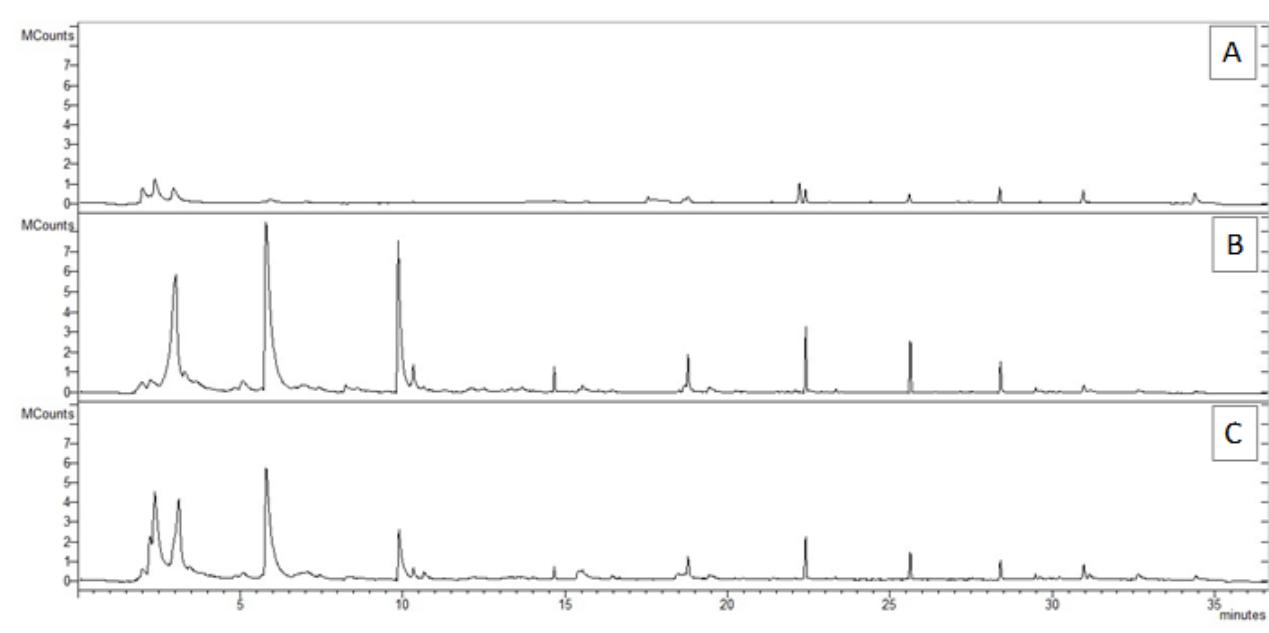


Supplementary Figure 1. Chromatograms from Malbec vine shoots after 6, 20 and 40 min heating time at 180 °C (A, B and C, respectively).



Supplementary Figure 2. Relative concentration, expressed as percentage, of volatile compounds with oenological interest obtained at 200 °C as heating temperature.



Supplementary Table 1. Identification of compounds detected in the volatile fraction sampled at 120 °C in the different varieties of vine shoots.

