

SUPPORTING INFORMATION

Identification and Characterization of GABA_A Receptor Modulatory Diterpenes from *Biota orientalis* which Decrease Locomotor Activity in Mice

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Switzerland

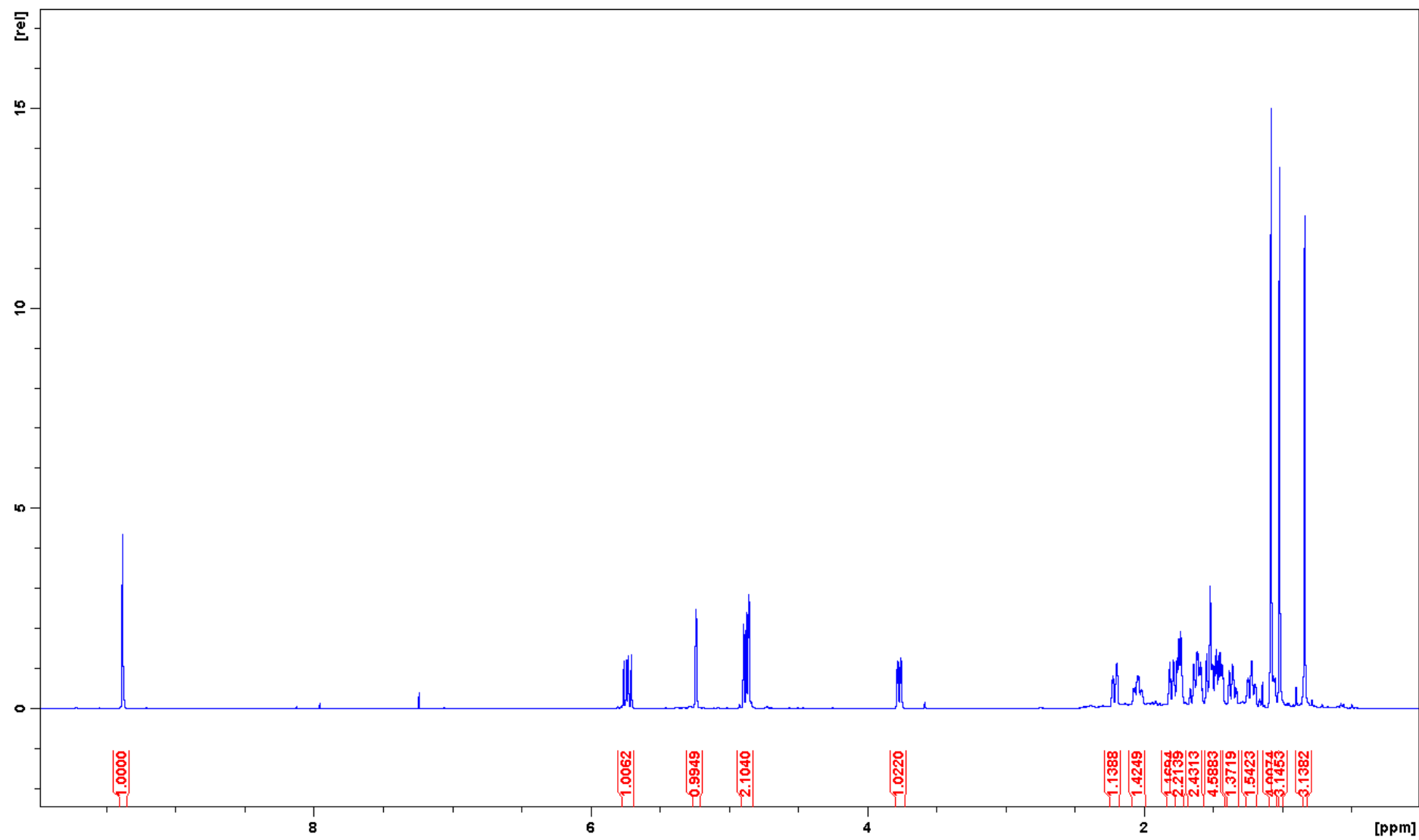
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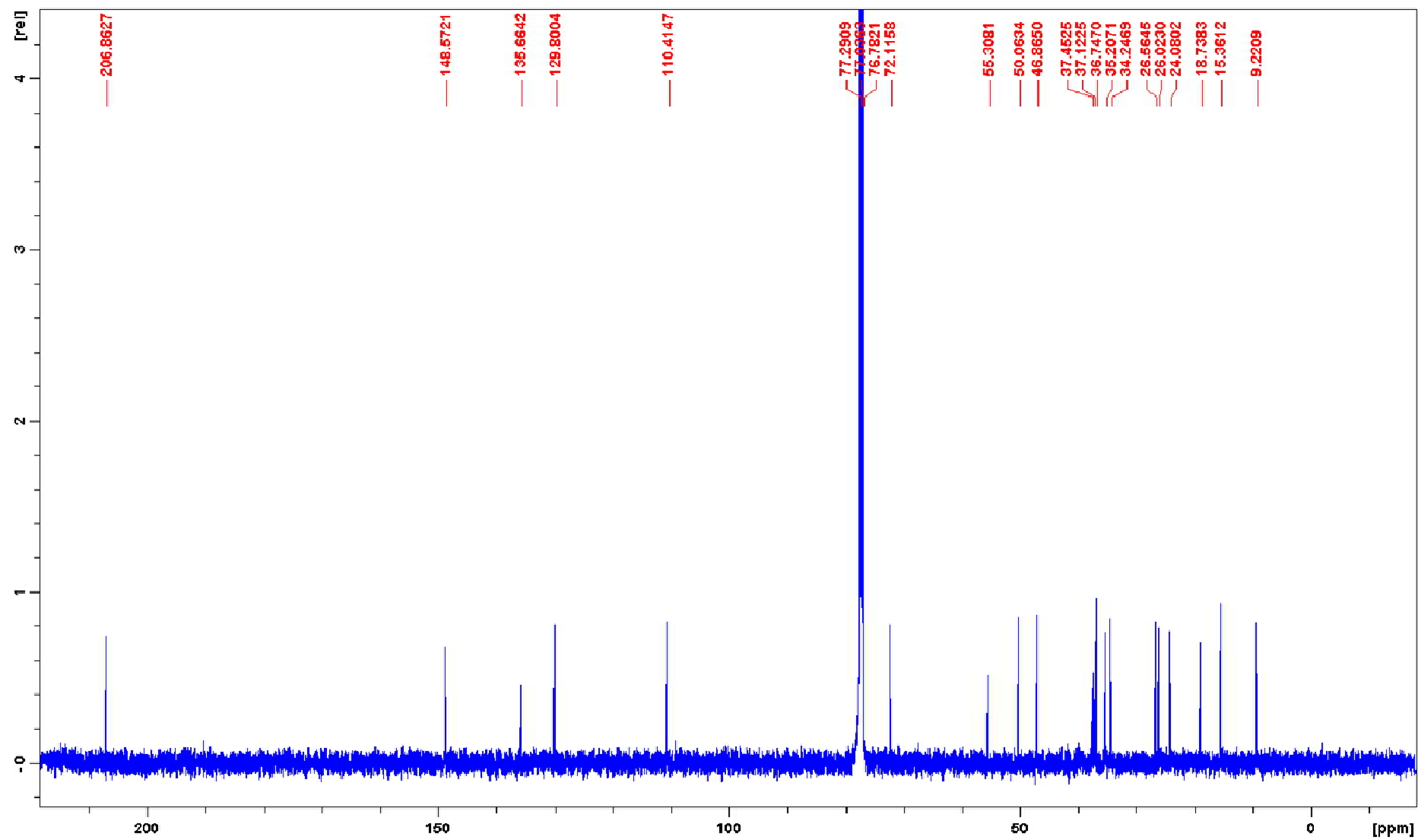
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address: matthias.hamburger@unibas.ch

