Electronic Supplementary Material (ESI) for Green Chemistry.

Supplementary information

A synthetic biology and green bioprocess approach to recreate agarwood sesquiterpenoid mixtures

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Supplementary Files

Files can be downloaded in the following link:

https://datadryad.org/stash/share/lSU89kHS9Poefgh9g65_v6Koerab9ZoBaYyGCcIri98

Supplementary File 1. GCxGC-TOF/MS data report of agarwood samples.

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Supplementary File 3. GC-TOF/MS raw data of agarwood samples.

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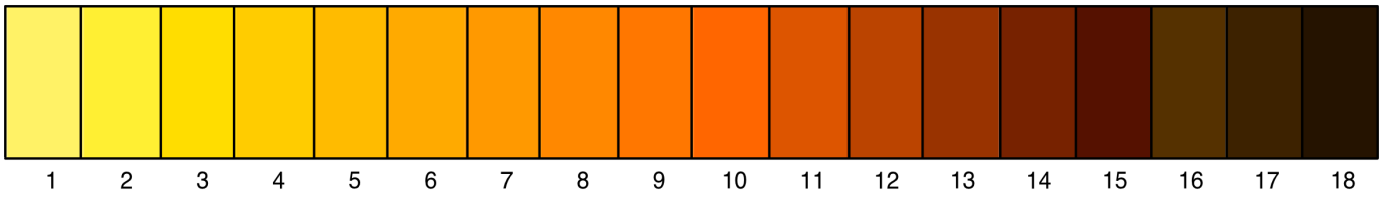
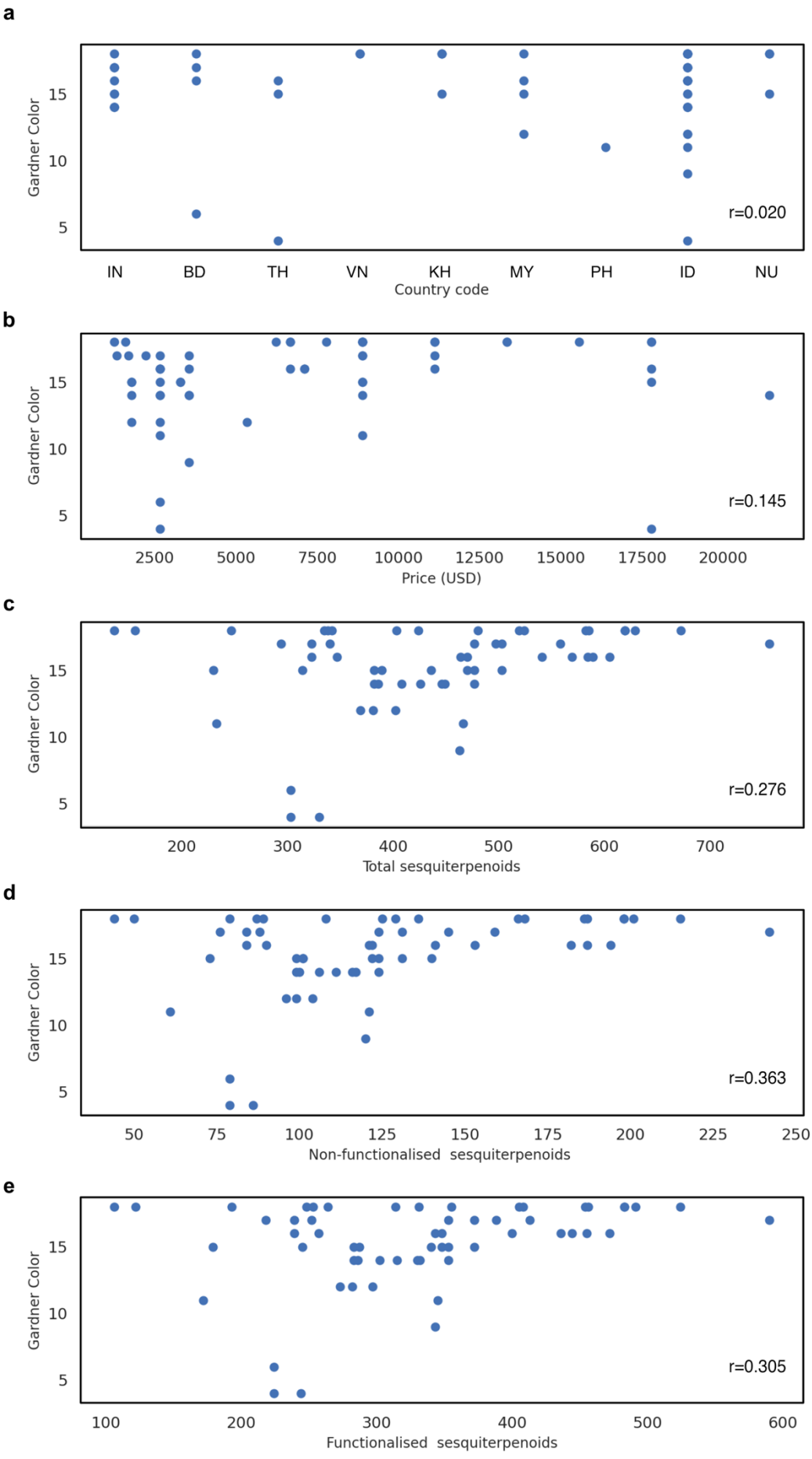


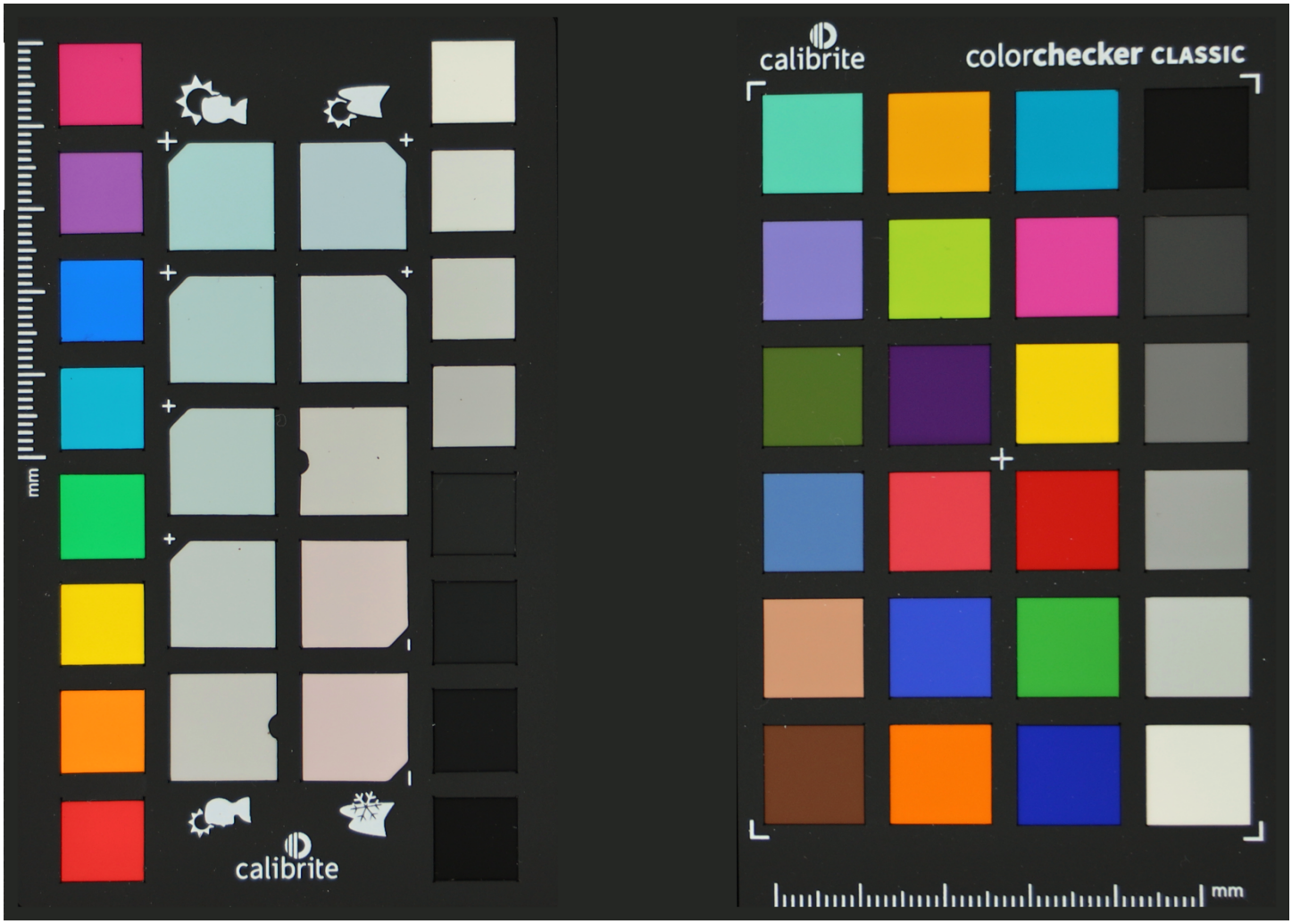
Supplementary Figure 1. Gardner Colour Scale.

Gardner Color Scale utilized for agarwood sample assessment. Displaying a progression from pale yellow (1) to dark red (18), this scale provides a standardized method for quantifying the color intensity of agarwood samples. Each number corresponds to a specific hue, enabling precise color matching and consistency evaluation. Analysis of sample images and assignment of color values according to the scale were conducted using ImageJ software (NIH, USA).


a
Gardner Color
15
10
5
r=0.020
IN
BD
TH
VN
KH
MY
PH
ID
NU
Country code
b
Gardner Color
15
10
5
r=0.145
2500
5000
7500
10000
12500
15000
17500
20000
Price (USD)
c
Gardner Color
15
10
5
r=0.276
200
300
400
500
600
700
Total sesquiterpenoids
d
Gardner Color
15
10
5
r=0.363
50
75
100
125
150
175
200
225
250
Non-functionalised sesquiterpenoids
e
Gardner Color
15
10
5
r=0.305
100
200
300
400
500
600
Functionalised sesquiterpenoids

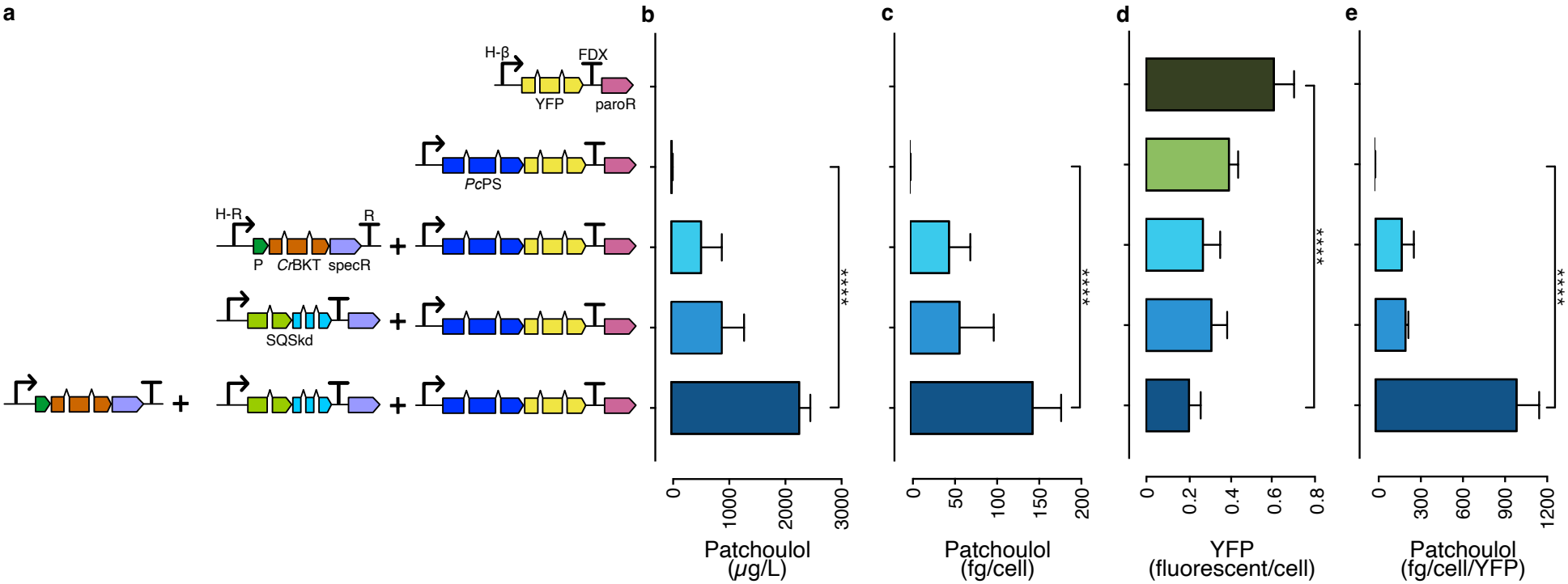
Supplementary Figure 2. Correlation of Agarwood Color Intensity.

a. presents a negligible correlation (r = -0.020) between Gardner Color values and the country of origin, implying no significant influence of geographical source on color intensity. **b.** indicates a slight positive correlation (r = 0.145) between color intensity and price, suggesting that more intense coloring could potentially command a higher market price, although the association is weak. **c.** reveals a mild positive correlation (r = 0.276) with total sesquiterpenoids content, while **d.** shows a moderate positive correlation (r = 0.363) with non-functionalised sesquiterpenoids content, and **e.** displays a similar positive correlation (r = 0.305) with functionalised sesquiterpenoids content, each indicating a trend towards darker colors with higher concentrations of these compounds. The correlations hint at a moderate influence of sesquiterpenoid content on the color intensity of agarwood, independent of its country of origin. Statistical performed using R Studio, and the complete set of values utlized for correlation coefficient analysis is available **in Supplementary Table 1**. Country codes are defined as follows: **IN** (India), **BD** (Bangladesh), **TH** (Thailand), **VN** (Vietnam), **KH** (Cambodia), **MY** (Malaysia), **PH** (Philippines), **ID** (Indonesia), **NU** (Unknown).



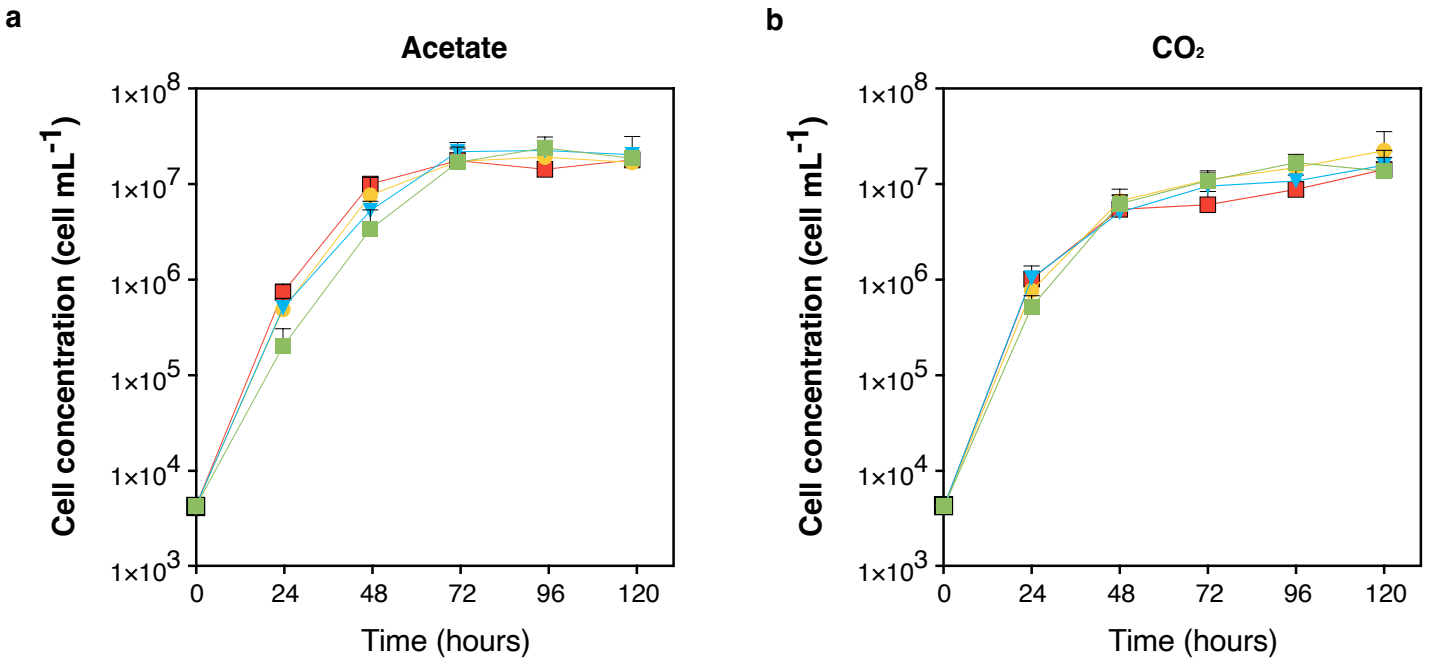
Supplementary Figure 3. Image of ColorChecker Passport.

Photograph of the ColorChecker Passport (CCPP2, Calibrite LLC, DE, USA) used for precise colour calibration. The calibration was achieved using the ColorChecker calibration software (Calibrite LLC, DE, USA) in conjunction with Adobe Lightroom (Adobe Inc., CA, USA) for colour correction profiling.

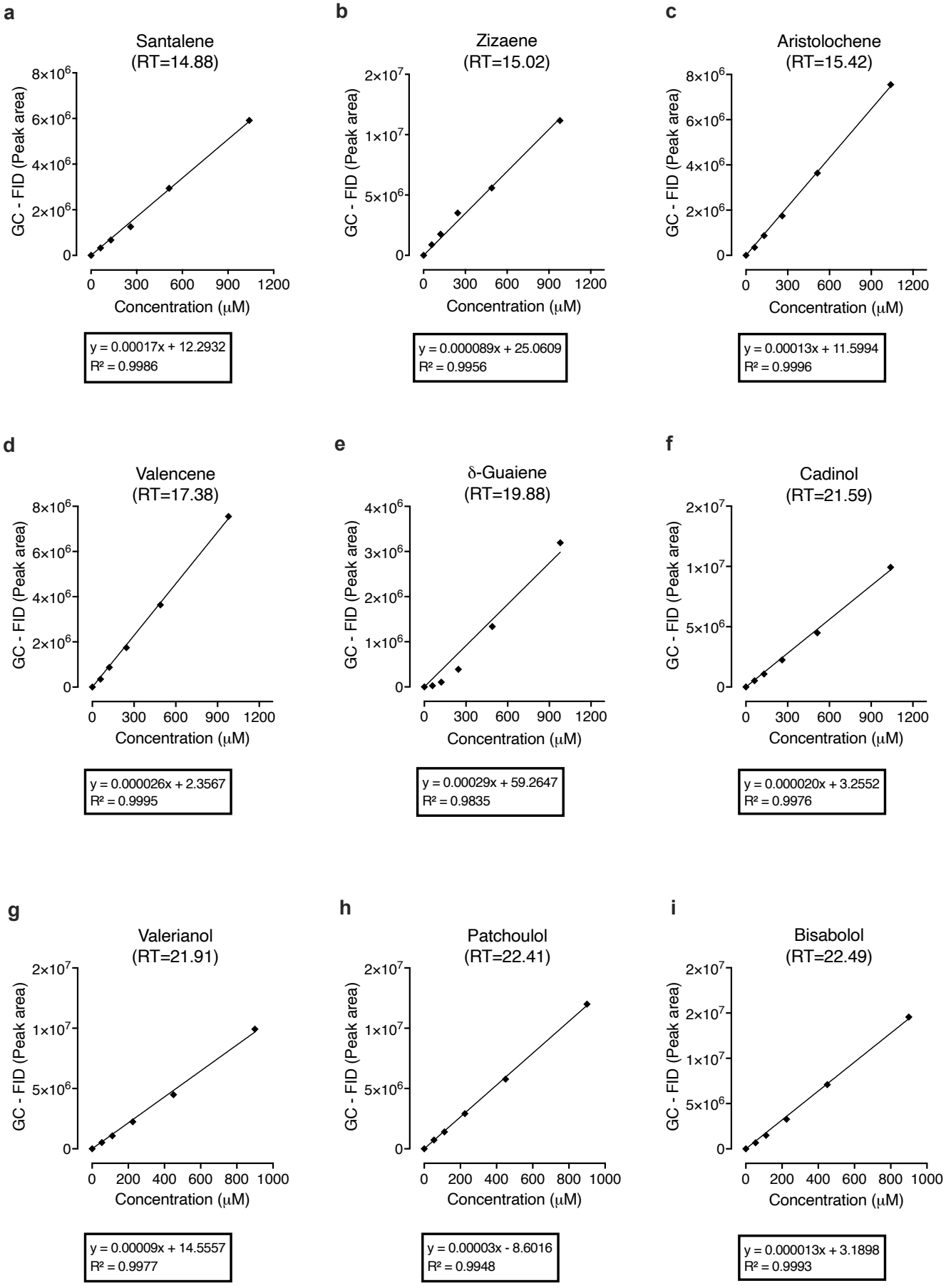


Supplementary Figure 4. Optimisation of *Chlamydomonas reinhardtii* metabolism for heterologous sesquiterpene production.

a. A variety of vectors, each containing algal-optimized genes such as mVenus (yellow fluorescent protein, YFP), PcPS-mVenus fusion, CrBKT, and CrSQS knockdown (k.d.), all integrated into the C. reinhardtii UPN22 parent strain. **b.** Patchoulol yields (μg/L) achieved with each engineered construct. **c.** Patchoulol yields (fg/cell) for each unique construct. **d.** Yellow fluorescent signal per cell for individual constructs. **e.** Patchoulol production for each construct normalised per cell by YFP fluorescence. **Definitions:** "k.d" refers to knock down; "*Pc*PS" stands for *Pogostemon cablin* patchoulol synthase; "*Cr*BKT" is *Chlamydomonas reinhardtii* β-carotene ketolase; "SQS" designates squalene synthase; "paroR" symbolises paromomycin resistance; "specR" identifies spectinomycin resistance; "H-β" represents the combined HSP70A-β tubulin promoter; "FDX" is the abbreviation for the ferredoxin 1 gene terminator; "P" indicates the photosystem I reaction centre subunit II. Statistical variations between groups were identified using ANOVA with Tukey's method for multiple comparisons. **Statistical significances:** *P < 0.05, **P < 0.01, ***P < 0.001. Comprehensive calculations, cell concentrations, and p-values are available in Supplementary Table 4.

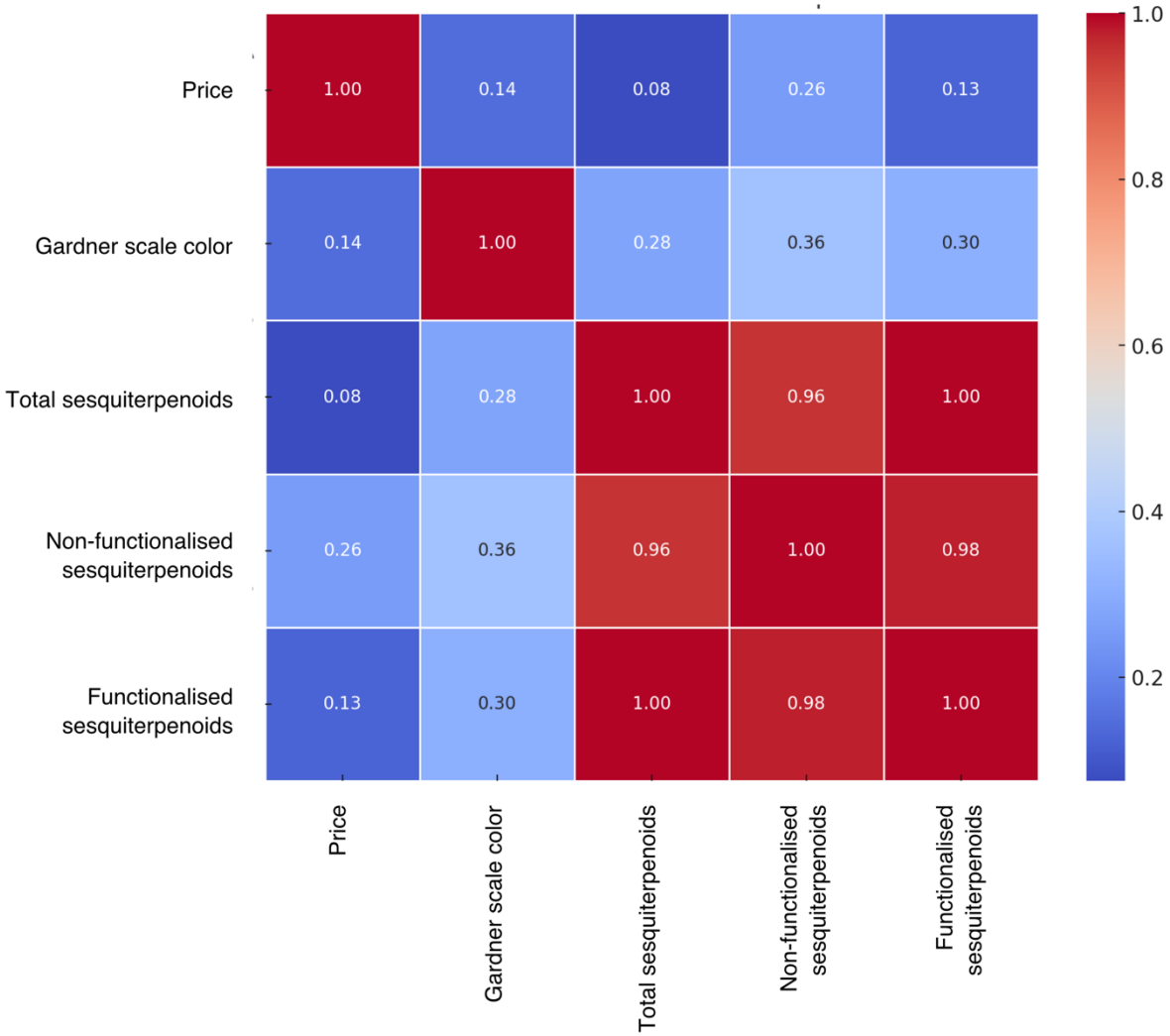


Supplementary Figure 5. Growth assessment of engineered *Chlamydomonas reinhardtii* engineered strains. Analysis of cell concentration over a 120-hour period under two distinct carbon sources: (a) acetate, and (b) carbon dioxide (CO_2). Four transformants from each cell line were assessed and compared to the parental strain, *C. reinhardtii* UPN22. Sampling was performed every 24 hours using an automated liquid handler (Opentrons Labworks Inc., NY, USA), with cell counts determined by flow cytometry (Thermo Fisher Scientific, MA, USA). Statistical differences between the groups were identified through ANOVA, utilising Tukey's method for multiple comparisons. Significance levels are marked as follows: $^{*}p < 0.05$, $^{**}p < 0.01$, $^{***}p < 0.001$.



Supplementary Figure 6. Calibration curves of sesquiterpenoid standards.

Calibration curves and calculations utilised purified standards, with concentrations ranging from 1–1200 µM in dodecane, of the following sesquiterpenoids: δ-guaiene (CAT#B942760), patchoulol (CAT#P206200), santalene (CAT#S15065), valerianol (CAT#V914000, Toronto Research Chemicals, ON, Canada), bisabolol (CAT#95426), valencene (CAT#06808), and cedrene (CAT#22133, Sigma-Aldrich, MO, USA). For compound identification, retention time acquisition, internal digital library calibration, and method development, we used a set of 12 microampules containing a standard terpene mixture, which covered 98 terpenes at 1.0 mM in methanol (CAT# MSITPN101, MetaSci, ON, Canada).



Supplementary Figure 7. Correlation matrix heatmap of agarwood samples.

The heatmap offers a comprehensive depiction of the Pearson correlation coefficients, showcasing the linear relationships between price, color, and sesquiterpenoid compound classifications found in the agarwood samples. There is a weak positive correlation (r = 0.14) between price and color, indicating that higher prices might be associated with more intense colors. There exists an inverse relationship (r = -0.08) between price and total sesquiterpenoid concentration, suggesting that while cost may not primarily depend on sesquiterpenoid content alone, it could still have some impact on pricing decisions to a lesser extent. The color demonstrates highly significant positive correlations with both non-functionalised (r = 0.96) and functionalised sesquiterpenoids (r = 0.98), implying a strong link between the intensity of color and the sesquiterpenoids.

Supplementary Table 1. Agarwood samples description.

