

Table S1. Compounds detected by HS SPME-GC-MS in resin samples, along with their corresponding peak integrations

Compound	Exper. RI	Quant mass[※]	Resin A_C	Resin A_N	Resin B_C	Resin B_N[*]
<i>α</i> -pinene [†]	1007	-	+++++	+++++	+++++	+++++
camphene	1046	93.1	8.48E+08	9.93E+08	1.30E+09	6.21E+08
<i>β</i> -pinene	1084	93.1	7.18E+08	9.83E+08	1.38E+09	9.67E+08
sabinene	1098	-	traces	traces	traces	traces
3-carene	1124	93.0	1.12E+08	5.42E+07	3.35E+08	2.47E+08
<i>β</i> -myrcene	1140	93.1	1.50E+09	2.72E+09	1.51E+09	1.20E+09
1,4-cineole	1154	-	traces	traces	traces	traces
limonene	1173	68.1	8.72E+08	9.51E+08	1.99E+09	1.51E+09
<i>β</i> -phellandrene	1180	93.0	1.49E+08	2.25E+08	2.03E+08	2.34E+08
eucalyptol	1181	43.2	8.99E+06	1.48E+07	3.49E+07	1.25E+07
<i>cis-β</i> -ocimene	1209	93.1	4.48E+07	5.38E+07	4.83E+07	3.53E+07
<i>γ</i> -terpinene	1216	93.1	3.08E+07	6.52E+07	1.34E+08	3.42E+07
<i>trans-β</i> -ocimene	1225	93.1	7.03E+07	8.48E+07	5.76E+07	7.12E+07
<i>p</i> -cymene	1237	119.0	3.99E+07	3.81E+08	1.12E+08	3.70E+07
<i>α</i> -terpinolene	1249	93.0	5.21E+08	4.87E+08	6.67E+08	4.19E+08
2-nonanone	1366	58.1	8.58E+07	9.48E+07	2.25E+08	2.17E+08
cyclosativene	1443	105.1	8.06E+07	1.47E+08	5.23E+07	4.21E+07
<i>α</i> -copaene	1459	119.0	4.03E+08	6.86E+08	2.57E+08	2.16E+08
2-nonanol	1506	45.2	5.60E+07	4.36E+07	7.01E+07	6.17E+07
linalool	1534	-	traces	traces	traces	traces
fenchol	1555	-	traces	traces	traces	traces
<i>β</i> -caryophyllene	1558	133.0	1.06E+09	1.08E+09	8.75E+08	6.20E+08
terpinen-4-ol	1573	71.1	4.52E+07	4.09E+07	9.76E+07	6.74E+06
2-undecanone	1577	58.1	2.40E+07	2.96E+07	3.86E+07	3.60E+07
<i>trans</i> -pinocarveol	1624	92.1	1.47E+07	1.59E+07	1.00E+07	1.38E+07
<i>α</i> -caryophyllene	1634	93.1	4.51E+08	4.46E+08	3.71E+08	2.48E+08
estragole	1645	148.0	2.35E+08	1.16E+08	3.50E+08	4.09E+08
<i>γ</i> -muurolene	1664	161.1	3.91E+07	7.21E+07	2.90E+07	2.25E+07
<i>trans</i> -verbenol	1665	109.0	3.11E+07	3.54E+07	1.61E+07	3.32E+07
endo-borneol	1690	95.1	3.42E+07	4.41E+07	6.20E+07	1.76E+07
<i>D</i> -germacrene	1691	161.1	1.90E+07	2.08E+08	2.96E+07	1.61E+07
<i>α</i> -terpineol	1698	59.1	7.11E+07	6.34E+07	4.63E+08	1.49E+07

α -muurolene	1713	105.0	6.80E+08	1.19E+09	4.24E+08	3.08E+08
δ -cadinene	1739	161.1	7.06E+07	1.28E+08	5.67E+07	3.55E+07
myrtenol	1778	79.1	1.62E+07	1.73E+07	1.18E+07	1.38E+07
trans-carveol	>1800 [‡]	109.0	9.67E+06	1.58E+07	9.15E+06	1.34E+07
cymen-8-ol	>1800	43.2	7.80E+06	6.60E+06	1.04E+07	1.02E+07
caryophyllene oxide	>1800	79.1	7.51E+06	1.15E+07	3.06E+06	2.94E+06
methyl eugenol	>1800	178.0	5.49E+06	2.15E+06	6.65E+06	6.26E+06
copaborneol	>1800	161.1	1.83E+07	2.73E+07	1.16E+07	8.36E+06

※: Fragment ion used for peak integration

†: Filament was turned off to avoid detector overloading due to α -pinene presence

‡: C₁₈ was the last detectable n-alkane (26.72 min)

*: Resins from forest A or B, harvested naturally (N) or conventionally (C)

Table S2. Compounds detected by HS SPME-GC-MS in Retsina samples ascribed to fermentation, maturation and aging process of wine

Compound	RI NIST (Polar)[※]	Identification method[†]
acetaldehyde (ethanal)	702±12	MS, RI
ethyl acetate	888±8	MS, RI
ethanol	932±8	MS, RI
isobutyl acetate	1012±8	MS, RI
ethyl butyrate	1035±8	MS, RI
isobutanol	1092±9	MS, RI
isoamyl acetate (isopentyl acetate)	1122±7	MS, RI
1-butanol	1142±11	MS, RI
methyl caproate (methyl hexanoate)	1184±7	MS, RI
isoamyl alcohol (isopentyl alcohol)	1209±9	MS, RI
ethyl caproate (ethyl hexanoate)	1233±9	MS, RI
hexyl acetate	1272±7	MS, RI
furfuryl ethyl ether	1291±N/A	MS, RI
ethyl lactate (ethyl 2-hydroxypropanoate)	1347±9	MS, RI
1-hexanol	1355±7	MS, RI
2-hexenol	1405±10	MS, RI

1,3-di-tert-butylbenzene	1427±7	MS, RI
ethyl caprylate (ethyl octanoate)	1435±6	MS, RI
furfural	1462±11	MS, RI
ethyl sorbate (ethyl hexa-2,4-dienoate)	1501±4	MS, RI
ethyl caprate (ethyl decanoate)	1638±9	MS, RI
diethyl succinate (diethyl butanedioate)	1680±9	MS, RI
2-phenylethyl acetate	1813±15	MS, RI
caproic acid (hexanoic acid)	1846±12	MS, RI
ethyl laurate (ethyl dodecanoate)	1841±9	MS, RI
phenethyl alcohol	1906±15	MS, RI
caprylic acid (octanoic acid)	2060±15	MS, RI
sorbic acid (2,4-hexadienoic acid)	2150±0	MS, RI
capric acid (decanoic acid)	2276±14	MS, RI
2,4-di-tert-butylphenol	2318±10	MS, RI
monoethyl succinate (monoethyl butanedioate)	2368±9	MS, RI
lauric acid (dodecanoic acid)	2497±11	MS, RI

※: Retention indices for polar columns according to NIST17 Mass Spectral Library

†: MS, mass spectrum; RI, retention indices (Kovats)

Table S3a. Compounds of resin origin in Retsina samples (detected by HS SPME-GC-MS) and their corresponding peak integrations[※]

Compound	Exper. RI (Kovats)	Quant mass [†]	s.01a-1	s.02a-1	s.03a-1	s.04a-1	s.05a-1	s.06a-1	s.07a-1	s.08a-1	s.09a-1
<i>α</i> -pinene	1007	93.0	4.81E+07	4.98E+07	4.71E+08	6.30E+07	4.15E+07	4.77E+07	5.82E+07	7.67E+07	3.28E+07
camphene	1046	93.0	2.45E+06	3.08E+06	4.47E+06	3.69E+06	4.42E+06	3.53E+06	5.84E+06	9.02E+06	7.95E+05
<i>β</i> -myrcene	1140	93.0	1.08E+06	9.34E+05	6.49E+06	1.13E+06	9.49E+05	1.19E+06	6.89E+05	1.01E+06	4.33E+05
1,4-cineole	1154	111.0	4.30E+05	5.14E+05	3.21E+06	3.08E+06	4.59E+05	3.93E+05	1.00E+07	1.55E+07	4.89E+04
limonene	1173	68.1	3.85E+06	3.23E+06	9.93E+06	5.57E+06	6.89E+06	6.24E+06	7.62E+06	1.22E+07	1.33E+06
<i>γ</i> -terpinene	1216	93.0	5.92E+05	7.47E+05	1.42E+06	9.63E+05	1.10E+06	7.92E+05	1.37E+06	2.47E+06	2.92E+05
<i>p</i> -cymene	1237	119.0	1.43E+06	2.05E+06	2.87E+06	2.70E+06	2.66E+06	2.63E+06	1.42E+06	2.19E+06	2.60E+05
<i>α</i> -terpinolene	1249	93.0	3.75E+06	3.85E+06	5.55E+06	4.41E+06	6.38E+06	5.13E+06	6.46E+06	1.12E+07	6.15E+05
2-nonanone	1366	58.1	4.48E+06	5.14E+06	8.64E+06	6.33E+06	6.97E+06	7.08E+06	6.20E+06	7.88E+06	6.13E+05
<i>α</i> -copaene	1459	119.0	8.72E+05	1.43E+06	2.58E+06	2.02E+06	2.97E+06	3.31E+06	4.93E+06	7.47E+06	1.89E+05
2-nonanol	1506	45.1	2.68E+07	2.63E+07	2.93E+07	2.48E+07	3.04E+07	3.18E+07	3.03E+07	3.60E+07	3.34E+06
linalool	1534	71.1	8.46E+05	1.47E+06	1.28E+06	1.17E+06	2.31E+06	2.94E+06	1.77E+06	2.51E+06	8.43E+05
fenchol	1555	81.1	8.62E+06	6.48E+06	1.39E+07	1.33E+07	1.51E+07	1.53E+07	2.96E+07	3.36E+07	5.60E+05
<i>β</i> -caryophyllene	1558	91.0	5.42E+06	6.09E+06	1.31E+07	7.14E+06	1.03E+07	1.18E+07	1.68E+07	2.17E+07	1.62E+05
terpinen-4-ol	1573	71.0	9.23E+06	9.43E+06	1.85E+07	1.73E+07	6.00E+06	6.66E+06	3.45E+07	4.66E+07	5.14E+05
estragole	1645	148.0	6.74E+06	8.45E+06	5.66E+06	5.39E+06	1.16E+07	1.28E+07	6.71E+06	8.67E+06	3.68E+05
endo-borneol	1690	95.0	1.02E+07	9.08E+06	1.61E+07	1.29E+07	1.04E+07	9.72E+06	1.82E+07	2.89E+07	4.54E+06
<i>α</i> -terpineol	1698	59.1	5.50E+07	5.29E+07	9.52E+07	9.02E+07	8.46E+07	9.06E+07	1.58E+08	2.07E+08	5.06E+06

