Table S1. Chemical composition of the six commercial essential oils (EOs) determined by GC–MS (relative peak area, %). Within each EO, compounds with an assigned retention index are listed in order of increasing RI, followed by compounds identified from mass spectra only.

No.	Compound	RI calc.[a]	RI lit.[b]	Peak area (%)	Identification[c]
Geranium (*Pelargonium graveolens*)					
1	α-Pinene	929	932	0.03	MS + RI
2	β-Pinene	975	974	0.34	MS + RI
3	β-Myrcene	986	988	0.39	MS + RI
4	α-Phellandrene	1006	1002	0.97	MS + RI
5	p-Cymene	1021	1020	0.37	MS + RI
6	Limonene	1027	1024	0.38	MS + RI
7	cis-Linalool oxide (furanoid)	1068	1065	0.12	MS + RI
8	Linalool	1100	1098	3.20	MS + RI
9	trans-Rose oxide	1122	1120	0.58	MS + RI
10	cis-Rose oxide	1127	1128	1.80	MS + RI
11	Menthone	1147	1152	3.30	MS + RI
12	Isomenthone	1156	1152	2.20	MS + RI
13	Menthol	1167	1165	0.51	MS + RI
14	α-Terpineol	1185	1189	0.85	MS + RI
15	Citronellol	1217	1225	37.50	MS + RI
16	Geraniol	1248	1255	6.20	MS + RI
17	Citronellyl formate	1268	1270	0.52	MS + RI
18	Geranyl formate	1303	1300	2.10	MS + RI
19	α-Cubebene	1347	1345	0.01	MS + RI
20	Citronellyl acetate	1356	1351	1.10	MS + RI
21	Geranyl acetate	1379	1380	0.87	MS + RI
22	β-Elemene	1387	1385	0.33	MS + RI
23	β-Cubebene	1387	1385	0.37	MS + RI
24	β-Bourbonene	1389	1387	2.60	MS + RI
25	β-Caryophyllene	1412	1418	0.59	MS + RI
26	γ-Elemene	1418	1420	0.54	MS + RI
27	Citronellyl pentanoate	1420	1420	0.89	MS + RI
28	Elemene isomer *	1424	1420	0.97	MS + RI (tentative)
29	α-Guaiene	1427	1437	0.09	MS + RI
30	Guaia-6,9-diene	1432	1435	0.68	MS + RI
31	Citronellyl propionate	1437	1437	1.50	MS + RI
32	trans-Calamenene	1449	1450	1.30	MS + RI
33	α-Humulene	1450	1450	0.09	MS + RI
34	Geranyl propionate	1454	1450	0.51	MS + RI
35	β-Selinene	1477	1480	0.64	MS + RI
36	γ-Muurolene	1489	1485	0.62	MS + RI
37	Viridiflorene	1489	1485	0.23	MS + RI
38	α-Muurolene	1492	1490	0.85	MS + RI
39	Germacrene D	1493	1480	0.53	MS + RI
40	γ-Cadinene	1511	1510	0.90	MS + RI
41	Citronellyl butanoate	1512	1515	1.40	MS + RI
42	δ-Cadinene	1521	1522	0.89	MS + RI
43	Germacrene B	1552	1550	0.78	MS + RI

