

# Characterization of Essential Oils from Seven *Salvia* taxa from Greece with Chemometric Analysis

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**Table S1.** Chemical compound contribution to each PCA component.

RI <sub>L</sub>	RI <sub>C</sub>	Compound	Component 1	Component 2	Component 3
921	920	tricyclene	0.990	0.074	0.029
924	923	$\alpha$ -thujene	-0.187	0.949	0.177
932	930	$\alpha$ -pinene	0.868	-0.070	0.413
946	945	camphene	0.926	-0.104	0.299
969	968	sabinene	-0.386	0.105	0.659
974	972	$\beta$ -pinene	0.739	-0.229	0.523
979	980	3-octanone	0.677	0.720	0.101
988	987	myrcene	0.200	0.507	-0.544
1002	1003	$\alpha$ -phellandrene	-0.038	0.974	0.122
1008	1007	$\delta$ -3-carene	0.031	0.925	0.126
1014	1013	$\alpha$ -terpinene	0.939	0.238	-0.007
1020	1023	p-cymene	0.386	0.278	0.218
1024	1025	limonene	-0.189	-0.232	-0.828
1025	1027	$\beta$ -phellandrene	-0.321	0.922	0.106
1026	1028	1,8-cineole	0.989	0.019	0.127
1032	1033	<i>cis</i> -ocimene	0.335	0.507	-0.413
1044	1043	<i>trans</i> -ocimene	-0.225	0.122	-0.760
1054	1053	$\gamma$ -terpinene	0.936	0.203	0.213
1065	1062	<i>cis</i> -sabinene hydrate	0.889	0.053	0.012
1067	1068	<i>cis</i> -linalool oxide	0.990	0.074	0.029
1086	1087	terpinolene	0.555	-0.072	-0.617
1095	1096	linalool	-0.191	-0.233	-0.825
1098	1099	<i>trans</i> -sabinene hydrate	0.990	0.074	0.029
1100	1101	nonanal	-0.357	0.895	-0.033
1101	1103	<i>cis</i> -thujone	0.975	0.033	0.118
1102	1105	isopentyl isovalerate	-0.317	-0.147	0.116
1112	1111	<i>trans</i> -thujone	0.910	0.060	0.086
1122	1120	$\alpha$ -campholenal	0.274	-0.469	0.743
1128	1126	<i>allo</i> -ocimene	0.705	0.082	0.051
1135	1131	<i>trans</i> -pinocarveol	0.270	-0.346	0.616
1140	1137	<i>trans</i> -verbenol	-0.207	-0.444	0.667
1141	1140	camphor	0.875	0.042	0.022
1145	1143	camphene hydrate	0.953	0.086	0.042
1149	1147	<i>neo</i> -3-thujanol	0.705	0.082	0.051
1155	1153	isoborneol	0.990	0.074	0.029
1158	1156	<i>trans</i> -pinocamphone	0.953	0.086	0.042

1160	1159	pinocarvone	-0.351	-0.497	0.696
1165	1163	borneol	0.954	0.034	0.062
1165	1166	nonanol	-0.321	0.922	0.106
1172	1170	<i>cis</i> -pinocamphone	0.638	-0.114	-0.623
1174	1172	terpinen-4-ol	0.895	0.210	-0.043
1179	1178	p-cymen-8-ol	0.990	0.074	0.029
1186	1183	$\alpha$ -terpineol	-0.147	-0.232	-0.829
1194	1191	myrtenol	0.853	-0.128	0.363
1195	1194	myrtenal	-0.012	-0.457	0.720
1201	1203	n-decanal	-0.321	0.922	0.106
1207	1205	<i>trans</i> -piperitol	0.990	0.074	0.029
1215	1216	<i>trans</i> -carveol	0.990	0.074	0.029
1226	1223	<i>cis</i> -carveol	0.573	0.014	-0.013
1227	1225	nerol	-0.189	-0.232	-0.828
1228	1230	bornyl formate	-0.207	-0.444	0.667
1254	1253	linalool acetate	-0.189	-0.233	-0.828
1266	1268	n-decanol	-0.321	0.922	0.106
1283	1279	iso-bornyl acetate	-0.207	-0.444	0.667
1284	1285	bornyl acetate	0.973	0.057	0.050
1289	1290	thymol	0.705	0.082	0.051
1289	1293	<i>trans</i> -sabinyol acetate	0.677	0.720	0.101
1295	1294	3-thujanol acetate	0.573	0.014	-0.013
1298	1296	carvacrol	0.953	0.086	0.042
1324	1320	myrtenyl acetate	0.953	0.086	0.042
1335	1332	$\delta$ -elemene	-0.207	-0.444	0.667
1339	1335	<i>trans</i> -carvyl acetate	0.705	0.082	0.051
1348	1350	$\alpha$ -cubebene	-0.474	0.686	0.172
1356	1353	eugenol	0.195	0.724	0.072
1359	1360	neryl acetate	-0.189	-0.232	-0.828
1373	1370	$\alpha$ -ylangene	0.031	0.925	0.126
1374	1373	isolekene	0.573	0.014	-0.013
1374	1375	$\alpha$ -copaene	-0.476	-0.401	0.430
1379	1378	geranyl acetate	-0.189	-0.232	-0.828
1387	1386	$\beta$ -bourbonene	-0.377	-0.121	0.149
1387	1388	$\beta$ -cubebene	-0.389	-0.136	0.030
1389	1390	$\beta$ -elemene	-0.520	-0.394	0.302
1408	1406	(Z)-caryophyllene	0.306	0.932	0.120
1409	1410	$\alpha$ -gurjunene	0.573	0.014	-0.013
1417	1415	(E)-caryophyllene	-0.417	0.491	0.234
1419	1417	$\beta$ -ylangene	0.573	0.014	-0.013