myrtenol	1778	79.0	9.81E+05	9.25E+05	1.26E+06	1.30E+06	1.72E+06	1.45E+06	1.41E+06	2.12E+06	2.16E+05
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Table S3b. Compounds of resin origin in Retsina samples (detected by HS SPME-GC-MS) and their corresponding peak integrations[✱]

Compound	Exper. RI (Kovats)	Quant mass [†]	s.01a-2	s.02a-2	s.03a-2	s.04a-2	s.05a-2	s.06a-2	s.07a-2	s.08a-2	s.09a-2
<i>α</i> -pinene	1007	93.0	5.52E+07	4.61E+07	1.38E+08	4.50E+07	3.89E+07	4.46E+07	5.51E+07	8.74E+07	1.27E+07
camphene	1046	93.0	2.97E+06	3.57E+06	3.53E+06	4.37E+06	3.67E+06	4.11E+06	6.71E+06	1.05E+07	2.90E+05
<i>β</i> -myrcene	1140	93.0	1.11E+06	1.09E+06	2.31E+06	7.85E+05	1.11E+06	1.23E+06	7.53E+05	1.16E+06	4.15E+05
1,4-cineole	1154	111.0	3.80E+05	5.61E+05	3.21E+06	2.91E+06	4.24E+05	3.88E+05	1.02E+07	1.44E+07	5.18E+04
limonene	1173	68.1	3.76E+06	4.37E+06	7.41E+06	5.97E+06	6.85E+06	6.24E+06	6.88E+06	1.26E+07	1.44E+06
<i>γ</i> -terpinene	1216	93.0	6.51E+05	9.38E+05	7.93E+05	8.67E+05	8.70E+05	7.73E+05	1.56E+06	2.42E+06	1.93E+05
<i>p</i> -cymene	1237	119.0	1.47E+06	2.02E+06	2.83E+06	2.78E+06	2.58E+06	2.83E+06	1.76E+06	2.49E+06	3.05E+05
<i>α</i> -terpinolene	1249	93.0	4.08E+06	4.94E+06	4.24E+06	4.54E+06	6.01E+06	5.52E+06	7.74E+06	1.16E+07	3.54E+05
2-nonanone	1366	58.1	4.39E+06	5.31E+06	7.85E+06	6.41E+06	6.71E+06	7.04E+06	6.49E+06	9.39E+06	7.34E+05
<i>α</i> -copaene	1459	119.0	1.58E+06	2.57E+06	2.74E+06	1.94E+06	2.87E+06	2.24E+06	7.81E+06	8.68E+06	1.66E+05
2-nonanol	1506	45.1	2.55E+07	3.09E+07	2.74E+07	2.46E+07	3.05E+07	3.29E+07	3.24E+07	3.84E+07	2.66E+06
linalool	1534	71.1	1.05E+06	1.42E+06	1.53E+06	1.77E+06	2.41E+06	3.18E+06	1.92E+06	2.90E+06	8.37E+05
fenchol	1555	81.1	9.54E+06	9.56E+06	1.53E+07	1.38E+07	1.49E+07	1.43E+07	3.44E+07	3.35E+07	4.69E+05
<i>β</i> -caryophyllene	1558	91.0	6.10E+06	7.31E+06	1.34E+07	9.02E+06	1.07E+07	1.04E+07	2.51E+07	2.78E+07	2.28E+05
terpinen-4-ol	1573	71.0	9.25E+06	1.04E+07	1.84E+07	1.71E+07	6.05E+06	6.80E+06	3.63E+07	4.85E+07	6.19E+05
estragole	1645	148.0	7.28E+06	7.84E+06	5.17E+06	5.19E+06	1.22E+07	1.38E+07	8.04E+06	5.95E+06	3.87E+05

endo-borneol	1690	95.0	8.30E+06	9.45E+06	1.13E+07	1.34E+07	1.34E+07	1.03E+07	2.29E+07	2.59E+07	1.62E+06
α -terpineol	1698	59.1	5.60E+07	6.06E+07	9.27E+07	8.85E+07	8.69E+07	8.31E+07	1.68E+08	2.12E+08	4.77E+06
myrtenol	1778	79.0	9.11E+05	1.07E+06	1.39E+06	1.35E+06	1.40E+06	1.42E+06	1.40E+06	1.64E+06	2.87E+05

Table S3c. Compounds of resin origin in Retsina samples (detected by HS SPME-GC-MS) and their corresponding peak integrations^{*}

Compound	Exper. RI (Kovats)	Quant mass [†]	s.01b-1	s.02b-1	s.03b-1	s.04b-1	s.05b-1	s.06b-1	s.07b-1	s.08b-1	s.09b-1
α -pinene	1007	93.0	9.40E+06	4.05E+07	1.91E+07	3.56E+07	9.73E+06	6.79E+07	1.63E+07	8.57E+07	2.01E+07
camphene	1046	93.0	2.39E+06	4.04E+06	2.90E+06	7.34E+06	4.15E+06	7.99E+06	8.17E+06	9.31E+06	3.97E+05
β -myrcene	1140	93.0	5.06E+05	1.50E+06	8.24E+05	9.96E+05	4.26E+05	1.65E+06	6.06E+05	2.28E+06	6.33E+05
1,4-cineole	1154	111.0	3.94E+05	5.73E+05	2.84E+06	3.71E+06	3.74E+05	4.59E+05	8.41E+06	1.36E+07	4.37E+04
limonene	1173	68.1	2.05E+06	5.66E+06	3.80E+06	5.15E+06	3.70E+06	9.47E+06	5.93E+06	1.29E+07	1.36E+06
γ -terpinene	1216	93.0	4.19E+05	1.32E+06	7.62E+05	9.65E+05	8.04E+05	9.96E+05	1.65E+06	1.76E+06	1.62E+05
<i>p</i> -cymene	1237	119.0	1.12E+06	2.12E+06	2.28E+06	3.28E+06	1.88E+06	2.53E+06	1.84E+06	2.59E+06	3.63E+05
α -terpinolene	1249	93.0	1.68E+06	8.13E+06	1.97E+06	5.54E+06	3.24E+06	1.05E+07	5.63E+06	1.16E+07	3.27E+05
2-nonanone	1366	58.1	2.45E+06	6.68E+06	4.57E+06	9.30E+06	3.75E+06	1.14E+07	3.36E+06	1.08E+07	7.49E+05
α -copaene	1459	119.0	1.01E+06	7.41E+05	1.92E+06	1.21E+06	1.71E+06	1.73E+06	4.17E+06	3.04E+06	2.23E+05
2-nonanol	1506	45.1	2.64E+07	3.59E+07	2.85E+07	3.32E+07	3.10E+07	4.46E+07	2.92E+07	5.12E+07	4.15E+06
linalool	1534	71.1	9.47E+05	1.31E+06	1.44E+06	1.17E+06	2.05E+06	3.17E+06	1.43E+06	2.19E+06	8.72E+05
fenchol	1555	81.1	8.74E+06	1.33E+07	1.57E+07	1.83E+07	1.32E+07	2.35E+07	2.79E+07	3.92E+07	5.84E+05
β -caryophyllene	1558	91.0	4.21E+06	4.18E+06	1.12E+07	7.33E+06	6.49E+06	9.24E+06	1.79E+07	2.08E+07	1.81E+05

terpinen-4-ol	1573	71.0	7.75E+06	1.05E+07	1.62E+07	1.82E+07	5.08E+06	7.83E+06	2.77E+07	4.62E+07	5.05E+05
estragole	1645	148.0	9.51E+06	1.23E+07	6.51E+06	7.18E+06	1.37E+07	1.96E+07	1.27E+07	1.99E+07	5.11E+05
endo-borneol	1690	95.0	9.10E+06	1.17E+07	1.54E+07	1.14E+07	1.20E+07	1.63E+07	1.85E+07	2.07E+07	1.78E+06
α -terpineol	1698	59.1	5.32E+07	9.09E+07	8.80E+07	1.14E+08	7.55E+07	1.49E+08	1.44E+08	2.43E+08	4.82E+06
myrtenol	1778	79.0	7.30E+05	1.04E+06	1.30E+06	1.85E+06	1.30E+06	1.90E+06	1.27E+06	1.87E+06	4.76E+05