No. Sample	Type	Origin (Country)	Code (Country)	Price (USD) (Kg or L)	Gardner color standard value	Total sesquiterpenoids (n=)	Non-functionalised sesquiterpenoids (n=)	Functionalised sesquiterpenoids (n=)
1	Agarwood	Philippines	PH	$ 8,888	11	233	61	172
2	Agarwood	Indonesia	ID	$ 3,555	9	463	120	343
3	Agarwood	Indonesia	ID	$ 2,666	11	466	121	345
4	Agarwood	Indonesia	ID	$ 2,666	12	402	104	297
5	Agarwood	Indonesia	ID	$ 7,111	16	541	141	400
6	Agarwood	Malaysia	MY	$ 3,288	15	503	131	372
7	Agarwood	Indonesia	ID	$ 2,666	14	408	106	302
8	Agarwood	Indonesia	ID	$ 8,888	14	386	100	286
9	Agarwood	Indonesia	ID	$ 1,688	17	503	131	372
10	Agarwood	Indonesia	ID	$ 2,666	4	303	79	224
11	Agarwood	Bangladesh	BD	$ 2,666	6	303	79	224
12	Agarwood	Malaysia	MY	$ 5,333	12	381	99	282
13	Agarwood	Indonesia	ID	$ 3,555	17	323	84	239
14	Agarwood	India	IN	$ 2,666	17	558	145	413
15	Agarwood	India	IN	$ 8,888	17	294	76	218
16	Agarwood	Thailand	TH	$ 17,777	4	330	86	244
17	Agarwood	Indonesia	ID	$ 3,555	16	589	153	436
18	Agarwood	Indonesia	ID	$ 7,111	16	347	90	257
19	Agarwood	Thailand	TH	$ 3,288	15	382	99	283
20	Agarwood	India	IN	$ 2,666	14	382	99	283
21	Agarwood	Indonesia	ID	$ 21,422	14	477	124	353
22	Agarwood	Indonesia	ID	$ 1,777	12	369	96	273
23	Agarwood	India	IN	$ 3,555	14	449	117	332
24	Agarwood	Indonesia	ID	$ 3,555	14	446	116	330
25	Agarwood	India	IN	$ 1,777	15	389	101	287
26	Agarwood	Indonesia	ID	$ 2,666	15	470	122	348
27	Agarwood	Indonesia	ID	$ 1,333	17	477	124	353
28	Agarwood	Indonesia	ID	$ 2,666	16	470	122	348
29	Agarwood	India	IN	$ 1,777	14	426	111	315

Supplementary Table 1. (Cont.)

No. Sample	Type	Origin (Country)	Code (Country)		Price (USD) (Kg or L)	Gardner color standard value	Total sesquiterpenoids (n=)	Non-functionalised sesquiterpenoids (n=)	Functionalised sesquiterpenoids (n=)
30	Agarwood	India	IN	$	2,666	16	464	121	343
31	Agarwood	Indonesia	ID	$	1,600	18	480	125	355
32	Agarwood	Indonesia	ID	$	2,222	17	340	88	252
33	Agarwood	Indonesia	ID	$	6,222	18	335	87	248
34	Agarwood	Indonesia	ID	$	1,777	15	477	124	353
35	Agarwood	Thailand	TH	$	2,666	16	323	84	239
36	Agarwood	Vietnam	VN	$	1,244	18	342	89	253
37	Distillate	Bangladesh	BD	$	8,888	17	497	159	388
38	Distillate	Bangladesh	BD	$	6,666	18	338	108	264
39	Distillate	Indonesia	ID	$	7,777	18	524	168	408
40	Distillate	Cambodia	KH	$	11,111	18	403	129	314
41	Distillate	Indonesia	ID	$	17,777	18	424	136	331
42	Distillate	Bangladesh	BD	$	11,111	16	584	187	455
43	Distillate	Malaysia	MY	$	17,777	18	582	186	454
44	Distillate	Cambodia	KH	$	8,888	18	629	201	491
45	Distillate	India	IN	$	11,111	17	756	242	590
46	Distillate	Unknown	NU	$	6,666	18	619	198	483
47	Distillate	Unknown	NU	$	8,888	18	672	215	524
48	Distillate	Indonesia	ID	$	13,333	18	585	187	456
49	Distillate	Indonesia	ID	$	13,333	18	519	166	405
50	Distillate	Cambodia	KH	$	8,888	15	314	101	245
51	Distillate	Vietnam	VN	$	8,888	18	247	79	193
52	Distillate	Indonesia	ID	$	6,666	16	605	194	472
53	Distillate	Cambodia	KH	$	8,888	18	619	198	483
54	Distillate	India	IN	$	17,777	15	436	140	340
55	Distillate	Malaysia	MY	$	17,777	16	569	182	444
56	Distillate	India	IN	$	11,111	18	156	50	122
57	Distillate	Indonesia	ID	$	15,555	18	136	44	106
58	Distillate	Unknown	NU	$	8,888	15	230	73	179

Supplementary Table 2. Sesquiterpenoids identified across agarwood (bakhour) samples using GCxGC-TOF/MS.

Compound Name	Mol. formula	Clas.	RT I (min)	RT II (sec)	MF	P (%)
Aromadendrene	$C_{15}H_{22}$	STP	34.70	2.64	772	94
α-Cubebene	$C_{15}H_{24}$	STP	34.70	2.22	714	68
4a,5-Dimethyl-3-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalen-1-ol	$C_{15}H_{24}O$	FSTP	34.70	2.62	654	48
β-Vatirenene	$C_{15}H_{22}$	STP	35.80	3.85	624	84
Germacrene A	$C_{15}H_{24}$	STP	37.30	2.44	633	85
β-copaene	$C_{15}H_{24}$	STP	37.30	2.42	674	92
1,5-Cyclodecadiene, 1,5-dimethyl-8-(1-methylethenyl)-, [S-(Z,E)]-	$C_{15}H_{24}$	STP	37.30	2.46	647	94
α-gurjunene	$C_{15}H_{24}$	STP	38.20	2.66	641	65
(2R,3R,3aR,6R,8aS)-3,7,7-Trimethyl-8-methyleneoctahydro-1H-3a,6-methanoazulen-2-ol	$C_{15}H_{24}O$	FSTP	38.70	3.17	654	82
muuroladiene	$C_{15}H_{24}$	STP	39.10	2.76	659	75
Caryophyllene	$C_{15}H_{24}$	STP	39.30	2.68	604	82
Patchouladiene	$C_{15}H_{22}$	STP	39.50	3.04	643	84
1H-Cycloprop[e]azulene, decahydro-1,1,4,7-tetramethyl-	$C_{15}H_{26}$	STP	39.90	2.36	662	86
4b,5,6,7,8,8a,9,10-Octahydro-1-methylphenanthrene	$C_{15}H_{20}$	FSTP	40.20	3.31	786	90
Cycloisolongifolol	$C_{15}H_{24}O$	FSTP	40.40	2.90	709	87
β-GURJUNENE	$C_{15}H_{24}$	STP	40.80	2.74	791	90
4,7-Methanoazulene, 1,2,3,4,5,6,7,8-octahydro-1,4,9,9-tetramethyl-, [1S-(1α,4α,7α)]-	$C_{15}H_{24}$	STP	40.80	2.76	665	82
Humulene	$C_{15}H_{24}$	STP	40.90	3.91	673	89
β-Selinene	$C_{15}H_{24}$	STP	40.90	2.58	693	94
α-bisabolene	$C_{15}H_{24}$	STP	41.30	2.92	603	90
Alloaromadendrene	$C_{15}H_{24}$	STP	41.30	2.98	716	94
Prezizaene	$C_{15}H_{24}$	STP	41.40	3.00	673	90
Calamene	$C_{15}H_{22}$	STP	41.60	3.09	650	87
1,4,6-Trimethyl-1,2,3,3a,4,7,8,8a-octahydro-4,7-ethanoazulene	$C_{15}H_{24}$	STP	41.70	2.88	706	54
2-Methyl-3-(3-methyl-but-2-enyl)-2-(4-methyl-pent-3-enyl)-oxetane	$C_{15}H_{26}O$	FSTP	41.90	2.68	688	17
Cadinene	$C_{15}H_{28}$	STP	42.10	2.38	514	65
(3S,6S)-6-Isopropyl-3-methyl-2-(propan-2-ylidene)-3-vinylcyclohexanone	$C_{15}H_{24}O$	FSTP	42.30	3.09	720	89
Diepicedrene oxide	$C_{15}H_{24}O$	FSTP	42.60	3.43	600	42

Supplementary Table 2. (Cont.)

Compound Name	Mol. formula	Class.	RT I (min.)	RT II (sec.)	MF	P (%)
(R,Z)-2-Methyl-6-(4-methylcyclohexa-1,4-dien-1-yl)hept-2-en-1-ol	$C_{15}H_{24}O$	FSTP	42.70	3.11	610	73
1H-Cycloprop[e]azulene, decahydro-1,1,4,7-tetramethyl-, [1aR-(1aα,4β,4aβ,7β,7aβ,7bα)]-	$C_{15}H_{26}$	STP	42.90	2.62	708	81
Caparratriene	$C_{15}H_{26}$	STP	43.10	2.60	700	83
Cycloisolongifolene	$C_{15}H_{24}$	STP	43.10	2.98	677	91
β-Guaiene	$C_{15}H_{24}$	STP	43.10	3.04	722	41
Aristolochene	$C_{15}H_{24}$	STP	43.10	3.00	641	43
Eremophilene	$C_{15}H_{24}$	STP	43.10	2.98	733	65
α-himachalene	$C_{15}H_{20}$	FSTP	43.30	3.59	777	41
β-Bisabolenol	$C_{15}H_{24}O$	FSTP	43.30	3.21	572	79
Eudesmatriene	$C_{15}H_{22}$	STP	43.40	3.17	825	72
2-(4a,8-Dimethyl-2,3,4,5,6,7-hexahydro-1H-naphthalen-2-yl)propan-2-ol	$C_{15}H_{26}O$	FSTP	43.40	2.94	752	76
10,11-Epoxycalamenene	$C_{15}H_{20}O$	FSTP	43.40	3.77	753	61
β-Vetispirene	$C_{15}H_{22}$	STP	43.50	3.17	588	38
(2R,8R,8aS)-8,8a-Dimethyl-2-(prop-1-en-2-yl)-1,2,3,7,8,8a-hexahydronaphthalene	$C_{15}H_{22}$	STP	43.50	3.13	752	56
6-Methyl-2-(4-methylcyclohex-3-en-1-yl)hepta-1,5-dien-4-ol	$C_{15}H_{24}O$	FSTP	43.70	4.27	708	38
1H-3a,7-Methanoazulene, octahydro-1,4,9,9-tetramethyl-	$C_{15}H_{26}$	STP	43.90	2.64	709	67
(3R,3aR,4aR,8aR,9aR)-3,8a-Dimethyl-5-methylene-3,3a,4,4a,5,6,9,9a-octahydronaphtho[2,3-b]furan-2(8aH)-one	$C_{15}H_{20}O_2$	FSTP	44.80	4.70	816	42
(3R,3aR,3bR,4S,7R,7aR)-4-Isopropyl-3,7-dimethyloctahydro-1H-cyclopenta[1,3]cyclopropa[1,2]benzen-3-ol	$C_{15}H_{26}O$	FSTP	44.90	2.98	824	84
Nivalenol	$C_{15}H_{20}O_7$	FSTP	45.20	3.55	769	61
Calamenene	$C_{15}H_{22}$	STP	45.30	3.41	625	80
Kessane	$C_{15}H_{26}O$	FSTP	45.80	3.37	959	71
Cubenene	$C_{15}H_{24}$	STP	45.80	3.08	449	77
1-Formyl-2,2-dimethyl-3-cis-(2-methyl-but-2-enyl)-6-methylidene-cyclohexane	$C_{15}H_{24}O$	FSTP	46.00	3.85	931	92
2,6-Dimethyl-10-methylene-12-oxatricyclo[7.3.1.0(1,6)]tridec-2-ene	$C_{15}H_{22}O$	FSTP	46.20	3.61	829	81
α-Calacorene	$C_{15}H_{20}$	FSTP	46.50	3.73	737	84
Nerolidol	$C_{15}H_{26}O$	FSTP	46.80	3.97	709	70
α-agorofuran	$C_{15}H_{24}O$	FSTP	46.90	3.99	735	71
2-Pentadecen-4-yne, (Z)-	$C_{15}H_{26}$	STP	46.90	5.22	720	51

Supplementary Table 2. (Cont.)

Compound Name	Mol. formula	Class.	RT I (min.)	RT II (sec.)	MF	P (%)
Longifolene	$C_{15}H_{20}$	FSTP	47.20	3.69	728	62
Aromadendran	$C_{15}H_{26}$	STP	47.40	4.25	754	77
Dihydroagarofurane	$C_{15}H_{26}O$	FSTP	47.50	3.47	754	90
4-Isopropyl-6-methyl-1-methylene-1,2,3,4-tetrahydronaphthalene	$C_{15}H_{20}$	FSTP	47.70	3.85	749	88
4(15)-Selinene-11,12-diol	$C_{15}H_{26}O_2$	FSTP	47.90	4.58	875	41
2-(4a,8-Dimethyl-2,3,4,4a,5,6-hexahydro-naphthalen-2-yl)-prop-2-en-1-ol	$C_{15}H_{22}O$	FSTP	48.20	4.86	774	81
Lanceol	$C_{15}H_{24}O$	FSTP	48.60	3.55	779	72
(5S,6R,7S,10R)-7-Isopropyl-2,10-dimethylspiro[4.5]dec-1-en-6-ol	$C_{15}H_{26}O$	FSTP	48.80	3.27	755	55
Neoisolongifolene	$C_{15}H_{22}$	STP	49.30	2.72	773	56
α-Santalol	$C_{15}H_{24}O$	FSTP	49.50	4.72	768	43
3,7-Cycloundecadien-1-ol, 1,5,5,8-tetramethyl-	$C_{15}H_{26}O$	FSTP	49.90	3.69	729	44
isoledene	$C_{15}H_{24}$	STP	50.10	3.47	672	36
β-Oplopenone	$C_{15}H_{24}O$	FSTP	50.10	3.49	803	60
Eudesmadien	$C_{15}H_{24}O$	FSTP	50.20	3.69	869	80
Taylorione	$C_{15}H_{22}O$	FSTP	50.50	3.95	594	40
Humulene epoxide I	$C_{15}H_{24}O$	FSTP	50.50	3.87	559	80
(1R,4S,5S)-1,8-Dimethyl-4-(prop-1-en-2-yl)spiro[4.5]dec-7-ene	$C_{15}H_{24}$	STP	51.00	4.03	579	90
2-((2S,4aR)-4a,8-Dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalen-2-yl)propan-2-ol	$C_{15}H_{26}O$	FSTP	51.10	3.75	509	60
γ-himachalene	$C_{15}H_{24}$	STP	51.10	4.17	564	81
4a(2H)-Naphthalenol, 1,3,4,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S,4R,4aS,8aR)-	$C_{15}H_{26}O$	FSTP	51.40	3.51	584	91
2(1H)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-7α-isopropyl-4aβ,8aβ-dimethyl-	$C_{15}H_{24}O$	FSTP	51.90	3.43	662	91
δ-Guaiene	$C_{15}H_{24}$	STP	52.00	3.75	669	93
β-Caryophyllene	$C_{15}H_{24}$	STP	52.10	4.09	574	32
τ-Cadinol	$C_{15}H_{26}O$	FSTP	52.10	3.71	640	42
Pogostol	$C_{15}H_{26}O$	FSTP	52.20	3.79	574	61
1H-Cycloprop[e]azulen-4-ol, decahydro-1,1,4,7-tetramethyl-, [1aR-(1aα,4β,4aβ,7α,7aβ,7bα)]-	$C_{15}H_{26}O$	FSTP	52.20	3.75	494	51
α-Guaiene	$C_{15}H_{24}$	STP	52.30	3.85	641	72
5β,7βH,10α-Eudesm-11-en-1α-ol	$C_{15}H_{26}O$	FSTP	52.40	0.42	651	48

Supplementary Table 2. (Cont.)

Compound Name	Mol. formula	Class.	RT I (min.)	RT II (sec.)	MF	P (%)
10s,11s-Himachala-3(12),4-diene	$C_{15}H_{24}$	STP	52.40	3.85	861	41
Rosifoliol	$C_{15}H_{26}O$	FSTP	52.50	4.05	591	51
Aristolene	$C_{15}H_{24}$	STP	52.50	4.19	731	58
Agarospirol	$C_{15}H_{26}O$	FSTP	52.80	4.07	525	37
Hedycaryol	$C_{15}H_{26}O$	FSTP	52.80	3.99	592	71
Maaliol	$C_{15}H_{26}O$	FSTP	52.80	4.09	690	56
Globulol	$C_{15}H_{26}O$	FSTP	52.80	4.31	634	59
Cubenol	$C_{15}H_{26}O$	FSTP	52.90	4.13	671	66
2-Naphthalenol, 2,3,4,4a,5,6,7-octahydro-1,4a-dimethyl-7-(2-hydroxy-1-methylethyl)	$C_{15}H_{26}O_2$	FSTP	52.90	4.52	593	77
β-BERGAMOTENE	$C_{15}H_{24}$	STP	52.90	4.48	700	58
Ledol	$C_{15}H_{26}O$	FSTP	52.90	5.81	735	65
1,2-Naphthalenedione, 3,8-dimethyl-5-(1-methylethyl)-	$C_{15}H_{16}O_2$	FSTP	53.00	4.58	835	31
Guaiol	$C_{15}H_{26}O$	FSTP	53.00	4.09	672	68
(1S,7S,8aR)-1,8a-Dimethyl-7-(prop-1-en-2-yl)-1,2,3,7,8,8a-hexahydronaphthalene	$C_{15}H_{22}$	STP	53.00	4.38	758	95
α-Bisabolol oxide B	$C_{15}H_{26}O_2$	FSTP	53.00	3.55	701	77
Terranol	$C_{15}H_{26}O$	FSTP	53.10	5.28	595	77
β-Longipinene	$C_{15}H_{24}$	STP	53.20	4.33	704	78
Cedrol	$C_{15}H_{26}O$	FSTP	53.30	4.33	712	91
α-coastal	$C_{15}H_{22}O$	FSTP	53.50	4.50	892	61
Zonarene	$C_{15}H_{24}$	STP	53.60	5.00	685	70
5-Azulenemethanol, 1,2,3,3a,4,5,6,7-octahydro-α,α,3,8-tetramethyl-, [3S-(3α,3aβ,5α)]-	$C_{15}H_{26}O$	FSTP	53.60	3.93	789	20
α-copaene	$C_{15}H_{24}O$	FSTP	53.90	4.44	552	41
Valerenal	$C_{15}H_{22}O$	FSTP	54.00	4.58	735	61
Sesquisabinene	$C_{15}H_{26}O$	FSTP	54.10	3.89	612	20
(3bR,4S,7aS)-7,7,8,8-Tetramethyloctahydro-2,3b-methanocyclopenta[1,3]cyclopropa[1,2]benzen-4-ol	$C_{15}H_{24}O$	FSTP	54.10	4.27	619	21
1-Buten-1-ol, 2-methyl-4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, formate, (E)-	$C_{15}H_{24}O_2$	FSTP	54.30	4.78	558	25
α.-Eudesmol	$C_{15}H_{24}O$	FSTP	54.60	4.21	641	31
Valerenol	$C_{15}H_{24}O$	FSTP	54.70	4.36	537	61

Supplementary Table 2. (Cont.)

Compound Name	Mol. formula	Class.	RT I (min.)	RT II (sec.)	MF	P (%)
α-isocomene	$C_{15}H_{24}$	STP	54.90	4.21	589	57
Acorenone B	$C_{15}H_{24}O$	FSTP	54.90	4.23	625	44
Valencene	$C_{15}H_{24}$	STP	54.90	4.21	602	49
Carvyl angelate	$C_{15}H_{22}O_2$	FSTP	55.00	3.77	641	34
Spathulenol	$C_{15}H_{24}O$	FSTP	55.00	4.33	641	61
Widdrenal	$C_{15}H_{22}O$	FSTP	55.00	4.42	605	72
Germacratrienol	$C_{15}H_{24}O$	FSTP	55.10	4.36	658	40
Epiprocurcumenol	$C_{15}H_{22}O$	FSTP	55.20	4.09	619	11
2,2,6-Trimethyl-1-(2-methyl-cyclobut-2-enyl)-hepta-4,6-dien-3-one	$C_{15}H_{22}O$	FSTP	55.20	4.09	694	61
2-((3R,3aR,3bS,4R,7R,7aS)-3,7-Dimethyloctahydro-1H-cyclopenta[1,3]cyclopropa[1,2]benzen-4-yl)propan-2-ol	$C_{15}H_{26}O$	FSTP	55.90	3.81	592	91
Solstitialin A	$C_{15}H_{20}O_5$	FSTP	56.00	4.82	714	59
Calarene epoxide	$C_{15}H_{24}O$	FSTP	56.10	5.24	725	51
α-Santalol	$C_{15}H_{24}O$	FSTP	56.10	4.05	760	42
α-cyperone	$C_{15}H_{20}O$	FSTP	56.60	4.38	459	55
2,2,5-Trimethyl-1-phenylhexa-3,4-dien-1-one	$C_{15}H_{18}O$	FSTP	56.80	4.82	627	64
6-Dehydropetasol	$C_{15}H_{20}O_2$	FSTP	56.80	4.86	683	41
(R)-1,5,8-Trimethyl-6,7,8,9-tetrahydronaphtho[2,1-b]furan	$C_{15}H_{18}O$	FSTP	57.20	4.72	714	4
Cycloseychellene	$C_{15}H_{24}$	STP	57.20	5.59	665	7
Elemol	$C_{15}H_{26}O$	FSTP	57.30	5.73	668	20
Thujopsene-l3	$C_{15}H_{24}$	STP	57.40	5.93	722	8
α-Hexylcinnamaldehyde	$C_{15}H_{20}O$	FSTP	57.50	4.44	726	20
Vetiselinenol	$C_{15}H_{24}O$	FSTP	57.50	4.52	692	4
Eudesmenol	$C_{15}H_{26}O$	FSTP	57.60	5.46	652	6
Khusimyl acid	$C_{15}H_{22}O$	FSTP	57.90	4.86	585	6
7-Isopropenyl-1,4a-dimethyl-4,4a,5,6,7,8-hexahydro-3H-naphthalen-2-one	$C_{15}H_{22}O$	FSTP	58.00	4.64	669	10
3,7-Cyclodecadien-1-one, 3,7-dimethyl-10-(1-methylethylidene)-, (E,E)-	$C_{15}H_{22}O$	FSTP	58.20	5.04	721	15
5(1H)-Azulenone, 2,4,6,7,8,8a-hexahydro-3,8-dimethyl-4-(1-methylethylidene)-, (8S-cis)-	$C_{15}H_{22}O$	FSTP	58.30	5.63	615	11
Valerenic acid	$C_{15}H_{22}O_2$	FSTP	58.60	5.73	741	9

Supplementary Table 2. (Cont.)

Compound Name	Mol. formula	Class.	RT I (min.)	RT II (sec.)	MF	P (%)
6-Isopropenyl-4,8a-dimethyl-4a,5,6,7,8,8a-hexahydro-1H-naphthalen-2-one	$C_{15}H_{22}O$	FSTP	58.70	5.14	676	13
1H-3a,7-Methanoazulene-6-methanol, 2,3,4,7,8,8a-hexahydro-3,8,8-trimethyl-, [3R-(3α,3aβ,7β,8aα)]-	$C_{15}H_{24}O$	FSTP	58.80	0.69	729	12
4-(3,3-Dimethyl-but-1-ynyl)-4-hydroxy-2,6,6-trimethylcyclohex-2-enone	$C_{15}H_{22}O_2$	FSTP	58.90	5.32	687	4
(S,Z)-2-Methyl-6-(p-tolyl)hept-2-en-1-ol	$C_{15}H_{22}O$	FSTP	58.90	4.94	677	9
7-(1,3-Dimethylbuta-1,3-dienyl)-1,6,6-trimethyl-3,8-dioxatricyclo[5.1.0.0(2,4)]octane	$C_{15}H_{22}O_2$	FSTP	59.40	4.98	652	6
Valerenic acid	$C_{15}H_{22}O_2$	FSTP	58.60	5.73	741	9
6-Isopropenyl-4,8a-dimethyl-4a,5,6,7,8,8a-hexahydro-1H-naphthalen-2-one	$C_{15}H_{22}O$	FSTP	58.70	5.14	676	13
1H-3a,7-Methanoazulene-6-methanol, 2,3,4,7,8,8a-hexahydro-3,8,8-trimethyl-, [3R-(3α,3aβ,7β,8aα)]-	$C_{15}H_{24}O$	FSTP	58.80	0.69	729	12
γ-Gurjunenepoxide	$C_{15}H_{24}O$	FSTP	59.50	4.64	690	19
(E,Z)-α-Farnesene	$C_{15}H_{24}$	STP	59.80	0.26	657	8
1(2H)Phenanthrenone, 3,4,4a,9,10,10a-hexahydro-4a-methyl-	$C_{15}H_{18}O$	FSTP	60.00	4.80	759	10
(R)-3-Methylene-6-((S)-1,2,2-trimethylcyclopentyl)cyclohex-1-ene	$C_{15}H_{24}$	STP	60.20	5.95	763	5
1H-Benzocyclohepten-7-ol, 2,3,4,4a,5,6,7,8-octahydro-1,1,4a,7-tetramethyl-, cis-	$C_{15}H_{26}O$	FSTP	60.30	5.93	674	12
Ylangenal	$C_{15}H_{22}O$	FSTP	60.40	5.77	516	22
Proximadiol	$C_{15}H_{28}O_2$	FSTP	60.60	5.16	711	23
3H-Cyclodeca[b]furan-2-one, 4,9-dihydroxy-6-methyl-3,10-dimethylene-3a,4,7,8,9,10,11,11a-octahydro-	$C_{15}H_{20}O_4$	FSTP	60.80	4.70	666	10
Nootkatone	$C_{15}H_{22}O$	FSTP	61.00	5.28	740	12
β-acoradienol	$C_{15}H_{24}O$	FSTP	61.00	4.23	689	29
2H-Cyclopropa[a]naphthalen-2-one, 1,1a,4,5,6,7,7a,7b-octahydro-1,1,7,7a-tetramethyl-, (1aα,7α,7aα,7bα)-	$C_{15}H_{22}O$	FSTP	61.00	5.20	703	29
Dehydrofukinone	$C_{15}H_{22}O$	FSTP	61.10	5.38	674	41
Caryophylladienol	$C_{15}H_{26}O$	FSTP	61.10	6.01	667	16
Elemadiol	$C_{15}H_{26}O_2$	FSTP	61.30	4.82	656	14
β-Eudesmol	$C_{15}H_{26}O$	FSTP	61.60	5.12	656	12
4,4-Dimethyl-3-(3-methylbut-2-enylidene)octane-2,7-dione	$C_{15}H_{24}O_2$	FSTP	61.70	5.63	584	7
4,6,6-Trimethyl-2-(3-methylbuta-1,3-dienyl)-3-oxatricyclo[5.1.0.0(2,4)]octane	$C_{15}H_{22}O$	FSTP	61.90	6.09	609	15
Cyperotundone	$C_{15}H_{22}O$	FSTP	62.10	4.88	677	7
2-Cyclohexene-1-carboxaldehyde, 2,6-dimethyl-6-(4-methyl-3-pentenyl)-	$C_{15}H_{24}O$	FSTP	62.20	4.33	618	25
6-Isopropenyl-4,8a-dimethyl-1,2,3,5,6,7,8,8a-octahydro-naphthalen-2-ol	$C_{15}H_{24}O$	FSTP	62.60	1.96	666	18

Supplementary Table 2. (Cont.)