1430	1428	$\beta$ -copaene	-0.403	0.901	0.090
1431	1430	$\beta$ -gurjunene	0.195	0.724	0.072
1434	1430	$\gamma$ -elemene	-0.207	-0.444	0.667
1439	1438	aromadendrene	0.195	0.724	0.072
1442	1440	6,9-guaiadiene	-0.207	-0.444	0.667
1452	1449	$\alpha$ -humulene	-0.245	0.812	0.206
1453	1453	geranylacetone	-0.207	-0.444	0.667
1454	1455	<i>trans</i> - $\beta$ -farnesene	-0.355	0.870	0.204
1458	1459	<i>allo</i> -aromadendrene	-0.207	-0.193	-0.098
1465	1460	<i>cis</i> -muurola-4(14),5-diene	-0.321	0.922	0.106
1478	1475	$\gamma$ -muurolene	-0.213	-0.192	-0.096
1480	1481	germacrene D	-0.707	-0.193	-0.067
1483	1482	$\alpha$ -amorphene	0.705	0.082	0.051
1487	1484	<i>trans</i> - $\beta$ -ionone	-0.321	0.922	0.106
1489	1486	$\beta$ -selinene	0.770	-0.096	-0.559
1493	1490	<i>trans</i> -muurola-4(14),5-diene	-0.321	0.922	0.106
1496	1497	viridiflorene	0.415	-0.380	0.658
1500	1499	bicyclogermacrene	-0.293	0.024	-0.074
1500	1501	$\alpha$ -muurolene	-0.453	0.772	-0.287
1505	1503	( <i>E,E</i> )- $\alpha$ -farnesene	-0.269	-0.521	0.391
1508	1506	germacrene A	-0.436	-0.456	0.493
1513	1510	$\gamma$ -cadinene	-0.420	0.809	0.168
1521	1520	<i>trans</i> -calamenene	0.031	0.925	0.126
1522	1523	$\delta$ -cadinene	-0.636	-0.334	0.690
1533	1530	10- <i>epi</i> -cubebol	0.031	0.925	0.126
1533	1532	<i>trans</i> -cadina-1,4-diene	-0.321	0.922	0.106
1537	1535	$\alpha$ -cadinene	0.031	0.925	0.126
1544	1540	$\alpha$ -calacorene	-0.243	-0.279	0.738
1548	1546	elemol	-0.189	-0.232	-0.828
1557	1550	1,5-epoxysalvial-4(14)-ene	-0.189	-0.232	-0.828
1559	1556	germacrene B	-0.207	-0.444	0.667
1561	1558	( <i>E</i> )-nerolidol	-0.321	0.922	0.106
1564	1566	$\beta$ -calacorene	-0.352	0.016	0.691
1574	1572	germacrene D-4-ol	-0.317	-0.147	0.116
1577	1575	spathulenol	-0.307	-0.073	-0.110
1582	1580	caryophyllene oxide	-0.522	-0.272	0.331