Table S3d. Compounds of resin origin in Retsina samples (detected by HS SPME-GC-MS) and their corresponding peak integrations[※]

Compound	Exper. RI (Kovats)	Quant mass [†]	s.01b-2	s.02b-2	s.03b-2	s.04b-2	s.05b-2	s.06b-2	s.07b-2	s.08b-2	s.09b-2
α -pinene	1007	93.0	1.08E+07	4.97E+07	2.18E+07	4.20E+07	1.17E+07	7.35E+07	1.38E+07	7.93E+07	2.38E+07
camphene	1046	93.0	2.46E+06	6.75E+06	3.08E+06	7.45E+06	4.34E+06	4.19E+06	7.47E+06	1.16E+07	4.69E+05
β -myrcene	1140	93.0	5.69E+05	1.60E+06	7.80E+05	1.12E+06	4.98E+05	1.64E+06	6.69E+05	2.28E+06	7.12E+05
1,4-cineole	1154	111.0	3.86E+05	5.44E+05	2.84E+06	3.61E+06	3.55E+05	4.43E+05	8.20E+06	1.49E+07	6.40E+04
limonene	1173	68.1	2.11E+06	5.85E+06	3.10E+06	7.62E+06	3.75E+06	8.98E+06	5.60E+06	1.24E+07	1.41E+06
γ -terpinene	1216	93.0	5.69E+05	1.33E+06	6.19E+05	1.27E+06	6.82E+05	1.08E+06	1.51E+06	2.03E+06	2.15E+05
<i>p</i> -cymene	1237	119.0	1.10E+06	2.07E+06	2.16E+06	3.50E+06	1.98E+06	2.35E+06	1.87E+06	2.95E+06	3.94E+05
α -terpinolene	1249	93.0	1.61E+06	7.94E+06	1.81E+06	7.16E+06	3.21E+06	1.04E+07	5.46E+06	1.45E+07	3.90E+05
2-nonanone	1366	58.1	2.34E+06	6.39E+06	4.30E+06	9.04E+06	3.37E+06	9.96E+06	3.19E+06	1.12E+07	8.97E+05
α -copaene	1459	119.0	8.43E+05	6.55E+05	1.77E+06	1.72E+06	3.07E+05	1.06E+06	3.53E+06	4.64E+06	2.20E+05
2-nonanol	1506	45.1	2.50E+07	3.50E+07	2.84E+07	3.29E+07	2.29E+07	3.90E+07	3.00E+07	5.34E+07	2.44E+06
linalool	1534	71.1	9.49E+05	1.10E+06	1.30E+06	1.53E+06	2.00E+06	2.90E+06	1.31E+06	2.82E+06	9.08E+05

fenchol	1555	81.1	7.85E+06	1.40E+07	1.50E+07	1.92E+07	9.44E+06	1.68E+07	2.90E+07	4.40E+07	6.29E+05
β -caryophyllene	1558	91.0	3.86E+06	4.11E+06	1.03E+07	9.63E+06	4.30E+06	6.34E+06	1.51E+07	2.76E+07	1.86E+05
terpinen-4-ol	1573	71.0	7.32E+06	1.03E+07	1.57E+07	1.81E+07	3.78E+06	6.44E+06	2.87E+07	4.91E+07	4.84E+05
estragole	1645	148.0	9.97E+06	1.43E+07	6.42E+06	8.11E+06	9.78E+06	1.03E+07	1.40E+07	2.34E+07	4.84E+05
endo-borneol	1690	95.0	8.49E+06	1.16E+07	1.09E+07	1.53E+07	8.58E+06	1.52E+07	1.64E+07	2.60E+07	1.49E+06
α -terpineol	1698	59.1	5.26E+07	9.15E+07	8.90E+07	1.15E+08	5.77E+07	1.23E+08	1.50E+08	2.62E+08	3.81E+06
myrtenol	1778	79.0	7.12E+05	1.12E+06	1.07E+06	1.98E+06	1.14E+06	1.85E+06	1.09E+06	2.17E+06	2.68E+05

Table S3e. Compounds of resin origin in Retsina samples (detected by HS SPME-GC-MS) and their corresponding peak integrations[✱]

Compound	Exper. RI (Kovats)	Quant mass [†]	s.01c-1	s.02c-1	s.03c-1	s.04c-1	s.05c-1	s.06c-1	s.07c-1	s.08c-1	s.09c-1
α -pinene	1007	93.0	1.17E+06	1.98E+06	5.12E+06	1.17E+07	3.50E+06	9.43E+06	2.52E+06	2.86E+06	1.82E+06
camphene	1046	93.0	3.71E+06	1.26E+07	4.02E+06	6.89E+06	1.00E+07	5.28E+06	9.91E+06	1.02E+07	2.60E+05
β -myrcene	1140	93.0	1.25E+05	2.22E+05	2.39E+05	2.72E+05	2.02E+05	3.04E+05	1.57E+05	2.00E+05	9.64E+04
1,4-cineole	1154	111.0	7.36E+05	2.38E+06	3.21E+06	2.97E+06	9.36E+05	1.00E+06	1.00E+07	1.47E+07	1.84E+05
limonene	1173	68.1	2.28E+06	3.08E+06	2.56E+06	2.87E+06	4.15E+06	3.05E+06	4.90E+06	6.23E+06	1.27E+06
γ -terpinene	1216	93.0	7.45E+05	1.61E+06	9.97E+05	9.16E+05	1.53E+06	7.58E+05	2.07E+06	2.47E+06	2.26E+05
<i>p</i> -cymene	1237	119.0	8.73E+05	1.33E+06	1.42E+06	1.38E+06	1.99E+06	1.35E+06	1.65E+06	2.62E+06	7.32E+05
α -terpinolene	1249	93.0	2.44E+06	5.30E+06	1.69E+06	9.79E+05	4.91E+06	2.98E+06	4.74E+06	5.56E+06	4.70E+05
2-nonanone	1366	58.1	8.10E+06	6.92E+06	7.19E+06	9.93E+06	1.27E+07	9.61E+06	9.23E+06	1.01E+07	3.13E+06

<i>α</i> -copaene	1459	119.0	2.97E+05	4.80E+05	3.22E+05	1.95E+05	4.69E+05	4.27E+05	2.47E+05	8.94E+05	2.19E+05
2-nonanol	1506	45.1	2.56E+07	2.42E+07	5.06E+06	1.99E+07	4.78E+07	5.21E+07	3.74E+07	5.13E+07	6.94E+06
linalool	1534	71.1	1.06E+06	1.02E+06	1.33E+06	2.51E+03	1.84E+06	2.58E+06	9.57E+05	1.75E+06	1.61E+06
fenchol	1555	81.1	1.90E+07	2.89E+07	1.31E+07	4.82E+06	3.23E+07	2.28E+07	3.35E+07	3.64E+07	2.62E+06
<i>β</i> -caryophyllene	1558	91.0	1.12E+06	2.60E+06	1.33E+06	1.77E+06	1.30E+06	1.52E+06	1.17E+06	2.99E+06	2.56E+05
terpinen-4-ol	1573	71.0	6.26E+06	7.37E+06	8.60E+06	9.51E+06	7.85E+06	6.69E+06	2.18E+07	4.06E+07	4.97E+05
estragole	1645	148.0	8.58E+06	1.32E+07	4.80E+06	7.86E+05	2.25E+07	2.36E+07	8.85E+06	2.21E+07	6.07E+06
endo-borneol	1690	95.0	1.46E+07	1.96E+07	1.82E+07	2.14E+07	2.27E+07	1.69E+07	2.16E+07	2.79E+07	1.40E+06
<i>α</i> -terpineol	1698	59.1	6.23E+07	9.78E+07	4.00E+07	7.54E+07	1.56E+08	1.11E+08	1.11E+08	2.05E+08	1.10E+07
myrtenol	1778	79.0	6.96E+05	2.23E+05	9.53E+05	1.01E+06	1.67E+06	1.55E+06	9.16E+05	1.49E+06	4.00E+05

Table S3f. Compounds of resin origin in Retsina samples (detected by HS SPME-GC-MS) and their corresponding peak integrations[✱]

Compound	Exper. RI (Kovats)	Quant mass[†]	s.01c-2	s.02c-2	s.03c-2	s.04c-2	s.05c-2	s.06c-2	s.07c-2	s.08c-2	s.09c-2
<i>α</i> -pinene	1007	93.0	8.34E+05	1.84E+06	1.57E+06	2.97E+06	1.96E+06	1.18E+07	6.30E+06	4.22E+06	5.38E+06
camphene	1046	93.0	5.79E+06	1.12E+07	4.84E+06	8.18E+06	9.21E+06	5.82E+06	9.54E+06	1.20E+07	5.47E+05
<i>β</i> -myrcene	1140	93.0	1.62E+05	3.80E+05	2.26E+05	2.35E+05	2.11E+05	4.14E+05	2.51E+05	1.71E+05	1.10E+05
1,4-cineole	1154	111.0	7.42E+05	2.41E+06	3.19E+06	3.88E+06	9.14E+05	9.14E+05	1.01E+07	1.60E+07	2.10E+05
limonene	1173	68.1	2.36E+06	4.89E+06	2.68E+06	3.23E+06	4.23E+06	3.05E+06	5.10E+06	6.76E+06	1.38E+06
<i>γ</i> -terpinene	1216	93.0	1.01E+06	1.71E+06	9.64E+05	3.79E+05	1.32E+06	7.98E+05	2.30E+06	2.88E+06	2.30E+05
<i>p</i> -cymene	1237	119.0	1.04E+06	1.65E+06	1.48E+06	1.69E+06	1.86E+06	1.36E+06	1.85E+06	2.76E+06	7.86E+05