Compound Name	Mol. formula	Class.	RT I (min.)	RT II (sec.)	MF	P (%)
Hexahydronaphthalenone	$C_{15}H_{22}O$	FSTP	62.60	5.83	708	11
Isovelleral	$C_{15}H_{20}O_2$	FSTP	62.70	5.77	572	94
6-(p-Tolyl)-2-methyl-2-heptenol, trans-	$C_{15}H_{22}O$	FSTP	62.70	0.99	675	18
1(2H)-Naphthalenone, octahydro-4,8a-dimethyl-6-(1-methylethenyl)-, (4α,4aβ,6α,8aβ)-	$C_{15}H_{24}O$	FSTP	63.00	0.87	608	65
Alloaromadendrene oxide	$C_{15}H_{24}O$	FSTP	63.00	5.08	639	10
Uvidin C	$C_{15}H_{26}O_2$	FSTP	63.10	5.85	553	13
Costal	$C_{15}H_{22}O$	FSTP	63.10	5.95	590	15
1,1,4,7-Tetramethyl-1a,2,3,4,6,7,7a,7b-octahydro-1H-cyclopropa[e]azulene	$C_{15}H_{24}$	STP	63.20	5.08	677	17
α-Farnesene	$C_{15}H_{24}$	STP	63.50	0.40	659	15
Isoaromadendrene epoxide	$C_{15}H_{24}O$	FSTP	63.50	5.24	529	32
2-((2R,4aR,8aR)-4a,8-Dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalen-2-yl)prop-2-en-1-ol	$C_{15}H_{24}O$	FSTP	63.50	5.20	580	40
4-Isopropyl-6-methyl-3,4,4a,7,8,8a-hexahydronaphthalene-1-carbaldehyde	$C_{15}H_{22}O$	FSTP	63.50	5.20	547	15
Bergamoto	$C_{15}H_{24}O$	FSTP	63.80	0.73	607	23
Silphiperfola-4,7(14)-diene	$C_{15}H_{22}$	STP	63.80	0.65	504	25
1-Cyclopropene-1-pentanol, α,ε,ε,2-tetramethyl-3-(1-methylethenyl)-	$C_{15}H_{26}O$	FSTP	63.90	5.54	698	15
Ledene oxide	$C_{15}H_{24}O$	FSTP	64.30	0.77	552	7
Carabrol	$C_{15}H_{22}O_3$	FSTP	64.30	4.72	549	14
ɣ-gurjunene	$C_{15}H_{24}$	STP	64.30	5.20	534	26
10-Epigazaniolide	$C_{15}H_{18}O_2$	FSTP	64.40	1.55	593	15
14-Hydroxycaryophyllene	$C_{15}H_{24}O$	FSTP	64.40	5.65	557	9
7-Tetracyclo[6.2.1.0(3.8)0(3.9)]undecanol, 4,4,11,11-tetramethyl-	$C_{15}H_{24}O$	FSTP	64.80	5.87	562	24
Isospathulenol	$C_{15}H_{24}O$	FSTP	65.50	5.50	653	29
2,4a,5,8a-Tetramethyl-1,2,3,4,4a,7,8,8a-octahydronaphthalen-1-yl formate (isomer 1)	$C_{15}H_{24}O_2$	FSTP	65.50	0.52	547	11
Cumanin	$C_{15}H_{22}O_4$	FSTP	66.50	1.88	528	20
11,11-Dimethyl-4,8-dimethylenebicyclo[7.2.0]undecan-3-ol	$C_{15}H_{24}O$	FSTP	66.70	0.58	598	5
(2S,4aR,8aR)-4a,8-Dimethyl-2-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,8a-octahydronaphthalene	$C_{15}H_{24}$	STP	66.80	0.65	549	46
α-Panasinsen	$C_{15}H_{24}$	STP	66.80	0.62	547	26
3-Cyclohexene-1-ethanol, α-ethenyl-α,3-dimethyl-6-(1-methylethylidene)-	$C_{15}H_{24}O$	FSTP	66.90	5.56	556	28

Supplementary Table 2. (Cont.)

Compound Name	Mol. formula	Class.	RT I (min.)	RT II (sec.)	MF	P (%)
2,3,3-Trimethyl-2-(3-methylbuta-1,3-dienyl)-6-methylenecyclohexanone	$C_{15}H_{22}O$	FSTP	66.90	6.19	686	19
Jaeskeanadiol	$C_{15}H_{26}O_2$	FSTP	67.00	1.09	590	60
Parthenolide	$C_{15}H_{20}O_3$	FSTP	67.00	6.13	614	31
Valerenolic acid	$C_{15}H_{22}O_3$	FSTP	67.00	5.57	556	91
7-(hydroxymethyl)-2,2,4-trimethyl-3,3a,4,8a-tetrahydro-1H-azulen-6-yl]methanol	$C_{15}H_{24}O_2$	FSTP	67.10	6.13	578	29
7-Oxabicyclo[4.1.0]heptane, 2,2,6-trimethyl-1-(3-methyl-1,3-butadienyl)-5-methylene-	$C_{15}H_{22}O$	FSTP	67.10	6.11	583	26
α-Bisabolene epoxide	$C_{15}H_{24}O$	FSTP	67.30	6.21	591	50
Aromadendrene oxide	$C_{15}H_{24}O$	FSTP	67.30	5.85	610	66
Squamulosone	$C_{15}H_{22}O$	FSTP	67.60	5.97	570	64
Verrucarol	$C_{15}H_{22}O_4$	FSTP	67.80	0.40	680	79
12-Hydroxy-6-epi-albrassitriol	$C_{15}H_{26}O_2$	FSTP	67.90	6.09	596	52
Curcumenol	$C_{15}H_{22}O_2$	FSTP	67.90	0.44	638	28
Shizukanolide	$C_{15}H_{18}O_2$	FSTP	68.20	0.18	600	30
Longiverbenone	$C_{15}H_{22}O$	FSTP	68.30	6.21	598	59
Asperilin	$C_{15}H_{20}O_3$	FSTP	68.30	5.75	619	65
Dihydrocolumellarin	$C_{15}H_{22}O_2$	FSTP	68.50	5.93	912	30
Solavetivone	$C_{15}H_{22}O$	FSTP	68.60	6.15	593	71
Occidentalol	$C_{15}H_{24}O$	FSTP	68.60	3.87	727	39
β-Cyclodihydrocostunolide	$C_{15}H_{22}O_2$	FSTP	68.70	0.62	565	66
Arctiol	$C_{15}H_{26}O_2$	FSTP	68.80	3.75	585	58
γ-Elemene	$C_{15}H_{24}$	STP	69.10	5.83	604	65
(2R,3R,4aR,5S,8aS)-2-Hydroxy-4a,5-dimethyl-3-(prop-1-en-2-yl)-2,3,4,4a,5,6-hexahydronaphthalen-1(8aH)-one	$C_{15}H_{22}O_2$	FSTP	69.10	0.36	605	35
α-Humulen-14-oic acid	$C_{15}H_{22}O_2$	FSTP	69.30	0.79	603	54
Nordeoxynivalenol	$C_{15}H_{22}O_3$	FSTP	69.30	1.33	654	33
Humulenol-II	$C_{15}H_{24}O$	FSTP	69.40	6.17	654	61
Velleral	$C_{15}H_{20}O_2$	FSTP	69.50	0.46	585	40
α-selinene	$C_{15}H_{24}O$	FSTP	69.60	6.19	628	19
(3R,3aR,5R,6R,7aR)-3,6-Dimethyl-5-(prop-1-en-2-yl)-6-vinylhexahydrobenzofuran-2(3H)-one	$C_{15}H_{22}O_2$	FSTP	69.70	5.81	638	48

Supplementary Table 2. (Cont.)

Compound Name	Mol. formula	Class.	RT I (min.)	RT II (sec.)	MF	P (%)
Calarene	$C_{15}H_{24}$	STP	69.70	4.07	609	71
4aH-Cycloprop[e]azulen-4a-ol, decahydro-1,1,4,7-tetramethyl-, [1aR-(1aα,4β,4aβ,7α,7aβ,7bα)]-	$C_{15}H_{26}O$	FSTP	70.10	1.39	479	25
Isoalantolactone	$C_{15}H_{20}O_2$	FSTP	70.50	1.27	610	18
Aromaticin	$C_{15}H_{20}O_2$	FSTP	70.60	6.19	694	37
(E)-6-Hydroxy-2-methyl-6-(4-methylphenyl)hept-2-enoic acid	$C_{15}H_{20}O_3$	FSTP	70.70	2.36	619	81
Ambrosin	$C_{15}H_{18}O_3$	FSTP	70.80	1.21	488	64
(2S)-2-((1R,3aR,4R,5S,7aS)-1,7a-Dimethyloctahydro-1H-1,2,4-(epimethanetriyl)inden-5-yl)propan-1-ol	$C_{15}H_{24}O$	FSTP	70.80	3.81	639	97
Reynosin	$C_{15}H_{20}O_3$	FSTP	70.80	0.69	493	81
β-Cyclocostunolide	$C_{15}H_{20}O_2$	FSTP	70.90	1.43	497	94
Velleral	$C_{15}H_{20}O_2$	FSTP	69.50	0.46	585	40
α-selinene	$C_{15}H_{24}O$	FSTP	69.60	6.19	628	19
6-(2-Hydroxypropan-2-yl)-4,8a-dimethyl-2,3,4,6,7,8-hexahydro-1H-naphthalen-1-ol	$C_{15}H_{26}O_2$	FSTP	71.30	1.90	641	44
2H-2,4a-Ethanonaphthalen-8(5H)-one, hexahydro-2,5,5-trimethyl-	$C_{15}H_{24}O$	FSTP	71.40	0.28	632	49
2,5-Dimethylbenzophenone	$C_{15}H_{14}O$	FSTP	71.40	0.69	738	20
4a,7-Methano-4aH-naphth[1,8a-b]oxirene, octahydro-4,4,8,8-tetramethyl-	$C_{15}H_{24}O$	FSTP	71.40	0.36	632	61
2,4-Dimethylbenzophenone	$C_{15}H_{14}O$	FSTP	71.40	0.69	654	22
(1S,4aR,7R)-1,4a-Dimethyl-7-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene	$C_{15}H_{24}$	STP	71.50	1.31	567	86
Bohlmann k2631	$C_{15}H_{20}O_2$	FSTP	71.50	1.35	668	18
Nootkaton epoxide	$C_{15}H_{22}O_2$	FSTP	71.70	1.09	682	21
11,13-Dihydrolactucin	$C_{15}H_{18}O_3$	FSTP	71.80	5.73	869	80
Isopetasol	$C_{15}H_{22}O_2$	FSTP	72.20	1.07	675	47
α-Eudesmol	$C_{15}H_{22}O_2$	FSTP	72.40	1.03	675	48
Limonenol	$C_{15}H_{24}O_2$	FSTP	72.70	1.96	535	83
Tourneforin	$C_{15}H_{18}O_3$	FSTP	72.80	2.34	782	42
1-Penten-3-one, 4-methyl-1-[2,6,6-trimethyl-2-cyclohexen-1-yl]-	$C_{15}H_{24}O$	FSTP	72.90	3.61	720	28
Spirafolide	$C_{15}H_{18}O_3$	FSTP	72.90	2.46	701	78
7-Methyl-3-methylidene-6-(3-oxobutyl)-4,7,8,8a-tetrahydro-3aH-cyclohepta[b]furan-2-one	$C_{15}H_{20}O_3$	FSTP	73.30	5.97	755	91
Hydroxymuurolene	$C_{15}H_{24}O$	FSTP	73.60	6.33	649	81

Supplementary Table 2. (Cont.)

Compound Name	Mol. formula	Class.	RT I (min.)	RT II (sec.)	MF	P (%)
Cedrandiol	$C_{15}H_{26}O_2$	FSTP	73.90	1.41	545	21
α-cedrene	$C_{15}H_{24}$	STP	74.00	2.04	698	82
4,7-Methanofuro[3,2-c]oxacycloundecin-6(4H)-one, 7,8,9,12-tetrahydro-3,11-dimethyl-	$C_{15}H_{18}O_3$	FSTP	74.00	3.09	717	72
Germacrene D	$C_{15}H_{24}$	STP	74.20	1.23	774	76
Phomenone	$C_{15}H_{20}O_4$	FSTP	74.20	0.89	525	94
Shyobunol	$C_{15}H_{26}O$	FSTP	75.40	0.54	710	93
1,8-Cyclopentadecadiyne	$C_{15}H_{22}$	STP	76.00	0.46	750	21
3-Oxo-10(14)-epoxyguai-11(13)-en-6,12-olide	$C_{15}H_{18}O_3$	FSTP	76.20	3.17	742	54
2,7-Cyclodecadiene-1-methanol, α,α,4,8-tetramethyl-	$C_{15}H_{26}O$	FSTP	76.60	1.43	546	91
Aureonitol	$C_{15}H_{20}O_3$	FSTP	76.70	4.60	551	92
7-Methoxy-3,4-dihydro-1(2H)-phenanthrenone	$C_{15}H_{14}O_2$	FSTP	77.20	2.12	488	48
Santamarine	$C_{15}H_{20}O_3$	FSTP	77.30	3.13	750	92
Spirafolide	$C_{15}H_{18}O_3$	FSTP	72.90	2.46	701	78
7-Methyl-3-methylidene-6-(3-oxobutyl)-4,7,8,8a-tetrahydro-3aH-cyclohepta[b]furan-2-one	$C_{15}H_{20}O_3$	FSTP	73.30	5.97	755	91
Hydroxymuurolene	$C_{15}H_{24}O$	FSTP	73.60	6.33	649	81
Cedrandiol	$C_{15}H_{26}O_2$	FSTP	73.90	1.41	545	21
α-cedrene	$C_{15}H_{24}$	STP	74.00	2.04	698	82
4,7-Methanofuro[3,2-c]oxacycloundecin-6(4H)-one, 7,8,9,12-tetrahydro-3,11-dimethyl-	$C_{15}H_{18}O_3$	FSTP	74.00	3.09	717	72
Graveolide	$C_{15}H_{20}O_3$	FSTP	77.30	2.12	549	81
1-n-Pentyladamantane	$C_{15}H_{26}$	STP	78.70	2.86	741	94
Ivalin	$C_{15}H_{20}O_4$	FSTP	79.20	1.61	552	51
Costunolide	$C_{15}H_{20}O_2$	FSTP	79.40	1.77	752	45
Achalensolide	$C_{15}H_{18}O_3$	FSTP	80.40	2.74	580	72
T-2 Tetraol	$C_{15}H_{22}O_6$	FSTP	80.70	1.31	836	32
Gazaniolide	$C_{15}H_{18}O_2$	FSTP	80.80	5.65	565	36
Cyperanic acid	$C_{15}H_{22}O_4$	FSTP	80.90	3.39	629	95
Pallensin	$C_{15}H_{20}O_4$	FSTP	82.10	2.52	544	40
Caryophyllene oxide	$C_{15}H_{24}O$	FSTP	82.40	3.65	717	36

Supplementary Table 2. (Cont.)

Compound Name	Mol. formula	Class.	RT I (min.)	RT II (sec.)	MF	P (%)
δ-Elemene	$C_{15}H_{24}$	STP	82.80	4.01	561	96
6-Hydroxy-5a,9-dimethyl-3-methylidene-4,5,6,7,9a,9b-hexahydro-3aH-benzo[g][1]benzofuran-2-one	$C_{15}H_{20}O_3$	FSTP	82.90	3.17	887	25
Achillin	$C_{15}H_{18}O_3$	FSTP	86.90	3.89	929	51
Achillicin	$C_{15}H_{18}O_3$	FSTP	86.90	4.11	729	32
5-[2-(Benzyloxy)ethyl]cyclohex-2-en-1-one	$C_{15}H_{18}O_2$	FSTP	87.40	4.03	831	95
Pentadecanal	$C_{15}H_{30}O$	FSTP	87.60	3.17	772	97
3,7,7-Trimethyl-8-(2-methyl-propenyl)-bicyclo[4.2.0]oct-2-ene	$C_{15}H_{24}$	STP	88.90	5.12	615	66
sesquithujene	$C_{15}H_{24}$	STP	91.80	3.67	541	71
2-Ethyl-5-methyl-2-phenyl-4-hexen-1-ol	$C_{15}H_{22}O$	FSTP	92.40	1.71	538	91
1-(2-Methylenecyclohexyl)-1-phenylethanol	$C_{15}H_{20}O$	FSTP	95.00	3.39	587	78
1-Cyclohexylnonene	$C_{15}H_{28}$	STP	95.10	3.27	580	40
1,4-Dimethyl 2-[(3,4-dimethoxyphenyl)methyl]butanedioate	$C_{15}H_{20}O_6$	FSTP	100.80	5.93	578	27
3-Pentadecanone	$C_{15}H_{30}O$	FSTP	101.10	3.37	572	97
1-Methylene-2b-hydroxymethyl-3,3-dimethyl-4b-(3-methylbut-2-enyl)-cyclohexane	$C_{15}H_{26}O$	FSTP	102.50	4.03	784	81
2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-, (Z,E)-	$C_{15}H_{26}O$	FSTP	102.60	3.99	769	52
2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-	$C_{15}H_{26}O$	FSTP	102.60	3.85	608	52
Ylangenol	$C_{15}H_{24}O$	FSTP	103.10	1.15	541	96
2-Pentadecanone	$C_{15}H_{30}O$	FSTP	104.60	3.49	441	26
1-Formyl-2,2,6-trimethyl-3-cis-(3-methylbut-2-enyl)-5-cyclohexene	$C_{15}H_{24}O$	FSTP	107.30	4.74	582	60
1,7-Dimethyl-4-(1-methylethyl)cyclodecane	$C_{15}H_{30}$	STP	108.90	3.11	530	43
7-Oxabicyclo[4.1.0]heptane, 1-(1,3-dimethyl-1,3-butadienyl)-2,2,6-trimethyl-, (E)-	$C_{15}H_{24}O$	FSTP	110.50	0.93	574	97
1H-Indene, 2,3,3a,4,7,7a-hexahydro-2,2,4,4,7,7-hexamethyl-	$C_{15}H_{26}$	STP	113.40	2.02	597	32
5,7-Decadien-3-yne, 2,9-dihydroxy-5-(1-hydroxy-1-methylethyl)-2,9-dimethyl-, (Z,E)-	$C_{15}H_{24}O_3$	FSTP	114.60	1.51	545	67
Guaiadiene	$C_{15}H_{24}$	STP	118.10	1.17	607	96
Anisole	$C_{15}H_{24}O$	FSTP	120.90	4.64	667	72

Supplementary Table 3. Sesquiterpenoids identified across agarwood distillates (Oudh) samples using GCxGC-TOF/MS.

Compound Name	Mol. formula	Clas.	RT I (min)	RT II (sec)	MF	P (%)
Aureonitol	$C_{15}H_{20}O_3$	FSTP	33.50	3.51	787	60
1,2-Dihydrothujopsene-(I1)	$C_{15}H_{26}$	STP	34.30	4.03	889	63
(8R,8aS)-8,8a-Dimethyl-2-(propan-2-ylidene)-1,2,3,7,8,8a-hexahydronaphthalene	$C_{15}H_{22}$	STP	36.60	2.78	832	95
Germacrene D	$C_{15}H_{24}$	STP	36.60	2.44	432	92
Copaene	$C_{15}H_{24}$	STP	36.70	2.46	799	56
α-Bergamotene	$C_{15}H_{24}$	STP	37.30	2.54	933	81
4b,5,6,7,8,8a,9,10-Octahydro-1-methylphenanthrene	$C_{15}H_{20}$	FSTP	37.90	3.25	471	79
(R)-1-Methyl-4-(6-methylhept-5-en-2-yl)cyclohexa-1,4-diene	$C_{15}H_{24}$	STP	38.00	3.09	662	71
isoledene	$C_{15}H_{24}$	STP	38.70	2.56	916	65
1H-Cycloprop[e]azulene, 1a,2,3,4,4a,5,6,7b-octahydro-1,1,4,7-tetramethyl-, [1aR-(1aα,4α,4aβ,7bα)]-	$C_{15}H_{24}$	STP	38.70	2.58	944	69
1H-Cyclopropa[a]naphthalene, decahydro-1,1,3a-trimethyl-7-methylene-, [1aS-(1aα,3aα,7aβ,7bα)]-	$C_{15}H_{24}$	STP	38.80	3.13	695	54
Cyperene	$C_{15}H_{24}$	STP	38.80	2.68	738	68
Bicyclo[5.3.0]decane, 2-methylene-5-(1-methylvinyl)-8-methyl-	$C_{15}H_{24}$	STP	39.00	2.64	712	64
α-Bergamotene	$C_{15}H_{24}$	STP	39.00	2.76	736	41
Cubenene	$C_{15}H_{24}$	STP	39.20	2.74	889	36
1H-3a,7-Methanoazulene, 2,3,4,7,8,8a-hexahydro-3,6,8,8-tetramethyl-, [3R-(3α,3aβ,7β,8aα)]-	$C_{15}H_{24}$	STP	39.30	2.78	588	81
Caryophyllene	$C_{15}H_{24}$	STP	39.40	2.72	947	83
6-Methyl-2-(4-methylcyclohex-3-en-1-yl)hepta-1,5-dien-4-ol	$C_{15}H_{24}O$	FSTP	39.60	2.94	655	24
3-methyl-5-(2,6-dimethylheptyl)-1,5-Pent-2-enolide	$C_{15}H_{26}O_2$	FSTP	39.60	3.97	734	19
Bicyclo[4.1.0]-3-heptene, 2-isopropenyl-5-isopropyl-7,7-dimethyl-	$C_{15}H_{24}$	STP	39.60	2.82	915	56
1,3,7,11-Cyclotetradecatetraene, 2-methyl-	$C_{15}H_{22}$	STP	39.80	3.13	733	62
γ-Elemene	$C_{15}H_{24}$	STP	40.10	3.55	790	48
β-Calarene	$C_{15}H_{24}$	STP	40.20	2.80	769	62
4a,5-Dimethyl-3-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalen-1-ol	$C_{15}H_{24}O$	FSTP	40.30	3.15	640	28
α-Guaiene	$C_{15}H_{24}$	STP	40.60	2.62	604	41
2-Pentadecen-4-yne, (Z)-	$C_{15}H_{26}$	STP	40.60	4.23	862	98
6,10-Dodecadien-1-yn-3-ol, 3,7,11-trimethyl-	$C_{15}H_{24}O$	FSTP	40.80	3.15	841	41
Caryophyllenyl alcohol	$C_{15}H_{26}O$	FSTP	41.00	3.67	754	72

Supplementary Table 3. (Cont.)

Compound Name	Mol. formula	Clas.	RT I (min)	RT II (sec)	MF	P (%)
Cycloisolongifolene	$C_{15}H_{24}$	STP	41.30	3.04	846	41
Humulene	$C_{15}H_{24}$	STP	41.40	2.88	588	44
6,10-Dodecadien-3-ol, 3,7,11-trimethyl-	$C_{15}H_{28}$	FSTP	41.50	2.32	666	29
1,5-Cyclodecadiene, 1,5-dimethyl-8-(1-methylethenyl)-, [S-(Z,E)]-	$C_{15}H_{24}$	STP	41.50	3.08	719	49
1R,3Z,9S-4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]undec-3-ene	$C_{15}H_{24}$	STP	41.50	2.84	630	50
Prezizaene	$C_{15}H_{24}$	STP	41.60	3.11	787	24
1H-3a,7-Methanoazulene, octahydro-1,4,9,9-tetramethyl-, (1α,3aα,4β,7α,8aβ)-	$C_{15}H_{26}$	STP	41.80	2.70	248	95
Rotundene	$C_{15}H_{24}$	STP	41.90	3.04	841	43
Alloaromadendrene	$C_{15}H_{24}$	STP	41.90	2.90	764	31
Aromandendrene	$C_{15}H_{24}$	STP	41.90	2.88	679	49
β-Caryophyllene	$C_{15}H_{24}$	STP	42.00	2.98	828	33
Sesquithujene	$C_{15}H_{24}$	STP	42.10	2.94	637	67
β-Acoradiene	$C_{15}H_{24}$	STP	42.30	2.94	706	33
(4R,4aS,6S)-4,4a-Dimethyl-6-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene	$C_{15}H_{24}$	STP	42.40	2.90	828	52
(R)-3-Methylene-6-((S)-1,2,2-trimethylcyclopentyl)cyclohex-1-ene	$C_{15}H_{24}$	STP	42.50	3.93	749	49
ɣ-Gurjunene	$C_{15}H_{24}$	STP	42.50	2.86	542	10
4a,8-Dimethyl-2-(prop-1-en-2-yl)-1,2,3,4,4a,5,6,7-octahydronaphthalene	$C_{15}H_{24}$	STP	42.60	2.84	545	42
Cedrene oxide	$C_{15}H_{24}O$	FSTP	42.70	3.57	661	33
Spathulenol	$C_{15}H_{24}O$	FSTP	42.70	3.55	722	14
β-Acoradienol	$C_{15}H_{24}O$	FSTP	42.70	3.19	616	27
α-Eremophilane	$C_{15}H_{28}$	STP	42.80	2.62	762	60
1,2,4-Metheno-1H-indene, octahydro-1,7a-dimethyl-5-(1-methylethyl)-, [1S-(1α,2α,3aβ,4α,5α,7aβ,8S*)]-	$C_{15}H_{24}$	STP	42.80	2.96	558	11
Cedrenol	$C_{15}H_{24}O$	FSTP	42.80	3.00	837	84
α-Amorphene	$C_{15}H_{24}$	STP	42.80	3.02	679	98
Zizanene	$C_{15}H_{24}$	STP	42.90	3.00	808	35
Muuroladiene	$C_{15}H_{24}$	STP	43.10	3.93	714	48
1,4-Dimethyl-7-(prop-1-en-2-yl)decahydroazulen-4-ol	$C_{15}H_{26}O$	FSTP	43.20	3.09	734	48
Aristolochene	$C_{15}H_{24}$	STP	43.20	3.02	833	65

Supplementary Table 3. (Cont.)

Compound Name	Mol. formula	Clas.	RT I (min)	RT II (sec)	MF	P (%)
Selinadiene	$C_{15}H_{24}$	STP	43.20	3.06	805	66
β-Selinene	$C_{15}H_{24}$	STP	43.40	3.06	785	41
Epoxycalamenene	$C_{15}H_{20}O$	FSTP	43.50	3.81	581	41
β-Vetispirene	$C_{15}H_{22}$	STP	43.60	3.21	659	91
β-Longipinene	$C_{15}H_{24}$	STP	43.70	3.08	731	42
δ-Guaiene	$C_{15}H_{24}$	STP	44.00	3.04	589	31
Valencene	$C_{15}H_{24}$	STP	44.00	2.92	811	21
α-Farnesene	$C_{15}H_{24}$	STP	44.00	3.65	690	81
Muurolane	$C_{15}H_{24}$	STP	44.00	2.96	511	62
Guaiadiene	$C_{15}H_{24}$	STP	44.40	3.25	759	53
Cuparene	$C_{15}H_{22}$	STP	44.50	3.75	649	91
α-Curcumene	$C_{15}H_{22}$	STP	44.60	3.69	462	59
1,1,4,7-Tetramethyldecahydro-1H-cyclopropa[e]azulene-4,7-diol	$C_{15}H_{26}O_2$	FSTP	44.70	3.31	752	69
Humulenol-II	$C_{15}H_{24}O$	FSTP	44.90	3.29	928	49
Nootkatene	$C_{15}H_{22}$	STP	45.10	3.23	769	21
γ-Muurolene	$C_{15}H_{24}$	STP	45.20	3.15	778	54
4aH-Cycloprop[e]azulen-4a-ol, decahydro-1,1,4,7-tetramethyl-, [1aR-(1aα,4β,4aβ,7α,7aβ,7bα)]-	$C_{15}H_{26}O$	FSTP	45.20	2.96	687	44
Carotol	$C_{15}H_{26}O$	FSTP	45.20	3.11	563	41
Caparratriene	$C_{15}H_{26}$	STP	45.30	4.38	770	61
α-Panasinsen	$C_{15}H_{24}$	STP	45.30	3.11	791	24
β-Cadinene	$C_{15}H_{24}$	STP	45.40	3.15	676	22
1-Isopropyl-4,7-dimethyl-1,2,3,5,6,8a-hexahydronaphthalene	$C_{15}H_{24}$	STP	45.40	3.06	607	95
Calamenene	$C_{15}H_{22}$	STP	45.50	3.47	634	12
1-Isopropyl-4,7-dimethyl-1,2,3,5,6,8a-hexahydronaphthalene	$C_{15}H_{24}$	STP	45.60	3.13	738	19
α-Muurolene	$C_{15}H_{24}O$	FSTP	45.60	3.63	745	52
γ-Vetivenene	$C_{15}H_{22}$	STP	45.70	3.37	530	10
Kessane	$C_{15}H_{26}O$	FSTP	45.80	3.29	652	12
Cyperene epoxide	$C_{15}H_{24}O$	FSTP	46.10	3.75	614	15

Supplementary Table 3. (Cont.)

