

Supplementary tables

Table 1S. Technological maturity stage of Chardonnay clones in vintages 2017 and 2018, Caldas (MG, Brazil).

Vintages	Clones	
	76	809
2017 Summer Vintage		
pH	3.22±0.03 ^A	3.27±0.00 ^B
Total soluble solids (°Brix)	17.43±0.15 ^A	16.90±0.00 ^B
Total acidity (g/L)	8.47±0.50 ^A	8.75±0.00 ^A
2018 Summer Vintage		
pH	3.11±0.02 ^A	3.14±0.01 ^B
Total soluble solids (°Brix)	17.00±0.37 ^A	17.00±0.00 ^A
Total acidity (g/L)	9.34±1.04 ^A	8.94±0.12 ^A

Source: Data obtained from the Enochemical Laboratory - EPAMIG Grape and Wine (Caldas/MG, Brazil). Values are expressed as the mean (n = 4) ± the standard deviation.

Evaluating each parameter in the same vintage, clones that do not share letters in the same line are significantly different (Tukey's method, $p < 0.05$).

Table 2S. Compounds identified in both clones (76 and 809) and harvests (2017 and 2018) from Chardonnay grapes to sparkling wines in the southeast of Brazil (Caldas, Minas Gerais): retention time (RT), NIST score, modified Kovats retention indexes (mKRI) obtained and from the literature, and the identification approach.

Classes and compounds	RT (min)	NIST Score	mKRI obtained	mKRI literature	Identification
Benzenoids					
Benzaldehyde	26.6	93.4	1537	1508	MS, RI
Benzeneacetaldehyde	27.4	88.3	1626	1646	MS, RI
Benzeneacetic acid, ethyl ester	26.0	90.1	1799	1779	MS, RI
Benzyl alcohol	35.6	82.7	1893	1877	MS, RI
Ethanone, 1-(2-hydroxy-5-methylphenyl)-	33.0	70.3	2213	2178	MS, RI
Styrene	14.2	98.0	1260	1241	MS, RI
Toluene	10.4	94.5	1047	1042	MS, RI
Carbonyls					
1-Octen-3-one	17.4	88.2	1280	1290	MS, RI
2,4-Heptadienal, (E,E)-	23.3	93.4	1459	1497	MS, RI
2,4-Hexadienal, (E,E)-	18.2	86.9	1376	1394	MS, RI
2,4-Nonadienal, (E,E)-	29.0	74.4	1662	1698	MS, RI
2,5-Furandicarboxaldehyde	37.6	91.6	1995	1996	MS, RI
2-Decenal, (E)-	25.9	91.0	1661	1643	MS, RI
2-Furancarboxaldehyde, 5-methyl-	21.7	73.0	1585	1570	MS, RI
2-Heptanone	12.2	85.2	1187	1184	MS, RI
2-Heptenal, (Z)-	18.1	97.0	1302	1287	MS, RI
2-Hexenal, (E)-	12.4	97.4	1196	1225	MS, RI
2-Nonanone	17.6	79.8	1397	1387	MS, RI
2-Nonenal, (E)-	24.5	84.4	1547	1542	MS, RI
2-Octenal, (E)-	21.4	95.3	1403	1434	MS, RI
2-Undecanone	22.3	82.6	1609	1599	MS, RI
3-Hexenal, (E)-	9.6	95.8	1144	1146	MS, RI
3-Hexenal, (Z)-	9.7	87.2	1150	1138	MS, RI