<i>α</i> -terpinolene	1249	93.0	2.72E+06	6.77E+06	1.87E+06	2.00E+06	5.07E+06	2.48E+06	4.94E+06	6.78E+06	8.23E+05
2-nonanone	1366	58.1	9.73E+06	8.03E+06	7.16E+06	1.05E+07	1.50E+07	8.77E+06	1.00E+07	1.12E+07	3.13E+06
<i>α</i> -copaene	1459	119.0	2.24E+05	3.12E+05	6.61E+05	4.65E+05	5.44E+05	1.84E+05	2.87E+05	6.43E+05	2.28E+05
2-nonanol	1506	45.1	3.92E+07	4.30E+07	2.17E+07	1.94E+07	4.98E+07	4.69E+07	4.38E+07	6.18E+07	7.35E+06
linalool	1534	71.1	1.25E+06	1.52E+06	1.27E+06	5.24E+05	1.98E+06	2.36E+06	1.26E+06	2.46E+06	1.40E+06
fenchol	1555	81.1	2.17E+07	3.21E+07	1.37E+07	1.53E+07	3.26E+07	2.20E+07	3.44E+07	4.37E+07	2.66E+06
<i>β</i> -caryophyllene	1558	91.0	6.68E+05	2.33E+06	1.36E+06	1.99E+06	2.21E+06	1.70E+06	1.31E+06	4.11E+06	2.33E+05
terpinen-4-ol	1573	71.0	8.56E+06	1.10E+07	1.07E+07	1.39E+07	8.11E+06	6.80E+06	2.57E+07	4.45E+07	1.08E+06
estragole	1645	148.0	1.22E+07	2.51E+07	8.72E+06	4.71E+06	2.08E+07	2.16E+07	1.69E+07	2.02E+07	3.87E+06
endo-borneol	1690	95.0	1.62E+07	2.21E+07	1.04E+07	2.60E+07	2.30E+07	1.57E+07	2.38E+07	1.80E+07	1.48E+06
<i>α</i> -terpineol	1698	59.1	1.01E+08	1.67E+08	5.73E+07	7.89E+07	1.56E+08	1.11E+08	1.58E+08	2.23E+08	1.22E+07
myrtenol	1778	79.0	9.89E+05	9.43E+05	1.25E+06	1.77E+06	1.77E+06	1.55E+06	1.07E+06	1.76E+06	4.93E+05

Table S3g. Compounds of resin origin in Retsina samples (detected by HS SPME-GC-MS) and their corresponding peak integrations[✱]

Compound	Exper. RI (Kovats)	Quant mass[†]	s.01-3M	s.02-3M	s.03-3M	s.04-3M	s.05-3M	s.06-3M	s.07-3M	s.08-3M	s.09-3M
<i>α</i> -pinene	1007	93.0	7.07E+06	1.33E+07	2.00E+06	2.51E+06	4.30E+06	9.10E+06	1.25E+06	3.47E+06	1.33E+08
camphene	1046	93.0	3.55E+06	6.85E+06	2.85E+06	5.27E+06	7.34E+06	3.68E+06	5.84E+06	6.98E+06	1.43E+06
<i>β</i> -myrcene	1140	93.0	1.73E+05	6.88E+04	2.35E+05	1.94E+05	1.49E+05	2.69E+05	1.01E+05	2.00E+05	1.21E+06
1,4-cineole	1154	111.0	8.72E+05	2.75E+06	3.38E+06	3.80E+06	1.07E+06	1.09E+06	1.08E+07	1.08E+07	1.87E+05
limonene	1173	68.1	2.40E+06	4.48E+06	2.60E+06	2.69E+06	3.43E+06	2.84E+06	4.41E+06	4.29E+06	2.17E+06

<i>γ</i> -terpinene	1216	93.0	7.80E+05	1.42E+06	9.60E+05	9.37E+05	9.87E+05	7.00E+05	2.19E+06	1.78E+06	3.38E+05
<i>p</i> -cymene	1237	119.0	1.18E+06	1.75E+06	1.60E+06	2.00E+06	1.59E+06	1.36E+06	2.00E+06	1.74E+06	8.59E+05
<i>α</i> -terpinolene	1249	93.0	1.93E+06	5.15E+06	1.57E+06	1.43E+06	3.40E+06	1.86E+06	4.19E+06	3.14E+06	7.38E+05
2-nonanone	1366	58.1	8.66E+06	7.76E+06	6.60E+06	1.13E+07	1.35E+07	8.95E+06	9.38E+06	6.28E+06	2.83E+06
<i>α</i> -copaene	1459	119.0	3.67E+05	4.63E+05	7.07E+05	5.71E+05	5.34E+05	3.26E+05	2.24E+05	4.58E+05	1.89E+05
2-nonanol	1506	45.1	3.62E+07	4.20E+07	2.26E+07	2.21E+07	4.68E+07	4.71E+07	4.10E+07	3.14E+07	5.20E+06
linalool	1534	71.1	9.15E+05	1.22E+06	1.17E+06	8.68E+05	1.58E+06	1.79E+06	1.37E+06	3.22E+06	1.10E+06
fenchol	1555	81.1	2.07E+07	3.55E+07	1.61E+07	1.41E+07	3.38E+07	2.22E+07	3.50E+07	2.40E+07	2.01E+06
<i>β</i> -caryophyllene	1558	91.0	1.23E+06	3.05E+06	1.31E+06	1.73E+06	2.40E+06	1.65E+06	1.24E+06	3.03E+06	2.51E+05
terpinen-4-ol	1573	71.0	7.44E+06	1.06E+07	9.69E+06	1.00E+07	7.96E+06	6.52E+06	2.40E+07	2.42E+07	3.93E+05
estragole	1645	148.0	1.19E+07	2.17E+07	9.53E+06	4.56E+06	1.59E+07	1.68E+07	1.41E+07	5.14E+06	4.13E+06
endo-borneol	1690	95.0	1.66E+07	2.63E+07	1.14E+07	1.84E+07	2.42E+07	1.71E+07	2.40E+07	3.25E+07	1.88E+06
<i>α</i> -terpineol	1698	59.1	8.32E+07	1.52E+08	4.95E+07	6.06E+07	1.28E+08	9.73E+07	1.32E+08	6.52E+07	9.53E+06
myrtenol	1778	79.0	8.84E+05	9.99E+05	9.95E+05	1.37E+06	1.36E+06	1.72E+06	9.84E+05	8.34E+05	7.92E+05

Table S3h. Compounds of resin origin in Retsina samples (detected by HS SPME-GC-MS) and their corresponding peak integrations*

Compound	Exper. RI (Kovats)	Quant mass [†]									
			s.01-6M	s.02-6M	s.03-6M	s.04-6M	s.05-6M	s.06-6M	s.07-6M	s.08-6M	s.09-6M
<i>α</i> -pinene	1007	93.0	2.05E+06	1.07E+06	2.68E+06	6.62E+06	5.95E+06	5.10E+06	2.95E+06	1.48E+06	1.79E+08
camphene	1046	93.0	3.41E+06	6.08E+06	2.35E+06	3.54E+06	5.13E+06	2.79E+06	4.00E+06	4.42E+06	5.45E+05
<i>β</i> -myrcene	1140	93.0	6.02E+04	6.77E+04	1.81E+05	2.62E+05	1.73E+05	1.93E+05	1.29E+05	2.43E+05	2.12E+06

1,4-cineole	1154	111.0	1.10E+06	2.67E+06	3.55E+06	4.55E+06	1.28E+06	1.16E+06	9.76E+06	1.28E+07	2.43E+05
limonene	1173	68.1	2.11E+06	3.70E+06	2.45E+06	2.55E+06	3.38E+06	2.46E+06	3.82E+06	4.87E+06	2.56E+06
γ -terpinene	1216	93.0	8.82E+05	1.52E+06	9.22E+05	3.70E+05	9.18E+05	5.51E+05	1.98E+06	8.29E+05	4.55E+05
<i>p</i> -cymene	1237	119.0	1.27E+06	2.09E+06	1.87E+06	1.93E+06	1.52E+06	1.23E+06	1.95E+06	1.35E+06	9.84E+05
α -terpinolene	1249	93.0	1.82E+06	4.15E+06	1.54E+06	1.14E+06	2.98E+06	1.34E+06	3.04E+06	3.02E+06	7.02E+05
2-nonanone	1366	58.1	7.56E+06	6.50E+06	6.33E+06	1.06E+07	1.24E+07	7.30E+06	8.09E+06	7.48E+06	2.88E+06
α -copaene	1459	119.0	1.88E+05	3.41E+05	7.73E+05	8.52E+05	5.45E+05	3.24E+05	3.31E+05	7.26E+05	2.17E+05
2-nonanol	1506	45.1	3.45E+07	3.36E+07	1.99E+07	2.76E+07	4.36E+07	3.27E+07	3.57E+07	3.39E+07	5.17E+06
linalool	1534	71.1	7.76E+05	1.19E+06	1.02E+06	2.55E+05	1.12E+06	9.67E+05	8.04E+05	1.09E+06	8.05E+05
fenchol	1555	81.1	1.99E+07	3.04E+07	1.46E+07	1.70E+07	3.23E+07	2.08E+07	3.18E+07	3.40E+07	2.43E+06
β -caryophyllene	1558	91.0	8.33E+05	2.26E+06	1.24E+06	1.92E+06	2.53E+06	1.58E+06	1.26E+06	3.39E+06	3.34E+05
terpinen-4-ol	1573	71.0	7.20E+06	8.62E+06	9.62E+06	1.34E+07	7.07E+06	5.50E+06	1.95E+07	2.52E+07	1.35E+06
estragole	1645	148.0	1.06E+07	1.38E+07	9.93E+06	5.01E+06	1.16E+07	1.30E+07	1.20E+07	1.18E+07	4.67E+06
endo-borneol	1690	95.0	1.58E+07	2.31E+07	9.06E+06	2.63E+07	2.46E+07	1.50E+07	2.18E+07	3.11E+07	2.33E+06
α -terpineol	1698	59.1	6.62E+07	1.06E+08	4.19E+07	5.53E+07	1.06E+08	5.52E+07	9.42E+07	8.87E+07	1.13E+07
myrtenol	1778	79.0	7.60E+05	8.14E+05	4.68E+05	8.97E+05	1.19E+06	1.14E+06	8.96E+05	7.68E+05	4.72E+05