Compound Name	Mol. formula	Clas.	RT I (min)	RT II (sec)	MF	P (%)
α-Cadinene	$C_{15}H_{24}$	STP	46.20	3.06	705	17
(4aR,8aS)-4a-Methyl-1-methylene-7-(propan-2-ylidene)decahydronaphthalene	$C_{15}H_{24}$	STP	46.30	3.21	621	26
Himachalene	$C_{15}H_{22}$	STP	46.30	3.65	586	18
4-Isopropyl-6-methyl-1-methylene-1,2,3,4-tetrahydronaphthalene	$C_{15}H_{20}$	FSTP	46.60	3.75	611	31
α-Calacorene	$C_{15}H_{20}$	FSTP	46.60	3.89	780	62
Cyclopentadecadiyne	$C_{15}H_{22}$	STP	46.80	5.65	754	36
Selina-3,7(11)-diene	$C_{15}H_{24}$	STP	46.80	3.19	743	35
Longiverbenone	$C_{15}H_{22}O$	FSTP	46.90	3.85	725	15
2-(4a,8-Dimethyl-1,2,3,4,4a,5,6,7-octahydro-naphthalen-2-yl)-prop-2-en-1-ol	$C_{15}H_{24}O$	FSTP	47.00	3.87	795	53
α-Agarofuran	$C_{15}H_{24}O$	FSTP	47.00	3.93	591	27
α-Calacorene	$C_{15}H_{20}$	FSTP	47.00	4.07	720	18
(3aS,8aS)-6,8a-Dimethyl-3-(propan-2-ylidene)-1,2,3,3a,4,5,8,8a-octahydroazulene	$C_{15}H_{24}$	STP	47.10	4.29	601	20
Coronene	$C_{15}H_{20}$	FSTP	47.30	3.75	793	77
Nerolidol	$C_{15}H_{26}O$	FSTP	47.40	3.08	724	43
1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (E)-	$C_{15}H_{26}O$	FSTP	47.40	3.00	666	14
Hydroxycaryophyllene	$C_{15}H_{24}O$	FSTP	47.70	3.59	702	13
α-Vetivone	$C_{15}H_{22}O$	FSTP	47.70	3.63	779	37
Bicyclo[4.4.0]dec-2-ene-4-ol, 2-methyl-9-(prop-1-en-3-ol-2-yl)-	$C_{15}H_{24}O_2$	FSTP	47.80	3.65	729	18
Bicyclo[4.4.0]dec-5-ene, 1,5-dimethyl-3-hydroxy-8-(1-methylene-2-hydroxyethyl-1)-	$C_{15}H_{24}O_2$	FSTP	47.80	3.79	817	69
4(15)-Selinene-11,12-diol	$C_{15}H_{26}O_2$	FSTP	48.00	4.76	684	18
1H-Cycloprop[e]azulene, decahydro-1,1,4,7-tetramethyl-, [1aR-(1aα,4β,4aβ,7β,7aβ,7bα)]-	$C_{15}H_{26}$	STP	48.10	4.40	702	14
2H-3,9a-Methano-1-benzoxepin, octahydro-2,2,5a,9-tetramethyl-, [3R-(3α,5aα,9α,9aα)]-	$C_{15}H_{26}O$	FSTP	48.30	4.80	652	12
4aH-cycloprop[e]azulen-4a-ol, decahydro-1,1,4,7-tetramethyl-	$C_{15}H_{26}O$	FSTP	48.30	3.69	722	28
(S,1Z,6Z)-8-Isopropyl-1-methyl-5-methylenecyclodeca-1,6-diene	$C_{15}H_{24}$	STP	48.40	4.31	758	66
2-(4a,8-Dimethyl-2,3,4,4a,5,6-hexahydro-naphthalen-2-yl)-prop-2-en-1-ol	$C_{15}H_{22}O$	FSTP	48.40	3.89	748	16
Isolongifolene	$C_{15}H_{20}$	FSTP	48.40	3.87	729	26
1H-3a,7-Methanoazulene, octahydro-1,4,9,9-tetramethyl-	$C_{15}H_{26}$	STP	48.60	4.48	750	26
2-((2R,4aR)-4a,8-Dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalen-2-yl)prop-2-en-1-ol	$C_{15}H_{24}O$	FSTP	48.90	3.93	759	14

Supplementary Table 3. (Cont.)

Compound Name	Mol. formula	Clas.	RT I (min)	RT II (sec)	MF	P (%)
1,4-Dihydrothujopsene-(I1)	$C_{15}H_{26}$	STP	49.00	0.46	861	28
Humulene epoxide I	$C_{15}H_{24}O$	FSTP	49.00	0.34	799	28
Humulene oxide II	$C_{15}H_{24}O$	FSTP	49.40	0.50	682	36
5-Azulenemethanol, 1,2,3,4,5,6,7,8-octahydro-α,α,3,8-tetramethyl-	$C_{15}H_{26}O$	FSTP	49.70	3.57	824	16
2-((2R,4aR,8aR)-4a,8-Dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalen-2-yl)prop-2-en-1-ol	$C_{15}H_{24}O$	FSTP	49.70	3.93	785	31
1,4-Methanoazulen-9-ol, decahydro-1,5,5,8a-tetramethyl-, [1R-(1α ..	$C_{15}H_{26}O$	FSTP	49.90	3.91	552	34
Isoaromadendrene epoxide	$C_{15}H_{24}O$	FSTP	50.00	3.79	794	24
(R)-3,5,8a-Trimethyl-7,8,8a,9-tetrahydronaphtho[2,3-b]furan-4(6H)-one	$C_{15}H_{18}O_2$	FSTP	50.10	4.72	720	13
α-Isocomene	$C_{15}H_{24}$	STP	50.10	4.42	769	17
α-cyperone	$C_{15}H_{20}O$	FSTP	50.60	4.60	873	43
4a(2H)-Naphthalenol, 1,3,4,5,6,8a-hexahydro-4,7-dimethyl-1-(1-methylethyl)-, (1S,4R,4aS,8aR)-	$C_{15}H_{26}O$	FSTP	50.70	3.63	783	35
2H-2,4a-Ethanonaphthalen-8(5H)-one, hexahydro-2,5,5-trimethyl-	$C_{15}H_{24}O$	FSTP	50.70	4.27	517	21
Neointermedeol	$C_{15}H_{26}O$	FSTP	50.70	3.75	612	65
1H-Benzocyclohepten-7-ol, 2,3,4,4a,5,6,7,8-octahydro-1,1,4a,7-tetramethyl-, cis-	$C_{15}H_{26}O$	FSTP	50.80	3.53	562	18
Cyperen-8-one	$C_{15}H_{22}O$	FSTP	50.90	4.34	803	12
Maaliol	$C_{15}H_{26}O$	FSTP	50.90	3.73	618	27
Junenol	$C_{15}H_{26}O$	FSTP	51.10	3.85	872	58
β-Guaiene	$C_{15}H_{24}$	STP	51.10	4.15	657	69
1,3a-Ethano-3aH-indene, 1,2,3,6,7,7a-hexahydro-2,2,4,7a-tetramethyl-, [1R-(1α,3aα,7aα)]-	$C_{15}H_{24}$	STP	51.30	5.46	615	48
2H-Cyclopropa[a]naphthalen-2-one, 1,1a,4,5,6,7,7a,7b-octahydro-1,1,7,7a-tetramethyl-, (1aα,7α,7aα,7bα)-	$C_{15}H_{22}O$	FSTP	51.30	4.68	757	16
β-Acorenol	$C_{15}H_{26}O$	FSTP	51.50	0.36	795	23
2-(4a,8-Dimethyl-2,3,4,5,6,7-hexahydro-1H-naphthalen-2-yl)propan-2-ol	$C_{15}H_{26}O$	FSTP	51.80	3.93	840	83
2-(4a,8-Dimethyl-2,3,4,5,6,7-hexahydro-1H-naphthalen-2-yl)propan-2-ol	$C_{15}H_{26}O$	FSTP	51.80	3.93	840	83
Aristolene	$C_{15}H_{24}$	STP	51.80	5.22	770	53
Curcumenol	$C_{15}H_{22}O_2$	FSTP	51.90	4.74	625	34
Zonarene	$C_{15}H_{24}$	STP	52.00	4.40	569	44
Agarospirol	$C_{15}H_{26}O$	FSTP	52.00	3.93	821	52
4,7-Methanoazulene, 1,2,3,4,5,6,7,8-octahydro-1,4,9,9-tetramethyl-, [1S-(1α,4α,7α)]-	$C_{15}H_{24}$	STP	52.00	4.50	823	59

Supplementary Table 3. (Cont.)

Compound Name	Mol. formula	Clas.	RT I (min)	RT II (sec)	MF	P (%)
1-Naphthalenol, 1,2,3,4,4a,7,8,8a-octahydro-1,6-dimethyl-4-(1-methylethyl)-, [1R-(1α,4β,4aβ,8aβ)]-	$C_{15}H_{26}O$	FSTP	52.10	3.77	831	38
γ-Gurjunenepoxide-(2)	$C_{15}H_{24}O$	FSTP	52.40	3.95	764	38
Rosifoliol	$C_{15}H_{26}O$	FSTP	52.50	3.99	604	45
Ambrosin	$C_{15}H_{18}O_3$	FSTP	52.60	4.54	548	82
β-Cyclocostunolide	$C_{15}H_{20}O_2$	FSTP	52.70	4.50	788	40
4a,trans-8a-Perhydro-cis-2-(2-hydroxy-2-propyl)-4a,cis-8-dimethylnaphthalene	$C_{15}H_{28}$	FSTP	52.80	3.75	807	34
β-Eudesmol	$C_{15}H_{24}O$	FSTP	52.80	4.19	674	32
2-Naphthalenemethanol, decahydro-α,α,4a-trimethyl-8-methylene-, [2R-(2α,4aα,8aβ)]-	$C_{15}H_{26}O$	FSTP	52.90	4.01	768	13
Guaiol	$C_{15}H_{26}O$	FSTP	52.90	4.07	788	52
α-Eudesmol	$C_{15}H_{26}O$	FSTP	53.00	4.27	592	47
Cubenol	$C_{15}H_{26}O$	FSTP	53.00	4.11	590	37
Viridiflorol	$C_{15}H_{26}O$	FSTP	53.10	3.95	798	16
Hedycaryol	$C_{15}H_{26}O$	FSTP	53.10	3.95	808	30
2-Furanmethanol, tetrahydro-α,α,5-trimethyl-5-(4-methyl-3-cyclohexen-1-yl)-, [2S-[2α,5β(R*)]]-	$C_{15}H_{26}O_2$	FSTP	53.20	3.55	709	19
Globulol	$C_{15}H_{26}O$	FSTP	53.30	4.56	807	23
Longipinene epoxide	$C_{15}H_{24}O$	FSTP	53.40	2.22	728	37
δ-Neoclovene	$C_{15}H_{26}$	STP	53.40	4.31	675	17
4-[(E)-5-Hydroxy-3-methylpent-3-enyl]-3,5,5-trimethylcyclohex-2-en-1-one	$C_{15}H_{24}O_2$	FSTP	53.40	0.60	808	24
Khusiol	$C_{15}H_{26}O$	FSTP	53.50	4.38	742	14
Patchouli alcohol	$C_{15}H_{26}O$	FSTP	53.50	4.38	746	17
5-Azulenemethanol, 1,2,3,3a,4,5,6,7-octahydro-α,α,3,8-tetramethyl-, [3S-(3α,3aβ,5α)]-	$C_{15}H_{26}O$	FSTP	53.60	3.99	663	63
2-Naphthalenemethanol, 1,2,3,4,4a,5,6,8a-octahydro-α,α,4a,8-tetramethyl-, (2α,4aα,8aα)-	$C_{15}H_{26}O$	FSTP	53.60	3.87	670	74
α-Bisabolene epoxide	$C_{15}H_{24}O$	FSTP	53.90	4.21	730	32
(7a-Isopropenyl-4,5-dimethyloctahydroinden-4-yl)methanol	$C_{15}H_{26}O$	FSTP	54.00	3.73	796	78
3-Cyclohexen-1-ol, 1-(1,5-dimethyl-4-hexenyl)-4-methyl-	$C_{15}H_{26}O$	FSTP	54.00	3.55	832	32
1H-3a,7-Methanoazulene, octahydro-1,4,9,9-tetramethyl-, (1α,3aα,4β,7α,8aβ)-	$C_{15}H_{26}$	STP	54.00	3.71	597	16
Guaiazulene	$C_{15}H_{18}$	STP	54.00	4.64	830	30
1H-Benzocycloheptene, 2,4a,5,6,7,8,9,9a-octahydro-3,5,5-trimethyl-9-methylene-, (4aS-cis)-	$C_{15}H_{24}$	STP	54.20	4.90	791	9

Supplementary Table 3. (Cont.)

Compound Name	Mol. formula	Clas.	RT I (min)	RT II (sec)	MF	P (%)
Germacraol	$C_{15}H_{24}O$	FSTP	54.20	4.44	783	11
2,6,10-Dodecatrien-1-ol, 3,7,11-trimethyl-	$C_{15}H_{26}O$	FSTP	54.30	3.51	572	22
Mustakone	$C_{15}H_{22}O$	FSTP	54.40	4.58	785	14
1-(1,3-Dimethyl-buta-1,3-dienyl)-3,7,7-trimethyl-2-oxa-bicyclo[3.2.0]hept-3-ene	$C_{15}H_{22}O$	FSTP	54.50	1.25	768	11
α-Bisabolol	$C_{15}H_{26}O$	FSTP	54.70	3.61	626	23
Epizizanone	$C_{15}H_{22}O$	FSTP	54.70	4.82	823	26
Taylorione	$C_{15}H_{22}O$	FSTP	54.90	4.84	819	33
Longifolene	$C_{15}H_{24}$	STP	55.00	5.00	816	30
1-Methylene-2b-hydroxymethyl-3,3-dimethyl-4b-(3-methylbut-2-enyl)-cyclohexane	$C_{15}H_{26}O$	FSTP	55.00	3.39	649	17
Alloaromadendrene oxide	$C_{15}H_{24}O$	FSTP	55.10	4.36	526	13
Aromadendrene oxide-(1)	$C_{15}H_{24}O$	FSTP	55.30	4.27	705	28
3,5,11-Eudesmatriene	$C_{15}H_{22}$	STP	55.30	5.20	809	16
Cyperotundone	$C_{15}H_{22}O$	FSTP	55.50	5.30	779	24
7-(1,3-Dimethylbuta-1,3-dienyl)-1,6,6-trimethyl-3,8-dioxatricyclo[5.1.0.0(2,4)]octane	$C_{15}H_{22}O_2$	FSTP	55.60	5.10	738	21
1H-Cyclopropa[a]naphthalene, 1a,2,6,7,7a,7b-hexahydro-1,1,7,7a-tetramethyl-, [1aR-(1aα,7α,7aα,7bα)]-	$C_{15}H_{22}$	STP	55.60	5.46	779	21
Eudesmatriene	$C_{15}H_{22}$	STP	55.70	5.63	789	18
4-isopropyl-1,6-dimethyl-1,2,3,4-tetrahydronaphthalene	$C_{15}H_{22}$	STP	55.70	5.48	548	21
2,4a,5,8a-Tetramethyl-1,2,3,4,4a,7,8,8a-octahydronaphthalen-1-yl formate (isomer 1)	$C_{15}H_{24}O_2$	FSTP	55.90	1.15	821	20
Eucalyptol	$C_{15}H_{22}O$	FSTP	56.00	4.58	785	17
2-((2R,4aR,8aR)-4a,8-Dimethyl-1,2,3,4,4a,5,6,8a-octahydronaphthalen-2-yl)acrylaldehyde	$C_{15}H_{22}O$	FSTP	56.00	4.66	737	16
1H-Cyclopropa[a]naphthalene, 1a,2,3,3a,4,5,6,7b-octahydro-1,1,3a,7-tetramethyl-, [1aR-(1aα,3aα,7bα)]-	$C_{15}H_{24}$	STP	56.10	5.04	585	16
Isocaryophyllene	$C_{15}H_{24}$	STP	56.20	1.25	725	32
4,6,6-Trimethyl-2-(3-methylbuta-1,3-dienyl)-3-oxatricyclo[5.1.0.0(2,4)]octane	$C_{15}H_{22}O$	FSTP	56.20	4.52	749	30
2-Pentanone, 4-cyclohexylidene-3,3-diethyl-	$C_{15}H_{26}O$	FSTP	56.20	3.65	772	23
2(1H)Naphthalenone, 3,5,6,7,8,8a-hexahydro-4,8a-dimethyl-6-(1-methylethenyl)-	$C_{15}H_{22}O$	FSTP	56.30	4.58	713	87
2-((2S,4aR)-4a,8-Dimethyl-1,2,3,4,4a,5,6,7-octahydronaphthalen-2-yl)propan-2-ol	$C_{15}H_{26}O$	FSTP	56.50	5.22	798	65
(R)-2-((4aS,8aR)-4a-Methyl-8-methylene-1,4,4a,5,6,7,8,8a-octahydronaphthalen-2-yl)propan-1-ol	$C_{15}H_{24}O$	FSTP	56.60	4.40	839	77
T-2 Tetraol	$C_{15}H_{22}O_6$	FSTP	56.70	4.96	583	14

Supplementary Table 3. (Cont.)

Compound Name	Mol. formula	Clas.	RT I (min)	RT II (sec)	MF	P (%)
Verrucarol	$C_{15}H_{22}O_4$	FSTP	56.70	4.86	812	22
Naphtho[1,2-b]furan-2-one, 2,3,3a,4,5,5a,6,7,9a,9b-decahydro-3,5a,9-trimethyl-7,9a-peroxy-	$C_{15}H_{20}O_4$	FSTP	56.70	3.67	672	12
Gossonorol	$C_{15}H_{22}O$	FSTP	56.90	5.83	751	19
6-Isopropenyl-4,8a-dimethyl-1,2,3,5,6,7,8,8a-octahydro-naphthalen-2-ol	$C_{15}H_{24}O$	FSTP	56.90	4.46	697	68
Sesquisabinene hydrate	$C_{15}H_{26}O$	FSTP	57.30	4.11	832	29
Ledol	$C_{15}H_{26}O$	FSTP	57.50	3.93	748	25
α-Santalol	$C_{15}H_{24}O$	FSTP	57.60	4.05	571	53
α-Vetivol	$C_{15}H_{24}O$	FSTP	57.60	4.44	804	18
Cadinene	$C_{15}H_{22}O$	FSTP	57.60	4.92	680	15
Valerenol	$C_{15}H_{24}O$	FSTP	57.60	4.46	846	33
1-Cyclopropene-1-pentanol, α,ε,ε,2-tetramethyl-3-(1-methylethenyl)-	$C_{15}H_{26}O$	FSTP	57.70	5.79	741	18
Khusimol	$C_{15}H_{24}O$	FSTP	57.80	4.86	770	29
1(2H)-Naphthalenone, 3,4,4a,5,6,7-hexahydro-4a,5-dimethyl-3-(1-methylethenyl)-, [3S-(3α,4aα,5α)]-	$C_{15}H_{22}O$	FSTP	57.90	5.30	748	42
7-Oxabicyclo[4.1.0]heptane, 1-(1,3-dimethyl-1,3-butadienyl)-2,2,6-trimethyl-, (E)-	$C_{15}H_{24}O$	FSTP	57.90	4.44	628	23
1-Naphthalenol, decahydro-1,4a-dimethyl-7-(1-methylethylidene)-, [1R-(1α,4aβ,8aα)]-	$C_{15}H_{26}O$	FSTP	58.00	4.52	797	16
7-Isopropenyl-1,4a-dimethyl-4,4a,5,6,7,8-hexahydro-3H-naphthalen-2-one	$C_{15}H_{22}O$	FSTP	58.20	4.82	702	16
β-Oplopenone	$C_{15}H_{24}O$	FSTP	58.50	3.06	672	72
Squamulosone	$C_{15}H_{22}O$	FSTP	58.80	5.28	610	36
Santalcamphor	$C_{15}H_{24}O_2$	FSTP	59.00	5.02	779	20
Calarene epoxide	$C_{15}H_{24}O$	FSTP	59.00	4.96	666	55
Epiglobulol	$C_{15}H_{26}O$	FSTP	59.20	4.86	605	22
1-Formyl-2,2-dimethyl-3-trans-(3-methyl-but-2-enyl)-6-methylidene-cyclohexane	$C_{15}H_{24}O$	FSTP	59.30	2.68	742	21
Isolongifolol	$C_{15}H_{26}O$	FSTP	59.40	4.21	745	20
Silphiperfoladiene	$C_{15}H_{22}$	STP	59.50	5.26	681	24
Arctiol	$C_{15}H_{26}O_2$	FSTP	59.70	3.95	739	21
6-(1-Hydroxymethylvinyl)-4,8a-dimethyl-3,5,6,7,8,8a-hexahydro-1H-naphthalen-2-one	$C_{15}H_{22}O_2$	FSTP	59.70	5.32	746	15
Parthenolide	$C_{15}H_{20}O_3$	FSTP	59.80	5.22	769	19
(E)-2-((8R,8aS)-8,8a-Dimethyl-3,4,6,7,8,8a-hexahydronaphthalen-2(1H)-ylidene)propan-1-ol	$C_{15}H_{24}O$	FSTP	60.00	4.94	687	30

Supplementary Table 3. (Cont.)

Compound Name	Mol. formula	Clas.	RT I (min)	RT II (sec)	MF	P (%)
2-Methyl-3-(3-methyl-but-2-enyl)-2-(4-methyl-pent-3-enyl)-oxetane	$C_{15}H_{26}O$	FSTP	60.00	2.84	772	27
5,6-Azulenedimethanol, 1,2,3,3a,8,8a-hexahydro-2,2,8-trimethyl-, (3aα,8β,8aα)-	$C_{15}H_{24}O_2$	FSTP	60.10	4.92	727	93
4,4-Dimethyl-3-(3-methylbut-3-enylidene)-2-methylenebicyclo[4.1.0]heptane	$C_{15}H_{22}$	STP	60.30	5.61	693	16
α-Isonootkatol	$C_{15}H_{24}O$	FSTP	60.40	5.52	754	16
Spiro[tricyclo[4.4.0.0(5,9)]decane-10,2'-oxirane], 1-methyl-4-isopropyl-7,8-dihydroxy-, (8S)-	$C_{15}H_{24}O_3$	FSTP	60.40	5.34	732	94
Bicyclo[5.2.0]nonane, 4-methylene-2,8,8-trimethyl-2-vinyl-	$C_{15}H_{24}$	STP	60.50	5.81	660	23
2,4a-Methanonaphthalen-7(4aH)-one, 1,2,3,4,5,6-hexahydro-1,1,5,5-tetramethyl-, (2s-cis)-	$C_{15}H_{22}O$	FSTP	60.60	4.88	733	41
Linderane	$C_{15}H_{16}O_4$	FSTP	60.70	5.63	790	27
Ylangenal	$C_{15}H_{22}O$	FSTP	60.90	5.12	775	20
3-Isopropyl-6,7-dimethyltricyclo[4.4.0.0(2,8)]decane-9,10-diol	$C_{15}H_{26}O_2$	FSTP	61.00	4.21	759	39
7-Oxabicyclo[4.1.0]heptane, 2,2,6-trimethyl-1-(3-methyl-1,3-butadienyl)-5-methylene-	$C_{15}H_{22}O$	FSTP	61.00	5.32	700	54
1H-3a,7-Methanoazulene-6-methanol, 2,3,4,7,8,8a-hexahydro-3,8,8-trimethyl-, [3R-(3α,3aβ,7β,8aα)]-	$C_{15}H_{24}O$	FSTP	61.10	4.34	593	24
Nootkatone	$C_{15}H_{22}O$	FSTP	61.20	5.26	768	53
1H-3a,7-Methanoazulene, 2,3,6,7,8,8a-hexahydro-1,4,9,9-tetramethyl-, (1α,3aα,7α,8aβ)-	$C_{15}H_{24}$	STP	61.20	4.46	854	96
4,4-Dimethyl-3-(3-methylbut-2-enylidene)octane-2,7-dione	$C_{15}H_{24}O_2$	FSTP	61.40	3.73	793	17
(5R,10R)-6,10-Dimethyl-2-(propan-2-ylidene)spiro[4.5]dec-6-en-8-one	$C_{15}H_{22}O$	FSTP	61.50	5.16	783	21
Cyperolactone	$C_{15}H_{22}O_2$	FSTP	61.70	5.52	595	30
Cumanin	$C_{15}H_{22}O_4$	FSTP	62.10	5.50	689	68
1,4-Methanonaphthalene, 6,7-diethyldecahydro-, cis-	$C_{15}H_{26}$	STP	62.30	3.91	624	69
5-Hydroxymethyl-1,1,4a-trimethyl-6-methylenedecahydronaphthalen-2-ol	$C_{15}H_{26}O_2$	FSTP	62.40	4.09	787	20
Uvidin C	$C_{15}H_{26}O_3$	FSTP	62.50	4.66	848	85
Cyperadione	$C_{15}H_{24}O_2$	FSTP	62.70	5.75	773	19
Ledene oxide-(I)	$C_{15}H_{24}O$	FSTP	62.70	3.21	787	14
Nootkaton epoxide	$C_{15}H_{22}O_2$	FSTP	62.80	5.65	477	42
(4aR,5S)-1-Hydroxy-4a,5-dimethyl-3-(propan-2-ylidene)-4,4a,5,6,7,8-hexahydronaphthalen-2(3H)-one	$C_{15}H_{22}O_2$	FSTP	63.20	5.22	722	13
Corymbolone	$C_{15}H_{24}O_2$	FSTP	63.70	5.59	774	17
Neoisolongifolene	$C_{15}H_{22}O$	FSTP	63.90	0.87	627	15
Cedrol	$C_{15}H_{26}O$	FSTP	64.10	5.56	789	12

Supplementary Table 3. (Cont.)

Compound Name	Mol. formula	Clas.	RT I (min)	RT II (sec)	MF	P (%)
2(3H)-Benzofuranone, 6-ethenylhexahydro-6-methyl-3-methylene-7-(1-methylethenyl)-, [3aS-(3aα,6α,7β,7aβ)]-	$C_{15}H_{20}O_2$	FSTP	64.20	5.75	822	27
5,7-Decadien-3-yne, 2,9-dihydroxy-5-(1-hydroxy-1-methylethyl)-2,9-dimethyl-, (Z,E)-	$C_{15}H_{24}O_3$	FSTP	64.50	4.15	774	43
7-Tetracyclo[6.2.1.0(3.8)0(3.9)]undecanol, 4,4,11,11-tetramethyl-	$C_{15}H_{24}O$	FSTP	64.50	0.77	776	21
1-Acetyl-4,6,8-trimethylazulene	$C_{15}H_{16}O$	FSTP	64.50	0.46	584	50
Clovanediol	$C_{15}H_{26}O_2$	FSTP	64.60	5.83	709	16
Psilostachyin B	$C_{15}H_{18}O_4$	FSTP	64.60	5.81	791	16
2-Cyclohexene-1-carboxaldehyde, 2,6-dimethyl-6-(4-methyl-3-pentenyl)-	$C_{15}H_{24}O$	FSTP	64.60	4.54	659	61
α-Hydroxyculmorin	$C_{15}H_{26}O_3$	FSTP	64.80	6.15	774	15
Shyobunone	$C_{15}H_{24}O$	FSTP	64.80	2.96	810	21
Solstitialin A	$C_{15}H_{20}O_5$	FSTP	64.90	0.22	664	23
3-Methoxymethyl-2,5,5,8a-tetramethyl-6,7,8,8a-tetrahydro-5H-chromene	$C_{15}H_{24}O_2$	FSTP	65.10	5.85	734	18
Callitrin	$C_{15}H_{22}O_2$	FSTP	65.40	5.42	799	36
1,4-Methanoazulen-3-ol, decahydro-1,5,5,8a-tetramethyl-, [1S-(1α,3β,3aβ,4α,8aβ)]-	$C_{15}H_{26}O$	FSTP	65.50	6.35	736	11
Valerenic acid	$C_{15}H_{22}O_2$	FSTP	65.70	5.57	901	20
8-Deoxylactucin	$C_{15}H_{16}O_4$	FSTP	66.30	1.01	687	34
1H-Indene, 2,3,3a,4,7,7a-hexahydro-2,2,4,4,7,7-hexamethyl-, trans-	$C_{15}H_{26}$	STP	66.30	2.98	757	14
5,9b-Dihydroxy-6,6,9a-trimethyl-5,5a,8,9-tetrahydro-3H-benzo[g][2]benzofuran-1,7-dione	$C_{15}H_{20}O_5$	FSTP	66.40	6.01	560	52
2(3H)-Benzofuranone, 6-ethenylhexahydro-3,6-dimethyl-7-(1-methylethenyl)-, [3S-(3α,3aα,6α,7β,7aβ)]-	$C_{15}H_{22}O_2$	FSTP	66.40	5.67	820	50
Asperilin	$C_{15}H_{20}O_3$	FSTP	66.60	6.13	766	25
Cubedol	$C_{15}H_{26}O$	FSTP	66.60	0.34	801	19
2(1H)-Naphthalenone, 4a,5,6,7,8,8a-hexahydro-6-[1-(hydroxymethyl)ethenyl]-4,8a-dimethyl-, [4ar-(4aα,6α,8aβ)]-	$C_{15}H_{22}O_2$	FSTP	66.70	0.32	632	15
Cyclolongifolene oxide	$C_{15}H_{22}O$	FSTP	66.90	1.43	793	32
Dihydrolactucin	$C_{15}H_{18}O_5$	FSTP	66.90	4.94	584	16
Carissone	$C_{15}H_{24}O_2$	FSTP	67.10	5.79	814	52
β-Cyclodihydrocostunolide	$C_{15}H_{22}O_2$	FSTP	67.40	6.49	746	72
Costunolide	$C_{15}H_{20}O_2$	FSTP	67.60	5.91	739	36
4-(3,3-Dimethyl-but-1-ynyl)-4-hydroxy-2,6,6-trimethylcyclohex-2-enone	$C_{15}H_{22}O_2$	FSTP	68.10	6.21	797	15
2,3,3-Trimethyl-2-(3-methylbuta-1,3-dienyl)-6-methylenecyclohexanone	$C_{15}H_{22}O$	FSTP	68.60	6.67	737	20

Supplementary Table 3. (Cont.)