No.	Compound	RI calc.[a]	RI lit.[b]	Peak area (%)	Identification[c]
44	Spathulenol	1572	1570	0.61	MS + RI
45	Caryophyllene oxide	1586	1585	3.70	MS + RI
46	2-Phenylethyl tiglate	1593	1587	1.70	MS + RI
47	epi-γ-Eudesmol	1612	1610	0.17	MS + RI
48	γ-Eudesmol	1622	1620	0.32	MS + RI
49	Citronellyl tiglate	1633	1632	1.00	MS + RI
50	Geranyl tiglate	1660	1661	1.80	MS + RI
	Unidentified compounds (sum)			10.06	
	Total identified: 89.94% | Total: 100.00%				
Patchouli (*Pogostemon cablin*)					
1	Eremophilene	1320	1322	1.30	MS + RI
2	β-Patchoulene	1380	1379	4.50	MS + RI
3	α-Cedrene	1419	1410	1.20	MS + RI
4	β-Caryophyllene	1431	1418	7.90	MS + RI
5	α-Guaiene	1434	1437	18.60	MS + RI
6	Seychellene	1444	1444	5.70	MS + RI
7	δ-Guaiene (α-bulnesene)	1508	1509	18.80	MS + RI
8	Guaiene isomer *	1509	1510	8.70	MS + RI (tentative)
9	Globulol	1576	1575	1.80	MS + RI
10	Viridiflorol	1611	1612	4.30	MS + RI
11	Patchoulol	1661	1654	22.70	MS + RI
12	2,3,3-Trimethyl-2-(3-methylbutyl)cyclohexanone *	1702	–	1.10	MS only (tentative)
	Unidentified compounds (sum)			3.40	
	Total identified: 96.60% | Total: 100.00%				
Pine (*Pinus sylvestris*)					
1	α-Pinene	930	932	39.20	MS + RI
2	Camphene	950	946	6.80	MS + RI
3	β-Pinene	984	974	12.60	MS + RI
4	α-Terpineol	1190	1189	8.10	MS + RI
5	Citronellol	1217	1225	1.10	MS + RI
6	Bornyl acetate	1278	1285	4.30	MS + RI
7	β-Caryophyllene	1430	1418	2.60	MS + RI
8	Germacrene D	1483	1480	6.20	MS + RI
9	β-Phellandrene *	–	–	11.60	MS only (tentative)
	Unidentified compounds (sum)			7.50	
	Total identified: 92.50% | Total: 100.00%				
Spruce (*Picea abies*)					
1	Tricyclene	918	921	0.03	MS + RI
2	α-Pinene	930	932	17.50	MS + RI
3	Camphene	950	946	6.50	MS + RI
4	Sabinene	968	969	0.01	MS + RI
5	β-Pinene	984	974	10.10	MS + RI
6	β-Myrcene	990	988	15.20	MS + RI
7	α-Phellandrene	1004	1002	0.04	MS + RI
8	δ-3-Carene	1012	1008	0.03	MS + RI
9	α-Terpinene	1012	1014	0.02	MS + RI

No.	Compound	RI calc.[a]	RI lit.[b]	Peak area (%)	Identification[c]
10	p-Cymene	1022	1020	0.05	MS + RI
11	Limonene	1023	1024	6.20	MS + RI
12	β-Phellandrene	1023	1025	0.05	MS + RI
13	1,8-Cineole (eucalyptol)	1026	1031	0.01	MS + RI
14	γ-Terpinene	1055	1059	0.01	MS + RI
15	Terpinolene	1086	1083	0.01	MS + RI
16	Linalool	1097	1098	0.03	MS + RI
17	Borneol	1160	1165	0.01	MS + RI
18	Bornyl acetate	1278	1285	10.10	MS + RI
19	δ-Cadinene	1522	1522	9.20	MS + RI
20	γ-Muurolene *	–	–	1.20	MS only (tentative)
21	α-Cadinol *	–	–	11.30	MS only (tentative)
22	τ-Muurolol *	–	–	3.10	MS only (tentative)
23	13-Epimanool *	–	–	7.80	MS only (tentative)
24	ent-Kaurenal *	–	–	1.50	MS only (tentative)
	Total identified: 100.00% | Total: 100.00%				
Coriander (*Coriandrum sativum*)					
1	α-Pinene	930	932	1.09	MS + RI
2	Camphene	950	946	0.13	MS + RI
3	β-Pinene	984	974	0.96	MS + RI
4	β-Myrcene	990	988	0.25	MS + RI
5	Limonene	1023	1024	1.33	MS + RI
6	γ-Terpinene	1055	1059	1.22	MS + RI
7	Linalool	1100	1098	73.92	MS + RI
8	Camphor	1135	1143	2.55	MS + RI
9	Borneol	1156	1165	0.81	MS + RI
10	Terpinen-4-ol	1173	1177	0.24	MS + RI
11	α-Terpineol	1190	1189	0.42	MS + RI
12	Geraniol	1248	1255	1.62	MS + RI
13	Geranyl acetate	1380	1380	4.44	MS + RI
14	β-Phellandrene *	–	–	0.12	MS only (tentative)
15	o-Cymene *	–	–	2.39	MS only (tentative)
16	α-Methyl-α-(4-methyl-3-pentenyl)oxiranemethanol *	–	–	0.48	MS only (tentative)
17	cis-Linalool oxide *	–	–	0.52	MS only (tentative)
18	Nonanal *	–	–	0.10	MS only (tentative)
19	2,6-Dimethyl-1,7-octadien-3-ol *	–	–	0.11	MS only (tentative)
20	Decanal *	–	–	0.32	MS only (tentative)
21	3,7-Dimethyl-2-octen-1-ol *	–	–	0.24	MS only (tentative)
22	2-Methyl-3-phenylpropanal *	–	–	1.67	MS only (tentative)
23	(R)-(−)-Carvone *	–	–	1.63	MS only (tentative)
24	(Z)-2-Decenal *	–	–	0.37	MS only (tentative)
25	(E)-2-Decen-1-ol *	–	–	0.12	MS only (tentative)
26	1-Decanol *	–	–	0.16	MS only (tentative)
27	2-Decanol *	–	–	0.17	MS only (tentative)
28	3-Caren-10-al *	–	–	0.55	MS only (tentative)
29	Carvacrol *	–	–	0.13	MS only (tentative)
30	Myrtenyl acetate *	–	–	0.09	MS only (tentative)