※: In most cases, noise level is between 10^5 and 10^6

†: Fragment ion used for peak integration

Table S4. Summary of fit for the five PLS-DA models for Retsina samples

Model 1: Sample grouping based on resin's origin (microclimate A vs B)				
Significant components:	1 st	2 nd	3 rd	Cumulative
R ² X (variance explained)	0.432	0.112	-	0.544
R ² Y (goodness of fit)	0.430	0.214	-	0.644
Q ² Y (predictivity)	0.363	0.033	-	0.396

Model 2: Sample grouping based on tapping method (natural vs conventional)				
Significant components:	1 st	2 nd	3 rd	Cumulative
R ² X (variance explained)	0.172	0.380	0.100	0.652
R ² Y (goodness of fit)	0.761	0.090	0.079	0.930
Q ² Y (predictivity)	0.670	0.124	0.085	0.879

Model 3: Sample grouping based on contact time with resin (short vs long)				
Significant components:	1 st	2 nd	3 rd	Cumulative
R ² X (variance explained)	0.352	0.164	-	0.516
R ² Y (goodness of fit)	0.290	0.302	-	0.592
Q ² Y (predictivity)	0.173	0.259	-	0.432

Model 4: Sample grouping based on contact time with resins of natural tapping				
Significant components:	1 st	2 nd	3 rd	Cumulative
R ² X (variance explained)	0.303	0.271	-	0.574
R ² Y (goodness of fit)	0.547	0.292	-	0.839
Q ² Y (predictivity)	0.316	0.344	-	0.660

Model 5: Sample grouping based on contact time with resins of conventional tapping				
Significant components:	1 st	2 nd	3 rd	Cumulative
R ² X (variance explained)	0.381	0.285	0.082	0.748
R ² Y (goodness of fit)	0.529	0.337	0.070	0.936
Q ² Y (predictivity)	0.374	0.385	0.027	0.786

Table S5. CV-ANOVA tables[※] of the five PLS-DA models for Retsina samples

Model 1: Sample grouping based on resin's origin (microclimate A vs B)						
	SS	DF	MS	F	<i>P</i>	SD
Total corrected	31	31	1			1
Regression	12.6996	4	3.1749	4.6842	5.31E-03	1.7818
Residual	18.3004	27	0.6778			0.8233

Model 2: Sample grouping based on tapping method (natural vs conventional)						
	SS	DF	MS	F	<i>P</i>	SD
Total corrected	31	31	1			1
Regression	27.0448	6	4.5075	28.4908	5.06E-10	2.1231
Residual	3.9552	25	0.1582			0.3978

Model 3: Sample grouping based on contact time with resin (short vs long)						
	SS	DF	MS	F	<i>P</i>	SD
Total corrected	31	31	1			1
Regression	12.1374	4	3.0343	4.3434	7.68E-03	1.7419
Residual	18.8626	27	0.6986			0.8358

Model 4: Sample grouping based on contact time with resins of natural tapping						
	SS	DF	MS	F	<i>P</i>	SD
Total corrected	15	15	1			1
Regression	9.2537	4	2.3134	4.4286	0.0224	1.5210
Residual	5.7463	11	0.5224			0.7228

Model 5: Sample grouping based on contact time with resins of conventional tapping						
	SS	DF	MS	F	<i>P</i>	SD
Total corrected	15	15	1			1
Regression	11.1153	6	1.8526	4.2920	0.0255	1.3611
Residual	3.8847	9	0.4316			0.6570

※: Sum of squares, SS; degrees of freedom, DF; mean squares, MS (=SS/DF); Standard deviation, SD ($=\sqrt{MS}$)

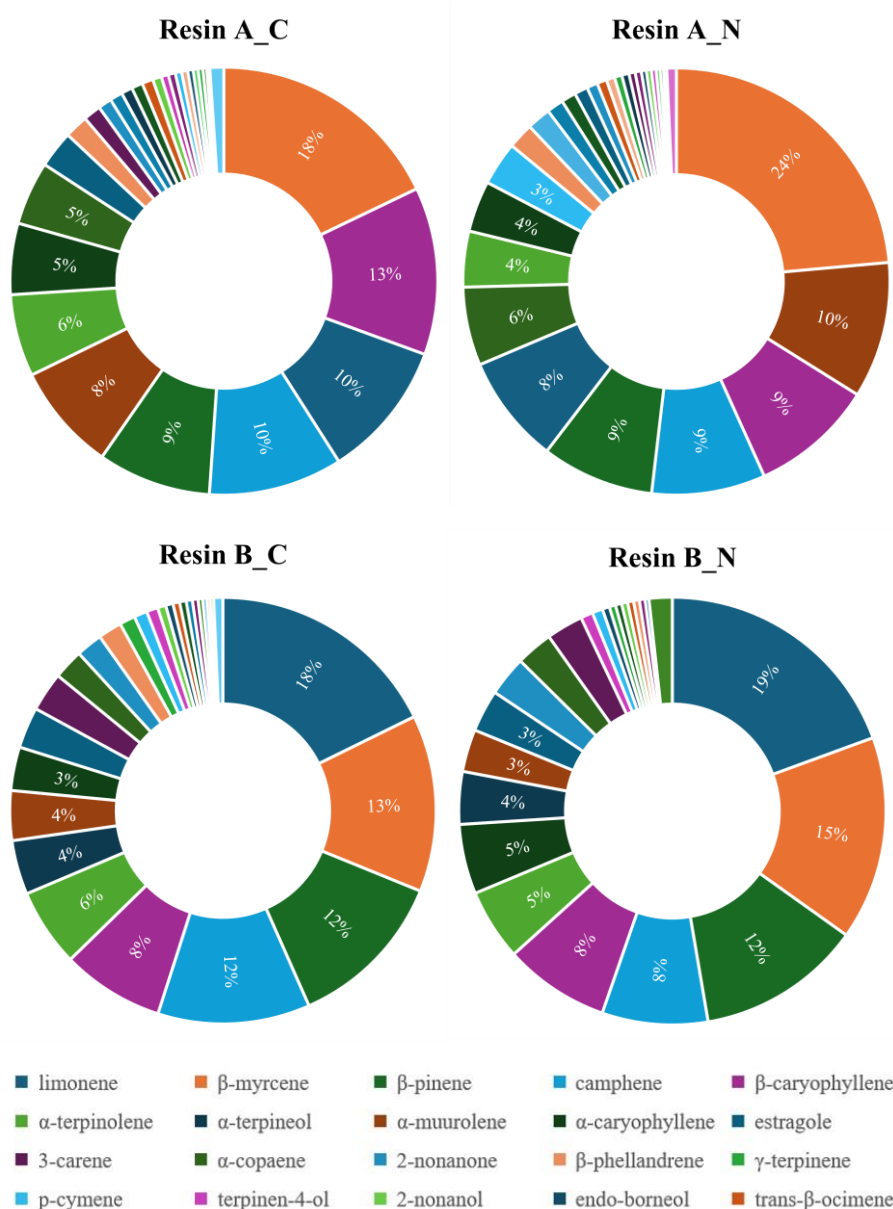


Figure S1. Sunburst charts depicting the relative abundance (percentage of peak area over the total area of TIC chromatogram, excluding α -pinene) of the compounds comprising the volatilome of the four resins: i) A_C (microclimate A, conventional method), ii) A_N (microclimate A, natural method), iii) B_C (microclimate B, conventional method) and iv) B_N (microclimate B, natural method)