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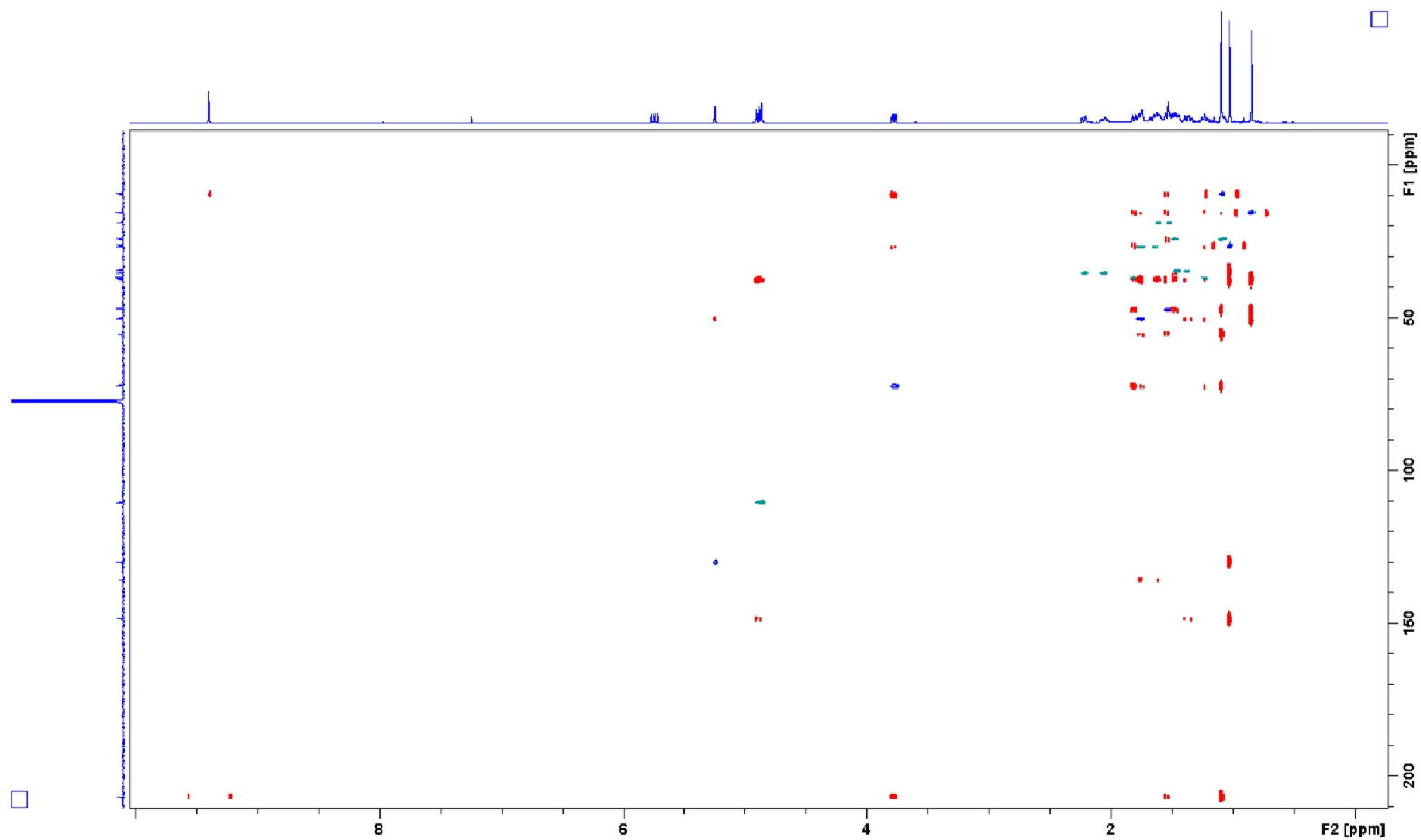
- S1.** ^1H NMR (500 MHz, CDCl_3) of sandaracopimaradienolal (**3**).
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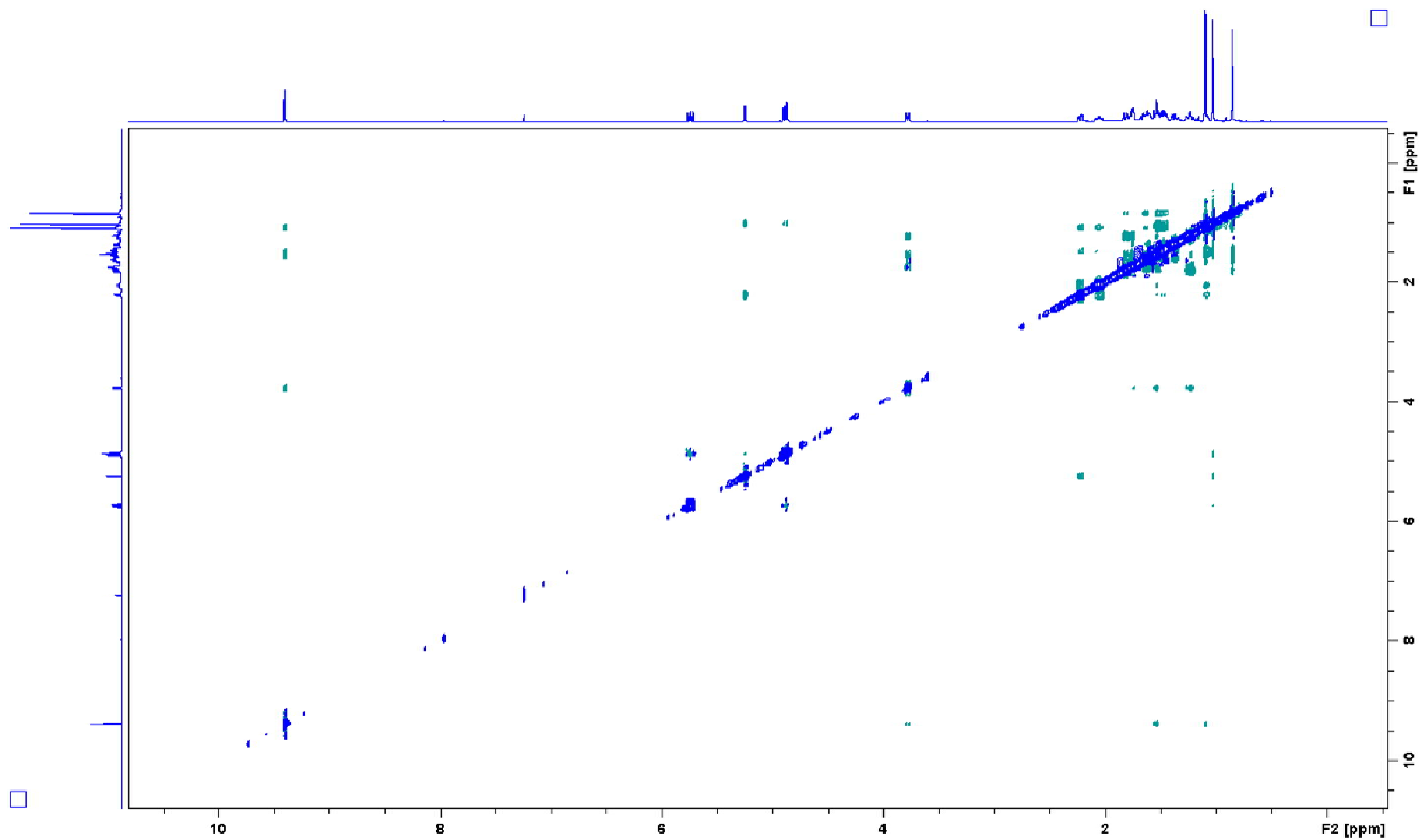
S1. ^1H NMR (500 MHz, CDCl_3) of sandaracopimaradienol (3).



S2. ¹³C NMR (125 MHz, CDCl₃) of sandaracopimaradienolal (**3**).



S3. DEPT-edited HSQC NMR (green/blue) and HMBC NMR (red) spectra of sandaracopimaradienolal (**3**), overlaid.