1590	1587	$\beta$ -copaen-4- $\alpha$ -ol	-0.207	-0.444	0.667
1592	1590	viridiflorol	0.867	-0.168	0.401
1594	1593	salvial-4(14)-en-1-one	-0.284	-0.163	-0.111
1602	1595	ledol	0.990	0.074	0.029
1608	1605	humulene epoxide II	-0.332	0.532	0.644
1627	1625	1- <i>epi</i> -cubenol	-0.459	0.302	0.162
1639	1636	caryophylla-4(12), 8(13)-dien-5 $\alpha$ -ol/or caryophylla-4(12), 8(13)-dien-5 $\beta$ -ol	-0.201	0.753	0.523
1640	1641	<i>epi</i> - $\alpha$ -muurolol	-0.206	0.949	0.116
1644	1645	$\alpha$ -muurolol	-0.317	-0.147	0.116
1649	1647	$\beta$ -eudesmol	-0.158	-0.233	-0.835
1652	1650	$\alpha$ -cadinol	-0.133	-0.234	-0.839
1652	1651	$\alpha$ -eudesmol	-0.482	0.737	-0.242
1660	1655	<i>cis</i> -calamenen-10-ol	-0.207	-0.444	0.667
1666	1662	14-hydroxy-( <i>Z</i> )- caryophyllene	0.031	0.925	0.126
1668	1666	<i>trans</i> -calamenen-10- ol	-0.207	-0.444	0.667
1691	1690	vulgarol B	-0.317	-0.147	0.116
1711	1715	valerenol	-0.382	-0.197	0.093
1826	1820	8,13-epoxy-15,16- dinorlab-12-ene	-0.223	-0.250	-0.826
1886	1882	(5 <i>E</i> ,9 <i>Z</i> )- farnesylacetone	-0.317	-0.147	0.116
1913	1911	(5 <i>E</i> ,9 <i>E</i> )- farnesylacetone	-0.321	0.922	0.106
1942	1948	phytol	-0.321	0.922	0.106
1987	1985	manool oxide	-0.189	-0.232	-0.828
2009	2006	13- <i>epi</i> -manool oxide	-0.289	-0.538	0.243
2056	2052	manool	0.822	-0.084	0.108
2149	2150	abienol	-0.189	-0.232	-0.828
2222	2218	sclareol	-0.189	-0.232	-0.828

RI<sub>c</sub> = calculated retention indices using an n-alkane standard solution C9–C24 in HP-5 MS column; RI<sub>L</sub> = literature retention indices.

**Table S2.** Clustered heat map of chemical compounds.

Compound	<i>Svert</i>	<i>Soff</i>	<i>Stom</i>	<i>Sath</i>	<i>Sarg</i>	<i>Sscl</i>	<i>Sampl</i>
( <i>E</i> )-caryophyllene	27.1	9.1	5.3	34.6	4.7	1.9	7.8
germacrene D	9.3	0.05	0	17.3	8	8.8	28.6

1,8-cineole	0	14.7	18.2	0.8	2.7	0	0
caryophyllene oxide	3.9	0.6	0.6	4.3	8.6	0.6	15
<i>cis</i> -thujone	0	11.1	17.9	0.1	2.2	0	0
$\alpha$ -humulene	14.6	5.8	1	8.6	0.9	0.1	0.05
linalool acetate	0	0	0	0.05	0	30.3	0
$\alpha$ -copaene	0.5	0.05	0.1	14.6	8.3	0.9	1.9
$\alpha$ -pinene	1.1	7	9.2	0.2	5.7	0.1	0
viridiflorol	0	7.2	8.5	0	5.7	0	0
linalool	0.05	0	0	0	0.1	19.9	0
spathulenol	2.2	0.05	0.05	0	0.2	0.6	14.6
borneol	0	9.4	6.7	0.05	0.7	0.05	0
$\delta$ -cadinene	2.1	0.05	0.3	4	6	0.3	3.3
$\beta$ -pinene	0.3	4.7	4.9	0.2	5	0.1	0
manool	0	8.5	3.5	0	2.1	0.7	0
salvial-4(14)-en-1-one	0.6	0	0	0.5	0	0.3	12
camphor	0	7.8	3.7	0.2	0.1	0	0
$\beta$ -phellandrene	10.3	0	0	0	0	0	0
germacrene B	0	0	0	0	8.9	0	0
$\alpha$ -terpineol	0.05	0.2	0.4	0.05	0.1	7.8	0
camphene	0.05	3.4	3.2	0.1	1.7	0.05	0
sclareol	0	0	0	0	0	7.1	0
$\beta$ -cubebene	0.4	0	0	5	0.4	0.2	0
$\beta$ -bourbonene	0.6	0	0.05	0.6	0.5	0	3.7
<i>trans</i> -thujone	0	1.4	3.7	0.1	0.2	0	0
myrcene	1.3	0.7	1	0.1	0.3	1.5	0
bornyl acetate	0	2	2.2	0.4	0	0	0
geranyl acetate	0	0	0	0	0	4.5	0
$\gamma$ -muurolene	0	0	0.2	0	0	0	4.2
humulene epoxide II	1.7	0.5	0.2	0.6	1.3	0	0
$\alpha$ -muurolene	0.7	0.05	0.1	0	0	0	3
iso-bornyl acetate	0	0	0	0	3.7	0	0
<i>allo</i> -aromadendrene	0	0.1	0.1	0	0	0	3.2
<i>cis</i> -ocimene	0.8	0.1	1.1	0	0	0.8	0
<i>trans</i> -ocimene	0.6	0.05	0.2	0	0.1	1.5	0
neryl acetate	0	0	0	0	0	2.4	0
p-cymene	0.4	0.05	1.1	0.7	0.1	0	0
$\beta$ -elemene	0.1	0	0	1.2	0.7	0.3	0.05
bicyclogermacrene	1.4	0	0	0.2	0	0.7	0
$\gamma$ -cadinene	1.2	0.05	0.1	0.7	0	0	0.05
$\gamma$ -terpinene	0.2	0.5	0.7	0.05	0.2	0.05	0
sabinene	0.5	0.05	0	0.05	0.8	0.05	0