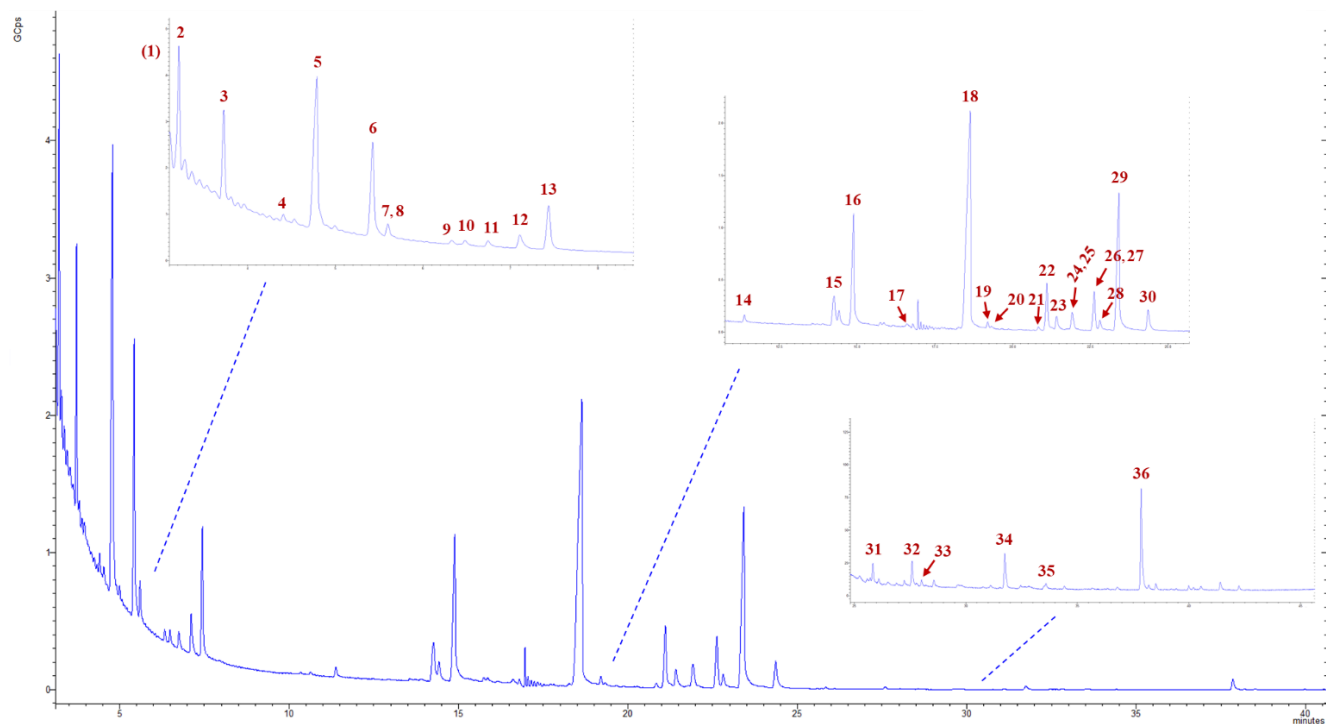


Figure S2. Representative HS SPME-GC-MS total ion chromatogram (TIC) of a resin sample. The numbers in the insets represent the following detected components: (1) α -pinene (prior to cutoff), (2) camphene, (3) β -pinene, (4) 3-carene, (5) β -myrcene, (6) limonene, (7) β -phellandrene, (8) eucalyptol, (9) *cis*- β -ocimene, (10) γ -terpinene, (11) *trans*- β -ocimene, (12) *p*-cymene, (13) α -terpinolene, (14) 2-nonanone, (15) cyclosativene, (16) α -copaene, (17) 2-nonanol, (18) β -caryophyllene, (19) terpinen-4-ol, (20) 2-undecanone, (21) *trans*-pinocarveol, (22) α -caryophyllene, (23) estragole, (24) γ -muurolene, (25) *trans*-verbenol, (26) *endo*-borneol, (27) *D*-germacrene, (28) α -terpineol, (29) α -muurolene, (30) δ -cadinene, (31) myrtenol, (32) *trans*-carveol, (33) cymen-8-ol, (34) caryophyllene oxide, (35) methyl eugenol, (36) copaborneol

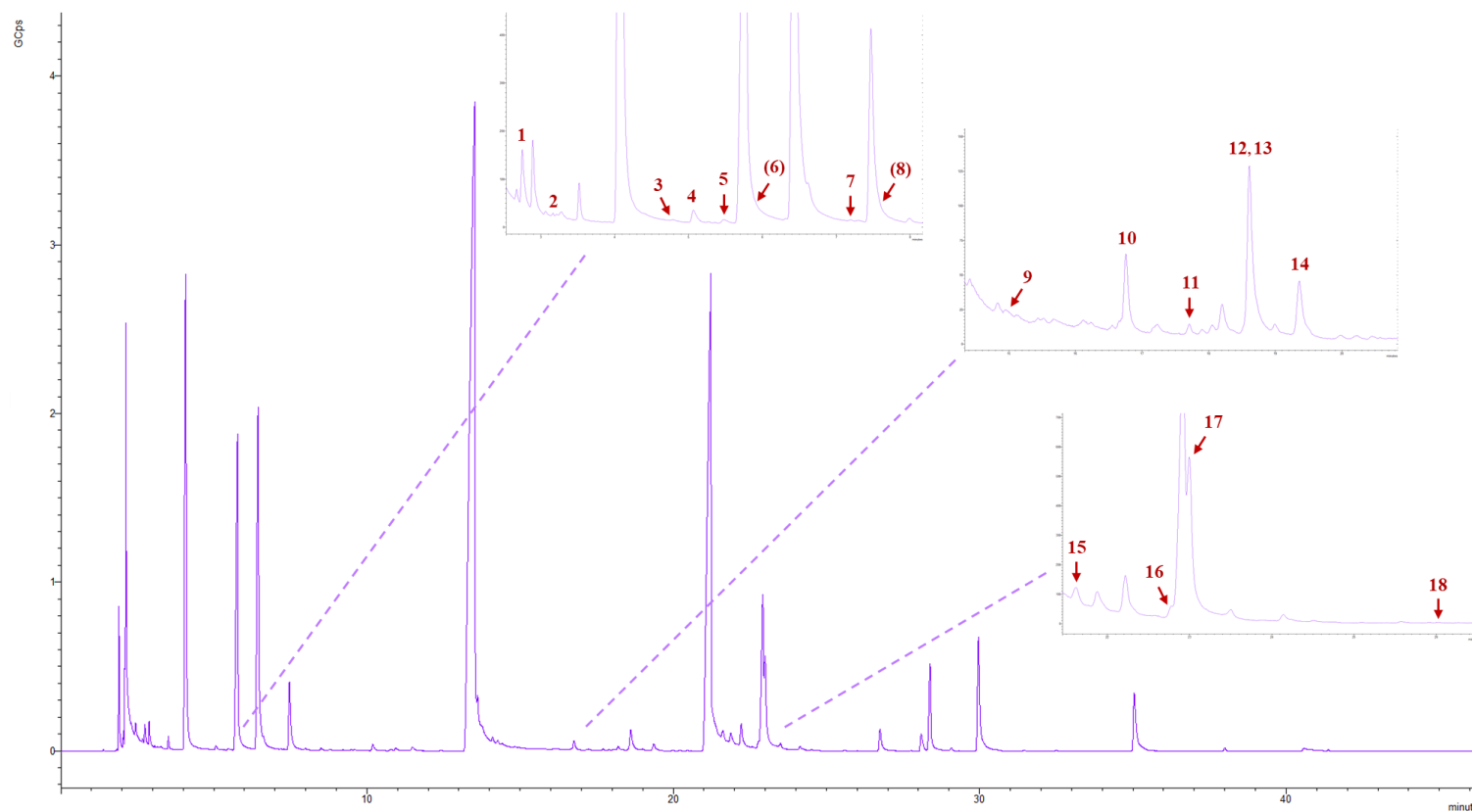


Figure S3. HS SPME-GC-MS total ion chromatogram (TIC) of a Retsina QC sample. The numbers in the insets represent the following detected components: (1) α -pinene, (2) camphene, (3) β -myrcene, (4) 1,4-cineole, (5) limonene, (6) γ -terpinene (surrounded by ethyl hexanoate), (7) *p*-cymene, (8) α -terpinolene (surrounded by ethyl acetate), (9) α -copaene, (10) 2-nonanol, (11) linalool, (12) fenchol, (13) β -caryophyllene, (14) terpinen-4-ol, (15) estragole, (16) endo-borneol, (17) α -terpineol, (18) myrtenol



Figure S4. RP-LC-TIMS-TOF MS total ion chromatograms (TICs) in ESI⁻, of samples from the same vinification protocol, collected at different vinification stages: i) intermediate point of fermentation (A), ii) end of fermentation (B), iii) end of maturation (C), iv) three months of aging (D) and v) six months of aging (E)