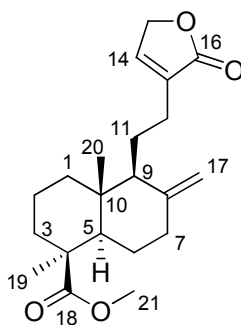


S4. NOESY NMR of sandaracopimaradienolal (**3**)

S5. Analytical data of pinusolide (**1**) (CAS = 31685-80-0)

Experimental data

m/z (ESI-ion trap, positive mode) ¹	$[M+H]^+$ 347.2; $[2M+Na]^+$ 715.3
m/z (ESI-TOF-MS, positive mode) ¹	$[M+Na]^+$ 369.2152; $[2M+Na]^+$ 715.4238
Sum formula	C ₂₁ H ₃₀ O ₄
UV $\lambda_{\max}$ [nm]	210



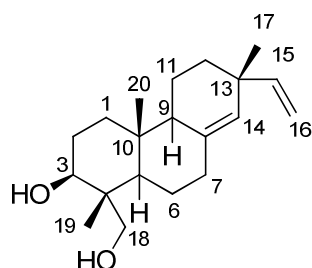
	δ_C (CDCl ₃) ^{a 2}	δ_H (I, m, J in Hz) (CDCl ₃) ²
1	39.7	1.81 (1H, m); 1.06 (1H, m)
2	20.2	1.83 (1H, m); 1.50 (1H, m)
3	38.6	2.16 (1H, m); 1.01 (1H, m)
4	45.3	-
5	56.9	1.59 (1H, dd, 12.6, 3.1)
6	26.5	1.97 (1H, m); 1.77 (1H, m)
7	39.1	2.40 (1H, m); 1.88 (1H, m)
8	148.0	-
9	56.3	1.60 (1H, br d, 10.8)
10	40.4	-
11	22.4	1.57 (1H, m); 1.76 (1H, m)
12	25.1	2.45 (1H, m); 2.10 (1H, m)
13	135.3	-
14	144.0	7.06 (1H, dd, 1.8)
15	70.2	4.73 (2H, dd, 4.3, 1.8)
16	175.2	-
17	107.3	4.87 (1H, br s); 4.56 (1H, br s)
18	178.7	-
19	29.1	1.16 (3H, s)
20	13.1	0.50 (3H, s)
21	51.4	3.58 (3H, s)

^a¹³C-Shifts from HSQC- and HMBC-NMR-experiments

S6. Analytical data of sandaracopimaradienediol (**2**) (CAS = 59219-64-6)

Experimental data

m/z (ESI-ion trap, positive mode)	$[2M+H]^+$ 609.3
m/z (ESI-TOF-MS, positive mode) ³	$[M+Na]^+$ 327.2313
Sum formula	$C_{20}H_{32}O_2$
UV λ_{max} [nm]	210



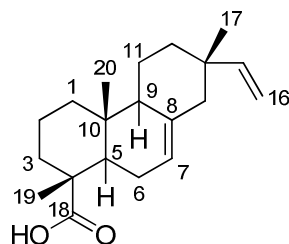
	δ_C (CDCl ₃) ^{a3}	δ_H (I, m, J in Hz) (CDCl ₃) ³
1	37.31	1.74 (1H, m); 1.15 (1H, m)
2	27.57	1.57 – 1.65 (2H, m)
3	77.03	3.66 (1H, m)
4	42.62	-
5	48.88	1.16 (1H, m)
6	22.75	1.38 – 1.45 (2H, m)
7	35.87	2.24 (1H, m); 2.02 (1H, m)
8	136.56	-
9	50.71	1.66 (1H, m)
10	38.34	-
11	19.12	1.58 (1H, m); 1.49 (1H, m)
12	34.93	1.45 (1H, m); 1.34 (1H, m)
13	37.68	-
14	129.45	5.21 (1H, s)
15	149.17	5.74 (1H, dd, 17.6, 10.6)
16	110.38	4.88 (1H, dd, 17.6, 1.22); 4.85 (1H, dd, 10.6, 1.22)
17	26.34	1.02 (3H, s)
18	71.88	3.66 (1H, d, 10.5); 3.40 (1H, d, 10.5)
19	11.74	0.90 (3H, s)
20	15.74	0.84 (3H, s)

^{a3}¹³C-shifts measured at 125.77 MHz.

S7. Analytical data of isopimaric acid (**4**) (CAS = 5835-26-7)

Experimental data

m/z (ESI-ion trap, negative mode) ⁴	$[M-H]^-$ 301.2 ; $[2M-H]^-$ 603.1
m/z (ESI-TOF-MS, negative mode)	$[M-H]^-$ 301.2174
Sum formula	$C_{20}H_{30}O_2$
UV λ_{max} [nm]	210



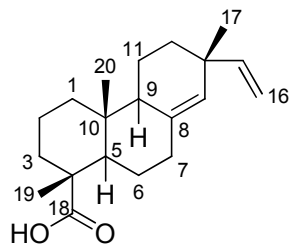
	δ_C (CDCl ₃) ^{a 5, 6}	δ_H (I, m, J in Hz) (CDCl ₃) ⁷
1	38.9	1.87 (1H, m); 1.14 (1H, m)
2	18.0	1.58 (2H, m)
3	37.0	1.81 (1H, m); 1.69 (1H, m)
4	46.2	-
5	45.3	1.98 (1H, m)
6	25.1	2.03 (1H, m); 1.73 (1H, m)
7	120.7	5.34 (1H, dd, 5.53, 1.30)
8	<i>n.d.</i>	-
9	52.0	1.78
10	35.1	-
11	20.0	1.59 (1H, m); 1.40 (1H, m)
12	36.0	1.51 (1H, m); 1.39 (1H, m)
13	<i>n.d.</i>	-
14	46.3	1.99 (1H, m); 1.94 (1H, m)
15	150.7	5.82 (1H, dd, 17.4, 10.8)
16	109.9	4.94 (1H, dd, 17.4, 0.8); 4.88 (1H, dd, 10.8, 0.8)
17	21.6	0.89 (3H, s)
18	185.9	-
19	17.2	1.30 (3H, s)
20	15.1	0.94 (3H, s)

^a¹³C-Shifts from HSQC- and HMBC-NMR-experiments

S8. Analytical data of sandaracopimaric acid (**5**) (CAS = 471-74-9)

Experimental data

m/z (ESI-ion trap, negative mode)	$[M-H]^-$ 301.2 ; $[2M-H]^-$ 603.1 ⁴
m/z (ESI-TOF-MS, negative mode)	$[M-H]^-$ 301.2174
Sum formula	C ₂₀ H ₃₀ O ₂
UV $\lambda_{\max}$ [nm]	210



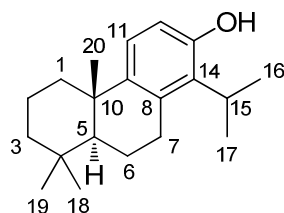
	δ_C (CDCl ₃) ^{a 5, 6}	δ_H (I, m, <i>J</i> in Hz) (CDCl ₃) ^{7, 8}
1	38.3	1.78 (1H, m); 1.15 (1H, m)
2	18.0	1.58 (2H, m)
3	37.0	1.81 (1H, m); 1.69 (1H, m)
4	47.9	-
5	48.8	1.94 (1H, m)
6	24.9	1.48 (1H, m); 1.31 (1H, m)
7	35.4	2.25 (1H, m); 2.15 (1H, m)
8	<i>n.d.</i>	-
9	50.7	1.83 (1H, m)
10	38.4	-
11	18.4	1.63 (1H, m); 1.49 (1H, m)
12	34.5	1.49 (1H, m); 1.40 (1H, m)
13	37.5	-
14	129.5	5.25 (1H, br s)
15	148.7	5.79 (1H, dd, 17.2, 10.7)
16	110.0	4.92 (1H, dd, 17.2, 1.2); 4.89 (1H, dd, 10.7, 1.2)
17	26.1	1.06 (3H, s)
18	185.9	-
19	16.7	1.23 (3H, s)
20	15.1	0.86 (3H, s)