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3-Pentanone	8.1	89.1	983	979	MS, RI
5-Hepten-2-one, 6-methyl-	20.9	96.2	1319	1340	MS, RI
Acetaldehyde	1.7	95.9	715	694	MS, RI
Acetoin	19.2	90.9	1296	1280	MS, RI
Acetone	3.5	65.4	808	821	MS, RI
Butanal, 2-methyl-	3.2	82.7	901	896	MS, RI
Butanal, 3-methyl-	3.3	93.6	907	900	MS, RI
Decanal	20.2	83.3	1464	1485	MS, RI
Furfural	19.3	97.8	1473	1460	MS, RI
Heptanal	13.3	94.5	1159	1181	MS, RI
Hexanal	7.8	97.6	1072	1078	MS, RI
Methyl Isobutyl Ketone	9.2	90.3	1009	1059	MS, RI
Nonanal	20.3	95.4	1369	1382	MS, RI
Octanal	14.6	95.8	1264	1287	MS, RI
Pentanal	4.5	97.4	964	974	MS, RI
Propanal, 2-methyl-	2.8	89.3	784	801	MS, RI
Esters					
1-Butanol, 3-methyl-, acetate	10.4	93.2	1125	1125	MS, RI
1-Butanol, 3-methyl-, propanoate	12.4	89.7	1196	1184	MS, RI
2-Butenoic acid, ethyl ester, (E)-	11.6	82.5	1170	1158	MS, RI
2-Furancarboxylic acid, ethyl ester	22.7	95.3	1633	1621	MS, RI
2-Hexen-1-ol, acetate, (E)-	16.2	77.4	1343	1315	MS, RI
2-Hexenoic acid, ethyl ester	16.5	75.5	1355	1336	MS, RI
3-Hexen-1-ol, acetate, (Z)-	15.6	93.3	1326	1309	MS, RI
3-Phenyl-1-propanol, acetate	28.9	73.6	1962	1944	MS, RI
4-Methyl-2-pentyl acetate	12.8	86.5	1108	1110	MS, RI
Acetic acid, 2-ethylhexyl ester	17.4	63.9	1392	1420	MS, RI
Acetic acid, 2-phenylethyl ester	26.6	96.7	1832	1825	MS, RI
Acetic acid, butyl ester	7.5	90.5	1082	1075	MS, RI
Acetic acid, heptyl ester	17.2	91.2	1382	1377	MS, RI
Acetic acid, hexyl ester	14.2	91.2	1279	1276	MS, RI
Acetic acid, phenylmethyl ester	32.0	85.8	1748	1708	MS, RI
Acetophenone	30.0	81.8	1637	1628	MS, RI
Anisole	16.6	73.4	1356	1355	MS, RI
Benzenepropanoic acid, ethyl ester	27.8	80.5	1901	1914	MS, RI
Benzoic acid, 2-methylpropyl ester	26.1	75.0	1807	1789	MS, RI
Benzoic acid, ethyl ester	23.7	77.5	1683	1644	MS, RI
Butanedioic acid, diethyl ester	23.8	94.1	1687	1687	MS, RI
Butanoic acid, 2-methyl-, ethyl ester	8.3	88.8	1061	1073	MS, RI
Butanoic acid, 3-methyl-, ethyl ester	8.7	90.3	1075	1082	MS, RI
Butanoic acid, 3-methylbutyl ester	14.4	77.3	1267	1259	MS, RI
Butanoic acid, ethyl ester	7.8	91.3	1045	1028	MS, RI
Butyrolactone	29.4	79.6	1652	1617	MS, RI
Decanoic acid, ethyl ester	23.1	94.6	1648	1633	MS, RI
Decanoic acid, methyl ester	22.2	79.2	1604	1586	MS, RI
Dodecanoic acid, ethyl ester	27.0	71.5	1856	1840	MS, RI
Ethyl 9-decenoate	24.1	95.1	1698	1689	MS, RI
Ethyl Acetate	3.8	94.9	882	885	MS, RI
Ethyl cinnamate	32.0	97.3	2153	2126	MS, RI