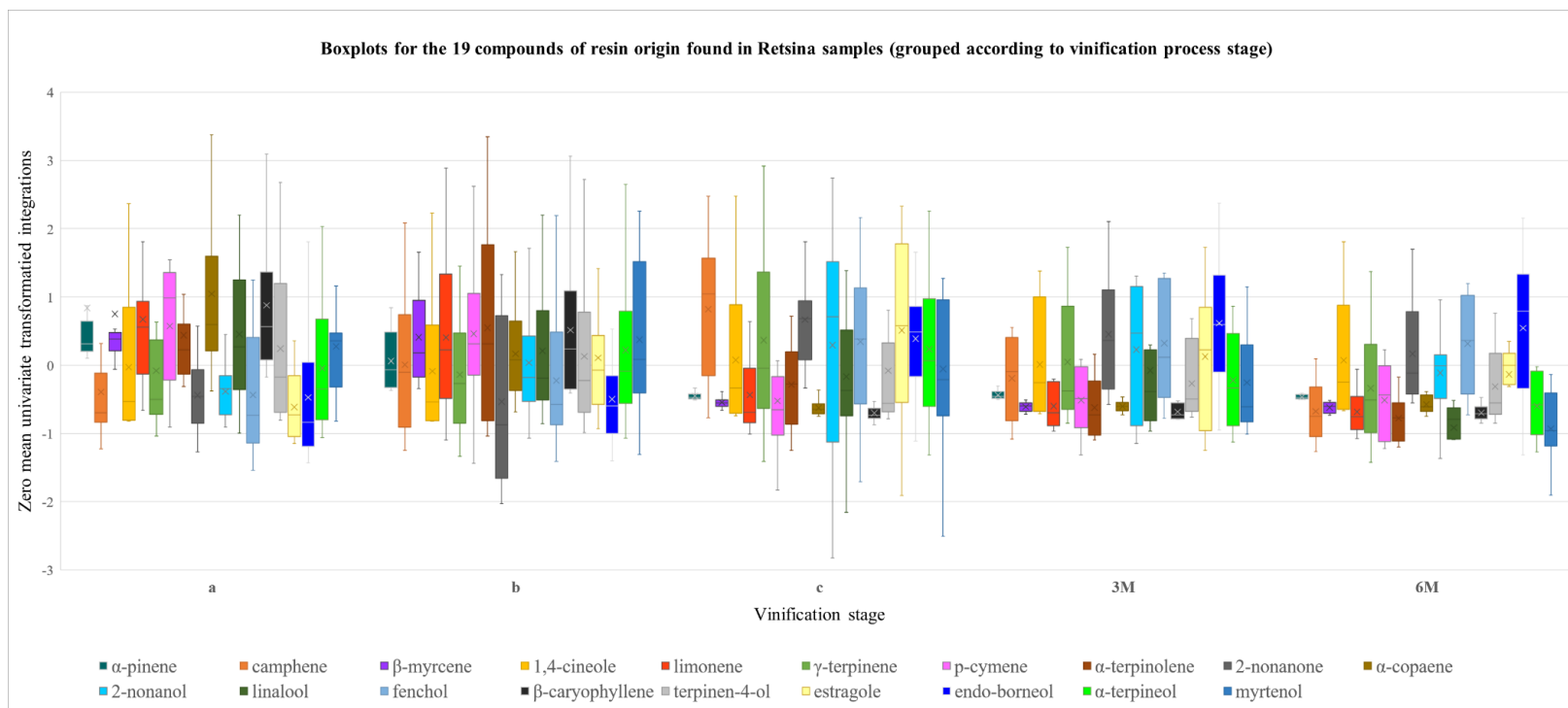


Figure S5. Boxplots for the 19 compounds of resin origin found in Retsina samples, grouped according to vinification process stage: i) intermediate point of fermentation (a), ii) end of fermentation (b), iii) end of maturation (c), iv) three months of aging (3M) and v) six months of aging (6M). A zero-mean univariate transformation has been applied to fit data of different magnitude in a unified chart. In each boxplot, the five whiskers correspond to Q_0 , Q_1 , Q_2 , Q_3 and Q_4 quartiles. The mean value is depicted with an “x” mark. For convenience of presentation, outliers are not shown here

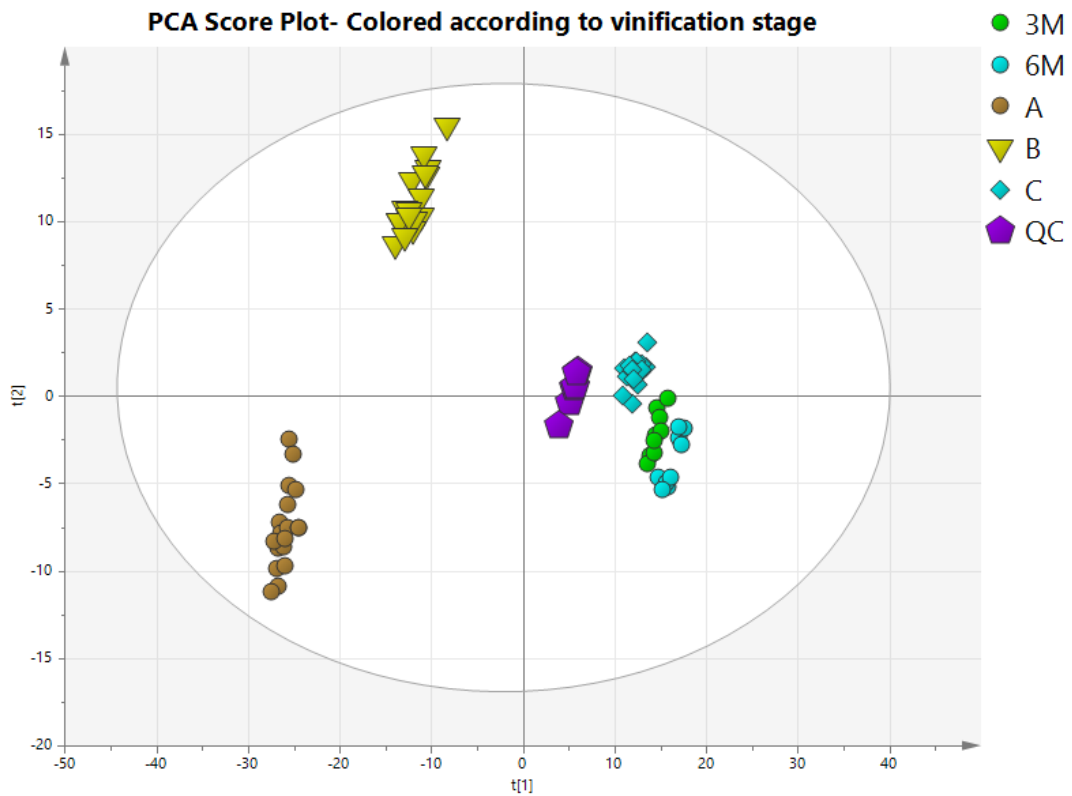


Figure S6. PCA score scatter plot of two first principal components for all Retsina samples (studied by LC-MS), colored according to vinification stage: i) intermediate point of fermentation (A), ii) end of fermentation (B), iii) end of maturation (C), iv) three months of aging (3M) and v) six months of aging (6M)