No.	Compound	RI calc.[a]	RI lit.[b]	Peak area (%)	Identification[c]
31	2-Dodecenal *	–	–	0.25	MS only (tentative)
32	Apiole *	–	–	1.54	MS only (tentative)
	Unidentified compounds (sum)			0.06	
	Total identified: 99.94% | Total: 100.00%				
Commercial eucalyptus EO (labelled "*Eucalyptus citriodora*")					
1	α-Pinene	930	932	8.44	MS + RI
2	Camphene	950	946	0.37	MS + RI
3	β-Pinene	984	974	0.01	MS + RI
4	β-Myrcene	990	988	7.78	MS + RI
5	1,8-Cineole (eucalyptol)	1026	1031	54.29	MS + RI
6	γ-Terpinene	1055	1059	1.73	MS + RI
7	Terpinen-4-ol	1173	1177	0.04	MS + RI
8	α-Terpineol	1190	1189	0.03	MS + RI
9	Citronellol	1217	1225	0.59	MS + RI
10	β-Caryophyllene	1430	1418	1.62	MS + RI
11	β-Phellandrene *	–	–	0.02	MS only (tentative)
12	p-Cymene *	–	–	10.10	MS only (tentative)
13	Citronellal *	–	–	1.62	MS only (tentative)
14	Pinocarvone *	–	–	0.01	MS only (tentative)
15	α-Cubebene *	–	–	0.01	MS only (tentative)
16	α-Copaene *	–	–	0.01	MS only (tentative)
17	Alloaromadendrene *	–	–	0.01	MS only (tentative)
18	α-Humulene *	–	–	0.01	MS only (tentative)
19	γ-Muurolene *	–	–	0.05	MS only (tentative)
20	α-Muurolene *	–	–	0.04	MS only (tentative)
21	Isoledene *	–	–	0.01	MS only (tentative)
22	4-epi-Cubebol *	–	–	0.01	MS only (tentative)
	Unidentified compounds (sum)			13.20	
	Total identified: 86.80% | Total: 100.00%				

[a] Linear retention index calculated with the Van den Dool and Kratz equation against a homologous series of n-alkanes on a 5%-phenyl-methylpolysiloxane column. [b] Literature retention index (Babushok et al., 2011). [c] Identification criteria (no authentic standards were analysed, so no compound is regarded as positively identified): MS + RI, mass spectrum matched with the NIST mass spectral library and calculated RI in agreement with literature data (putative identification); MS + RI (tentative), RI in agreement but the mass spectrum not sufficiently specific to distinguish closely related isomers; MS only (tentative), mass spectrum match only, no RI assigned. Tentative identifications are additionally marked with an asterisk (*) after the compound name. –, not determined.

Babushok, V.I.; Linstrom, P.J.; Zenkevich, I.G. Retention Indices for Frequently Reported Compounds of Plant Essential Oils. J. Phys. Chem. Ref. Data 2011, 40, 043101.