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Heptanoic acid, ethyl ester	16.2	80.2	1337	1328	MS, RI
Hexadecanoic acid, ethyl ester	33.8	80.3	2267	2252	MS, RI
Hexanoic acid, 2-methylpropyl ester	16.6	86.4	1359	1347	MS, RI
Hexanoic acid, ethyl ester	13.7	93.2	1240	1223	MS, RI
Hexanoic acid, methyl ester	12.3	92.6	1191	1184	MS, RI
Hexanoic acid, propyl ester	15.9	84.4	1321	1339	MS, RI
Isobutyl acetate	7.1	93.8	1023	1020	MS, RI
Isopentyl hexanoate	19.3	97.1	1467	1464	MS, RI
Isopropyl myristate	36.7	71.6	2047	2041	MS, RI
Isopropyl palmitate	33.5	76.0	2250	2232	MS, RI
n-Caprylic acid isobutyl ester	21.2	73.7	1562	1561	MS, RI
Nonanoic acid, ethyl ester	20.9	91.3	1547	1547	MS, RI
n-Propyl acetate	5.8	76.7	984	952	MS, RI
Octanoic acid, 3-methylbutyl ester	23.5	95.3	1666	1658	MS, RI
Octanoic acid, ethyl ester	18.9	97.4	1457	1428	MS, RI
Octanoic acid, methyl ester	17.6	90.2	1394	1378	MS, RI
Pentanedioic acid, diethyl ester	25.8	84.7	1790	1780	MS, RI
Pentanoic acid, 4-methyl-, ethyl ester	12.4	86.8	1193	1197	MS, RI
Pentanoic acid, ethyl ester	10.8	80.0	1139	1139	MS, RI
Phenethyl hexanoate	32.7	80.0	2194	2164	MS, RI
Phenylethyl butyrate	29.2	83.2	1986	1968	MS, RI
Propanoic acid, 2-hydroxy-, ethyl ester	16.5	91.3	1354	1340	MS, RI
Propanoic acid, 2-methyl-, ethyl ester	5.6	84.0	971	975	MS, RI
Propyl octanoate	20.6	92.2	1530	1514	MS, RI
Tetradecanoic acid, ethyl ester	30.6	74.9	2064	2027	MS, RI
Higher Alcohols					
1-Pentanol	14.0	89.3	1252	1255	MS, RI
1-Butanol	14.6	89.7	1159	1157	MS, RI
1-Butanol, 3-methyl-	13.2	98.7	1223	1208	MS, RI
1-Decanol	25.5	96.8	1773	1769	MS, RI
1-Heptanol	24.5	95.2	1442	1441	MS, RI
1-Hexanol	17.2	95.3	1365	1357	MS, RI
1-Hexanol, 2-ethyl-	25.5	97.4	1498	1484	MS, RI
1-Hexen-3-ol	18.2	91.1	1264	1225	MS, RI
1-Nonanol	30.1	96.3	1671	1666	MS, RI
1-Octanol	21.4	96.5	1569	1546	MS, RI
1-Octen-3-ol	21.9	96.6	1436	1456	MS, RI
1-Propanol	8.0	95.6	1053	1030	MS, RI
1-Propanol, 2-methyl-	9.7	98.4	1104	1077	MS, RI
2-Heptanol	17.9	94.6	1298	1294	MS, RI
2-Hexen-1-ol, (E)-	23.1	97.6	1419	1410	MS, RI
2-Hexen-1-ol, (Z)-	20.6	96.5	1382	1420	MS, RI
2-Nonen-1-ol, (E)-	31.5	75.5	1727	1713	MS, RI
2-Octen-1-ol, (E)-	26.6	92.5	1577	1590	MS, RI
2-Undecanol	24.6	77.4	1729	1706	MS, RI
3-Hexen-1-ol, (E)-	21.8	87.5	1344	1366	MS, RI
3-Hexen-1-ol, (Z)-	22.4	96.9	1353	1390	MS, RI
5-Hepten-2-ol, 6-methyl-	24.7	84.8	1475	1468	MS, RI
Phenylethyl Alcohol	36.4	96.4	1930	1912	MS, RI