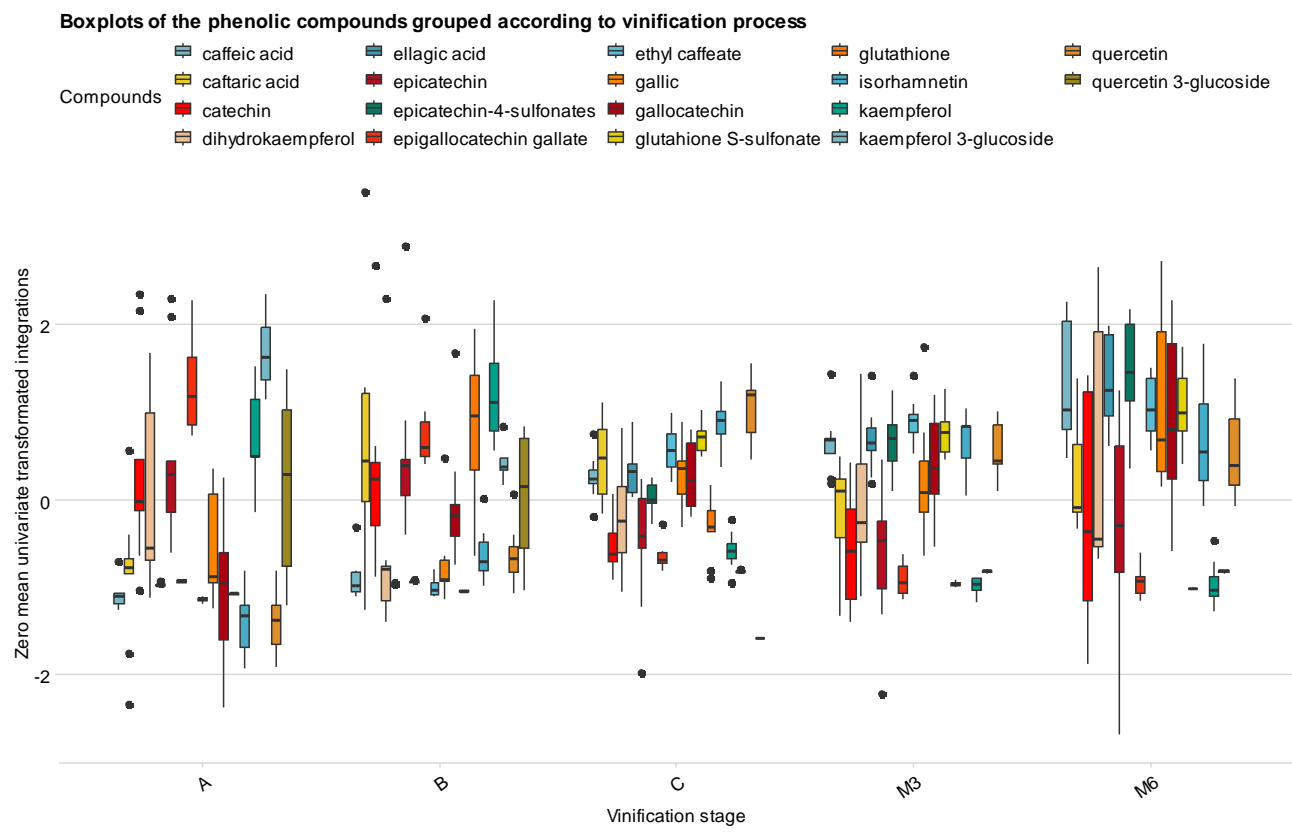
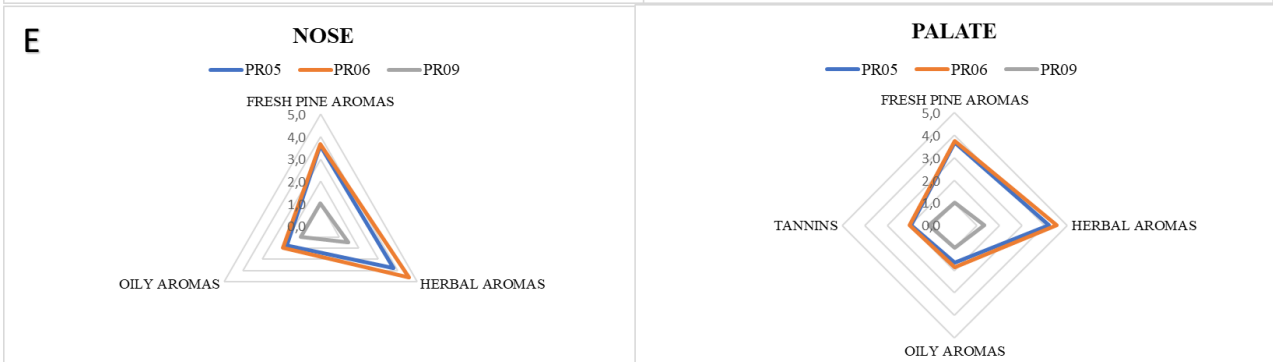
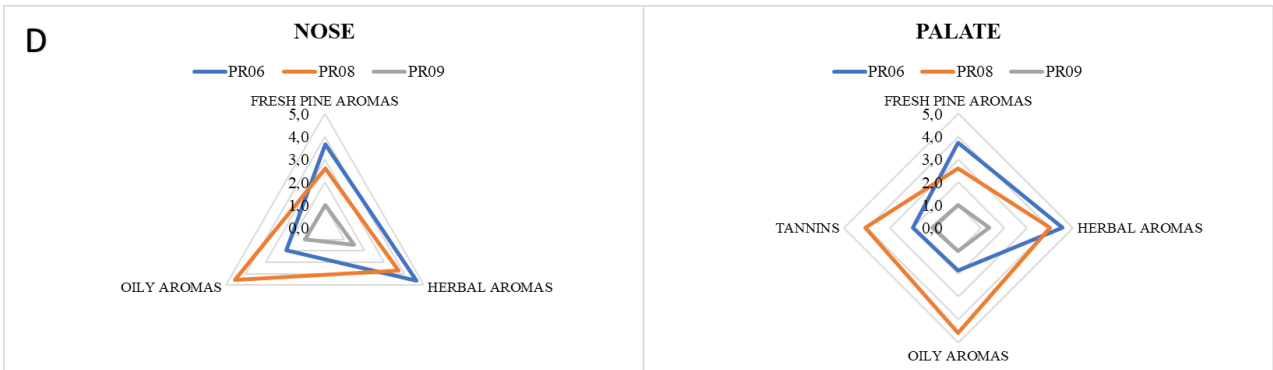
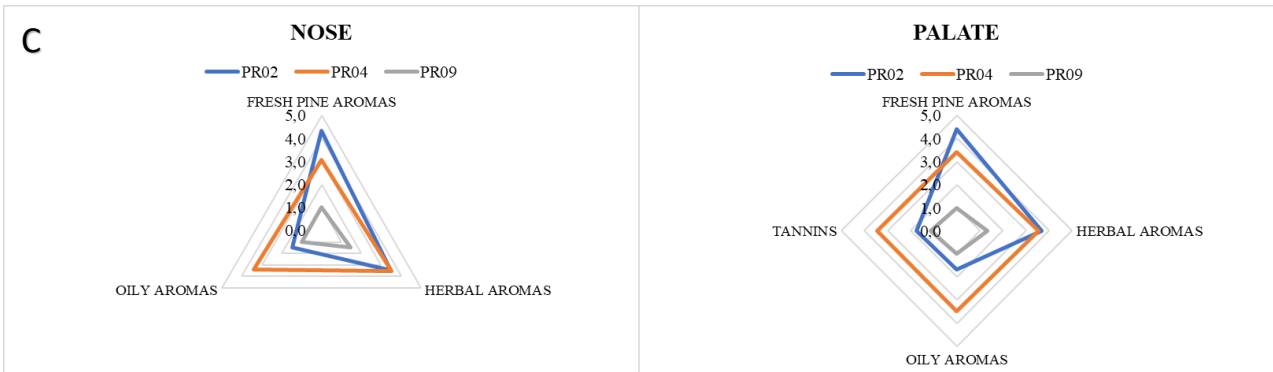
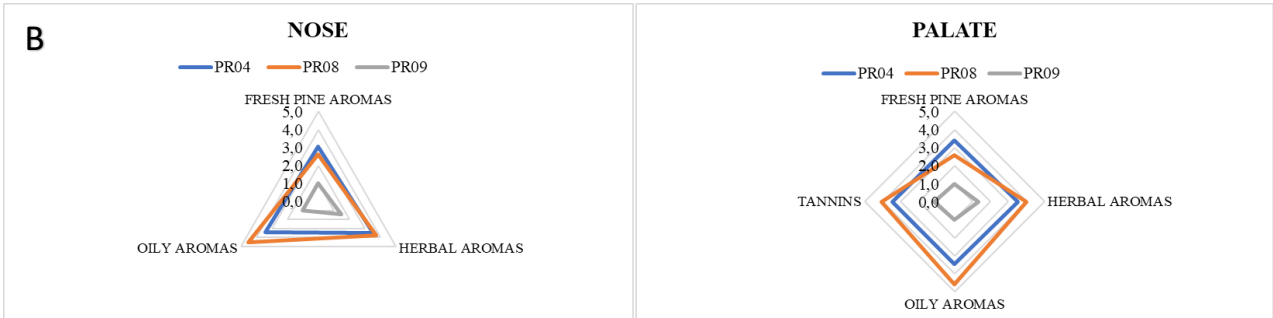
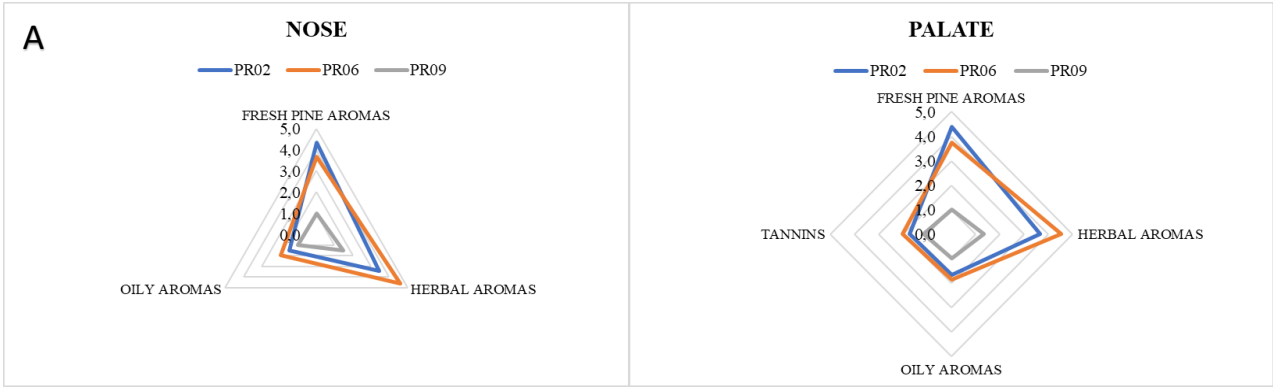


Figure S7. Boxplots of detected polyphenols grouped according to vinification process stage: i) intermediate point of fermentation (a), ii) end of fermentation (b), iii) end of maturation (c), iv) three months of aging (3M) and v) six months of aging (6M). A zero-mean univariate transformation has been applied to fit data of different magnitude in a unified chart



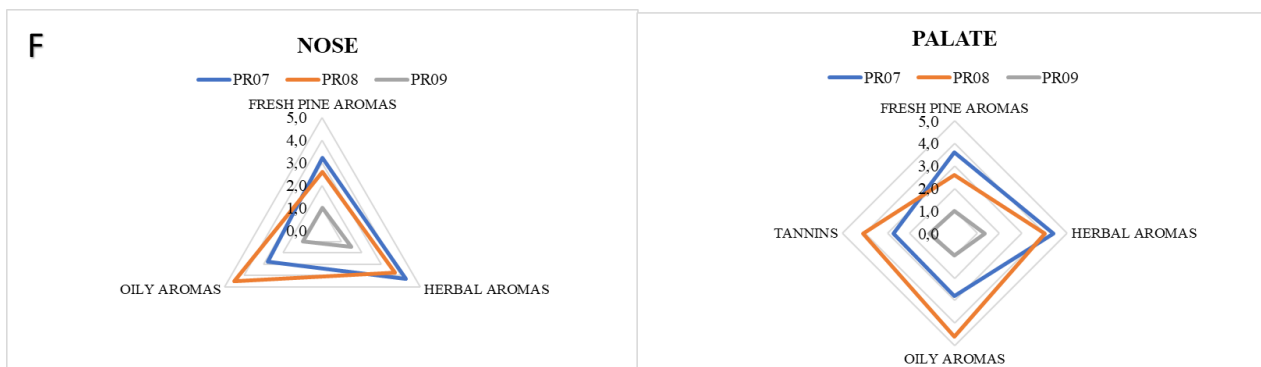


Figure S8. Organoleptic differences in nose and palate between: i) resins from different pine forests (microclimate A *vs* B) and harvested (A) naturally (PR02 *vs* PR06), or (B) conventionally (PR04 *vs* PR08), both for long extraction time in the must, ii) resins obtained through different methods (harvested naturally *vs* conventionally) from (C) pine forest A (PR02 *vs* PR04), and from (D) pine forest B (PR06 *vs* PR08), both for long extraction time in the must, and iii) different extraction times (short *vs* long) for resins harvested from pine forest B (E) naturally (PR05 *vs* PR06), or (F) conventionally (PR07 *vs* PR08)