioate (No. 119)	1795	1798	4.0	1.6 ± 0.3
W	2-phenylethyl acetate (No. 125, Co26)	1837	1819	7.3	10.5 ± 0.9
X	phenylethyl alcohol (No. 63, Co29)	1908	1916	5.5	5.5 ± 0.6
Y	1-dodecanol (No. 64)	1965	1969	3.4	2.5 ± 0.2
Z	octanoic acid (No. 11)	2082	2075	4.5	2.3 ± 0.4

[a]r designation of the odoriferous region by capital letters, as in Table 2; [b]number of compound is according to Table S4 and Cox informs if the compound is coeluting with other one(s), where x is the coelution number also according to Table S4; [c]experimental retention index (RI) calculated using *n*-alkanes (C9-C24) in DB-Wax (100% polyethyleneglycol) for both GC-O (RI_{OSME}) and GC-FID (RI_{FID}) analyses. In GC-O, the retention time of the maximum intensity of the odor peak was used in RI calculation; [d]intensity (I, evaluated in a 10 cm scale anchored at the left and right extremities by the intensity terms "none" and "strong", respectively) was obtained as an average intensity of the consensual aromagram constructed after the analyses of the sample by 5 judges in 3 replicates; [e]OSME area ± standard deviation: corresponds to the percentage of area of an odoriferous compound in relation to the sum of the area of all compounds detected when the OSME technique was used to obtain information on the volatiles determined by GC-O, through a sensory panel.

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