^a¹³C-Shifts from HSQC- and HMBC-NMR-experiments

S9. Analytical data of totarol (**6**) (CAS = 511-15-9)

Experimental data

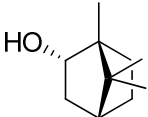
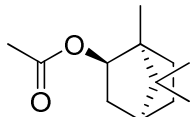
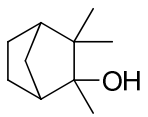
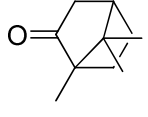
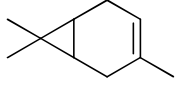
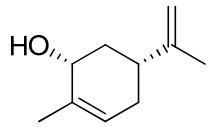
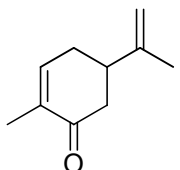
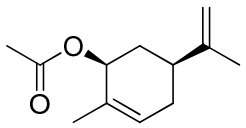
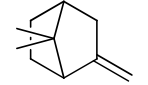
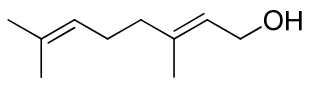
m/z (ESI-ion trap, negative mode)	$[M-H]^-$ 285.3
m/z (ESI-TOF-MS, negative mode) ⁹	$[M-H]^-$ 285.2248
Sum formula	C ₂₀ H ₃₀ O
UV $\lambda_{\max}$ [nm] ¹⁰	210; 280

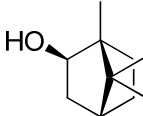
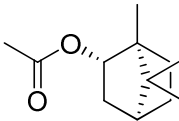
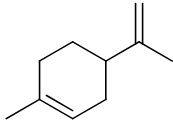
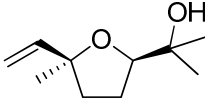
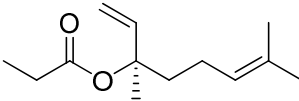
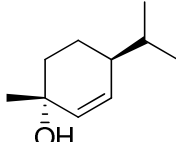
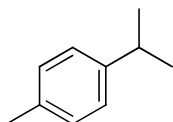
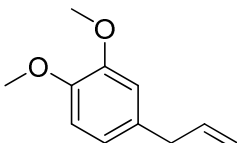
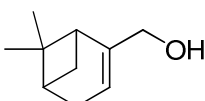
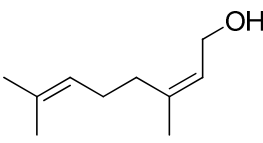


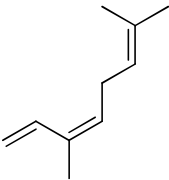
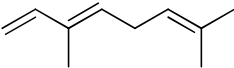
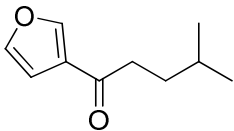
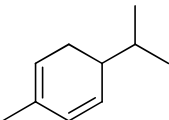
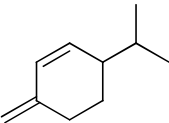
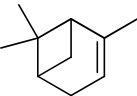
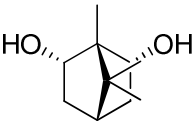
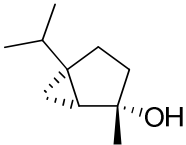
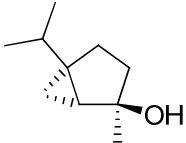
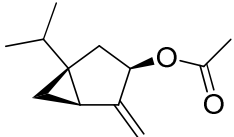
	δ_C (CDCl ₃) ^{a 9, 11}	δ_H (I, m, J in Hz) (CDCl ₃) ¹¹
1	39.6	2.25 (1H, br d, 12.7); 1.37 (1H, m)
2	19.5	1.75 (1H, m); 1.61 (1H, m)
3	41.7	1.49 (1H, br d, 13.3); 1.23 (1H, ddd, 13.3, 13.3, 3.1)
4	33.2	-
5	49.7	1.29 (1H, dd, 12.6, 2.0)
6	19.3	1.94 (1H, br dd, 12.6, 7.7); 1.69 (1H, m)
7	28.6	2.96 (1H, dd, 17.2, 6.7); 2.78 (1H, ddd, 17.2, 10.1, 7.7)
8	133.7	-
9	143.2	-
10	37.6	-
11	122.9	7.00 (1H, d, 8.5)
12	114.3	6.51 (1H, d, 8.4)
13	151.8	-
14	131.1	-
15	27.1	3.32 (1H, sept, 7.2)
16/17	20.5	1.38 (3H, d, 7.2) and 1.36 (3H, d, 7.2)
18	33.2	0.98 (3H, s)
19	21.6	0.95 (3H, s)
20	25.1	1.20 (3H, s)

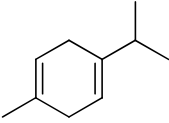
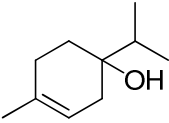
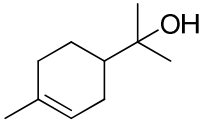
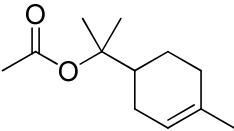
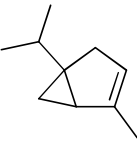
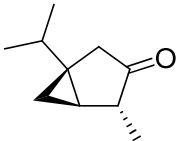
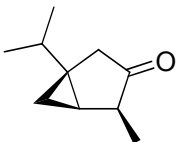
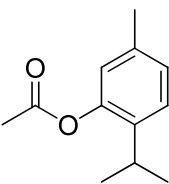
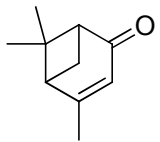
^a¹³C-Shifts from HSQC- and HMBC-NMR-experiments

S10. Monoterpenes isolated from *Biota orientalis*

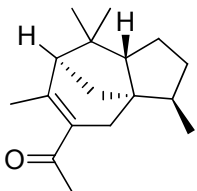
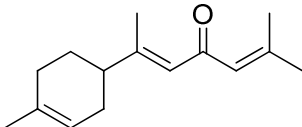
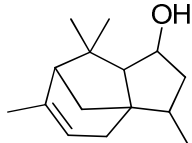
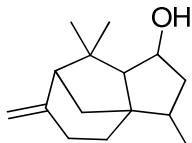
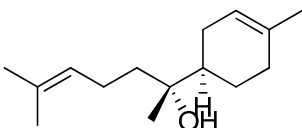
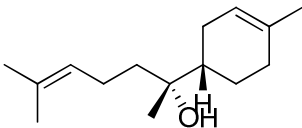
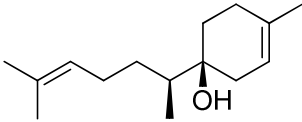
<i>Trivial name</i>	<i>CAS number</i>	<i>Sum formula</i>	<i>MW</i>	<i>Structure</i>	<i>Ref.</i>
Borneol	507-70-0	C ₁₀ H ₁₈ O	154.25		12
Bornyl acetate	76-49-3	C ₁₂ H ₂₀ O ₂	196.29		13
Camphene hydrate	465-31-6	C ₁₀ H ₁₈ O	154.25		12
Camphor	76-22-2	C ₁₀ H ₁₆ O	152.23		12
Δ ³ -Carene	13466-78-9	C ₁₀ H ₁₆	136.23		12
<i>cis</i> -Carveol	1197-06-4	C ₁₀ H ₁₆ O	152.23		12
Carvone	99-49-0	C ₁₀ H ₁₄ O	150.22		12
<i>cis</i> -Carvyl acetate	1205-42-1	C ₁₂ H ₁₈ O ₂	194.27		12
α-Fenchene	471-84-1	C ₁₀ H ₁₆	136.23		14
Geraniol	106-24-1	C ₁₀ H ₁₈ O	154.25		12