terpinolene	0.1	0.4	0.3	0	0.1	0.5	0
nerol	0	0	0	0	0	1.3	0
$\beta$ -copaene	1	0	0	0.2	0	0.05	0
$\alpha$ -cubebene	0.6	0	0.05	0.5	0	0	0.05
$\gamma$ -elemene	0	0	0	0	1.2	0	0
8,13-epoxy-15,16-dinorlab-12-ene	0	0	0	0.1	0	1	0
$\alpha$ -terpinene	0.1	0.3	0.5	0.05	0	0.05	0
6,9-guaiadiene	0	0	0	0	1	0	0
$\alpha$ -thujene	0.7	0.1	0.1	0.05	0.05	0	0
$\alpha$ -phellandrene	0.7	0.1	0.2	0	0	0	0
$\beta$ -eudesmol	0	0.05	0	0	0	0.9	0
germacrene A	0	0	0	0.5	0.4	0.05	0
terpinen-4-ol	0.1	0.2	0.4	0.05	0.05	0.1	0
caryophylla-4(12), 8(13)-dien-5 $\alpha$ -ol/ or caryophylla-4(12), 8(13)-dien-5 $\beta$ -ol	0.4	0.1	0.1	0.1	0.2	0	0
$\alpha$ -cadinol	0.4	0	0.05	0.2	0	0.2	0
( <i>E,E</i> )- $\alpha$ -farnesene	0	0	0	0	0.6	0.2	0
<i>trans</i> - $\beta$ -farnesene	0.7	0	0	0	0.1	0	0
$\alpha$ -calacorene	0.1	0	0.05	0.05	0	0	0
<i>epi</i> - $\alpha$ -muurolol	0.6	0	0.1	0	0	0	0
14-hydroxy-( <i>Z</i> )- caryophyllene	0.4	0	0.2	0	0	0	0
$\alpha$ -eudesmol	0	0.05	0	0	0	0.5	0
limonene	0	0	0	0	0	0.4	0
bornyl formate	0	0	0	0	0.4	0	0
viridiflorene	0	0.1	0.1	0	0.2	0	0
isopentyl isovalerate	0	0	0	0.4	0	0	0
tricyclene	0	0.2	0.2	0	0	0	0
aromadendrene	0.2	0.2	0	0	0	0	0
<i>cis</i> -muurola-4(14),5- diene	0.4	0	0	0	0	0	0
<i>trans</i> - $\beta$ -ionone	0.4	0	0	0	0	0	0
nonanal	0.3	0	0	0	0	0.05	0
$\beta$ -calacorene	0.1	0	0	0	0.2	0	0
1- <i>epi</i> -cubenol	0.1	0	0	0.2	0	0	0
<i>trans</i> -pinocamphone	0	0.1	0.2	0	0	0	0
$\alpha$ -ylangene	0.2	0	0.1	0	0	0	0
<i>trans</i> -calamenene	0.2	0	0.1	0	0	0	0
$\beta$ -copaen-4- $\alpha$ -ol	0	0	0	0	0.3	0	0

