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GC-MS olfactometry reveals sesquiterpenes α-humulene and δ-cadinene significantly influence the aroma of treated *Aquilaria malaccensis* essential oil

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Table S1 Metabolite profiling of volatiles extracted from treated agarwood and healthy *A. malaccensis* essential oil obtained via hydrodistillation technique in comparison with volatiles identified from wood samples using SPME technique

No.	Compounds [a]	Volatiles extracted from wood samples by SPME technique		Essential oil from hydrodistillation technique	
		Percentage [b]			
		Treated agarwood	Healthy tree	Treated agarwood	Healthy tree
	Sesquiterpenes and aromatics	[e]**86.94**	**1.04**	**80.61**	**0.29**
1	β-Caryophyllene	[c] 8.92	-	0.05	-
2	α-Humulene	13.33	[d] -	0.23	-
3	δ-Guaiene	10.41	-	2.03	-
4	δ-Cadinene	4.09	-	1.47	-
5	β-Elemene	-	-	0.08	-
6	10-Epi-γ-Eudesmol	-	-	13.39	-
7	(-)-Aristolene	-	-	9.10	-
8	Cis-Z-α-bisabolene epoxide	-	-	1.05	-
9	Longipinocarveol trans	-	-	2.18	-
10	β-Guaiene	-	-	0.54	-
11	Isolongifolen-9-one	-	-	0.33	-
12	Isolongifolenone	-	-	0.25	-
13	Benzylacetone	-	-	5.68	-
14	Vitispirane	-	-	0.06	-
15	α-Copaene	12.49	-	0.06	-
16	1H Cyclopenta[1,3]cyclopropa[1,2] benzene, octahydro-7-methyl-3-methylene-4-(1-methylethyl)-, [3aS-(3aà,3bá,4á,7à,7aS*)]-	7.19	-	-	-
17	α-Cedrene	-	-	0.42	-
18	α-Guaiene	3.99	-	0.52	-
19	β-Patchoulene	4.57	-	-	-
20	1H-Cycloprop[e]azulene, decahydro-1,1,7-trimethyl-4-methylene-, [1aR-(1aà,4aá,7à,7aá,7bà)]-	-	-	0.11	-
21	Spiro[4.5]dec-7-ene, 1,8-dimethyl-4-(1-methylethenyl)-, [1S-(1à,4á,5à)]-	-	–	0.22	-
22	Germacrene D	6.71	-	-	-
23	α-Muurolene	4.26	–	0.43	–
24	Isoaromadendrene epoxide	-	–	2.51	–
25	Squalene	2.13	-	-	-
26	α-Curcumene	–	–	0.84	–
27	γ-Muurolene	–	–	0.62	–
28	β-Maaliene	–	–	0.09	-
29	Elemol	–	-	2.23	-
30	Bicyclo[4.4.0]dec-2-ene-4-ol, 2-methyl-9-(prop-1-en-3-ol-2-yl)	–	–	1.55	-
31	α-Gurjunene	–	–	8.84	-