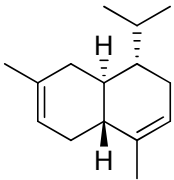
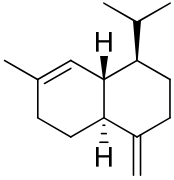
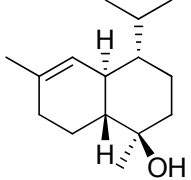
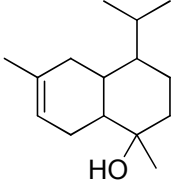
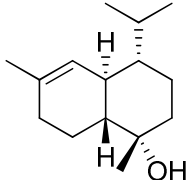
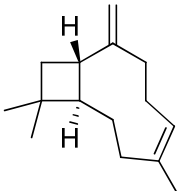
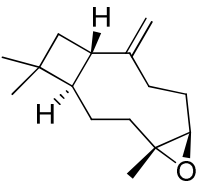
<i>Trivial name</i>	<i>CAS number</i>	<i>Sum formula</i>	<i>MW</i>	<i>Structure</i>	<i>Ref.</i>
Isoborneol	124-76-5	C ₁₀ H ₁₈ O	154.25		12
Isobornyl acetate	125-12-2	C ₁₂ H ₂₀ O ₂	196.29		12
α -Limonene	138-86-3	C ₁₀ H ₁₆	136.23		12
Linalool oxide	5989-33-3	C ₁₀ H ₁₈ O ₂	170.25		12
Linalyl propionate	144-39-8	C ₁₃ H ₂₂ O ₂	210.31		12
trans- <i>p</i> -Menth-2-en-1-ol	29803-82-5	C ₁₀ H ₁₈ O	154.25		12
<i>p</i> -Methyl-cumene (<i>p</i> -Cymene)	99-87-6	C ₁₀ H ₁₄ O	134.22		12
Methyleugenol	93-15-2	C ₁₁ H ₁₄ O ₂	178.23		12
Myrtenol	515-00-4	C ₁₀ H ₁₆ O	152.23		12
β -Nerol (<i>cis</i> -Geraniol)	106-25-2	C ₁₀ H ₁₈ O	154.25		12

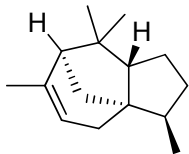
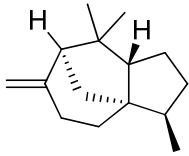
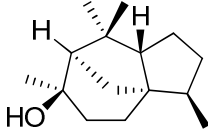
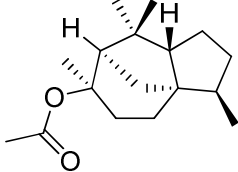
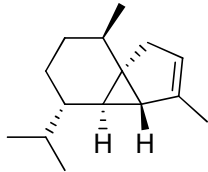
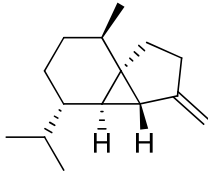
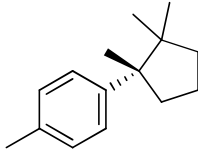
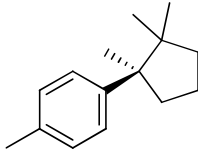
<i>Trivial name</i>	<i>CAS number</i>	<i>Sum formula</i>	<i>MW</i>	<i>Structure</i>	<i>Ref.</i>
<i>cis</i> -β-Ocimene	3338-55-4	C ₁₀ H ₁₆	136.23		12
<i>trans</i> -β-Ocimene	3779-61-1	C ₁₀ H ₁₆	136.23		12
Perilla ketone	553-84-4	C ₁₀ H ₁₄ O ₂	166.22		12
α-Phellandrene	99-83-2	C ₁₀ H ₁₆	136.23		12
β-Phellandrene	555-10-2	C ₁₀ H ₁₆	136.23		13
α-Pinene	80-56-8	C ₁₀ H ₁₆	136.23		12
Platydiol	70630-07-8	C ₁₀ H ₁₈ O ₂	170.25		4
<i>cis</i> -Sabinene hydrate (<i>cis</i> -4-Thujanol)	15537-55-0	C ₁₀ H ₁₈ O	154.25		12
<i>trans</i> -Sabinene hydrate (<i>trans</i> -4-Thujanol)	17699-16-0	C ₁₀ H ₁₈ O	154.25		12
Sabinyl acetate	53833-85-5	C ₁₂ H ₁₈ O ₂	194.27		12

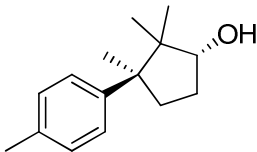
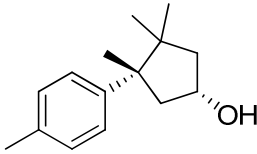
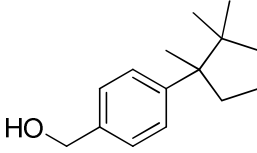
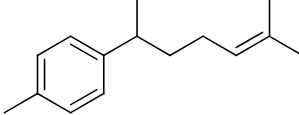
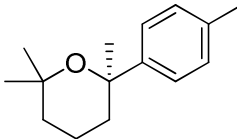
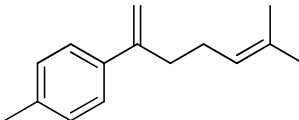
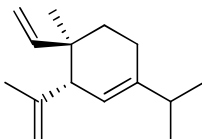
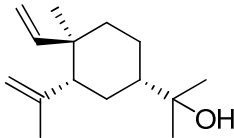
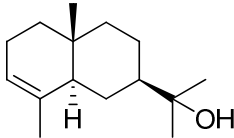
<i>Trivial name</i>	<i>CAS number</i>	<i>Sum formula</i>	<i>MW</i>	<i>Structure</i>	<i>Ref.</i>
γ -Terpinene	99-85-4	C ₁₀ H ₁₆	136.23		12
4-Terpineol	562-74-3	C ₁₀ H ₁₈ O	154.25		12
α -Terpineol	98-55-5	C ₁₀ H ₁₈ O	154.25		12
α -Terpinyl acetate	80-26-2	C ₁₂ H ₂₀ O ₂	196.29		12
α -Thujene	2867-05-2	C ₁₀ H ₁₆	136.23		13
α -Thujone	546-80-5	C ₁₀ H ₁₆ O	152.23		14
β -Thujone	471-15-8	C ₁₀ H ₁₆ O	152.23		14
Thymol acetate	528-79-0	C ₁₂ H ₁₆ O ₂	192.25		12
Verbenone	80-57-9	C ₁₀ H ₁₄ O	150.22		12

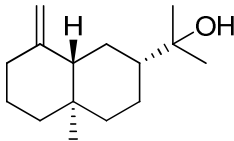
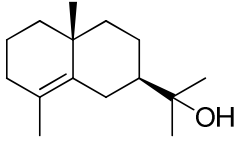
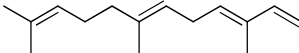
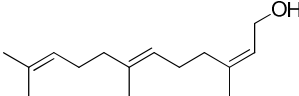
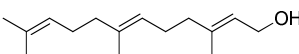
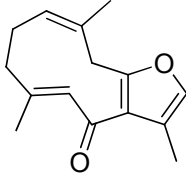
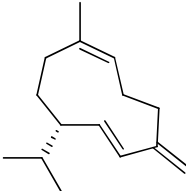
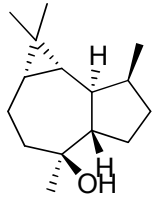
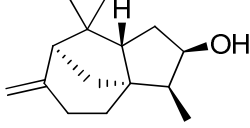
S11. Sesquiterpenes isolated from *Biota orientalis*