Vine shoots 120 °C						
Compound	Mass	RI (Ri)	Formula	Characteristic fragments	Red wine varieties	White wine varieties
Difluorochloromethane	86	292 (258)	CHClF ₂	51, 67, 85	✓	✓
Trichloromethane	118	642 (601)	CHCl ₃	83, 50, 118	✓	
3-Methoxybutan-2-ol	104	677 (692)	C ₅ H ₁₂ O ₂	59, 71, 89	✓	✓
3,4-Dimethyl-1-penten-3-ol	112	755 (742)	C ₇ H ₁₂ O	79, 43, 97		✓
Hexanal	100	784 (806)	C ₆ H ₁₂ O	56, 72, 82	✓	✓
1,3,5-Trioxacycloheptane	104	835 (806)	C ₄ H ₈ O ₃	73, 61, 104	✓	
1,2-Butanediol	90	790 (824)	C ₄ H ₁₀ O ₂	59, 89, 61	✓	✓
2-Hydroxypropionamide	89	872 (891)	C ₃ H ₇ NO ₂	61, 55, 74	✓	
3-Pyridinol	95	915 (895)	C ₅ H ₅ NO	95, 68, 67		✓
4-Pyridinol	95	921 (895)	C ₅ H ₅ NO	95, 67, 55		✓
2,7-Dimethyl-3,5-octadiene	138	955 (903)	C ₁₀ H ₁₈	95, 81, 67		✓
4,6-Dimethyl-2-heptanone	142	912 (924)	C ₉ H ₁₈ O	58, 69, 85		✓
Oxybis dichloromethane	182	980 (987)	C ₂ H ₂ Cl ₄ O	83, 85, 50		✓
1,1-Dimethoxyheptane	160	1055 (1004)	C ₉ H ₂₀ O ₂	75, 55, 97	✓	
Cyclopentanecarboxylic acid	114	1036 (1017)	C ₆ H ₁₀ O ₂	73, 86, 114		✓
2,3-Dimethylcyclohexanol	128	1022 (1030)	C ₈ H ₁₆ O	95, 81, 110	✓	
2-Pentylfuran	138	998 (1040)	C ₉ H ₁₄ O	81, 53, 138	✓	✓
Benzeneacetaldehyde	120	1102 (1081)	C ₈ H ₈ O	91, 65, 120		✓
Propanoic acid hexyl ester	158	1062 (1083)	C ₉ H ₁₈ O ₂	57, 75, 84	✓	
3-Undecyne	152	1156 (1132)	C ₁₁ H ₂₀	67, 81, 120		✓
5-Hydroxymethylfurfural	126	1185 (1163)	C ₆ H ₆ O ₃	97, 126, 69		✓
2-Isopropyl-5-methylcyclohexanol	156	1202 (1164)	C ₁₀ H ₂₀ O	71, 81, 95		✓
6-Nonen-1-ol	142	1189 (1167)	C ₉ H ₁₈ O	67, 55, 82		✓
Decanal	156	1232 (1204)	C ₁₀ H ₂₀ O	57, 70, 82		✓
Copaene	204	1186 (1221)	C ₁₅ H ₂₄	105, 119, 161	✓	
7-Methoxy-3,7-dimethyloctanal	186	1243 (1230)	C ₁₁ H ₂₂ O ₂	73, 55, 69		✓
1-Formyl-4-hydroxymethylcyclohexane	142	1281 (1273)	C ₈ H ₁₄ O ₂	81, 67, 95	✓	
Benzeneacetic acid, α -oxomethyl ester	164	1271 (1296)	C ₉ H ₈ O ₃	105, 77, 51		✓
1-Undecanol	172	1388 (1357)	C ₁₁ H ₂₄ O	55, 69, 83		✓
Vanillin	152	1412 (1392)	C ₈ H ₈ O ₃	152, 81, 123		✓
3,5-Dimethoxyacetophenone	180	1426 (1407)	C ₁₀ H ₁₂ O ₃	165, 180, 137		✓
Vanillyl methyl ketone (Guaiacylacetone)	180	1530 (1538)	C ₁₀ H ₁₂ O ₃	137, 180, 122		✓
Syringaldehyde	182	1602 (1581)	C ₉ H ₁₀ O ₄	182, 111, 167		✓
Methoxyeugenol	194	1611 (1581)	C ₁₁ H ₁₄ O ₃	194, 91, 119		✓
1-Hexadecyne	222	1633 (1609)	C ₁₆ H ₃₀	81, 67, 55		✓
2,6-bis(1,1-Dimethylethyl)-2,5-cyclohexadiene-1,4-dione	220	1678 (1633)	C ₁₄ H ₂₀ O ₂	177, 220, 135		✓