Compound Name	Mol. formula	Clas.	RT I (min)	RT II (sec)	MF	P (%)
Dihydrocolumellarin	$C_{15}H_{22}O_2$	FSTP	68.60	6.03	663	27
Cedrandiol	$C_{15}H_{26}O_2$	FSTP	68.70	6.61	782	28
Zizanoic acid	$C_{15}H_{22}O_2$	FSTP	69.40	3.17	656	32
4-(Hydroxymethyl)-3,4a,8,8-tetramethyl-1,2,5,6,7,8a-hexahydronaphthalene-1,2-diol	$C_{15}H_{26}O_3$	FSTP	69.90	0.50	704	15
2-((2R,4aR,8aS)-4a-Methyl-8-methylenedecahydronaphthalen-2-yl)acrylaldehyde	$C_{15}H_{22}O$	FSTP	70.00	0.32	697	10
Furanoeremophilone	$C_{15}H_{20}O_2$	FSTP	70.40	0.67	775	23
Columellarin	$C_{15}H_{20}O_2$	FSTP	71.00	6.33	706	24
1-Formyl-2,2,6-trimethyl-3-cis-(3-methylbut-2-enyl)-5-cyclohexene	$C_{15}H_{24}O$	FSTP	71.50	3.69	823	61
5,6-Azulenedicarboxaldehyde, 1,2,3,3a,8,8a-hexahydro-2,2,8-trimethyl-, (3aα,8α,8aα)-(-)-	$C_{15}H_{20}O_2$	FSTP	71.70	1.09	698	37
2-Acetoxy-1,1,10-trimethyl-6,9-epidioxydecalin	$C_{15}H_{24}O_4$	FSTP	71.90	6.25	553	39
Lapachol	$C_{15}H_{14}O_3$	FSTP	71.90	6.19	732	44
3α,4α,9β,11-Diepoxymuurolan-10-ol	$C_{15}H_{24}O_3$	FSTP	72.20	6.07	779	39
Naphtho[2,3-b]furan-2(4H)-one, 4a,5,6,7,8,8a,9,9a-octahydro-3,8a-dimethyl-5-methylene-	$C_{15}H_{20}O_2$	FSTP	72.20	0.56	686	99
Reynosin	$C_{15}H_{20}O_3$	FSTP	73.10	0.79	492	44
Spirojatamol	$C_{15}H_{26}O$	FSTP	73.50	5.65	787	37
Hydroxyvalerenic acid	$C_{15}H_{22}O_3$	FSTP	73.80	0.65	756	22
Cyperanic acid	$C_{15}H_{22}O_4$	FSTP	73.90	5.89	639	68
Nonanophenone	$C_{15}H_{22}O$	FSTP	74.00	0.89	749	40
Gansongone	$C_{15}H_{22}O$	FSTP	74.10	1.33	728	29
Humulaneol	$C_{15}H_{26}O$	FSTP	75.20	4.21	789	83
1H-3a,7-Methanoazulene, octahydro-3,8,8-trimethyl-6-methylene-, [3R-(3α,3aβ,7β,8aα)]-	$C_{15}H_{24}$	STP	75.40	1.63	714	25
2H-Cyclopentacyclooctene, 4,5,6,7,8,9-hexahydro-1,2,2,3-tetramethyl-	$C_{15}H_{24}$	STP	76.60	4.33	745	43
Alantolactone	$C_{15}H_{20}O_3$	FSTP	76.60	5.36	775	37
Naphtho[2,3-b]furan-2(3H)-one, 4a,5,6,7,8,8a-hexahydro-3,8a-dimethyl-5-methylene-	$C_{15}H_{18}O_2$	FSTP	76.90	0.89	740	29
Ageratriol	$C_{15}H_{24}O_3$	FSTP	76.90	4.86	634	47
α-Santalol	$C_{15}H_{24}O$	FSTP	78.40	4.13	612	47
Dihydroartemisinin	$C_{15}H_{22}O_3$	FSTP	78.90	1.77	794	52
Lanceol	$C_{15}H_{24}O$	FSTP	78.90	4.27	695	38

Supplementary Table 3. (Cont.)

Compound Name	Mol. formula	Clas.	RT I (min)	RT II (sec)	MF	P (%)
4,11-Dimethyl-8-(propan-2-yl)-5,12-dioxatricyclo[9.1.0.04,6]dodecan-7-ol	$C_{15}H_{26}O_3$	FSTP	79.00	4.13	699	67
β-Copaenol	$C_{15}H_{24}O$	FSTP	79.10	4.07	595	27
2H-2,4a-Ethanonaphthalene, 1,3,4,5,6,7-hexahydro-2,5,5-trimethyl-	$C_{15}H_{24}$	STP	79.50	4.54	583	46
Thujopsene	$C_{15}H_{24}$	STP	80.30	3.95	588	34
Hinesol	$C_{15}H_{26}O$	FSTP	82.00	4.09	593	40
Himachaladiene	$C_{15}H_{24}$	STP	83.60	4.15	716	31
α-Selinene	$C_{15}H_{24}$	STP	84.00	4.15	670	15
[5-(Hydroxymethyl)-2,5,8a-trimethyl-1,4,4a,6,7,8-hexahydronaphthalen-1-yl]methanol	$C_{15}H_{26}O_2$	FSTP	84.20	0.52	794	29
3,4,8,8-Tetramethyl-4,5,6,7,8,8a-hexahydro-1H-3a,7-methanoazulen-4-ol	$C_{15}H_{24}O$	FSTP	85.90	4.74	769	21
5β,7βH,10α-Eudesm-11-en-1α-ol	$C_{15}H_{26}O$	FSTP	86.60	4.21	747	16
Limonenol	$C_{15}H_{24}O_2$	FSTP	86.80	4.36	633	15
β-Santalol	$C_{15}H_{24}O$	FSTP	86.80	4.27	755	54
1,4-Methano-1H-indene, octahydro-4-methyl-8-methylene-7-(1-methylethyl)-, [1S-(1α,3aβ,4α,7α,7aβ)]-	$C_{15}H_{24}$	STP	86.80	1.71	671	42
9-(3,3-Dimethyloxiran-2-yl)-2,7-dimethylnona-2,6-dien-1-ol	$C_{15}H_{26}O_2$	FSTP	87.10	4.48	681	28
Eudesmaol	$C_{15}H_{24}O$	FSTP	87.40	3.97	712	44
6S-2,3,8,8-Tetramethyltricyclo[5.2.2.0(1,6)]undec-2-ene	$C_{15}H_{24}$	STP	89.50	5.20	644	29
Hydroxy albrassitriol	$C_{15}H_{26}O_4$	FSTP	89.70	2.44	702	53
1,7-Dimethyl-4-(1-methylethyl)cyclodecane	$C_{15}H_{30}$	STP	92.40	4.86	667	25
Picrotoxinin	$C_{15}H_{16}O_6$	FSTP	94.80	3.69	625	84
Isopetasol	$C_{15}H_{22}O_2$	FSTP	96.70	4.96	630	88
3H-Cyclodeca[b]furan-2-one, 4,9-dihydroxy-6-methyl-3,10-dimethylene-3a,4,7,8,9,10,11,11a-octahydro-	$C_{15}H_{20}O_4$	FSTP	100.80	4.29	681	44
2H-Cyclopropa[g]benzofuran, 4,5,5a,6,6a,6b-hexahydro-4,4,6b-trimethyl-2-(1-methylethenyl)-	$C_{15}H_{22}O$	FSTP	103.50	5.14	776	69
Coronopilin	$C_{15}H_{20}O_4$	FSTP	107.30	5.50	632	89
3-Oxo-10(14)-epoxyguai-11(13)-en-6,12-olide	$C_{15}H_{18}O_4$	FSTP	110.90	4.36	750	30
Longipinocarveol	$C_{15}H_{24}O$	FSTP	111.10	4.96	695	32
1H-Indene, 2,3,3a,4,7,7a-hexahydro-2,2,4,4,7,7-hexamethyl-	$C_{15}H_{26}$	STP	113.50	5.28	622	80
4-Hydroxy-5-(5-hydroxypentan-2-yl)-6-methyl-3-methylidene-3a,4,7,7a-tetrahydro-1-benzofuran-2-one	$C_{15}H_{22}O_4$	FSTP	114.50	4.56	690	67
2,4a,8,8-Tetramethyldecahydrocyclopropa[d]naphthalene	$C_{15}H_{26}$	STP	116.40	4.25	766	71

Supplementary Table 3. (Cont.)

Compound Name	Mol. formula	Clas.	RT I (min)	RT II (sec)	MF	P (%)
γ-Himachalene	$C_{15}H_{24}$	STP	116.70	5.00	742	79
Spiro[4.5]decan-7-one, 1,8-dimethyl-8,9-epoxy-4-isopropyl-	$C_{15}H_{24}O_2$	FSTP	119.60	4.80	597	54
1,5,9,9-Tetramethyl-2-oxatricyclo[6.4.0.0(4,8)]dodecane	$C_{15}H_{26}O$	FSTP	122.90	4.05	690	44

Supplementary Table 4. Terpenoid standard mixture analysed using GCxGC-TOF/MS.

Compound Name	Molecular formula	Classification	RT I (min)	RT II (min)	MF	P (%)
Butanoic acid, 3-methyl-, 1-ethenyl-1,5-dimethyl-4-hexenyl ester	C15H26O2	Sesquiterpenoid	12.00	1.07	726	73
Camphene	C10H16	Monoterpenoid	12.50	1.29	879	88
Bicyclo[3.1.1]heptane, 6,6-dimethyl-2-methylene-, (1S)-	C10H16	Monoterpenoid	13.60	1.43	780	78
β-Myrcene	C10H16	Monoterpenoid	13.90	1.37	780	78
Bicyclo[3.1.0]hex-2-ene, 4-methylene-1-(1-methylethyl)-	C10H14	Monoterpenoid	14.20	1.57	603	60
Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)-	C10H16	Monoterpenoid	14.70	1.63	883	88
5-Isopropyl-2-methylbicyclo[3.1.0]hexan-2-ol #	C10H18O	Monoterpenoid	15.20	1.61	543	54
p-Cymene	C10H14	Monoterpenoid	15.60	1.86	572	57
Limonene	C10H16	Monoterpenoid	15.80	1.63	951	95
Eucalyptol	C10H18O	Monoterpenoid	16.00	1.85	676	68
3-Carene	C10H16	Monoterpenoid	16.50	1.65	937	94
γ-Terpinene	C10H16	Monoterpenoid	17.20	1.85	896	90
Bicyclo[3.1.0]hexan-2-ol, 2-methyl-5-(1-methylethyl)-, (1α,2α,5α)-	C10H18O	Monoterpenoid	17.70	2.00	838	84
Cyclohexene, 1-methyl-4-(1-methylethylidene)-	C10H16	Monoterpenoid	18.80	1.98	918	92
Fenchone	C10H16O	Monoterpenoid	19.00	2.56	949	95
3-Octanol, 3,7-dimethyl-	C10H22O	Monoterpenoid	19.10	1.73	949	95
Fenchol	C10H18O	Monoterpenoid	20.40	2.44	883	88
1-Pentene, 5-(2,2-dimethylcyclopropyl)-2-methyl-4-methylene-	C12H20	Ketone	21.00	2.64	592	59
1,2-Dihydrolinalool	C10H20O	Monoterpenoid	21.10	2.12	840	84
cis-Verbenol	C10H16O	Monoterpenoid	21.90	2.72	789	79
(+)-2-Bornanone	C10H16O	Monoterpenoid	22.20	3.23	867	87
Cyclohexanol, 5-methyl-2-(1-methylethenyl)-	C10H18O	Monoterpenoid	22.20	2.48	978	98
Cyclohexanone, 5-methyl-2-(1-methylethyl)-, cis-	C10H18O	Monoterpenoid	22.60	2.68	938	94
Isoborneol	C10H18O	Monoterpenoid	22.90	2.90	935	93
endo-Borneol	C10H18O	Monoterpenoid	23.40	2.96	946	95
Cyclohexanol, 5-methyl-2-(1-methylethyl)-, [1S-(1α,2α,5β)]-	C10H20O	Monoterpenoid	23.70	2.50	764	76
Terpinen-4-ol	C10H18O	Monoterpenoid	24.00	2.74	930	93

Supplementary Table 4. (Cont.)

Compound Name	Molecular formula	Classification	RT I (min)	RT II (min)	MF	P (%)
α-Terpineol	C10H18O	Monoterpenoid	24.80	2.92	935	93
Estragole	C10H12O	Monoterpenoid	25.20	3.43	796	80
Bicyclo[3.1.1]hept-2-ene-2-methanol, 6,6-dimethyl-	C10H16O	Monoterpenoid	25.20	3.09	883	88
Bicyclo[3.1.1]hept-3-en-2-one, 4,6,6-trimethyl-	C10H14O	Monoterpenoid	26.00	3.89	630	63
2,6-Octadiene, 1-(1-ethoxyethoxy)-3,7-dimethyl-	C14H26O2	Ketone	26.80	2.76	885	89
Cyclohexanone, 5-methyl-2-(1-methylethenyl)-	C10H16O	Monoterpenoid	27.80	3.53	845	85
Carvone	C10H14O	Monoterpenoid	28.00	3.75	925	93
Bicyclo[3.1.1]heptan-3-one, 2-hydroxy-2,6,6-trimethyl-	C10H16O2	Monoterpenoid	28.50	4.17	529	53
2-Cyclohexen-1-one, 3-methyl-6-(1-methylethyl)-	C10H16O	Monoterpenoid	28.70	3.75	938	94
Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, acetate, (1S-endo)-	C12H20O2	Ketone	30.70	2.96	895	89
Phenol, 2-methyl-5-(1-methylethyl)-	C10H14O	Monoterpenoid	30.90	3.71	757	76
Cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate, (1α,2α,5β)-	C12H22O2	Ketone	30.90	2.54	841	84
Phenol, 2-methyl-5-(1-methylethyl)-	C10H14O	Monoterpenoid	31.50	3.83	908	91
Bicyclo[2.2.1]heptane-2,3-dione, 1,7,7-trimethyl-, (1S)-	C10H14O2	Monoterpenoid	31.80	5.38	973	97
Santolina alcohol	C10H18O	Monoterpenoid	31.80	3.97	929	93
(1R,2R,3S,5R)-(-)-2,3-Pinanediol	C10H18O2	Monoterpenoid	33.00	4.34	908	91
Bicyclo[2.2.1]heptane, 2-chloro-2,3,3-trimethyl-	C10H17Cl	Monoterpenoid	33.40	2.40	886	89
6-Octen-1-ol, 3,7-dimethyl-, acetate	C12H22O2	Ketone	34.30	2.58	797	80
Geranyl isovalerate	C15H26O2	Sesquiterpenoid	35.10	2.88	809	81
4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-, acetate	C12H20O2	Ketone	36.20	3.00	995	100
α-Damascone	C13H20O	Ketone	37.20	3.45	834	83
1,3-Cyclohexadiene, 5-(1,5-dimethyl-4-hexenyl)-2-methyl-, [S-(R*,S*)]-	C15H24	Sesquiterpenoid	38.70	2.64	644	64
Caryophyllene	C15H24	Sesquiterpenoid	39.10	2.68	923	92
cis-β-Farnesene	C15H24	Sesquiterpenoid	40.80	2.40	901	90
Humulene	C15H24	Sesquiterpenoid	41.20	2.84	903	90
3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	C13H20O	Ketone	42.80	3.61	849	85
1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (Z,E)-	C15H24	Sesquiterpenoid	43.00	2.58	877	88

Supplementary Table 4. (Cont.)

Compound Name	Molecular formula	Classification	RT I (min)	RT II (min)	MF	P (%)
1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (Z,E)-	C15H24	Sesquiterpenoid	43.80	2.58	846	85
(E)-β-Farnesene	C15H24	Sesquiterpenoid	44.00	2.60	855	85
Butylated Hydroxytoluene	C15H24O	Sesquiterpenoid	44.30	3.35	953	95
1-Isopropyl-4,7-dimethyl-1,2,3,5,6,8a-hexahydronaphthalene	C15H24	Sesquiterpenoid	45.10	2.96	980	98
1,5-Diphenyl-2H-1,2,4-triazoline-3-thione	C14H11N3S	Ketone	46.00	2.74	885	89
(E)-β-Farnesene	C15H24	Sesquiterpenoid	47.00	3.57	953	95
1,6,10-Dodecatrien-3-ol, 3,7,11-trimethyl-, (E)-	C15H26O	Sesquiterpenoid	47.10	2.92	898	90
Caryophyllene oxide	C15H24O	Sesquiterpenoid	48.80	3.69	954	95
Cedrol	C15H26O	Sesquiterpenoid	50.00	3.87	838	84
Cyclopentaneacetic acid, 3-oxo-2-(2-pentenyl)-, methyl ester, [1α,2α(Z)]-	C13H20O3	Ketone	52.00	4.72	957	96
α-Bisabolol	C15H26O	Sesquiterpenoid	54.00	3.53	970	97
2-Butenoic acid, 2-methyl-, 3,7-dimethyl-2,6-octadienyl ester, (E,Z)-	C15H24O2	Sesquiterpenoid	54.60	3.49	788	79
1-Methylene-2b-hydroxymethyl-3,3-dimethyl-4b-(3-methylbut-2-enyl)-cyclohexane	C15H26O	Sesquiterpenoid	55.90	3.39	912	91
Cyclopropane, 1-methyl-2-(3-methylpentyl)-	C10H20	Monoterpenoid	56.00	1.81	931	93
Azulene, 1,4-dimethyl-7-(1-methylethyl)-	C15H18	Sesquiterpenoid	59.20	5.14	915	91
Nootkatone	C15H22O	Sesquiterpenoid	60.80	5.14	811	81
Neophytadiene	C20H38	Diterpenoid	61.60	2.08	948	95
(E,E)-7,11,15-Trimethyl-3-methylene-hexadeca-1,6,10,14-tetraene	C20H32	Diterpenoid	65.60	2.84	879	88
3,7,11,15-Tetramethyl-2-hexadecen-1-ol	C20H40O	Diterpenoid	66.90	2.44	835	83
1-Methylene-2b-hydroxymethyl-3,3-dimethyl-4b-(3-methylbut-2-enyl)-cyclohexane	C15H26O	Sesquiterpenoid	68.00	2.98	602	60
Musk ketone	C14H18N2O5	Ketone	69.30	5.93	954	95
Phytol	C20H40O	Diterpenoid	74.50	2.90	935	93
α-Santonin	C15H18O3	Sesquiterpenoid	79.60	3.11	631	63
2-Methyl-3-(3-methyl-but-2-enyl)-2-(4-methyl-pent-3-enyl)-oxetane	C15H26O	Sesquiterpenoid	101.10	3.61	499	50
Supraene	C30H50	Triterpenoid	101.40	3.55	881	88
Squalene	C30H50	Triterpenoid	101.70	3.65	690	69

Supplementary Table 5. *Chlamydomonas reinhardtii* metabolism optimisation to produce heterologous sesquiterpenes.

Construct transformed	Cell concentration (cells/L)			Patchoulol titer (μg/L)					Patchoulol titer (fg/cell)				
	n	Mean	SD	n	Mean	SD	Fold change	p-value	n	Mean	SD	Fold change	p-value
PcPS_YFP	2.1E+10	2.3E+10	4.5E+09	77	119	37	-	-	3.7	5.4	2.1	-	-
	2.1E+10			109					5.3				
	2.0E+10			165					8.4				
	2.9E+10			125					4.3				
PcPS_YFP + CrBKT	2.2E+10	2.2E+10	2.1E+08	969	906	126	8	0.0003	44.6	41.2	5.9	8	0.0114
	2.2E+10			993					45.3				
	2.2E+10			719					32.6				
	2.2E+10			941					42.4				
PcPS_YFP + SQSkd	2.2E+10	2.3E+10	2.1E+08	1502	1622	174	14	<0.0001	67.1	71.7	7.8	12	0.0110
	2.3E+10			1809					80.3				
	2.3E+10			1729					76.2				
	2.3E+10			1449					63.4				
PcPS_YFP + CrBKT + SQSkd	2.3E+10	2.8E+10	3.7E+09	2171	2215	272	21	<0.0001	110.7	132.7	41.1	25	<0.0001
	2.6E+10			2385					156.4				
	2.9E+10			2074					87.1				
	3.1E+10			2231					176.7				

Supplementary Table 6. List of plasmids.

Construct number	Construct name	Gene name	Product	Gene length (bp)	Protein size (kDa)	Intron copies (i1RBCS2)	Reporter (FP)	Selection (Antibiotic Resistance)
01	P007	*mVenus*	Yellow fluorescent protein	1004	27	3	YFP	Paromomycin
02	P117	*Sa*SS	Santalene	2441	92	5	YFP	Paromomycin
03	P118	*Cl*SS	Santalene	2387	91	5	YFP	Paromomycin
04	P119	*Cc*SS	Santalene	2393	91	5	YFP	Paromomycin
05	P124	*Cz*ZS	Zizaene	2399	91	4	YFP	Paromomycin
06	P125	*Cz*ZS	Zizaene	2390	91	4	YFP	Paromomycin
07	P107	*Pe*AS	Aristolochene	1446	65	3	YFP	Paromomycin
08	P108	*Pc*AS	Aristolochene	1470	66	3	YFP	Paromomycin
09	P109	*Pc*AS	Aristolochene	1521	68	3	YFP	Paromomycin
10	P110	*Pr*AS	Aristolochene	1470	66	3	YFP	Paromomycin
11	P120	*Cs*VS	Valencene	2378	91	5	YFP	Paromomycin
12	P121	*Cn*VS	Valencene	2501	96	5	YFP	Paromomycin
13	P111	*Ac*DGSI	δ-guaiene	2375	91	5	YFP	Paromomycin
14	P112	*Ac*DGSII	δ-guaiene	2375	91	5	YFP	Paromomycin
15	P113	*Ac*DGSIII	δ-guaiene	2375	91	5	YFP	Paromomycin
16	P114	*As*DGSI	δ-guaiene	2375	95	5	YFP	Paromomycin
17	P115	*As*DGSII	δ-guaiene	2375	91	5	YFP	Paromomycin
18	P116	*As*DGSIII	δ-guaiene	2375	91	5	YFP	Paromomycin
19	P126	*La*CS	τ-Cadinol	2426	92	5	YFP	Paromomycin
20	P122	*Cs*VL	Valerioanol	2453	94	5	YFP	Paromomycin
21	P123	*Ch*VL	Valerioanol	2396	91	5	YFP	Paromomycin
22	P139	ispA_*Pc*PS(C415F_H454A)	Patchoulol	3707	122	8	YFP	Paromomycin
23	P140	*Pc*PS(C415F_H454A)	Patchoulol	2378	72	6	YFP	Paromomycin
24	P127	*Cc*BS	Bisabolol	2468	93	5	YFP	Paromomycin
25	B005	mTFP1	Cyan-green florescent protein	1140	27	3	TFP	Bleomycin
26	B036	*ClSS*	Santalene	1650	91	5	BFP	Bleomycin
27	B039	*CzZS*	Zizaene	2399	91	4	BFP	Bleomycin
28	B033	*PcAS*	Aristolochene	1078	67	3	BFP	Bleomycin
29	B037	*CnVS*	Valencene	1764	96	5	BFP	Bleomycin

Supplementary Table 6. (Cont.)

Construct number	Construct name	Gene name	Product	Gene length (bp)	Protein size (kDa)	Intron copies (i1RBCS2)	Reporter (FP)	Selection (Antibiotic Resistance)
30	B034	*AcDGSI*	δ-guaiene	1638	91	5	BFP	Bleomycin
31	B035	*AsDGSIII*	δ-guaiene	1638	91	5	BFP	Bleomycin
32	B040	*LaCS*	τ-Cadinol	1662	92	5	BFP	Bleomycin
33	B038	*ChVL*	Valerioanol	1659	91	5	BFP	Bleomycin
34	B031	ispA_*Pc*PS(C415F_H454A)	Patchoulol	3707	122	8	BFP	Bleomycin
35	B032	*Pc*PS(C415F_H454A)	Patchoulol	2378	72	6	BFP	Bleomycin
36	B041	*Cc*BS	Bisabolol	1704	93	5	BFP	Bleomycin
37	P011	*Pc*PS	Patchoulol	2097	72	5	YFP	Paromomycin
38	MS021	BKT	Ketocarotenoids	2419	93	3	-	Spectinomycin
39	S001	SQSkd	Squalene synthase knock-down	1382	30	3	gLuc	Spectinomycin

Supplementary Table 7. Sesquiterpenoid quantifications (Single transformation).

Sesquiterpenoid	Construct transformed	Cell concentration (cells/L)			Product titer (μg/L culture)			Product titer (fg/cell)		
		n	Mean	SD	n	Mean	SD	n	Mean	SD
Santalene	3	2.3E+10	2.3E+10	2.1E+09	78	64	10	3.4	2.7	0.5
		2.1E+10			55			2.7		
		2.6E+10			58			2.3		
		2.4E+10			63			2.6		
Zizaene	6	2.5E+10	2.5E+10	4.1E+09	503	416	77	19.8	16.6	2.5
		3.1E+10			448			14.5		
		2.2E+10			324			14.7		
		2.2E+10			390			17.4		
Aristolochene	9	1.9E+10	1.7E+10	2.4E+09	32	25	6	1.6	1.4	0.2
		1.7E+10			29			1.7		
		1.9E+10			22			1.2		
		1.4E+10			18			1.3		
Valencene	12	2.3E+10	2.3E+10	0.0E+00	57	52	5	2.4	2.5	0.1
		2.3E+10			54			2.5		
		2.3E+10			52			2.6		
		2.3E+10			46			2.5		
δ-Guaiene	13	2.1E+10	2.1E+10	3.4E+08	26	25	4	1.3	1.2	0.2
		2.1E+10			30			1.4		
		2.1E+10			21			1.0		
		2.1E+10			22			1.0		
δ-Guaiene	18	2.1E+10	2.5E+10	3.2E+09	1747	1447	312	83.6	60.3	20.4
		2.4E+10			1668			70.9		
		2.7E+10			1279			46.8		
		2.7E+10			1094			39.9		
τ-Cadinol	19	2.1E+10	2.4E+10	2.6E+09	30	43	14	1.4	1.8	0.6
		2.7E+10			37			1.4		
		2.2E+10			43			2.0		
		2.4E+10			62			2.6		
Valerianol	21	2.2E+10	2.0E+10	1.9E+09	40	41	13	1.8	2.1	0.6
		1.8E+10			44			2.4		
		2.0E+10			56			2.7		
		1.8E+10			25			1.4		
Patchoulol	22	2.4E+10	2.1E+10	2.6E+09	1813	1729	132	77.1	82.1	4.4
		2.3E+10			1871			80.4		
		1.9E+10			1618			83.5		
		1.8E+10			1614			87.5		
Bisabolol	24	2.2E+10	2.2E+10	9.6E+08	28	21	5	1.3	1.0	0.3
		2.1E+10			23			1.1		
		2.3E+10			19			0.8		
		2.3E+10			15			0.6		

Supplementary Table 8. Sesquiterpenoid quantifications (Double transformation).