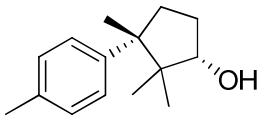
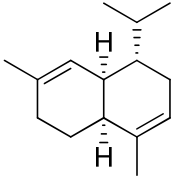
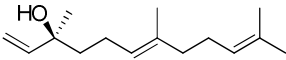
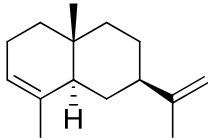
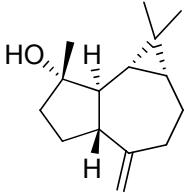
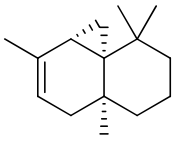
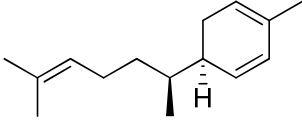
Trivial name	CAS number	Sum formula	MW	Structure	Ref.
Acetylcedrene	32388-55-9	C ₁₇ H ₂₆ O	246.39		12
<i>trans</i> - α -Atlantone	32207-08-2	C ₁₅ H ₂₂ O	218.33		12
α -Biotol	19902-30-8	C ₁₅ H ₂₄ O	220.35		15
β -Biotol	19902-26-2	C ₁₅ H ₂₄ O	220.35		15
α -Bisabolol	515-69-5	C ₁₅ H ₂₆ O	222.37		12
<i>epi</i> - α -Bisabolol	78148-59-1	C ₁₅ H ₂₆ O	222.37		12
β -Bisabolol	15352-77-9	C ₁₅ H ₂₆ O	222.37		12

<i>Trivial name</i>	<i>CAS number</i>	<i>Sum formula</i>	<i>MW</i>	<i>Structure</i>	<i>Ref.</i>
β -Cadinene	523-47-7	$C_{15}H_{24}$	204.35		12
γ -Cadinene	39029-41-9	$C_{15}H_{24}$	204.35		12
α -Cadinol	481-34-5	$C_{15}H_{26}O$	222.37		12
β -Cadinol	481-33-4	$C_{15}H_{26}O$	222.37		12
τ -Cadinol	5937-11-1	$C_{15}H_{26}O$	222.37		12
β -Caryophyllene	87-44-5	$C_{15}H_{24}$	204.35		12
β -Caryophyllene oxide (Caryophyllene oxide)	1139-30-6	$C_{15}H_{24}O$	220.35		12

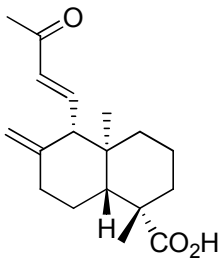
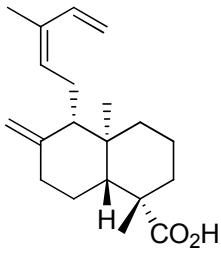
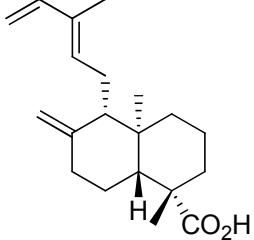
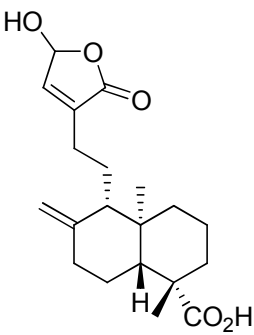
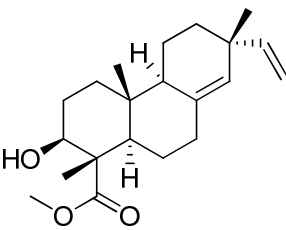
<i>Trivial name</i>	<i>CAS number</i>	<i>Sum formula</i>	<i>MW</i>	<i>Structure</i>	<i>Ref.</i>
α -Cedrene	469-61-4	$C_{15}H_{24}$	204.35		12
β -Cedrene	546-28-1	$C_{15}H_{24}$	204.35		12
α -Cedrol	77-53-2	$C_{15}H_{26}O$	222.37		4, 12
Cedryl acetate	77-54-3	$C_{17}H_{28}O_2$	264.40		12
α -Cubebene	17699-14-8	$C_{15}H_{24}$	204.35		12
β -Cubebene	13744-15-5	$C_{15}H_{24}$	204.35		12
(-)-Cuparene	56324-31-3	$C_{15}H_{22}$	202.34		12
(+)-Cuparene	16982-00-6	$C_{15}H_{22}$	202.34		12

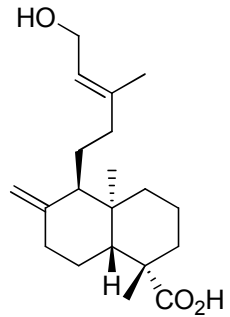
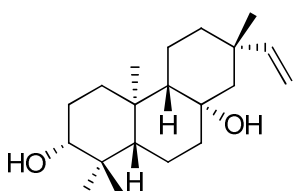
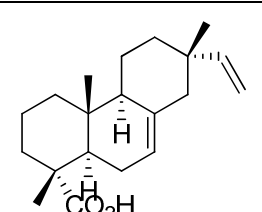
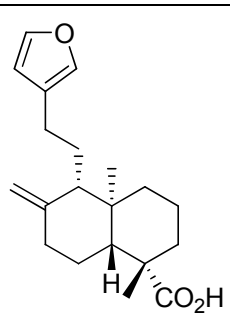
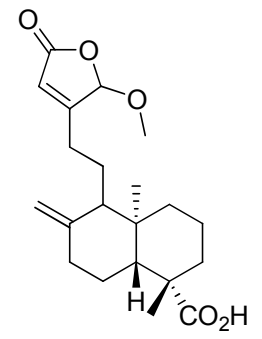
<i>Trivial name</i>	<i>CAS number</i>	<i>Sum formula</i>	<i>MW</i>	<i>Structure</i>	<i>Ref.</i>
α -Cuparenol	21730-88-1	C ₁₅ H ₂₂ O	218.33		15
β -Cuparenol	24887-33-0	C ₁₅ H ₂₂ O	218.33		15
γ -Cuparenol	4584-25-2	C ₁₅ H ₂₂ O	218.33		15
Curcumene	644-30-4	C ₁₅ H ₂₂	202.34		12
Curcumene ether	24048-43-9	C ₁₅ H ₂₂ O	218.33		16
Dehydro- α -curcumene	4999-58-0	C ₁₅ H ₂₀	200.32		17
δ -Elemene	20307-84-0	C ₁₅ H ₂₄	204.35		12
α -Elemol	639-99-6	C ₁₅ H ₂₆ O	222.37		12
α -Eudesmol	473-16-5	C ₁₅ H ₂₆ O	222.37		12

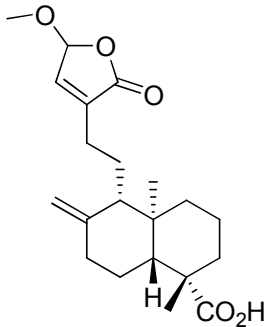
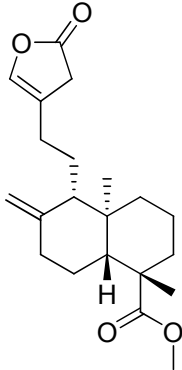
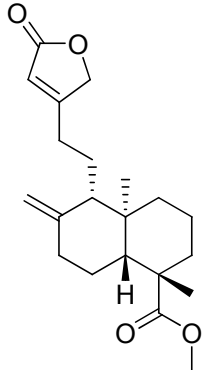
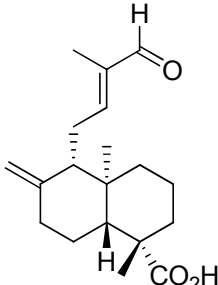
<i>Trivial name</i>	<i>CAS number</i>	<i>Sum formula</i>	<i>MW</i>	<i>Structure</i>	<i>Ref.</i>
β -Eudesmol	473-15-4	C ₁₅ H ₂₆ O	222.37		12
γ -Eudesmol	1209-71-8	C ₁₅ H ₂₆ O	222.37		12
Farnesene	502-61-4	C ₁₅ H ₂₄	204.35		18
<i>cis,trans</i> -Farnesol	3790-71-4	C ₁₅ H ₂₆ O	222.37		12
<i>trans</i> -Farnesol/ <i>E,E</i> -Farnesol	106-28-5	C ₁₅ H ₂₆ O	222.37		12
Furanodienone	24268-41-5	C ₁₅ H ₁₈ O ₂	230.30		12
Germacrene D	23986-74-5	C ₁₅ H ₂₄	204.35		12
Globulol	489-41-8	C ₁₅ H ₂₆ O	222.37		12
β -Isobiotol	24048-41-7	C ₁₅ H ₂₄ O	220.35		16