<i>cis</i> -calamenen-10-ol	0	0	0	0	0.3	0	0
<i>trans</i> -calamenen-10-ol	0	0	0	0	0.3	0	0
germacrene D-4-ol	0	0	0	0.3	0	0	0
valerenol	0	0	0	0.2	0	0	0.05
<i>cis</i> -pinocamphone	0	0.05	0.1	0	0	0.1	0
<i>trans</i> -pinocarveol	0	0	0.1	0.05	0.1	0	0
$\alpha$ -campholenal	0	0.05	0.05	0.05	0.1	0	0
manool oxide	0	0	0	0	0	0.2	0
geranylacetone	0	0	0	0	0.2	0	0
myrtenal	0	0	0.05	0.05	0.1	0	0
myrtenol	0	0.05	0.1	0	0.05	0	0
$\alpha$ -muurolol	0	0	0	0.2	0	0	0
ledol	0	0.1	0.1	0	0	0	0
( <i>Z</i> )-caryophyllene	0.1	0.05	0.05	0	0	0	0
<i>trans</i> -muurola-4(14),5-diene	0.2	0	0	0	0	0	0
( <i>E</i> )-nerolidol	0.2	0	0	0	0	0	0
phytol	0.2	0	0	0	0	0	0
13- <i>epi</i> -manool oxide	0	0	0	0	0.1	0.05	0
$\beta$ -selinene	0	0.05	0.05	0	0	0.05	0
pinocarvone	0	0	0	0.05	0.1	0	0
camphene hydrate	0	0.05	0.1	0	0	0	0
carvacrol	0	0.05	0.1	0	0	0	0
myrtenyl acetate	0	0.05	0.1	0	0	0	0
<i>cis</i> -sabinene hydrate	0	0.1	0.05	0	0	0	0
3-octanone	0.05	0.05	0.05	0	0	0	0
thymol	0.05	0.05	0.05	0	0	0	0
$\delta$ -3-carene	0.1	0	0.05	0	0	0	0
<i>trans</i> -cadina-1,4-diene	0.1	0	0.05	0	0	0	0
$\alpha$ -cadinene	0.1	0	0.05	0	0	0	0
1,5-epoxysalvial-4(14)-ene	0	0	0	0	0	0.1	0
$\delta$ -elemene	0	0	0	0	0.1	0	0
vulgarol B	0	0	0	0.1	0	0	0
(5 <i>E</i> ,9 <i>Z</i> )-farnesylacetone	0	0	0	0.1	0	0	0
<i>trans</i> -sabinyol acetate	0	0	0.1	0	0	0	0
<i>cis</i> -linalool oxide	0	0.05	0.05	0	0	0	0
<i>trans</i> -sabinene hydrate	0	0.05	0.05	0	0	0	0



isoborneol	0	0.05	0.05	0	0	0	0
p-cymen-8-ol	0	0.05	0.05	0	0	0	0
<i>trans</i> -piperitol	0	0.05	0.05	0	0	0	0
<i>trans</i> -carveol	0	0.05	0.05	0	0	0	0
eugenol	0.05	0.05	0	0	0	0	0
$\beta$ -gurjunene	0.05	0.05	0	0	0	0	0
decanal	0.1	0	0	0	0	0	0
(5 <i>E</i> ,9 <i>E</i> )- farnesylacetone	0.1	0	0	0	0	0	0
elemol	0	0	0	0	0	0.05	0
abienol	0	0	0	0	0	0.05	0
<i>trans</i> -verbenol	0	0	0	0	0.05	0	0
<i>allo</i> -ocimene	0	0	0.05	0	0	0	0
<i>neo</i> -3-thujanol	0	0	0.05	0	0	0	0
<i>trans</i> -carvyl acetate	0	0	0.05	0	0	0	0
$\alpha$ -amorphene	0	0	0.05	0	0	0	0
<i>cis</i> -carveol	0	0.05	0	0	0	0	0
3-thujanol acetate	0	0.05	0	0	0	0	0
isolekene	0	0.05	0	0	0	0	0
$\alpha$ -gurjunene	0	0.05	0	0	0	0	0
$\beta$ -ylangene	0	0.05	0	0	0	0	0
nonanol	0.05	0	0	0	0	0	0
decanol	0.05	0	0	0	0	0	0
10- <i>epi</i> -cubebol	0.05	0	0	0	0	0	0

Sath: *S. aethiopis*, Sampl: *S. amplexicaulis*, Sarg: *S. argentea*, Svert: *S. verticillata* subsp. *verticillata*,  
Soff: *S. officinalis* subsp. *officinalis*, Sscl: *S. sclarea*, Stom: *S. tomentosa*