Sesquiterpenoid	Construct transformed	Cell concentration (cells/L)			Product titer (μg/L culture)			Product titer (fg/cell)		
		n	Mean	SD	n	Mean	SD	n	Mean	SD
Santalene	3+26	2.1E+10 2.7E+10 2.4E+10 2.2E+10	2.4E+10	2.7E+09	211 257 269 265	250	27	10.0 9.4 11.3 11.9	11	1.1
Zizaene	6+27	2.4E+10 2.4E+10 2.5E+10 2.4E+10	2.4E+10	6.0E+08	739 625 659 547	642	80	30.4 25.9 26.2 23.1	26	3.0
Aristolochene	9+28	2.2E+10 1.4E+10 8.4E+09 1.2E+10	1.4E+10	6.0E+09	36 39 47 30	38	7	1.6 2.8 5.5 2.6	3	1.7
Valencene	12+29	2.4E+10 2.2E+10 2.0E+10 1.8E+10	2.1E+10	2.5E+09	332 309 292 319	313	17	14.3 13.3 12.5 13.7	13	0.7
δ-Guaiene	13+30	2.1E+10 2.2E+10 2.3E+10 2.3E+10	2.2E+10	9.3E+08	54 67 57 36	53	13	2.5 3.0 2.5 1.6	2	0.6
δ-Guaiene	18+31	2.3E+10 2.7E+10 2.3E+10 2.3E+10	2.4E+10	1.8E+09	3236 2092 2861 2580	2692	482	137.8 78.1 122.0 113.0	113	25.3
τ-Cadinol	19+32	2.6E+10 2.5E+10 2.4E+10 2.6E+10	2.5E+10	8.7E+08	374 434 363 425	399	36	14.5 17.1 14.9 16.1	16	1.2
Valerianol	21+33	2.6E+10 2.9E+10 2.1E+10 2.1E+10	2.4E+10	4.0E+09	446 494 640 573	538	85	17.1 17.3 31.0 27.8	23	7.2
Patchoulol	22+34	2.6E+10 2.4E+10 2.1E+10 2.7E+10	2.4E+10	2.6E+09	3007 2578 2625 2858	2767	201	116.9 107.7 127.2 107.6	115	9.3
Bisabolol	24+35	2.2E+10 2.5E+10 2.3E+10 2.5E+10	2.4E+10	1.5E+09	330 293 256 219	275	48	15.0 11.7 11.1 8.8	12	2.6

Supplementary Table 9. Summary of sesquiterpenoids quantification.

Sesquiterpenoid	Titer (μg/cell)				Titer (fg/cell)				Fold change
	Single transformation		Double transformation		Single transformation		Double transformation		
	Mean	SD	Mean	SD	Mean	SD	mean	SD	
Santalene	63.5	10.4	250.5	26.9	2.7	0.5	10.6	1.1	3.9
Zizaene	416.3	76.8	642.3	79.5	16.6	2.5	26.4	3.0	1.6
Aristolochene	25.1	6.3	38.1	6.8	1.4	0.2	3.1	1.7	2.2
Valencene	52.4	4.7	313.1	16.9	2.5	0.1	13.4	0.7	5.4
δ-Guaiene	1447.0	311.5	2692.4	482.2	60.3	20.4	112.7	25.3	1.9
τ-Cadinol	43.2	13.9	398.8	35.8	1.8	0.6	15.7	1.2	8.7
Valerianol	41.3	12.5	538.2	85.4	2.1	0.6	23.3	7.2	11.1
Patchoulol	1729.1	132.4	2766.9	201.4	82.1	4.4	114.8	9.3	1.4
Bisabolol	21.2	5.5	274.9	47.8	1.0	0.3	11.7	2.6	11.7

Supplementary Table 10. Concentrated algal-produced sesquiterpenoids identified in ethanol using GCxGC-TOF/MS.

Compound Name	Molecular formula	Classification	RT I (min)	RT II (min)	MF	P (%)
α-Santalene	$C_{15}H_{24}$	STP	31.20	2.72	888	89
Aromadendrene	$C_{15}H_{22}$	STP	34.70	2.64	821	82
α-Cubebene	$C_{15}H_{24}$	STP	36.30	2.42	752	75
β-Bourbonene	$C_{15}H_{24}$	STP	36.90	2.54	718	72
β-Elemene	$C_{15}H_{24}$	STP	37.20	2.50	728	73
β-copaene	$C_{15}H_{24}$	STP	37.30	2.42	775	78
α-gurjunene	$C_{15}H_{24}$	STP	38.20	2.66	744	74
Isocaryophyllene	$C_{15}H_{24}$	STP	39.10	2.76	737	74
Caryophyllene	$C_{15}H_{24}$	STP	39.30	2.68	752	75
Seychellene	$C_{15}H_{24}$	STP	40.60	3.15	758	76
β-Santalene	$C_{15}H_{24}$	STP	41.30	2.74	695	69
Alloaromadendrene	$C_{15}H_{24}$	STP	41.30	2.98	739	74
Zizaene	$C_{15}H_{24}$	STP	41.40	3.00	761	76
Cadinene	$C_{15}H_{28}$	STP	42.10	2.38	904	90
α-Curcumene	$C_{15}H_{22}$	STP	42.50	3.04	815	82
α-Farnesene	$C_{15}H_{24}$	STP	42.90	3.11	910	91
β-Guaiene	$C_{15}H_{24}$	STP	43.10	3.04	765	76
Aristolochene	$C_{15}H_{24}$	STP	43.10	3.00	774	77
Eremophilene	$C_{15}H_{24}$	STP	43.10	2.98	797	80
Rosiglitazone	$C_{15}H_{24}$	STP	44.60	3.09	693	69
Humulene	$C_{15}H_{24}$	STP	47.90	3.91	823	82
α-Santalol	$C_{15}H_{24}O$	FSTP	49.50	4.72	774	77
α-Guaiene	$C_{15}H_{24}$	STP	50.40	2.60	748	75
γ-himachalene	$C_{15}H_{24}$	STP	51.10	4.17	812	81
β-Caryophyllene	$C_{15}H_{24}$	STP	52.10	4.09	791	79
β-Longipinene	$C_{15}H_{24}$	STP	53.20	4.33	591	59
α-Santalol	$C_{15}H_{24}O$	FSTP	53.70	3.85	828	83

Supplementary Table 10. (Cont.)

Compound Name	Molecular formula	Classification	RT I (min)	RT II (min)	MF	P (%)
α-copaene	$C_{15}H_{24}O$	FSTP	53.90	4.44	690	69
α-Eudesmol	$C_{15}H_{24}O$	FSTP	54.60	4.21	702	70
Valencene	$C_{15}H_{24}$	STP	54.90	4.21	814	81
Elemol	$C_{15}H_{24}O$	FSTP	57.30	5.73	805	81
δ-Guaiene	$C_{15}H_{24}$	STP	59.67	3.75	779	78
Nootkatone	$C_{15}H_{22}O$	FSTP	61.00	5.28	830	83
α-Patchoulene	$C_{15}H_{24}$	STP	61.40	3.04	737	74
τ-Cadinol	$C_{15}H_{24}O$	FSTP	62.10	3.71	843	84
ɣ-gurjunene	$C_{15}H_{24}$	STP	64.30	5.20	894	89
Valerianol	$C_{15}H_{24}O$	FSTP	64.70	4.36	658	66
α-Selinene	$C_{15}H_{24}O$	FSTP	69.60	6.19	949	95
Patchouli alcohol	$C_{15}H_{24}O$	FSTP	73.20	4.52	865	86
α-bisabol	$C_{15}H_{24}$	STP	78.30	2.92	866	87
α-Bisabolol oxide B	$C_{15}H_{26}O_2$	FSTP	81.00	3.55	676	68
δ-Elemene	$C_{15}H_{24}$	STP	82.80	4.01	865	86

Supplementary Table 11. Sesquiterpenoids identified after hydroboration-oxidation reaction using GCxGC-TOF/MS.

Compound Name	Molecular formula	Classification	RT I (min)	RT II (min)	MF	P (%)
α-Bisabolol oxide B	$C_{15}H_{26}O_2$	FSTP	31.20	2.72	888	89
α-Santalene	$C_{15}H_{24}$	STP	31.20	2.72	834	83
α-cedrene	$C_{15}H_{24}$	STP	34.00	2.04	1005	101
Zizaene	$C_{15}H_{24}$	STP	34.40	3.00	883	88
Aromadendrene	$C_{15}H_{22}$	STP	34.70	2.64	888	89
β-Vatirenene	$C_{15}H_{22}$	STP	35.80	3.85	728	73
α-Cubebene	$C_{15}H_{24}$	STP	36.30	2.42	775	78
β-Bourbonene	$C_{15}H_{24}$	STP	36.90	2.54	744	74
β-Elemene	$C_{15}H_{24}$	STP	37.20	2.50	737	74
Germacrene A	$C_{15}H_{24}$	STP	37.30	2.44	752	75
β-copaene	$C_{15}H_{24}$	STP	37.30	2.42	758	76
Isocaryophyllene	$C_{15}H_{24}$	STP	39.10	2.76	910	91
Caryophyllene	$C_{15}H_{24}$	STP	39.30	2.68	797	80
Patchouladiene	$C_{15}H_{22}$	STP	39.50	3.04	693	69
Cycloisolongifolol	$C_{15}H_{24}O$	FSTP	40.40	2.90	812	81
Seychellene	$C_{15}H_{24}$	STP	40.60	3.15	591	59
Humulene	$C_{15}H_{24}$	STP	40.90	3.91	702	70
β-Selinene	$C_{15}H_{24}$	STP	40.90	2.58	805	81
β-Santalene	$C_{15}H_{24}$	STP	41.30	2.74	779	78
Alloaromadendrene	$C_{15}H_{24}$	STP	41.30	2.98	843	84
α-Patchoulene	$C_{15}H_{24}$	STP	41.40	3.04	658	66
α-gurjunene	$C_{15}H_{24}$	STP	41.40	3.00	761	76
Cadinene	$C_{15}H_{28}$	STP	42.10	2.38	804	80
α-Farnesene	$C_{15}H_{24}$	STP	42.90	3.11	811	81
β-Guaiene	$C_{15}H_{24}$	STP	43.10	3.04	813	81
α-coastal	$C_{15}H_{22}O$	FSTP	43.10	3.00	895	89

Supplementary Table 11. (Cont.)

Compound Name	Molecular formula	Classification	RT I (min)	RT II (min)	MF	P (%)
Aristolochene	$C_{15}H_{24}$	STP	43.10	3.00	815	82
Eremophilene	$C_{15}H_{24}$	STP	43.10	2.98	768	77
α-himachalene	$C_{15}H_{20}$	FSTP	43.30	3.59	783	78
β-Bisabolenol	$C_{15}H_{24}O$	FSTP	43.30	3.21	763	76
Eudesmatriene	$C_{15}H_{22}$	STP	43.40	3.17	821	82
α-agorofuran	$C_{15}H_{24}O$	FSTP	46.90	3.99	838	84
Longifolene	$C_{15}H_{20}$	FSTP	47.20	3.69	841	84
Aromadendran	$C_{15}H_{26}$	STP	47.40	4.25	842	84
Neoisolongifolene	$C_{15}H_{22}$	STP	49.30	2.72	848	85
α-Santalol	$C_{15}H_{24}O$	FSTP	49.50	4.72	849	85
isoledene	$C_{15}H_{24}$	STP	50.10	3.47	852	85
Humulene epoxide I	$C_{15}H_{24}O$	FSTP	50.50	3.87	856	86
γ-himachalene	$C_{15}H_{24}$	STP	51.10	4.17	859	86
δ-Guaiene	$C_{15}H_{24}$	STP	52.00	3.75	864	86
β-Caryophyllene	$C_{15}H_{24}$	STP	52.10	4.09	866	87
τ-Cadinol	$C_{15}H_{26}O$	FSTP	52.10	3.71	867	87
α-Guaiene	$C_{15}H_{24}$	STP	52.30	3.85	872	87
Aristolene	$C_{15}H_{24}$	STP	52.50	4.19	875	88
Agarospirol	$C_{15}H_{26}O$	FSTP	52.80	4.07	877	88
Alloaromadendrenol	$C_{15}H_{26}O$	FSTP	52.80	4.07	986	99
Globulol	$C_{15}H_{26}O$	FSTP	52.80	4.31	880	88
Cubenol	$C_{15}H_{26}O$	FSTP	52.90	4.13	881	88
Ledol	$C_{15}H_{26}O$	FSTP	52.90	5.81	884	88
Guaiol	$C_{15}H_{26}O$	FSTP	53.00	4.09	886	89
β-Longipinene	$C_{15}H_{24}$	STP	53.20	4.33	892	89
Cedrol	$C_{15}H_{26}O$	FSTP	53.30	4.33	894	89
α-Santalol	$C_{15}H_{24}O$	FSTP	53.70	3.85	898	90

Supplementary Table 11. (Cont.)

Compound Name	Molecular formula	Classification	RT I (min)	RT II (min)	MF	P (%)
α.Eudesmol	$C_{15}H_{24}O$	FSTP	54.60	4.21	904	90
Valerenol	$C_{15}H_{24}O$	FSTP	54.70	4.36	851	85
Valerianol	$C_{15}H_{24}O$	FSTP	54.70	4.36	868	87
α-Curcumene	$C_{15}H_{22}$	STP	54.90	4.21	750	75
Valencene	$C_{15}H_{24}$	STP	54.90	4.21	911	91
Agidol	$C_{15}H_{22}O$	FSTP	57.00	5.00	990	99
Elemol	$C_{15}H_{26}O$	FSTP	57.30	5.73	928	93
Eudesmenol	$C_{15}H_{26}O$	FSTP	57.60	5.46	933	93
Aromadendrenol	$C_{15}H_{26}O$	FSTP	58.00	3.59	977	98
Valerenic acid	$C_{15}H_{22}O_2$	FSTP	58.60	5.73	937	94
γ-Gurjunenepoxide	$C_{15}H_{24}O$	FSTP	59.50	4.64	943	94
α-Hexylcinnamaldehyde	$C_{15}H_{20}O$	FSTP	59.67	3.75	930	93
Ylangenal	$C_{15}H_{22}O$	FSTP	60.40	5.77	949	95
Nootkatone	$C_{15}H_{22}O$	FSTP	61.00	5.28	951	95
β-acoradienol	$C_{15}H_{24}O$	FSTP	61.00	4.23	953	95
Caryophylladienol	$C_{15}H_{26}O$	FSTP	61.10	6.01	957	96
β-Eudesmol	$C_{15}H_{26}O$	FSTP	61.60	5.12	959	96
α-isocomene	$C_{15}H_{24}$	STP	62.10	3.71	909	91
Alloaromadendrene oxide	$C_{15}H_{24}O$	FSTP	63.00	5.08	968	97
Isoaromadendrene epoxide	$C_{15}H_{24}O$	FSTP	63.50	5.24	864	86
ɣ-gurjunene	$C_{15}H_{24}$	STP	64.30	5.20	982	98
α-cyperone	$C_{15}H_{20}O$	FSTP	64.70	4.36	923	92
Curcumenol	$C_{15}H_{28}O$	FSTP	64.70	4.07	988	99
Bourbonenol	$C_{15}H_{26}O$	FSTP	65.00	3.21	989	99
Cumanin	$C_{15}H_{22}O_4$	FSTP	66.50	1.88	988	99
α-Panasinsen	$C_{15}H_{24}$	STP	66.80	0.62	991	99
Valerenolic acid	$C_{15}H_{22}O_3$	FSTP	67.00	5.57	935	94

Supplementary Table 11. (Cont.)

Compound Name	Molecular formula	Classification	RT I (min)	RT II (min)	MF	P (%)
Aromadendrene oxide	$C_{15}H_{24}O$	FSTP	67.30	5.85	940	94
γ-Elemene	$C_{15}H_{24}$	STP	69.10	5.83	954	95
Humulenol-II	$C_{15}H_{24}O$	FSTP	69.40	6.17	975	97
α-selinene	$C_{15}H_{24}O$	FSTP	69.60	6.19	951	95
Farnesenol	$C_{15}H_{26}O$	FSTP	69.60	6.19	970	97
Nootkaton epoxide	$C_{15}H_{22}O_2$	FSTP	71.70	1.09	922	92
α-Eudesmol	$C_{15}H_{22}O_2$	FSTP	72.40	1.03	961	96
α-copaene	$C_{15}H_{24}O$	FSTP	73.20	4.52	898	90
Gurjunenol	$C_{15}H_{28}O$	FSTP	73.20	4.52	981	98
Patchouli alcohol	$C_{15}H_{24}O$	FSTP	73.20	4.52	865	86
Hydroxymuurolene	$C_{15}H_{24}O$	FSTP	73.60	6.33	958	96
Cedrandiol	$C_{15}H_{26}O_2$	FSTP	73.90	1.41	958	96
Copaenol	$C_{15}H_{26}O$	FSTP	78.00	4.07	980	98
α-bisabol	$C_{15}H_{24}$	STP	78.30	2.92	866	87
Santalenol	$C_{15}H_{26}O$	FSTP	78.30	2.92	985	99
Cadinol	$C_{15}H_{26}O$	FSTP	81.00	3.17	987	99
Santalol	$C_{15}H_{26}O$	FSTP	81.00	3.55	976	98
Caryophyllene oxide	$C_{15}H_{24}O$	FSTP	82.40	3.65	950	95
Seychellene alcohol	$C_{15}H_{22}O$	FSTP	82.80	4.01	984	98
δ-Elemene	$C_{15}H_{24}$	STP	82.80	4.01	951	95
Ylangenol	$C_{15}H_{24}O$	FSTP	83.10	2.98	966	97
Zizaenol	$C_{15}H_{26}O$	FSTP	85.20	4.58	986	99
Caryophyllene alcohol	$C_{15}H_{26}O$	FSTP	86.00	4.19	982	98

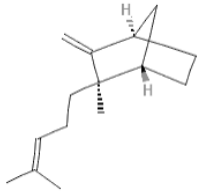
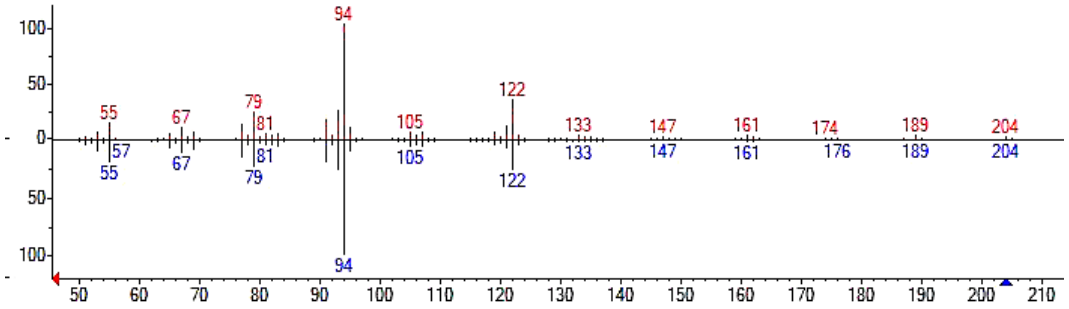
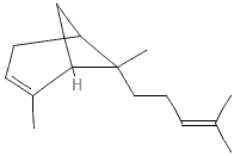
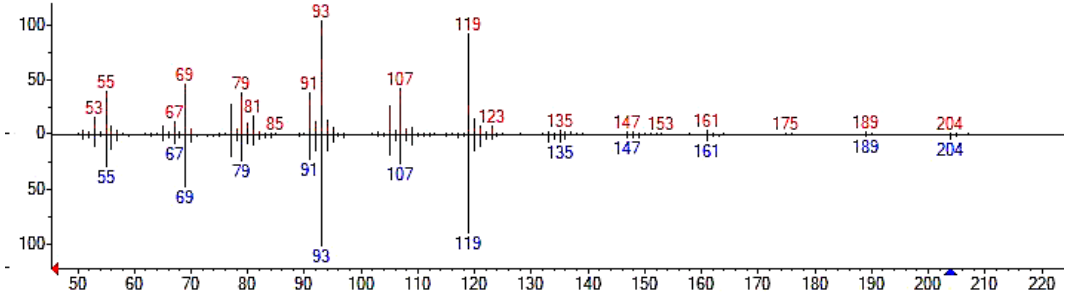
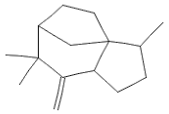
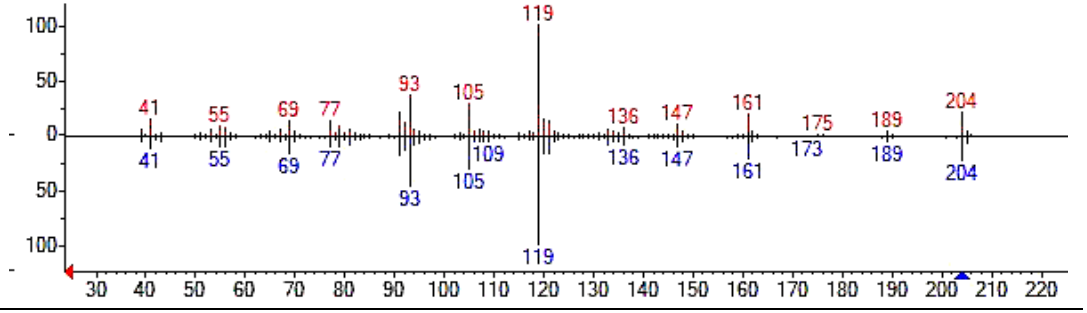
Supplementary Table 12. Common sesquiterpenoids identified using GCxGC-TOF/MS in alga-derivate mixture, agarwood and agarwood distillate samples.

Compound Name	Molecular formula	Classification	Algal	Distillate	Agarwood
α-Santalol	$C_{15}H_{24}O$	FSTP	0.56%	2.12%	2.69%
Agarospirol	$C_{15}H_{26}O$	FSTP	3.44%	5.53%	1.37%
Alloaromadendrene	$C_{15}H_{24}$	STP	3.96%	1.82%	4.19%
Alloaromadendrene oxide	$C_{15}H_{24}O$	FSTP	4.19%	4.65%	2.60%
Aristolene	$C_{15}H_{24}$	STP	4.27%	2.09%	1.47%
Aristolochene	$C_{15}H_{24}$	STP	1.73%	3.25%	3.02%
Cadinene	$C_{15}H_{28}$	STP	3.04%	1.84%	2.28%
Caryophyllene	$C_{15}H_{24}$	STP	3.52%	2.51%	0.63%
Cedrandiol	$C_{15}H_{26}O_2$	FSTP	4.18%	0.72%	3.28%
Cedrol	$C_{15}H_{26}O$	FSTP	2.05%	3.44%	3.68%
Cubenol	$C_{15}H_{26}O$	FSTP	2.54%	4.20%	1.81%
Cumanin	$C_{15}H_{22}O_4$	FSTP	1.96%	0.78%	2.62%
Curcumenol	$C_{15}H_{28}O$	FSTP	1.62%	2.38%	4.31%
Globulol	$C_{15}H_{26}O$	FSTP	0.13%	0.28%	3.98%
Guaiol	$C_{15}H_{26}O$	FSTP	2.75%	1.64%	2.64%
Humulene	$C_{15}H24$	STP	2.36%	5.59%	3.24%
Humulene epoxide I	$C_{15}H_{24}O$	FSTP	0.67%	0.60%	1.04%
Humulenol-II	$C_{15}H_{24}O$	FSTP	2.85%	4.75%	4.30%
Isoaromadendrene epoxide	$C_{15}H_{24}O$	FSTP	0.47%	2.98%	2.04%
isoledene	$C_{15}H_{24}$	STP	2.54%	0.63%	1.34%
Ledol	$C_{15}H_{26}O$	FSTP	2.73%	0.73%	3.98%
Longifolene	$C_{15}H_{20}$	FSTP	2.45%	2.50%	0.33%
Neoisolongifolene	$C_{15}H_{22}$	STP	3.18%	3.96%	3.14%
Nootkaton epoxide	$C_{15}H_{22}O_2$	FSTP	1.90%	3.81%	2.38%
Nootkatone	$C_{15}H_{22}O$	FSTP	0.31%	3.43%	2.57%
Valencene	$C_{15}H_{24}$	STP	0.36%	1.23%	0.86%

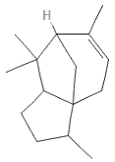
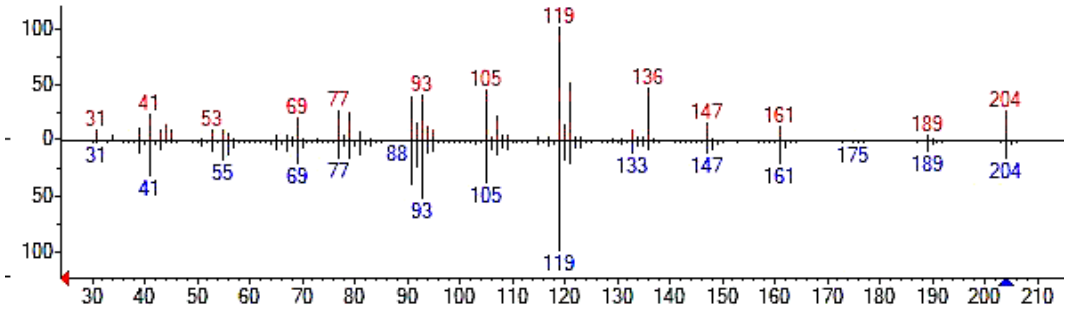
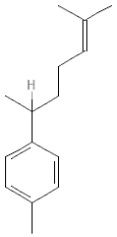
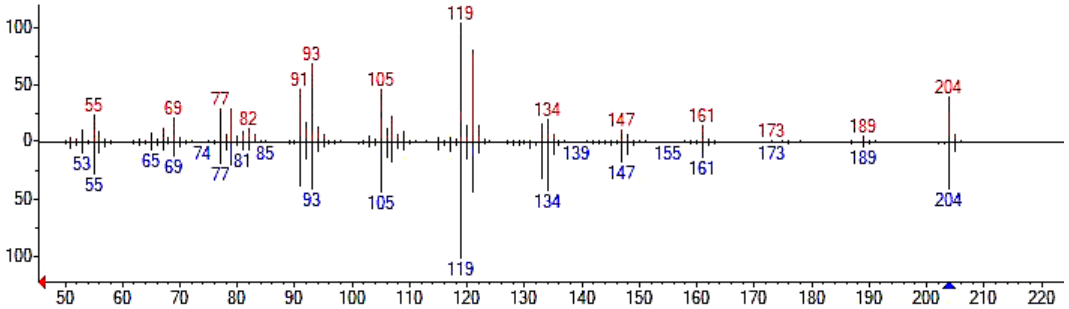
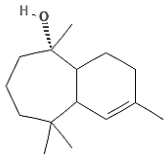
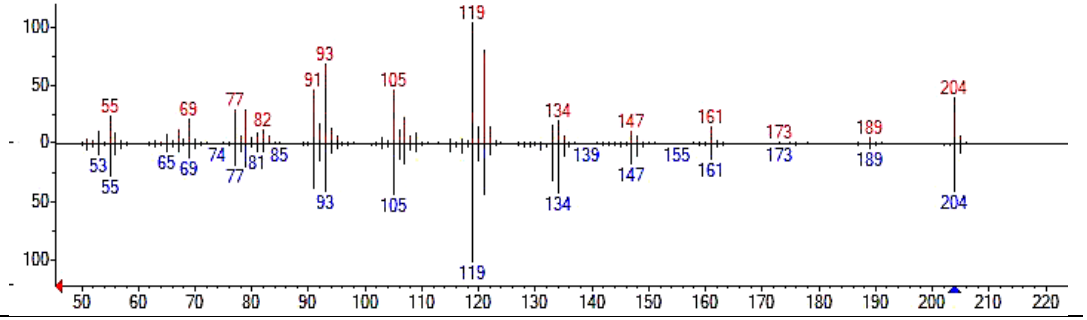
Supplementary Table 12. (Cont.)

