

In Vitro and In Silico Pharmacological and Cosmeceutical Potential of Ten Essential Oils from Aromatic Medicinal Plants from the Mascarene Islands

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Table S1. Percentage yields and chemical composition of major components of the studied essential oils (EOs).

EOs	% Yield (w/w) ^a	Major EO components ^b
CAF	0.24	Limonene (84.3%), 9-octadecanoic acid (3.9%), germacrene D (2.5%), myrcene (2.3%)
CAL	0.17	Sabinene (38.1%), citronellal (13.7%), (<i>E</i>)- β -ocimene (11.6%), citronellyl acetate (5.2%), terpinen-4-ol (5.1%), γ -terpinene (4.0%), β -pinene (3.0%), myrcene (3.2%), limonene (2.6%), α -terpinene (2.3%), α -pinene (2.0%)
CC	0.73	1,8-cineole (54.0%), sabinene (14.6%), α -terpineol (9.8%), α -pinene (4.8%), terpinen-4-ol (3.4%), β -pinene (3.5%)
CL	1.21	Turmerone (31.4%), ar-turmerone (16.1%), turmerol (14.6%), terpinolene (11.0%), α -zingiberene (5.2%), β -sesquiphellandrene (4.8%), β -caryophyllene (3.5%)
MC	0.35	Octanoic acid (78.9%), hexanoic acid (11.3%), [octanoic acid, methyl ester] (5.4%)
PA	0.23	Carvacrol (17.9%), δ -3-carene (15.2%), camphor (12.9%), <i>p</i> -cymene (9.9%), γ -terpinene (6.6%), β -caryophyllene (6.1%), β -selinene (4.2%), α -terpinene (4.1%), <i>trans</i> - β -bergamotene (4.0%)
PC	0.09	Myristicin (40.3%), 1,3,8- <i>p</i> -dimenthatriene (17.9%), β -phellandrene (15.0%), myrcene (4.2%), α , <i>p</i> -dimethylstyrene (3.7%), terpinolene (2.6%), limonene (2.5%)
PS	0.77	Myrcene (62.2%), germacrene D (7.8%), limonene (3.4%), 9-octadecanoic acid (3.1%), β -phellandrene (2.9%), δ -cadinene (2.9%)
SC	0.03	(<i>E</i>)- β -ocimene (24.4%), (<i>Z</i>)- β -ocimene (10.7%), α -guaiene (12.6%), β -selinene (9.7%), myrcene (7.8%), δ -guaiene (7.2%), selin-11-en-4 α -ol (3.8%), α -selinene (3.1%)
SS	0.04	β -pinene (21.3%), α -pinene (8.9%), γ -terpinene (7.9%), limonene (7.7%), <i>p</i> -cymene (5.9%), β -selinene (3.8%), selin-11-en-4 α -ol (3.6%), β -caryophyllene (3.5%), α -selinene (3.4%), δ -cadinene (2.9%), 1-epi-cubenol (2.2%), terpinolene (2.1%), α -terpineol (2.1%)

CAL: *Citrus aurantium* leaf, CAF: *Citrus aurantium* fruit (peel), CC: *Cinnamomum camphora*; CL: *Curcuma longa*, MC: *Morinda citrifolia*, PA: *Plectranthus amboinicus*, PC: *Petroselinum crispum*; PS: *Pittosporum senacia*; SC: *Syzygium coriaceum*; SS: *Syzygium samarangense*; ^aw/w per 100 g of plant materials; ^bidentified by GC-MS/GC-FID [1,2].