4-(3-Hydroxy-1-propenyl)-2-methoxyphenol (Coniferyl alcohol)	180	1622 (1653)	C ₁₀ H ₁₂ O ₃	137, 124, 180	✓	
6-Methyl-2,4-di-tert-butyl-phenol	220	1660 (1668)	C ₁₅ H ₂₄ O	205, 220, 57	✓	
1-Heptadecyne	236	1688 (1709)	C ₁₇ H ₃₂	81, 67, 55		✓
6,10,14-Trimethyl-2-pentadecanone	268	1791 (1754)	C ₁₈ H ₃₆ O	58, 71, 109		✓
9,12-Tetradecadien-1-ol, acetate	252	1814 (1795)	C ₁₆ H ₂₈ O ₂	67, 81, 95	✓	✓
1-Octadecyne	250	1776 (1808)	C ₁₈ H ₃₄	81, 67, 55		✓
2-Methyl-7-octadecyne	264	1869 (1863)	C ₁₉ H ₃₆	81, 67, 95		✓
Hexadecanoic acid methyl ester (Methyl palmitate)	270	1891 (1878)	C ₁₇ H ₃₄ O ₂	74, 87, 55	✓	✓
1,2-Benzenedicarboxylic acid, butyl 2-methylpropyl ester	278	1986 (1972)	C ₁₆ H ₂₂ O ₄	149, 223, 104		✓
Hexadecanoic acid ethyl ester (Ethyl palmitate)	284	1993 (1978)	C ₁₈ H ₃₆ O ₂	43, 73, 60	✓	✓
3,7,11,15-Tetramethyl-2-hexadecen-1-ol (Phytol)	296	2071 (2045)	C ₂₀ H ₄₀ O	81, 95, 123		✓
9,12-Octadecadien-1-ol	266	2096 (2069)	C ₁₈ H ₃₄ O	67, 55, 81		✓
9,12,15-Octadecatrien-1-ol	264	2044 (2077)	C ₁₈ H ₃₂ O	79, 67, 55		✓
Linolelaidic acid methyl ester	294	2045 (2093)	C ₁₉ H ₃₄ O ₂	67, 55, 81	✓	✓

Supplementary Table 2. Identification of compounds detected in the volatile fraction sampled at 120 °C in the different varieties of oak wood.