Compound Name	Molecular formula	Classification	RT I (min)	RT II (min)	MF
Valerenic acid	$C_{15}H_{22}O_2$	FSTP	2.88%	1.23%	0.46%
Valerenol	$C_{15}H_{24}O$	FSTP	1.86%	5.52%	3.82%
Ylangenal	$C_{15}H_{22}O$	FSTP	2.43%	3.79%	1.23%
α-Farnesene	$C_{15}H_{24}$	STP	4.10%	0.96%	2.66%
α-Guaiene	$C_{15}H_{24}$	STP	3.47%	3.71%	0.13%
α-Panasinsen	$C_{15}H_{24}$	STP	0.13%	1.48%	3.75%
α-Santalol	$C_{15}H_{24}O$	FSTP	1.20%	2.68%	3.17%
β-Caryophyllene	$C_{15}H_{24}$	STP	3.70%	2.67%	0.07%
β-Eudesmol	$C_{15}H_{26}O$	FSTP	2.75%	1.72%	3.14%
β-Guaiene	$C_{15}H_{24}$	STP	3.46%	1.43%	3.07%
β-Longipinene	$C_{15}H_{24}$	STP	3.86%	0.95%	1.25%
β-Selinene	$C_{15}H_{24}$	STP	0.43%	0.67%	3.33%
γ-Elemene	$C_{15}H_{24}$	STP	3.55%	3.73%	4.34%
δ-Elemene	$C_{15}H_{24}$	STP	2.07%	0.83%	1.16%
δ-Guaiene	$C_{15}H_{24}$	STP	4.34%	1.16%	2.62%

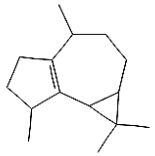
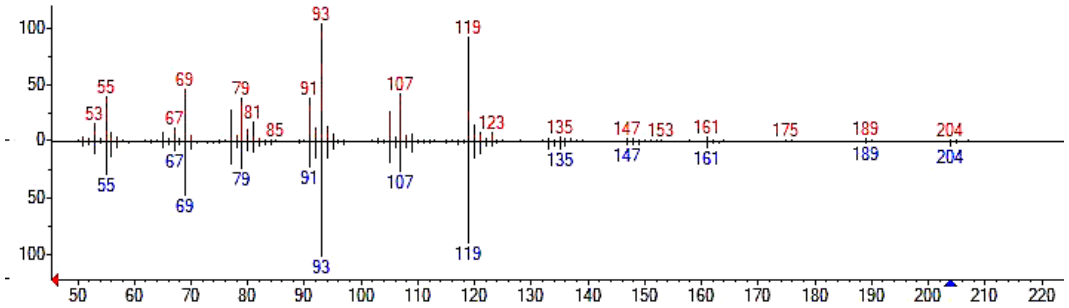
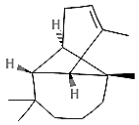
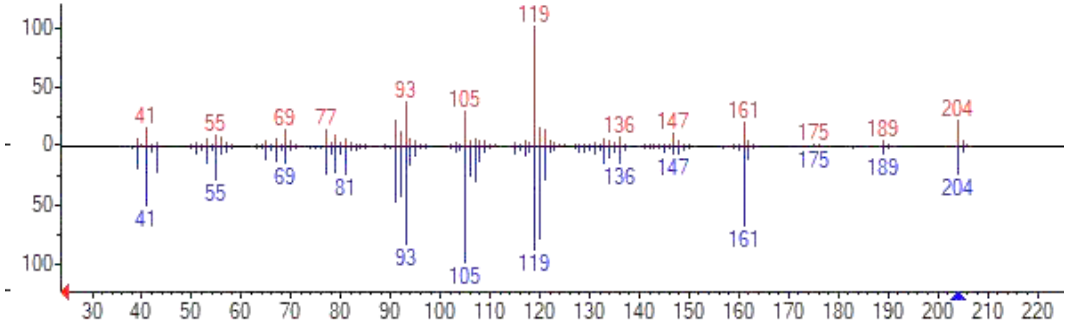
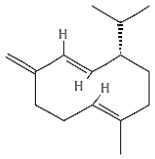
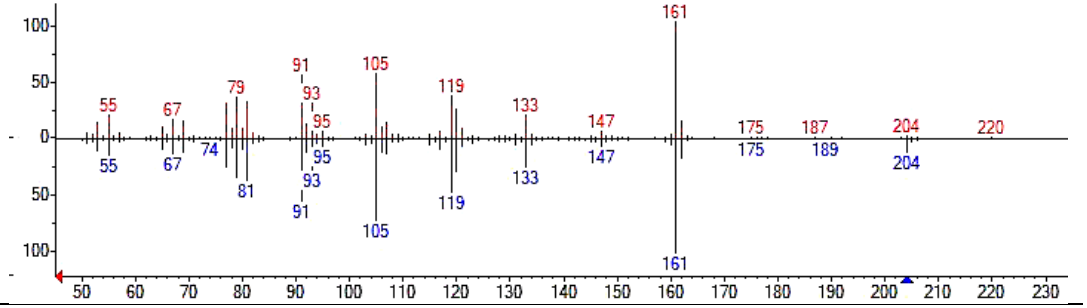
Supplementary Table 13. Mass spectra of sesquiterpenoids identified by GC – MS.

Compound Name	Molecular formula	Structure	Mass spectra
Santalene	$C_{15}H_{24}$		
Bergamotene	$C_{15}H_{24}$		
Zizaene	$C_{15}H_{24}$		

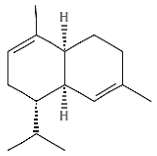
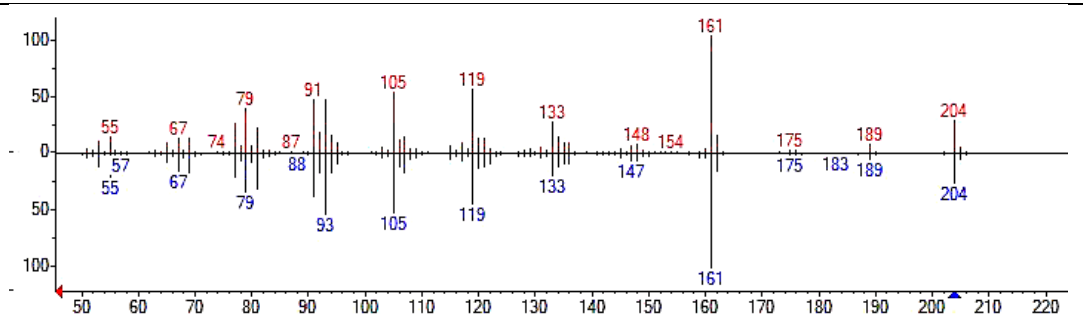
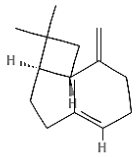
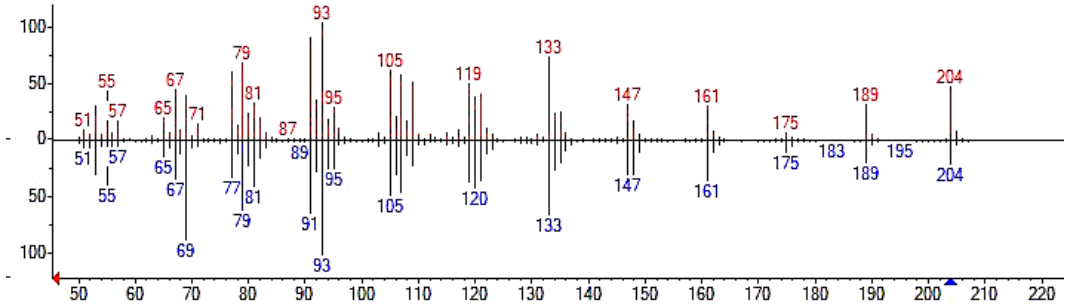
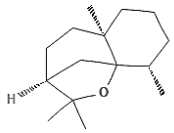
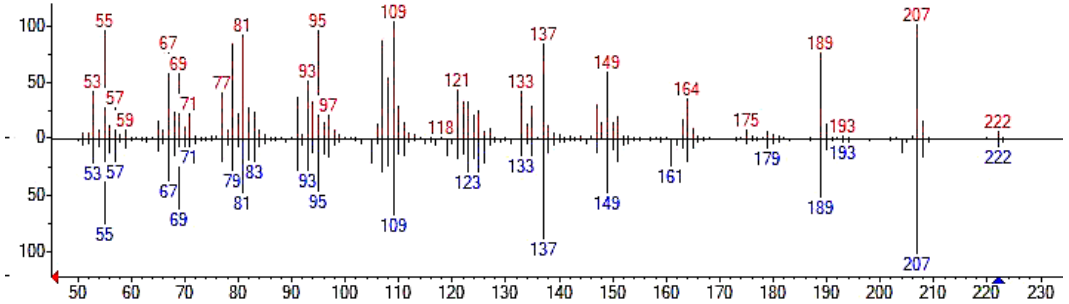
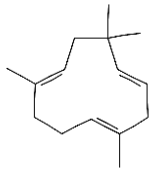
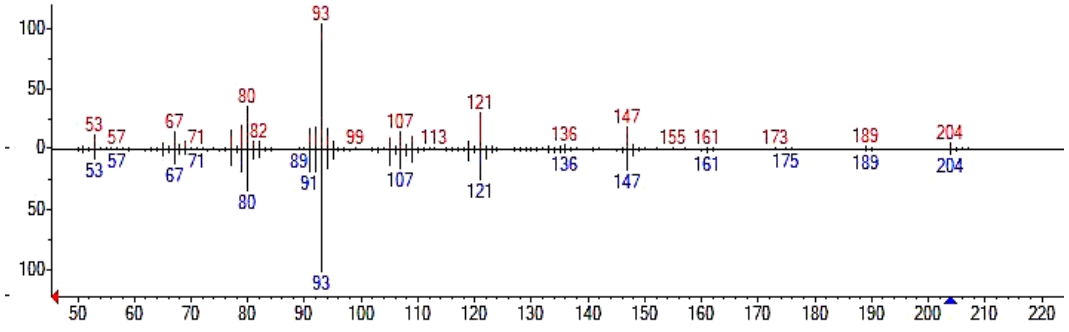
Supplementary Table 13. (Cont.)

Compound Name	Molecular formula	Structure	Mass spectra
Cedrene	$C_{15}H_{24}$		
Curcumene	$C_{15}H_{22}$		
Himalachene	$C_{15}H_{24}$		

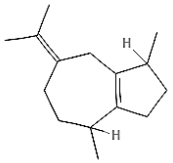
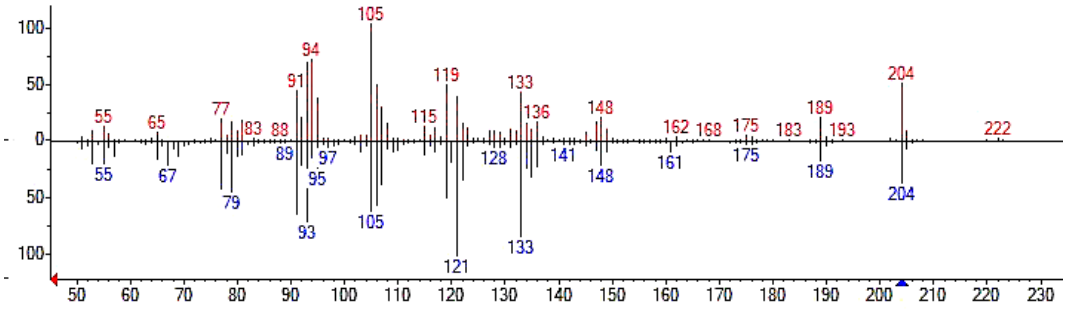
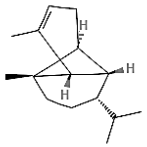
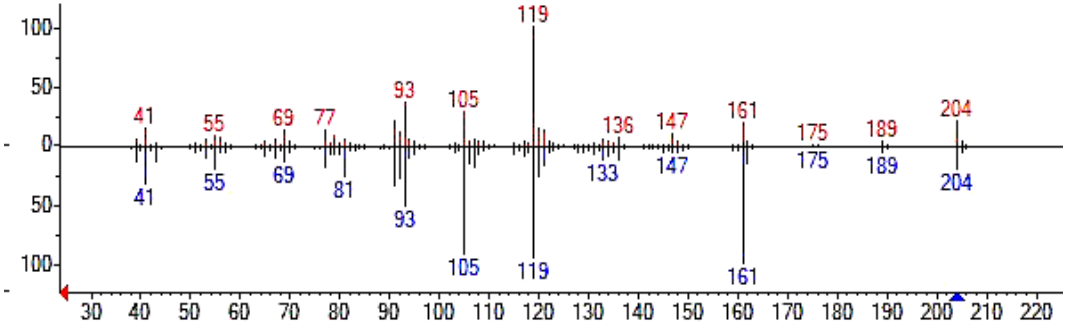
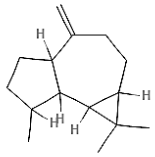
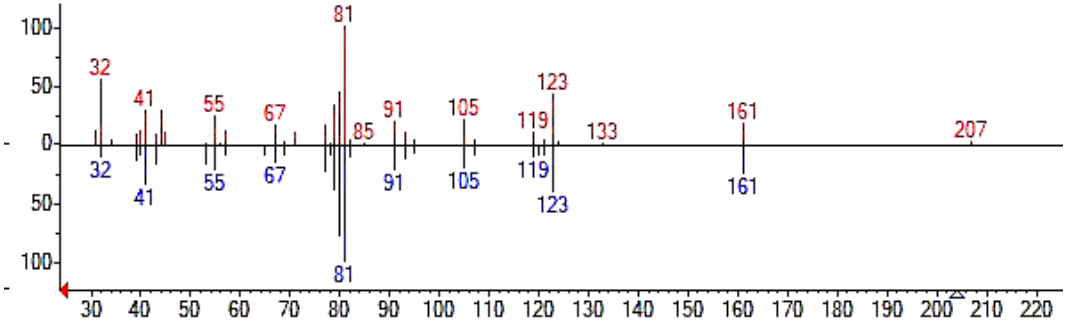
Supplementary Table 13. (Cont.)

Compound Name	Molecular formula	Structure	Mass spectra
Isoledene	$C_{15}H_{24}$		
Longipinene	$C_{15}H_{24}$		
Germacrene D	$C_{15}H_{24}$		

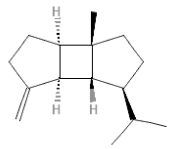
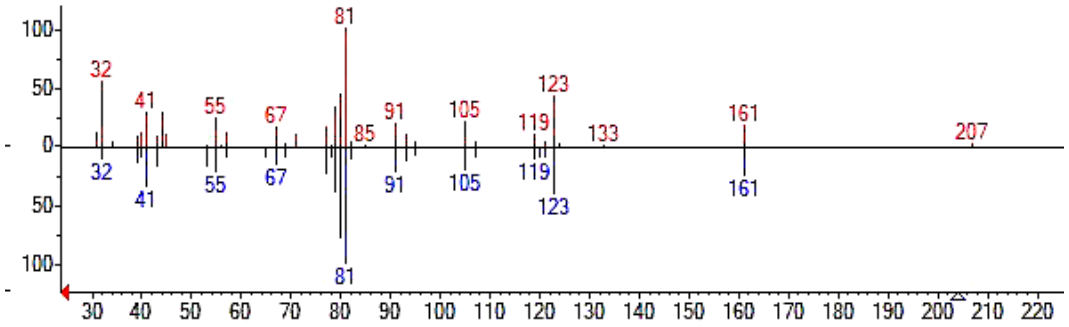
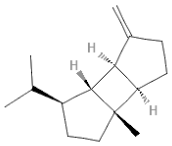
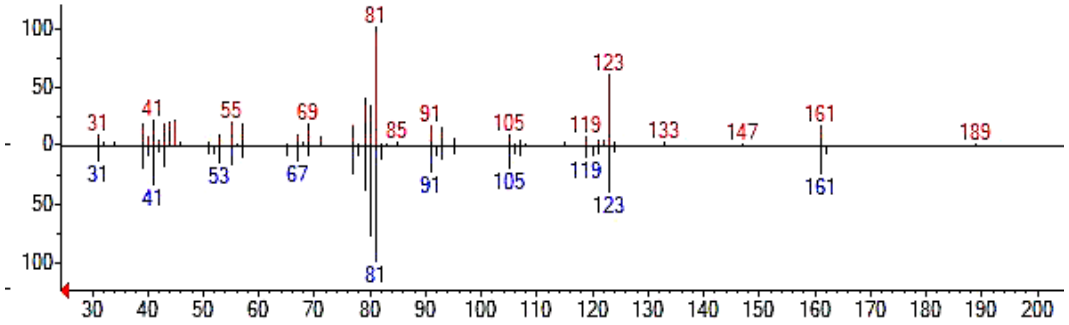
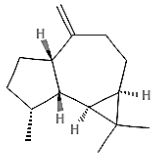
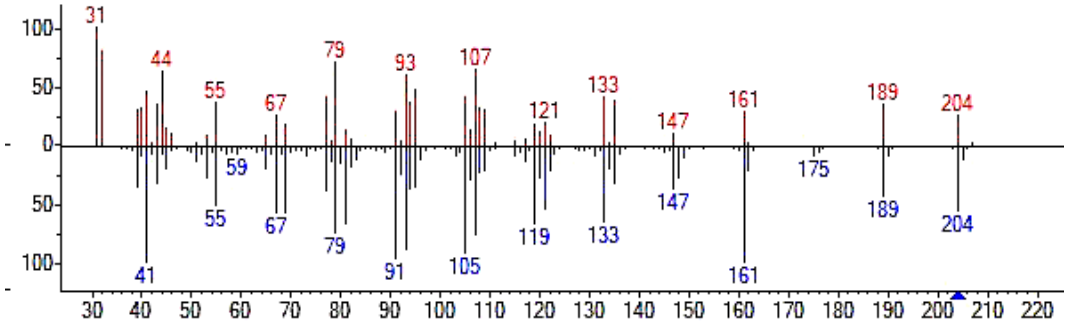
Supplementary Table 13. (Cont.)

Compound Name	Molecular formula	Structure	Mass spectra
γ-Muurolene	$C_{15}H_{24}$		
Caryophyllene	$C_{15}H_{24}$		
β-Agarofuran	$C_{15}H_{26}O$		
α-Humulene	$C_{15}H_{24}$		

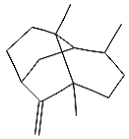
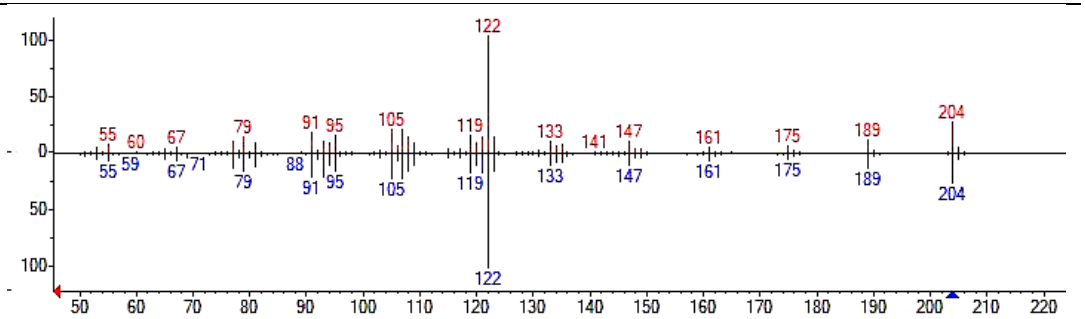
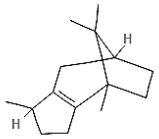
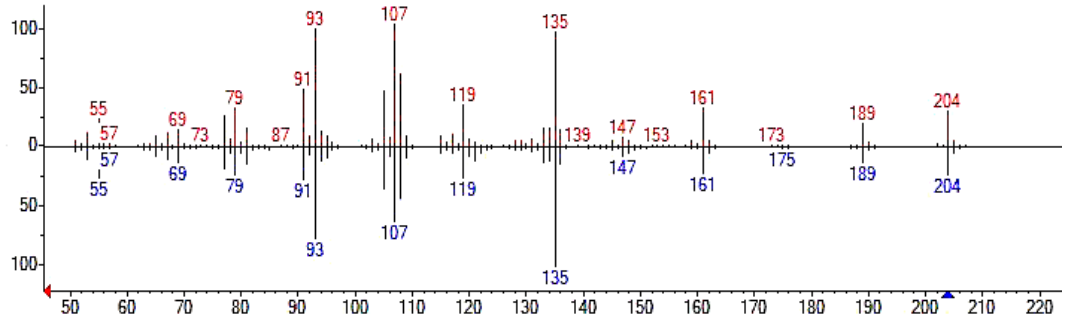
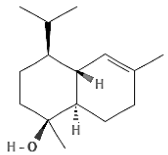
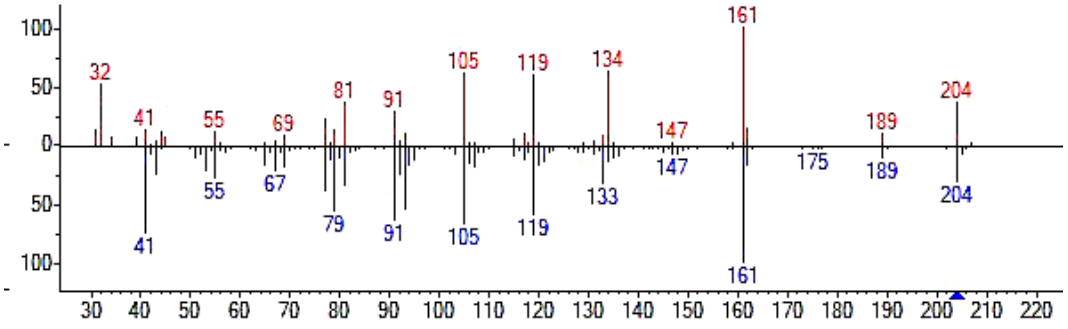
Supplementary Table 13. (Cont.)

Compound Name	Molecular formula	Structure	Mass spectra
α-Guaiene	$C_{15}H_{24}$		
Copaene	$C_{15}H_{24}$		
Aromadendrene	$C_{15}H_{24}$		

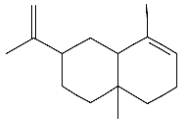
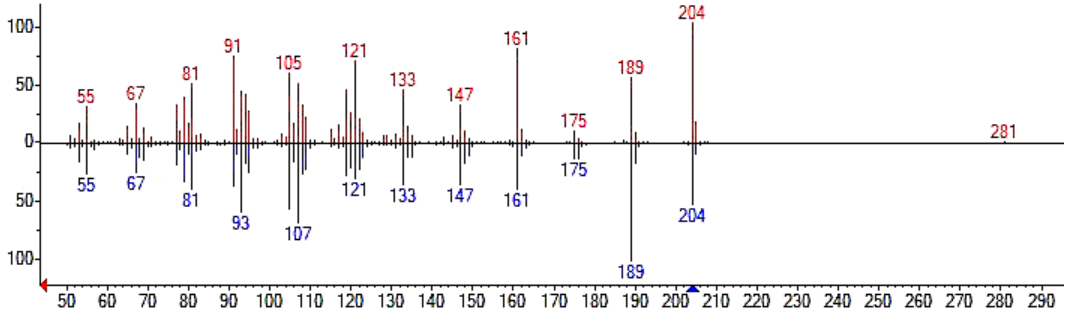
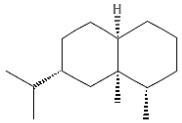
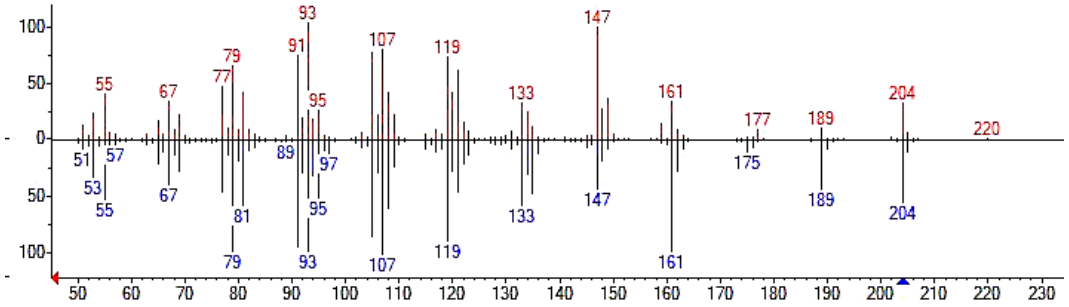
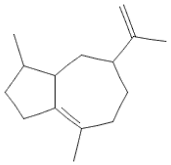
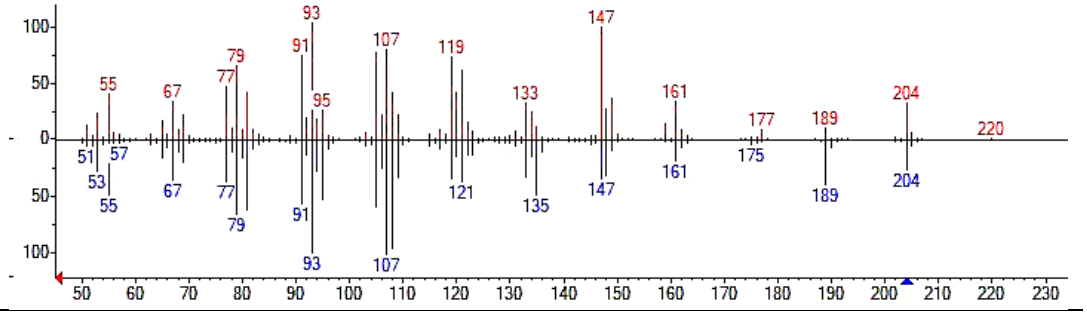
Supplementary Table 13. (Cont.)

Compound Name	Molecular formula	Structure	Mass spectra
β-Bourbonene	$C_{15}H_{24}$		
α-Bourbonene	$C_{15}H_{24}$		
Alloaromadendrene	$C_{15}H_{24}$		

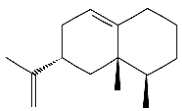
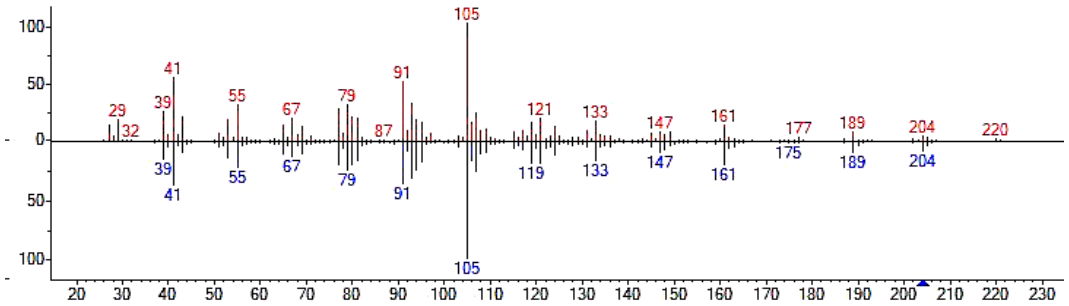
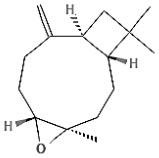
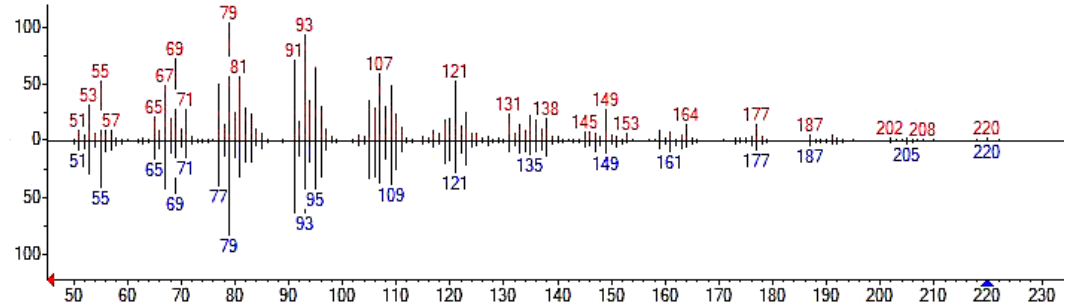
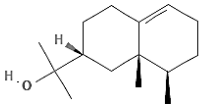
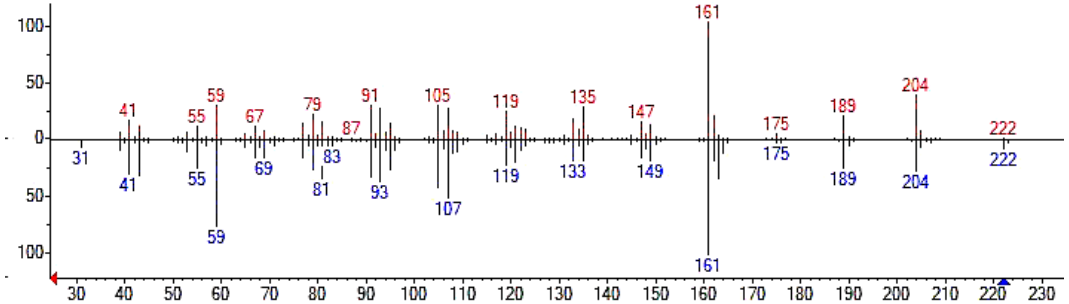
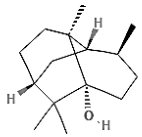
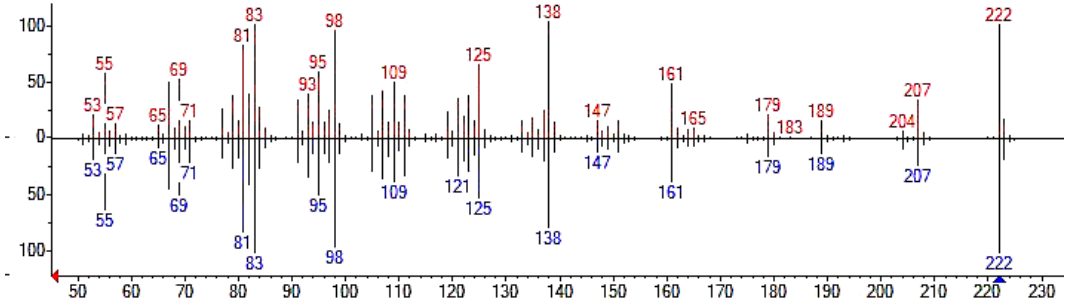
Supplementary Table 13. (Cont.)