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Volatile Fatty Acids					
2-Hexenoic acid, (E)-	32.8	91.5	1954	1933	MS, RI
9-Decenoic acid	35.1	84.6	2354	2348	MS, RI
Acetic acid	24.3	99.4	1460	1465	MS, RI
Butanoic acid	23.0	88.5	1638	1637	MS, RI
Butanoic acid, 3-methyl-	30.5	80.0	1684	1666	MS, RI
Dodecanoic acid	37.3	83.8	2499	2502	MS, RI
Hexanoic acid	27.0	97.8	1854	1857	MS, RI
Hexanoic acid, 2-ethyl-	37.1	92.5	1962	1963	MS, RI
n-Decanoic acid	34.0	86.9	2283	2281	MS, RI
n-Hexadecanoic acid	43.5	76.1	2928	2923	MS, RI
Nonanoic acid	37.1	80.7	2178	2169	MS, RI
Octanoic acid	30.7	83.7	2072	2070	MS, RI
Propanoic acid, 2-methyl-	27.8	88.6	1579	1581	MS, RI
Tetradecanoic acid	40.0	85.9	2715	2715	MS, RI
Volatile Phenols					
2-Ethylhexyl salicylate ¹	34.6	97.2	2322	NF	MS
n-Hexyl salicylate	33.3	76.8	2234	2203	MS, RI
Phenol	38.1	86.0	2017	2008	MS, RI
Volatile Sulfurs					
Carbon disulfide	2.4	82.7	685	733	MS, RI
Dimethyl sulfide	1.9	83.3	748	777	MS, RI
Sulfur dioxide	3.0	76.1	847	882	MS, RI
Ethers					
1-Propanol, 3-ethoxy-	17.5	90.6	1388	1378	MS, RI
3(2H)-Thiophenone, dihydro-2-methyl-	20.9	70.9	1548	1518	MS, RI
Terpenoids					
(E,Z)-alloocimene	21.9	90.3	1382	1372	MS, RI
(Z)-Dehydroxylinalool oxide	12.8	81.4	1209	1199	MS, RI
cis-Linalool oxide	24.2	90.7	1421	1444	MS, RI
cis-β-Ocimene	18.0	91.7	1260	1235	MS, RI
Citral	29.7	82.7	1715	1733	MS, RI
Citronellol	25.6	93.7	1779	1755	MS, RI
Citronellyl acetate	23.5	87.6	1672	1645	MS, RI
Cymene	18.6	77.1	1278	1260	MS, RI
Dehydrolinalool	28.8	90.5	1620	1648	MS, RI
Dihydromyrcenol	24.9	87.8	1479	1470	MS, RI
Eucalyptol	11.7	83.0	1175	1211	MS, RI
Farnesene	30.1	79.9	1710	1692	MS, RI
Geranic acid	39.6	86.0	2363	2347	MS, RI
Geraniol	32.4	97.2	1862	1847	MS, RI
Geranylacetone	27.3	88.8	1869	1862	MS, RI
Isoterpinolene	15.0	84.0	1291	1270	MS, RI
Limonene	16.1	91.9	1203	1185	MS, RI
Linalool	24.7	98.8	1557	1552	MS, RI
Linaloyl oxide	9.9	86.9	1107	1096	MS, RI
L-rose oxide ¹	16.7	81.1	1361	NF	MS
Menthol	27.2	71.9	1599	1631	MS, RI
Nerol	31.3	93.5	1815	1781	MS, RI

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Nerol oxide	19.5	95.3	1484	1469	MS, RI
β -Damascenone	26.8	94.0	1841	1834	MS, RI
β -Myrcene	14.8	98.9	1160	1164	MS, RI
β -Phellandrene	13.8	84.7	1158	1162	MS, RI
β -Thujene	10.0	88.3	1082	1117	MS, RI
trans-Geranic acid methyl ester	31.1	82.4	1707	1677	MS, RI
trans-Linalool oxide (furanoid)	21.7	91.1	1458	1452	MS, RI
trans- β -Ocimene	17.4	96.5	1250	1242	MS, RI
α -Terpineol	24.3	96.2	1716	1680	MS, RI

NF: Not found; MS: compound identified by MS spectra (similarity $\geq 70\%$); RI: compound identified by comparing Kovats retention indices from the literature (accepted standard deviation of RI not exceeding 50 (Ilc *et al.*, 2016)).

¹ 2-Ethylhexyl salicylate and L-rose oxide compounds were tentatively identified based on the fragmentation profile similarity compared to NIST library and score.