27	Octanoic acid, methyl ester	1391	-	-	-	-	5.4	-	-	-	-	-
28	3-Octanol	1391	-	-	-	-	-	0.1	-	-	-	-
29	1,3,8- <i>p</i> -dimenthatriene	1403	-	-	-	tr	-	-	17.9	-	-	-
30	Rosefuran	1404	-	-	-	-	-	-	-	tr	-	-
31	α -Fenchone	1408	-	-	-	-	-	0.2	-	-	-	-
32	Perillen	1426	-	-	-	-	-	-	-	0.1	-	-
33	Octanoic acid, ethyl ester	1436	-	-	-	-	0.1	-	-	-	-	-
34	α , <i>p</i> -dimethylstyrene	1447	-	-	-	0.3	-	0.1	3.7	-	-	tr
35	1-Octen-3-ol	1450	-	-	-	-	-	0.6	-	-	-	-
36	α -Cubebene	1465	-	-	-	-	-	0.1	-	0.1	0.1	0.2
37	Longipinene	1479	-	-	-	-	-	-	-	0.1	-	-
38	Citronellal	1486	-	13.7	-	-	-	-	-	-	-	-
39	Bicycloelemene	1489	1.1	0.8	-	-	-	-	-	0.1	-	-
40	Cycloisosativene	1491	-	-	-	-	-	-	-	-	-	-
41	(<i>E</i>)- β -Ocimene epoxide	1492	-	-	-	-	-	-	-	-	0.1	-
42	α -Ylangene	1493	-	-	-	-	-	-	-	-	-	0.2
43	α -Copaene	1501	-	-	-	-	-	1.1	0.1	2.1	0.1	1.5
44	Decanal	1503	0.4	-	-	-	-	-	-	-	-	-
45	β -Bourbonene	1531	-	-	-	-	-	-	-	-	0.2	tr
46	Camphor	1535	-	-	-	-	-	12.9	-	-	-	-
47	α -Gurjunene	1540	-	-	-	-	-	-	-	-	0.1	tr
48	Linalool	1548	0.2	0.2	-	-	-	0.3	-	-	0.1	0.5
49	β -Cubebene	1549	-	-	-	-	-	-	-	0.7	-	-
50	1-Nonene-3-ol	1550	0.2	-	-	-	-	-	-	-	-	-
51	Octanol	1557	-	-	-	-	-	-	-	-	-	tr
52	<i>trans</i> - α -Bergamotene	1577	-	-	-	-	-	tr	-	-	-	-
53	Isopulegol	1582	-	-	-	-	-	-	-	-	-	0.3
54	Fenchol	1592	-	-	-	-	-	-	-	-	-	0.8
55	<i>trans</i> - β -Bergamotene	1593	-	-	-	-	-	4.0	-	0.1	-	-
56	Bornyl acetate	1593	-	-	-	-	-	-	-	-	-	-
57	Decanoic acid, methyl ester	1597	-	-	-	-	0.3	-	-	-	-	-
58	β -Elemene	1601	0.4	0.5	-	-	-	0.1	1.2	0.8	-	0.1

59	α -Guaiene	1602	-	-	-	-	-	-	-	-	12.6	-
60	Terpinen-4-ol	1612	0.3	5.1	3.4	-	-	-	-	-	-	-
61	β -Caryophyllene	1614	-	-	-	3.5	-	6.1	-	0.8	0.4	3.5
62	Aromadendrene	1624	-	-	-	-	-	-	-	tr	-	tr
63	γ -Elemene	1650	0.4	0.5	-	-	-	-	0.4	-	0.1	0.1
64	(E)-2-Decenal	1658	0.5	-	-	-	-	-	-	-	-	-
65	Alloaromodendrene	1664	-	-	-	-	-	-	-	0.1	-	0.2
66	Citronellyl acetate	1665	-	5.2	-	-	-	-	-	-	-	-
67	(Z)- β -Farnesene	1670	-	-	-	0.3	-	0.1	tr	0.1	-	-
68	Muurola-4,11-diene	1673	-	-	-	-	-	-	-	-	0.1	-
69	δ -Terpineol	1681	-	-	0.7	-	-	-	-	-	-	-
70	α -Humulene	1689	0.1	0.2	1.0	0.6	-	1.6	-	0.3	0.7	0.3
71	Selina-4,11-diene	1689	-	-	-	-	-	-	-	-	1.0	-
72	(E)- β -Farnesene	1695	-	-	-	tr	-	0.1	-	-	-	-
73	Cryptone	1695	-	-	-	-	-	-	0.1	-	-	-
74	γ -muurolene	1704	-	-	-	-	-	-	-	0.2	0.6	1.2
75	α -Terpineol	1706	0.3	-	9.8	-	-	0.2	-	-	-	2.1
76	Borneol	1715	-	-	0.2	-	-	-	-	-	-	1.0
77	Chamigrene	1723	-	-	-	-	-	-	-	-	-	-
78	Germacrene D	1729	2.5	0.5	0.2	-	-	-	-	7.8	-	-
79	α -Zingiberene	1730	-	-	-	5.2	-	-	-	-	-	-
80	δ -Guaiene	1732	-	-	-	-	-	-	-	-	7.2	-
81	β -Bisabolone	1738	-	-	-	0.8	-	0.3	tr	0.4	-	-
82	α -Muurolene	1740	-	-	-	-	-	-	-	0.5	-	-
83	β -Selinene	1743	-	0.2	-	-	-	4.2	-	-	9.7	3.8
84	α -Selinene	1747	-	-	-	-	-	0.7	-	-	3.1	3.4
85	Geranial	1750	tr	-	-	-	-	-	-	-	-	-
86	(E,E)- α -Farnesene	1752	-	-	-	-	-	-	-	-	0.1	0.2
87	Bicyclogermacrene	1754	-	0.3	0.1	-	-	-	-	1.1	-	-
88	Geranyl acetate	1763	-	-	-	-	-	-	-	-	1.6	-
89	Citronellol	1768	-	1.8	-	-	-	-	-	-	-	0.6
90	δ -Cadinene	1773	0.2	-	-	-	-	1.4	0.1	2.9	1.0	2.9