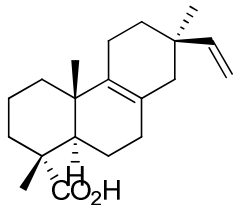
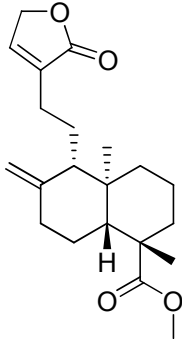
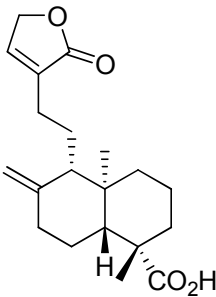
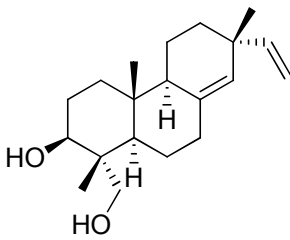
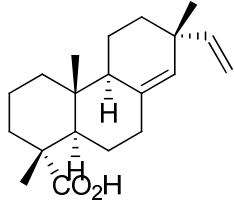
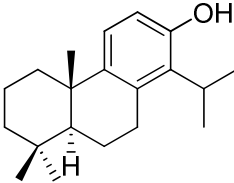
<i>Trivial name</i>	<i>CAS number</i>	<i>Sum formula</i>	<i>MW</i>	<i>Structure</i>	<i>Ref.</i>
α -Isocuparenol	21730-87-0	C ₁₅ H ₂₂ O	218.33		15
α -Muurolene	10208-80-7	C ₁₅ H ₂₄	204.35		12
Nerolidol	7212-44-4	C ₁₅ H ₂₆ O	222.37		12
α -Selinene	473-13-2	C ₁₅ H ₂₄	204.35		12
Spathulenol	6750-60-3	C ₁₅ H ₂₄ O	220.35		12
Thujopsene	470-40-6	C ₁₅ H ₂₄	204.35		12
Zingiberene	495-60-3	C ₁₅ H ₂₄	204.35		12

S12. Diterpenes isolated from *Biota orientalis*

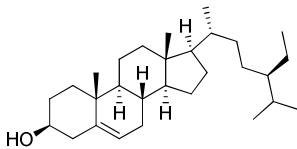
Trivial name	CAS number	Sum formula	MW	Structure	Ref.
14,15-bisnor-13-oxo-8(17),11(<i>E</i>)-labdadiene-19-oic acid	98531-41-0	C ₁₈ H ₂₆ O ₃	290.40		4
<i>cis</i> -Communic acid	1231-35-2	C ₂₀ H ₃₀ O ₂	302.45		4
<i>trans</i> -Communic acid	10178-32-2	C ₂₀ H ₃₀ O ₂	302.45		4
15-Hydroxy-pinusolidic acid	131737-65-0	C ₂₀ H ₂₈ O ₅	348.43		4
3-Hydroxy-sandaracopimaric acid methyl ester	151384-98-4	C ₂₁ H ₃₂ O ₃	332.48		19

<i>Trivial name</i>	<i>CAS number</i>	<i>Sum formula</i>	<i>MW</i>	<i>Structure</i>	<i>Ref.</i>
Isocupressic acid	1909-91-7	C ₂₀ H ₃₂ O ₃	320.47		19
<i>Ent</i> -isopimara-15-en-3 α ,8 α -diol	462122-56-1	C ₂₀ H ₃₄ O ₂	306.48		20
Isopimaric acid	5835-26-7	C ₂₀ H ₃₀ O ₂	302.45		4
Lambertianic acid (Daniellic acid)	4966-13-6	C ₂₀ H ₂₈ O ₃	316.43		20
16-Methoxy labda-8(17),13-dien-15,19-dioic acid butenolide	303176-48-9	C ₂₁ H ₃₀ O ₅	362.46		19

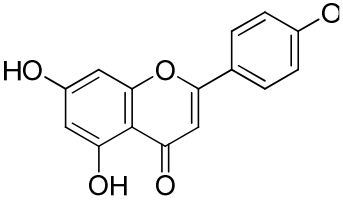
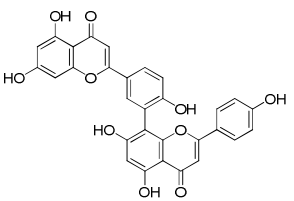
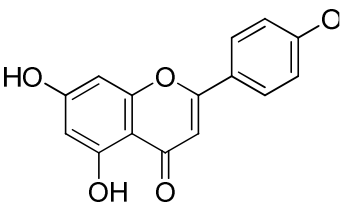
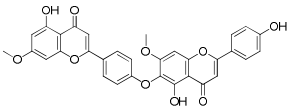
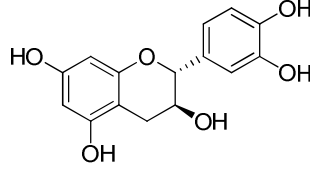
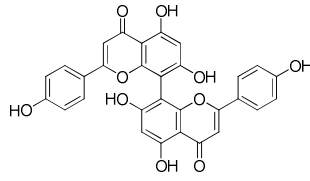
<i>Trivial name</i>	<i>CAS number</i>	<i>Sum formula</i>	<i>MW</i>	<i>Structure</i>	<i>Ref.</i>
15-Methoxypinulosidic acid	769928-72-5	C ₂₁ H ₃₀ O ₅	362.46		20
Methyl 8(17),13(16)-labdadiene-16,15-olide-18-oate	443965-67-1	C ₂₁ H ₃₀ O ₄	346.46		21
Methyl 8(17),13-labdadiene-16,15-olide-18-oate	130464-01-6	C ₂₁ H ₃₀ O ₄	346.46		21
15-norlabda-8(17),12(E)-diene-14-carboxyaldehyde-19-oic-acid	144125-18-8	C ₁₉ H ₂₈ O ₃	304.42		4

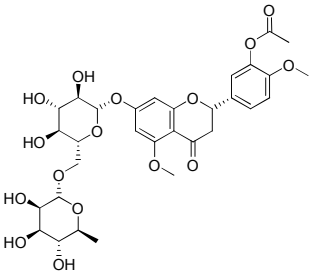
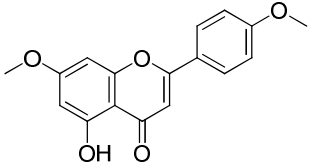
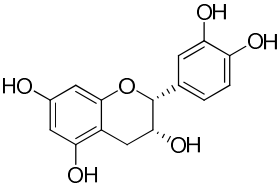
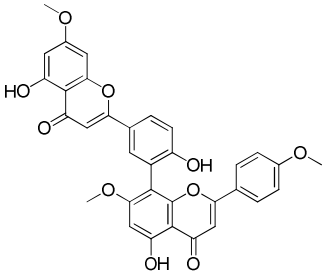
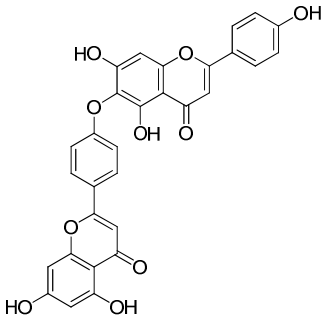
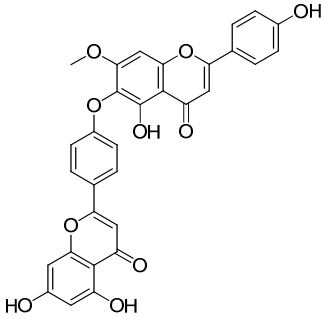
<i>Trivial name</i>	<i>CAS number</i>	<i>Sum formula</i>	<i>MW</i>	<i>Structure</i>	<i>Ref.</i>
8,15-Pimaradien-18-oic acid	7715-76-6	C ₂₀ H ₃₀ O ₂	302.45		4
Pinusolide	31685-80-0	C ₂₁ H ₃₀ O ₄	346.46		4
Pinusolidic acid	40433-82-7	C ₂₀ H ₂₈ O ₄	332.43		4
Sandaraco-pimaradienediol	59219-64-6	C ₂₀ H ₃₂ O ₂	304.47		22
Sandaracopimaric acid	471-74-9	C ₂₀ H ₃₀ O ₂	302.45		4
Totarol	511-15-9	C ₂₀ H ₃₀ O	286.45		23