Oak wood 120 °C						
Compound	Mass	RI (Ri)	Formula	Characteristic fragments	French oak	American oak
Propiolonitrile	51	580 (563)	C ₃ HN	51, 50, 52		✓
Trichloromethane	118	633 (601)	CHCl ₃	83, 85, 50	✓	✓
Hexanal	100	785 (806)	C ₆ H ₁₂ O	56, 72, 82		✓
Furfural	96	836 (831)	C ₅ H ₄ O ₂	96, 95, 67	✓	✓
2,5-Dimethyl-2-hexanol	130	823 (844)	C ₈ H ₁₈ O	59, 69, 97	✓	✓
4-Pyridinol	95	910 (895)	C ₅ H ₅ NO	95, 67, 55		✓
Methyl 2-furoate	126	932 (909)	C ₆ H ₆ O ₃	95, 126, 68		✓
3-Methyl-6-hepten-1-ol	128	1016 (985)	C ₈ H ₁₆ O	55, 67, 95		✓
Octanal	128	1023 (1005)	C ₈ H ₁₆ O	56, 69, 84		✓
1-Ethynyl-1-cyclohexanol	124	1055 (1028)	C ₈ H ₁₂ O	81, 68, 95	✓	
2-Pentylfuran	138	1071 (1040)	C ₉ H ₁₄ O	81, 53, 138		✓
5-Hydroxymethylfurfural	126	1182 (1163)	C ₆ H ₆ O ₃	97, 126, 69		✓
1-Formyl-3,5,6-trimethyl-3-cyclohexene	152	1194 (1163)	C ₁₀ H ₁₆ O	121, 81, 67		✓
2,6-Dimethyl-2-octen-8-ol	156	1185 (1179)	C ₁₀ H ₂₀ O	69, 81, 55	✓	
3-Allyl-2,6,6-trimethylbicyclo[3.1.1]heptane	178	1150 (1187)	C ₁₃ H ₂₂	83, 69, 55	✓	
1-Cyclohexyl-1-butanol	156	1209 (1241)	C ₁₀ H ₂₀ O	55, 95, 73		✓
5-Butyldihydro-4-methyl-2(3H)-furanone (<i>cis</i> -Oak lactone)	156	1226 (1245)	C ₉ H ₁₆ O ₂	99, 71, 87	✓	✓
Vanillin	152	1369 (1392)	C ₈ H ₈ O ₃	151, 109, 81		✓
3,4,5-Trimethoxyphenol	184	1499 (1468)	C ₉ H ₁₂ O ₄	169, 184, 141		✓
2,6-Dimethyl-2-octen-8-ol butyrate	226	1487 (1501)	C ₁₄ H ₂₆ O ₂	81, 69, 95	✓	
δ-Undecalactone	184	1526 (1503)	C ₁₁ H ₂₀ O ₂	99, 71, 55	✓	
Vanillyl methyl ketone (Guaiacylacetone)	180	1506 (1538)	C ₁₀ H ₁₂ O ₃	137, 180, 122	✓	
Dodecanoic acid	200	1562 (1570)	C ₁₂ H ₂₄ O ₂	60, 73, 129	✓	
Methoxyeugenol	194	1566 (1581)	C ₁₁ H ₁₄ O ₃	194, 91, 119	✓	
Syringaldehyde	182	1583 (1581)	C ₉ H ₁₀ O ₄	182, 167, 139	✓	
3-(4-Hydroxy-3-methoxyphenyl)- 2-propenal (Coniferaldehyde)	178	1623 (1599)	C ₁₀ H ₁₀ O ₃	178, 135, 107	✓	
Acetosyringone	196	1639 (1628)	C ₁₀ H ₁₂ O ₄	181, 196, 153	✓	
Homovanillic acid	182	1644 (1659)	C ₉ H ₁₀ O ₄	137, 182, 122	✓	
6-Methyl-2,4-di-tert-butyl-phenol	220	1654 (1668)	C ₁₅ H ₂₄ O	205, 220, 57	✓	
9,12-Tetradecadien-1-ol	210	1659 (1672)	C ₁₄ H ₂₆ O	68, 81, 55	✓	
6,10,14-Trimethyl-2-pentadecanone	268	1779 (1754)	C ₁₈ H ₃₆ O	58, 71, 109		✓
Ferulic acid	194	1772 (1767)	C ₁₀ H ₁₀ O ₄	194, 179, 133		✓
14-Methyl-8-hexadecenal	252	1858 (1843)	C ₁₇ H ₃₂ O	55, 70, 83		✓

2-Methyl-7-octadecyne	264	1881 (1863)	C ₁₉ H ₃₆	81, 67, 95	✓	✓
Hexadecanoic acid methyl ester (Methyl palmitate)	270	1861 (1878)	C ₁₇ H ₃₄ O ₂	74, 87, 55	✓	✓
9-Hexadecenoic acid methyl ester	268	1897 (1886)	C ₁₇ H ₃₂ O ₂	55, 69, 74		✓
3,7,11,15-Tetramethyl-1-hexadecen-3-ol (Isophytol)	296	1915 (1899)	C ₂₀ H ₄₀ O	71, 57, 82		✓
Hexadecanoic acid ethyl ester (Ethyl palmitate)	284	1990 (1978)	C ₁₈ H ₃₆ O ₂	43, 73, 60	✓	✓
3,7,11,15-Tetramethyl-2-hexadecen-1-ol (Phytol)	296	2091 (2045)	C ₂₀ H ₄₀ O ₈	81, 95, 123		✓
Methyl octadecadienoate	294	2122 (2093)	C ₁₉ H ₃₄ O ₂	67, 81, 95		✓
9,12-Octadecadienoic acid (Linoleic acid)	280	2211 (2183)	C ₁₈ H ₃₂ O ₂	67, 81, 55	✓	✓
1,2-Benzenedicarboxylic acid butyl cyclohexyl ester	304	2263 (2299)	C ₁₈ H ₂₄ O ₄	149, 55, 223	✓	