32	Agarospirol	-	-	0.50	-
33	α-Cadinol	-	-	19.40	-
34	Ledene oxide-(II)	-	-	1.15	-
35	Dehydroaromadendrene	-	-	1.01	-
36	Cedran-diol, 8S,14-	-	-	0.95	-
37	2(1H)Naphthalenone, 3,5,6,7,8,8a-hexahydro-4,8a-dimethyl-6-(1-methylethenyl)-	-	-	0.34	-
38	Dibenzylacetone	-	-	0.71	-
39	Isopropyl tetradecanoate	-	-	-	0.05
40	Hexadecanoic acid, methyl ester	-	1.04	-	0.04
41	2-Ethyhexyl (2E)-3-(4-Methoxyphenyl)-2-Propenoate	-	-	-	0.13
42	1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester	-	-	0.91	-
43	1,2-Benzenedicarboxylic acid, mono(2-ethylhexyl) ester	-	-	0.76	-
44	3-Octadecenoic acid, methyl ester	-	-	-	0.07
45	1,2- Benzenedicarboxylic acid, diisooctyl ester	1.41	-	-	-
46	Hexanedioic acid, dioctyl ester	5.75	-	-	-
47	Hexadecanoic acid, tert-butyldimethylsilyl ester	1.69	-	-	-
	Fatty acids	**13.06**	**58.45**	**12.57**	**98.69**
48	Tetradecanoic acid	–	1.98	-	1.85
49	Pentadecanoic acid	–	1.22	1.67	0.61
50	Cis-9-Hexadecenoic acid	–	–	0.11	1.32
51	Hexadecanoic acid	13.06	20.41	8.76	26.26
52	9-Hexadecenoic acid	-	1.69	-	-
53	Oleic acid	-	28.47	0.99	54.16
54	1,2-Benzenedicarboxylic acid	-	2.01	-	-
55	Decanoic acid	-	-	-	0.26
56	Dodecanoic acid	-	-	-	4.53
57	9-Octadecenoic acid (Z)-	-	-	-	0.01
58	14-Pentadecenoic acid	-	-	-	0.46
59	Cis-10-Heptadecenoic acid	-	-	-	0.86
60	Heptadecanoic acid	-	-	0.12	0.74
61	Octadecanoic acid	-	2.67	–	7.63
62	Octanoic acid	-	-	0.72	-
63	Nonanoic acid	-	-	0.12	-
64	9, 12- Octadecadienoic acid	-	-	0.08	-
	Alcohol derivatives	**0**	**0**	**4.88**	**0.18**
65	1-Hexadecanol	-	-	-	0.01
66	Hexadecen-1-ol, trans-9-	-	-	-	0.12
67	Phenol, 2,4-bis(1-phenylethyl)-	-	-	-	0.05
68	Benzenepropanol	-	-	0.06	-
69	2-(4a,8-Dimethyl-1,2,3,4,4a,5,6,7-octahydro-naphthalen-2-yl)-prop-2-en-1-ol	-	-	1.49	-
70	3-Cyclohexen-1-ol, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-	-	-	2.82	-
71	2-Methyl-4-(2,6,6-trimethylcyclohex-1-enyl)but-2-en-1-ol	-	-	0.51	-
	Alkanes/ Alkenes	**0**	**38.46**	**0.47**	**0.3**
72	4,6,6-Trimethyl-2-(3-Methyl-Buta-1,3-Dienyl)-3-Oxa-Tricyclo[5.1.0.0	-	-	0.40	-

	2,4]Ocatane				
73	Tetracosane	-	-	-	0.07
74	Heptadecane	-	-	-	0.04
75	Octadecane	-	-	-	0.04
76	Hexadecane, 2,6,10,14-Tetramethyl	-	-	-	0.04
77	Nonadecane	-	-	-	0.03
78	Hexacosane	-	-	-	0.08
79	2,6,10,14,18-Pentamethyl-2,6,10,14,18-eicosapentaene	-	38.46	-	-
80	Benzene, 1,1'-(2-pentene-1,5-diyl)bis-	-	-	0.07	-
	Aldehydes/ Ketones	**0**	**0.30**	**1.30**	**0.47**
81	Dodecanal	-	-	-	0.02
82	Tetradecanal	-	0.30	-	0.08
83	Hexadecanal	-	-	-	0.02
84	2-Pentadecanone, 6,10,14-trimethyl-	-	-	-	0.02
85	Cyclopentadecanone, 2-hydroxy-	-	-	-	0.29
86	7,9-Di-tert-butyl-1-oxaspiro(4,5)deca-6,9-diene-2,8-dione	-	-	-	0.03
87	2-(3-Isopropyl-4-methyl-pent-3-en-1-ynyl)-2-methyl-cyclobutanone	-	-	1.30	-
	Others	-	**1.75**	**0.17**	**0.07**
88	4,8,12,16-Tetramethylheptadecan-4-olide	-	-	-	0.07
89	Hexadecanamide	-	1.75	-	-
90	9-Octadecenamide	-	-	0.17	-
	Total	**100.00**	**100.00**	**100.00**	**100.00**

[a] Compounds identified by GC-MS Software using NIST and Wiley-Adams mass spectral library; [b] Percentage of each component is calculated as peak area of compound divided by peak area of total ion chromatogram and times 100; [c] The results are the mean of at least 3 experiments; [d] Not detected; [e] total for each groups of volatiles