91	γ -Cadinene	1779	-	-	-	-	-	0.1	-	1.1	0.5	0.8
92	β -Sesquiphellandrene	1783	-	-	-	4.8	-	0.1	0.5	0.1	-	-
93	7-epi- α -Selinene	1784	-	-	-	-	-	-	-	-	0.2	-
94	ar-Curcumene	1787	-	-	-	1.9	-	-	-	-	-	-
95	p-Methyl acetophenone	1800	-	-	-	-	-	-	0.2	-	-	-
96	Nerol	1806	0.1	-	-	-	-	-	-	-	-	-
97	α -Cadinene	1811	-	-	-	-	-	-	-	0.3	-	-
98	Hexanoic acid	1846	-	-	-	-	11.3	-	-	-	-	-
99	Calamenene	1854	-	-	-	-	-	0.2	-	0.1	0.2	0.7
100	Germacrene B	1856	0.3	0.3	-	-	-	-	0.2	-	-	-
101	<i>p</i> -Cymen-8-ol	1861	-	-	-	0.3	-	tr	-	-	-	tr
102	Carvacryl acetate	1887	-	-	-	-	-	0.1	-	-	-	-
103	α -Calacorene	1943	-	-	-	-	-	tr	-	-	0.1	0.2
104	Caryophyllene oxide	2017	-	-	-	0.1	-	0.9	-	-	0.1	1.3
105	Carotol	2042	-	-	-	-	-	-	1.9	-	-	-
106	(<i>E</i>)-Nerolidol	2051	-	-	-	0.4	-	tr	-	-	0.4	-
107	Octanoic acid	2062	-	-	-	-	78.9	-	-	-	-	-
108	Cubenol	2081	-	-	-	-	-	0.1	-	-	0.4	1.1
109	1-epi-Cubenol	2088	-	-	-	-	-	0.2	-	-	0.6	2.2
110	Guaiol	2103	-	-	-	-	-	-	-	-	0.1	-
111	Spathulenol	2147	-	-	-	-	-	-	-	0.3	-	-
112	T-Cadinol	2193	-	-	-	-	-	-	-	0.4	0.7	1.2
113	Thymol	2196	-	-	-	-	-	0.3	-	-	-	-
114	Turmerone	2206	-	-	-	31.4	-	-	-	-	-	-
115	T-Muurolol	2208	-	-	-	-	-	0.3	-	0.5	1.0	0.9
116	δ -Cadinol	2218	-	-	-	-	-	-	-	-	0.2	0.7
117	α -Muurolol	2222	-	-	-	-	-	-	-	-	0.1	0.2
118	Carvacrol	2227	-	-	-	-	-	17.9	-	-	-	-
119	2-Heptadecanone	2240	-	-	-	-	-	-	-	0.5	-	-
120	Elemicin	2242	-	-	-	-	-	-	1.7	-	-	-
121	α -Eudesmol	2246	-	-	-	-	-	-	-	-	-	0.4
122	α -Cadinol	2254	-	-	-	-	-	0.4	-	1.2	0.8	1.9

123	Guaia-6,10(14)-diene	2261	-	-	-	-	-	-	-	-	0.6	-
124	Turmerol	2270	-	-	-	14.6	-	-	-	-	-	-
125	Decanoic acid	2273	-	-	-	-	1.7	-	-	-	-	-
126	Selin-11-en-4 α -ol	2279	-	-	-	-	-	-	-	-	3.8	3.6
127	α -Turmerone	2282	-	-	-	16.1	-	-	-	-	-	-
128	Myristicin	2291	-	-	-	-	-	0.2	40.3	0.3	0.2	-
129	Apiol	2508	-	-	-	-	-	-	1.5	-	-	-
130	9-Octadecanoic acid	3200	3.9	-	1.2	-	-	-	-	3.1	-	-
Total identified (%)^d			99.5	99.6	99.6	94.2	99.3	98.0	98.6	98.1	92.6	95.8

CAL: *Citrus aurantium* leaf, CAF: *Citrus aurantium* fruit (peel), CC: *Cinnamomum camphora*; CL: *Curcuma longa*, MC: *Morinda citrifolia*,

PA: *Plectranthus amboinicus*, PC: *Petroselinum crispum*; PS: *Pittosporum senacia*; SC: *Syzygium coriaceum*; SS: *Syzygium samarangense*.

^a Relative retention indices (RRI) calculated against *n*-alkanes (C8-C30).

^b Not detected.

^c Trace (<0.1%).

^d % components identified within EOs.

References

- [1] Jugreet, B.S., Mahomoodally, M.F., Sinan, K.I., Zengin, G. and Abdallah, H.H. Chemical variability, pharmacological potential, multivariate and molecular docking analyses of essential oils obtained from four medicinal plants. *Ind Crops Prod* **2020**, 150, p.112394.
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