Compound Name	Molecular formula	Structure	Mass spectra
Seychellene	$C_{15}H_{24}$		
Patchoulene	$C_{15}H_{24}$		
Cadinol	$C_{15}H_{26}O$		

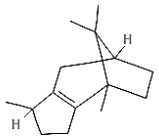
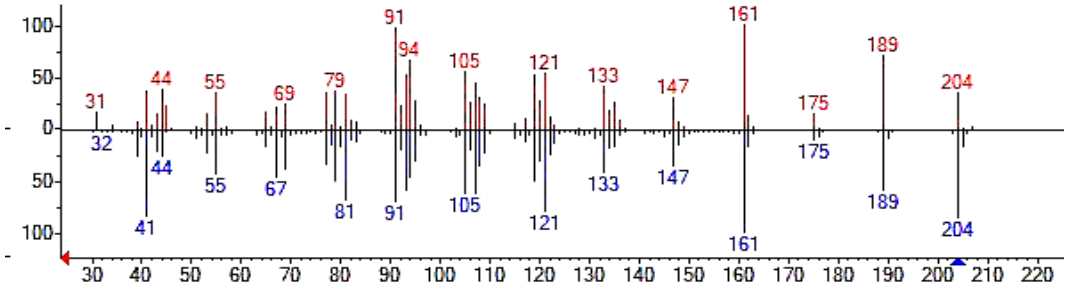
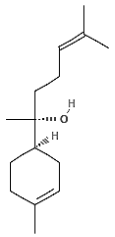
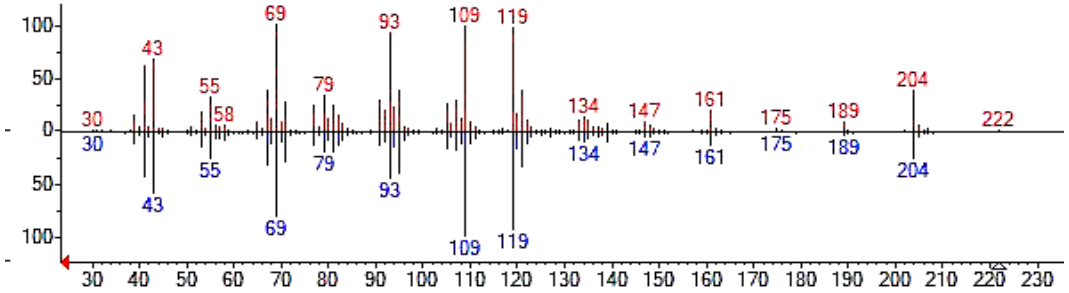
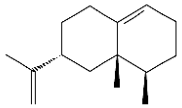
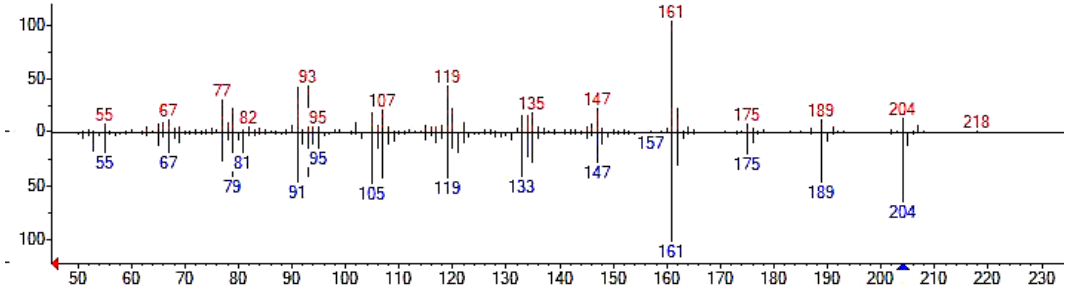
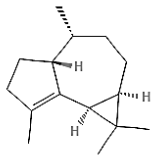
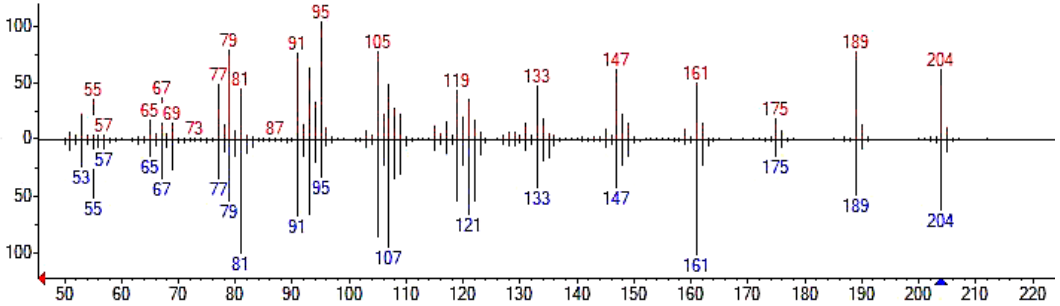
Supplementary Table 13. (Cont.)

Compound Name	Molecular formula	Structure	Mass spectra
Selinene	$C_{15}H_{24}$		
Eremophilane	$C_{15}H_{24}$		
δ-Guaiene	$C_{15}H_{24}$		

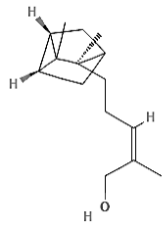
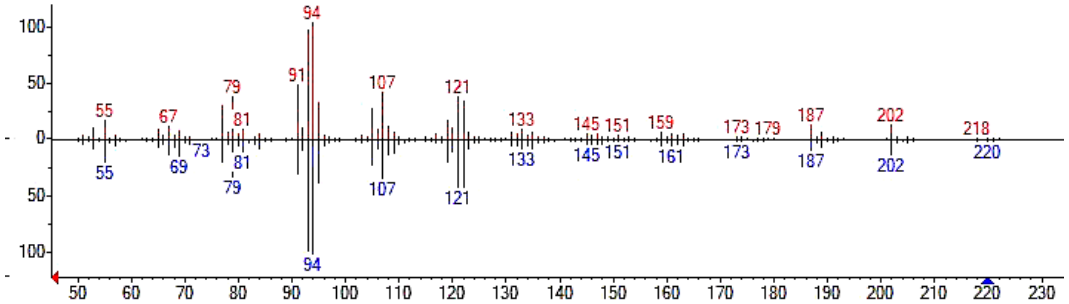
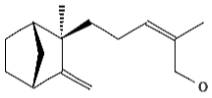
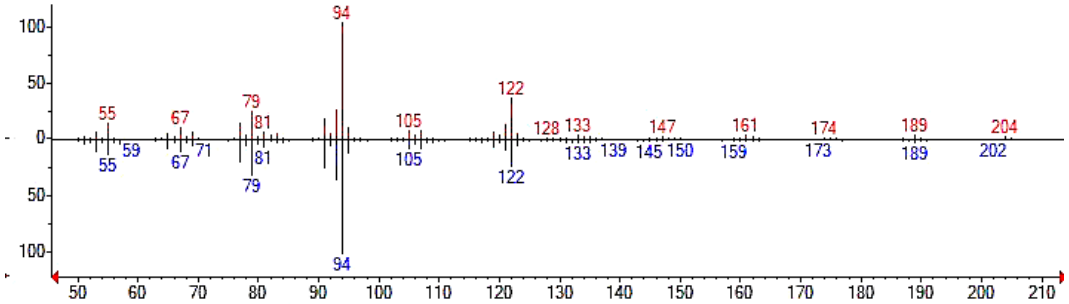
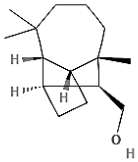
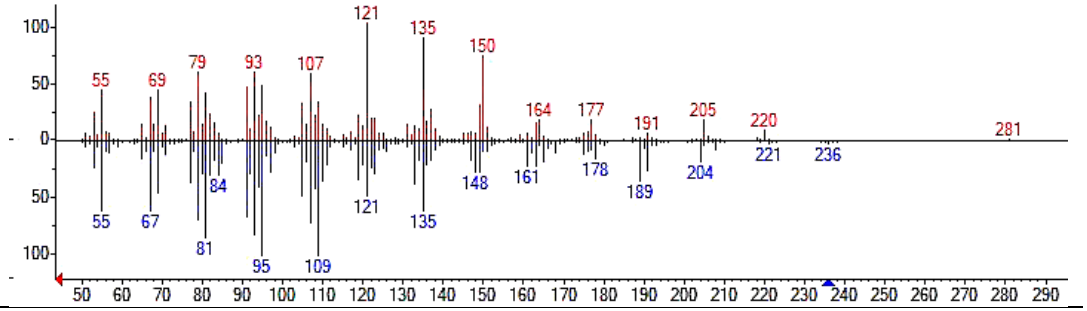
Supplementary Table 13. (Cont.)

Compound Name	Molecular formula	Structure	Mass spectra
Aristolochene	$C_{15}H_{24}$		
Caryophyllene oxide	$C_{15}H_{24}O$		
Valerianol	$C_{15}H_{26}O$		
Patchoulol	$C_{15}H_{26}O$		

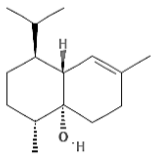
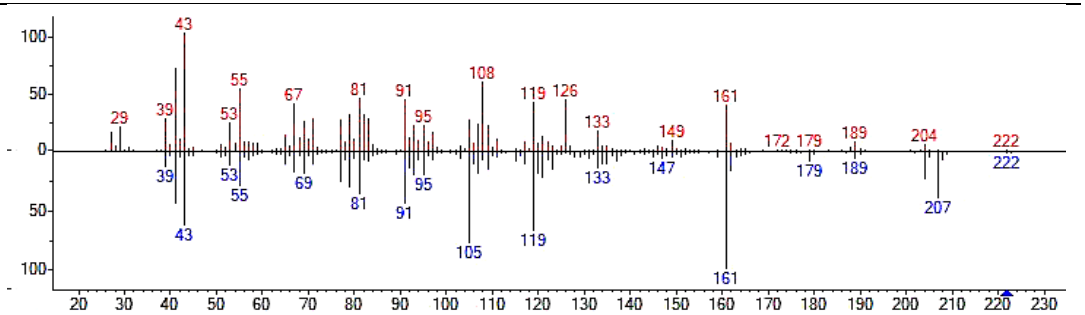
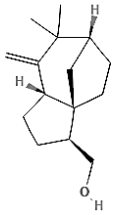
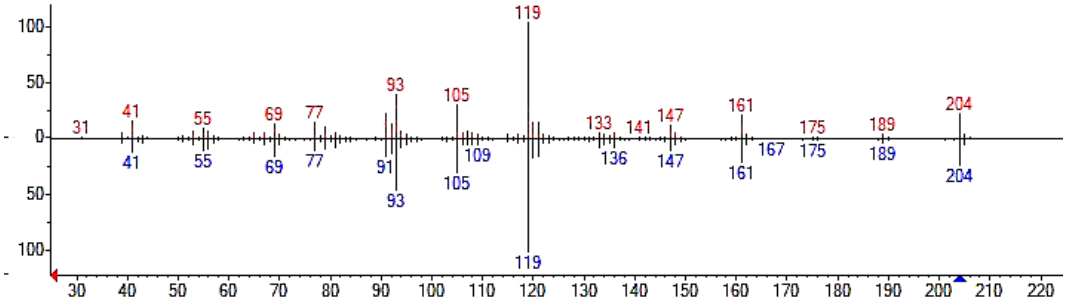
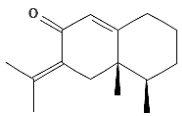
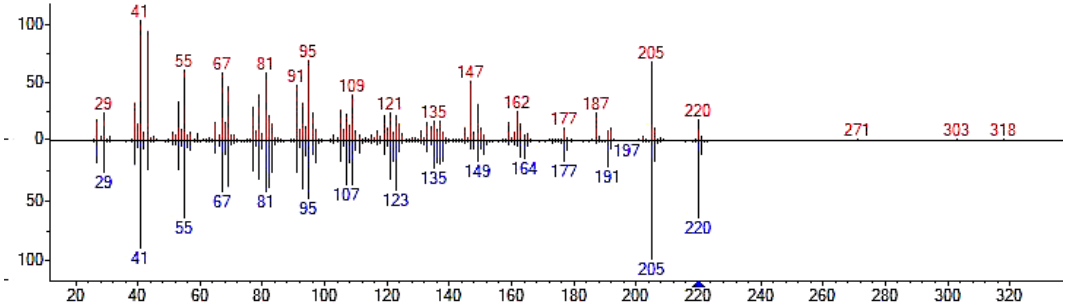
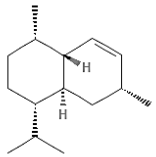
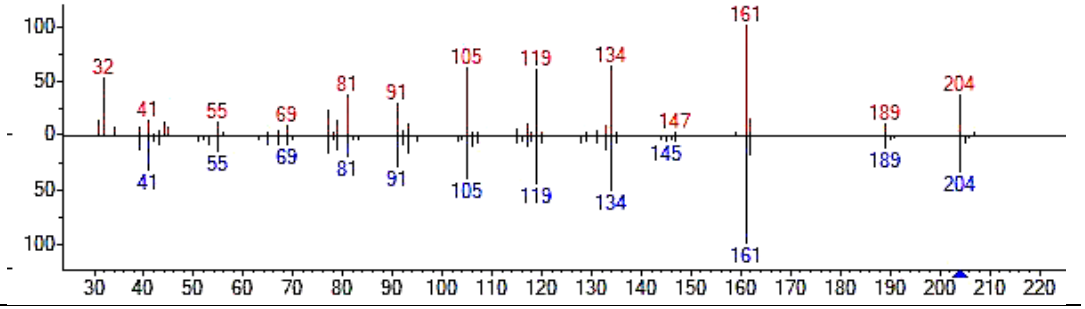
Supplementary Table 13. (Cont.)

Compound Name	Molecular formula	Structure	Mass spectra
Patchoulene	$C_{15}H_{24}$		
Bisabolol	$C_{15}H_{26}O$		
Valencene	$C_{15}H_{24}$		
Gurjunene	$C_{15}H_{24}$		

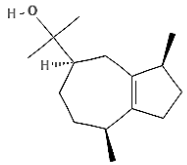
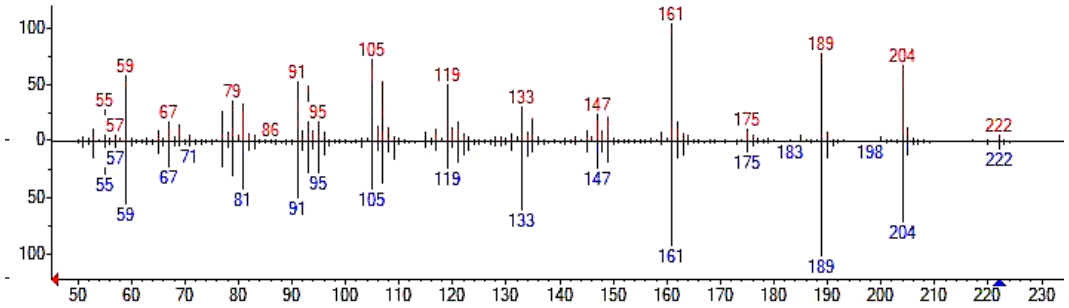
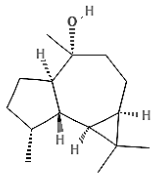
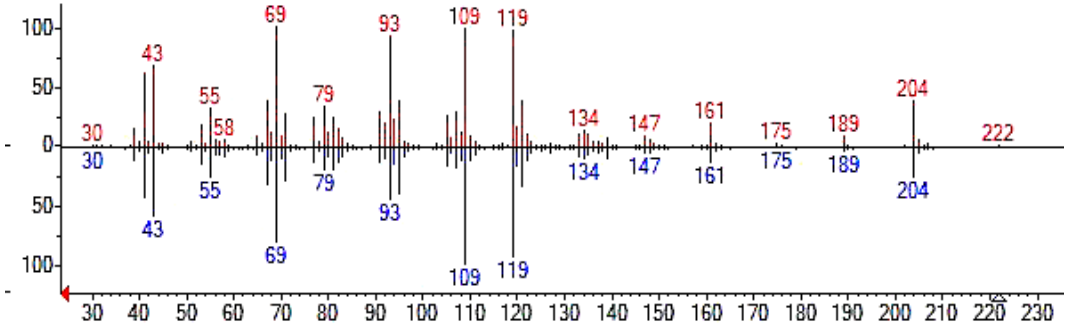
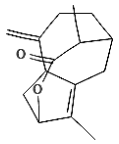
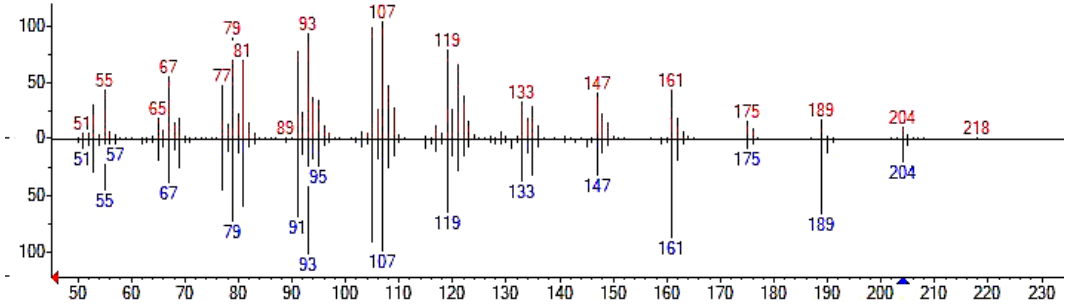
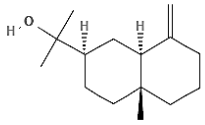
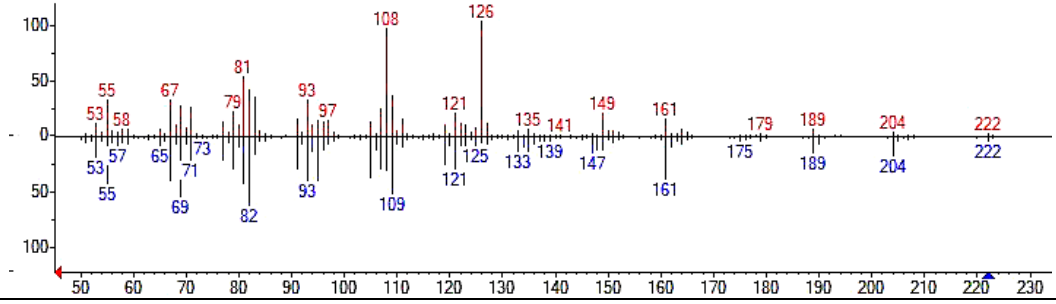
Supplementary Table 13. (Cont.)

Compound Name	Molecular formula	Structure	Mass spectra
α-Santalol	$C_{15}H_{24}O$		
β-Santalol	$C_{15}H_{24}O$		
Isolongifolol	$C_{16}H_{28}O$		

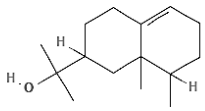
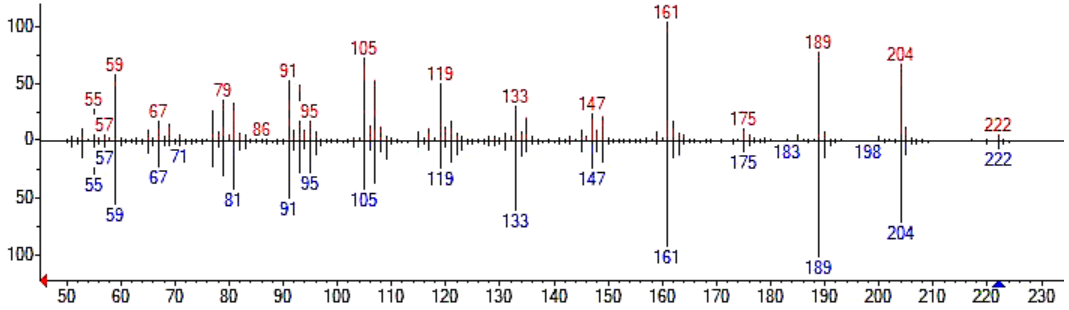
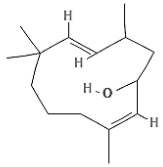
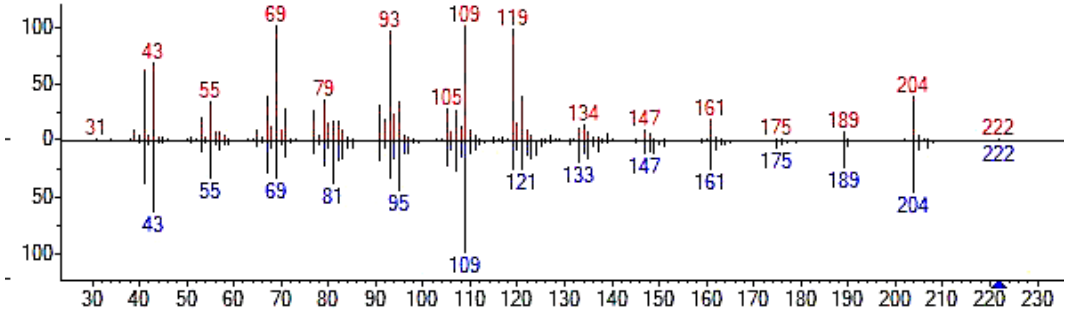
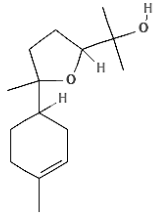
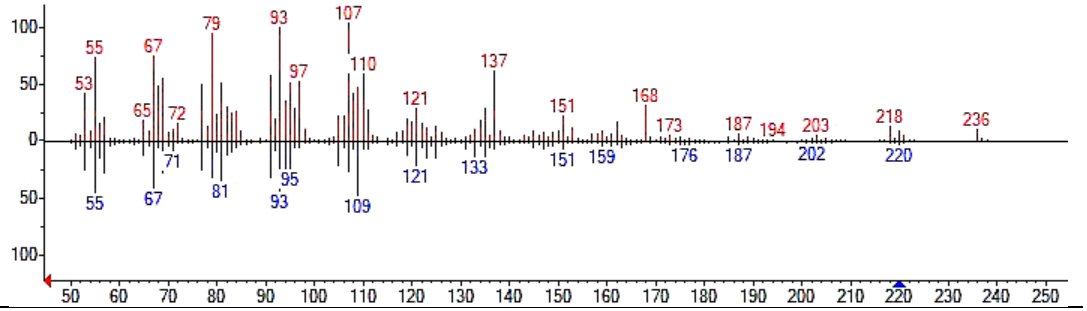
Supplementary Table 13. (Cont.)

Compound Name	Molecular formula	Structure	Mass spectra
Cubenol	$C_{15}H_{26}O$		
Khusimol	$C_{15}H_{24}O$		
Dihydrokaranone	$C_{15}H_{22}O$		
Cadinene	$C_{15}H_{24}$		

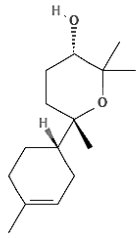
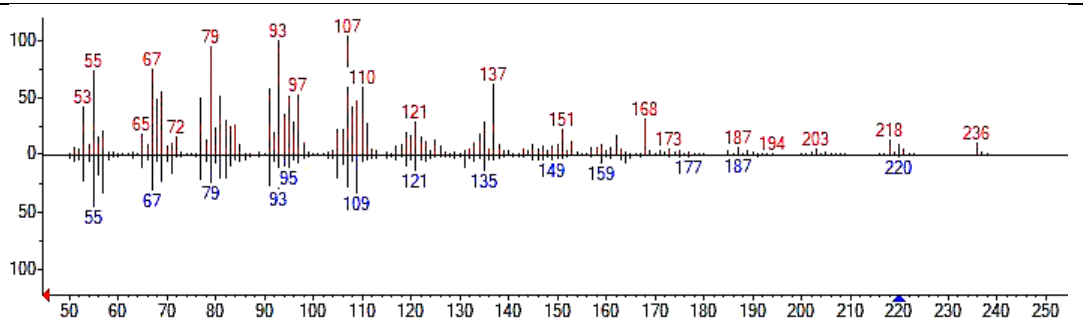
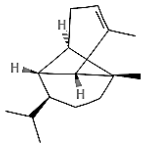
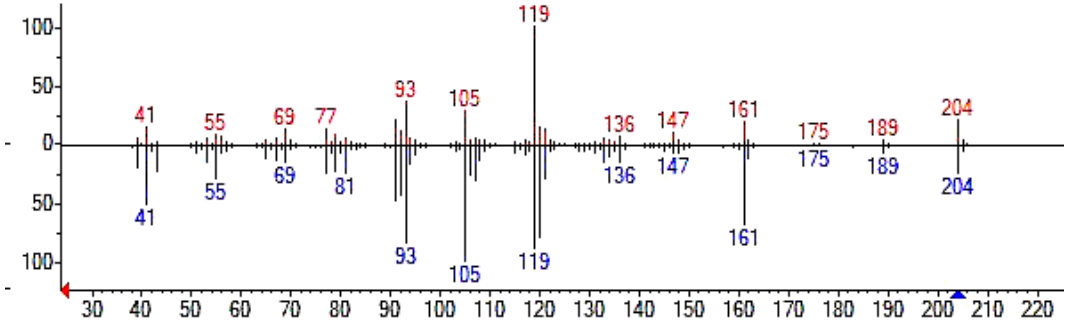
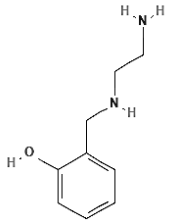
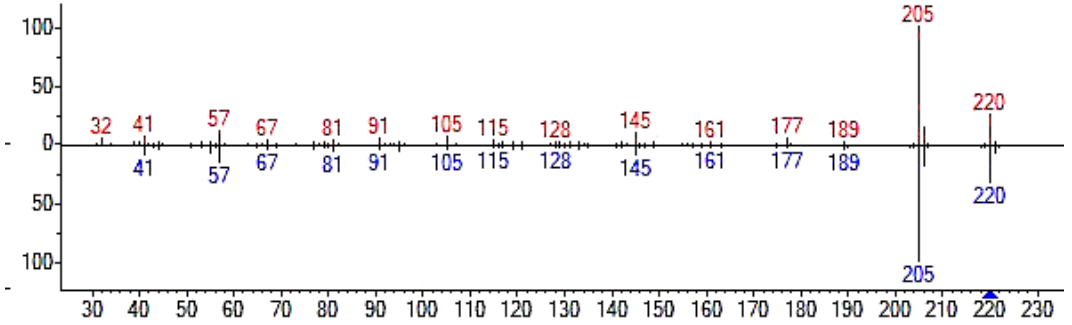
Supplementary Table 13. (Cont.)

Compound Name	Molecular formula	Structure	Mass spectra
Guaiol	$C_{15}H_{26}O$		
Globulol	$C_{15}H_{26}O$		
Guaia-1(10),11-dien-15,2-olide	$C_{15}H_{20}O_2$		
Eudesmol	$C_{15}H_{26}0$		

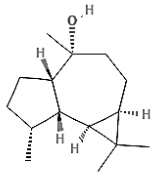
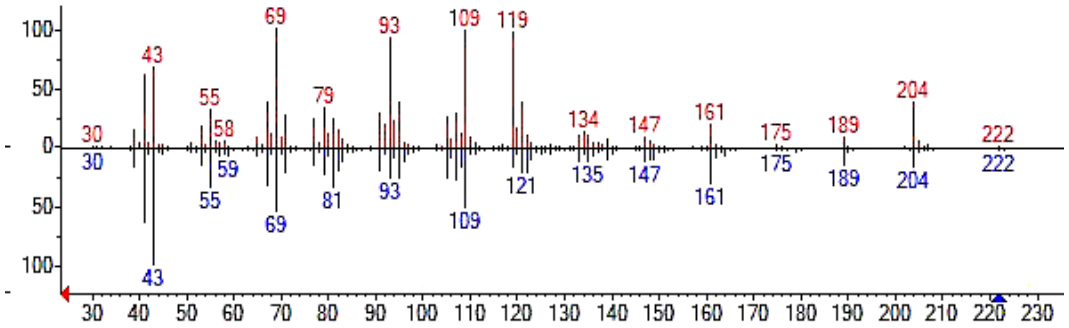
Supplementary Table 13. (Cont.)

Compound Name	Molecular formula	Structure	Mass spectra
Jinkoheremol	$C_{15}H_{26}O$		
Humulane-1,6-dien-3-ol	$C_{15}H_{26}O$		
Bisabolol oxide B	$C_{15}H_{26}O_2$		

Supplementary Table 13. (Cont.)

Compound Name	Molecular formula	Structure	Mass spectra
Bisabolol oxide A	$C_{15}H_{26}O_2$		
Ylangene	$C_{15}H_{24}$		
Agidol	$C_{15}H_{24}O$		

Supplementary Table 13. (Cont.)

Compound Name	Molecular formula	Structure	Mass spectra
Ledol	$C_{15}H_{26}O$		
Aromadendrene oxide	$C_{15}H_{24}O$