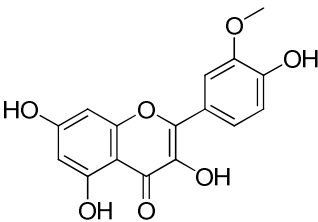
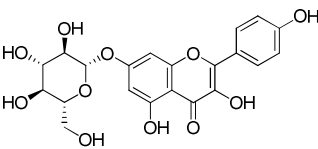
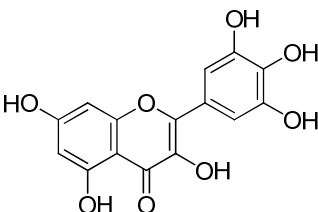
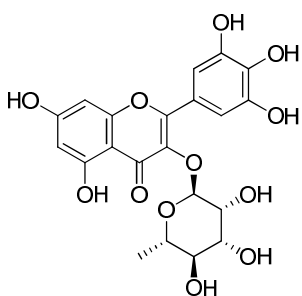
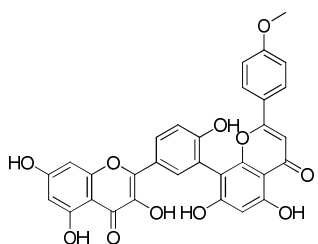
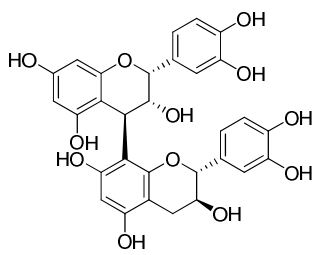
S13. Steroles isolated from *Biota orientalis*

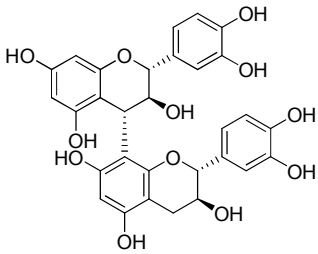
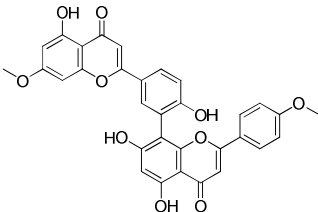
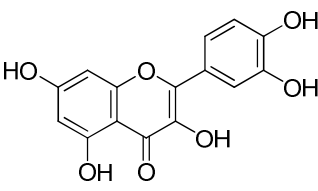
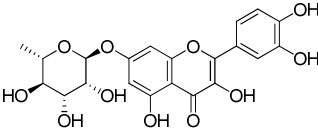
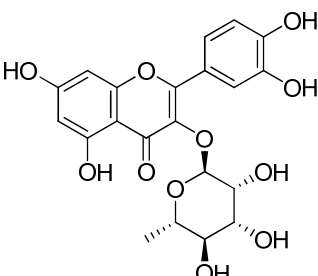
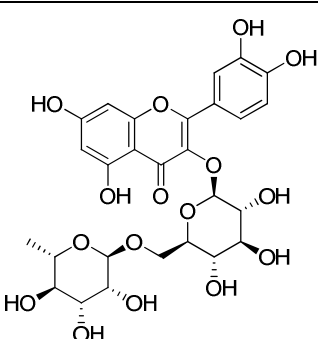
<i>Trivial name</i>	<i>CAS number</i>	<i>Sum formula</i>	<i>MW</i>	<i>Structure</i>	<i>Ref.</i>
β -Sitosterol	83-46-5	C ₂₉ H ₅₀ O	414.71		4

S14. Flavonoids isolated from *Biota orientalis*

Trivial name	CAS number	Sum formula	MW	Structure	Ref.
Acacetin	480-44-4	C ₁₆ H ₁₂ O ₅	284.26		19
Amentoflavone	1617-53-4	C ₃₀ H ₁₈ O ₁₀	538.46		24
Apigenin	520-36-5	C ₁₅ H ₁₀ O ₅	270.24		19, 25
Chamecyparin	20931-35-5	C ₃₂ H ₂₂ O ₁₀	566.51		19
(+)-Catechin	154-23-4	C ₁₅ H ₁₄ O ₆	290.27		26
Cupressuflavone	3952-18-9	C ₃₀ H ₁₈ O ₁₀	538.46		27, 28

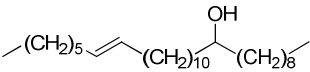
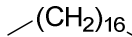
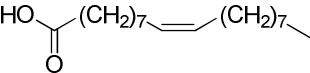
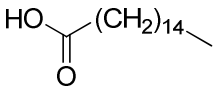
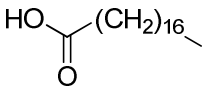
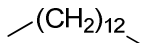
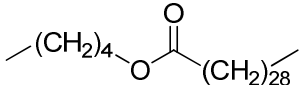
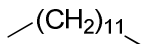
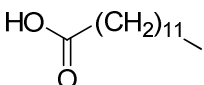
<i>Trivial name</i>	<i>CAS number</i>	<i>Sum formula</i>	<i>MW</i>	<i>Structure</i>	<i>Ref.</i>
5,4'-dimethyl 3'-acetyl eriodicytol 70.β rutinoside	752259-33-9	C ₃₁ H ₃₈ O ₁₆	666.62		29
4',7-Dimethyl- apigenin	5128-44-9	C ₁₇ H ₁₄ O ₅	298.29		4
(-)-Epicatechin	490-46-0	C ₁₅ H ₁₄ O ₆	290.27		26
Heveaflavone	23132-13-0	C ₃₃ H ₂₄ O ₁₀	580.54		19
Hinokiflavone	19202-36-9	C ₃₀ H ₁₈ O ₁₀	538.46		28
Isocryptomerin	20931-58-2	C ₃₁ H ₂₀ O ₁₀	552.48		19

<i>Trivial name</i>	<i>CAS number</i>	<i>Sum formula</i>	<i>MW</i>	<i>Structure</i>	<i>Ref.</i>
Isorhamnetin	480-19-3	C ₁₆ H ₁₂ O ₇	316.26		25
Kaempferol 7-O-glucoside	16290-07-6	C ₂₁ H ₂₀ O ₁₁	448.38		27
Myricetin	529-44-2	C ₁₅ H ₁₀ O ₈	318.24		25
Myricitrine	17912-87-7	C ₂₁ H ₂₀ O ₁₂	464.38		27
Podocarpusflavone	22136-74-9	C ₃₁ H ₂₀ O ₁₀	552.48		28
Procyanidin B1	20315-25-7	C ₃₀ H ₂₆ O ₁₂	578.52		26

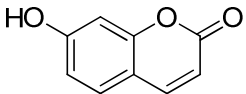
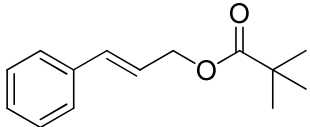
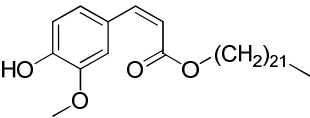
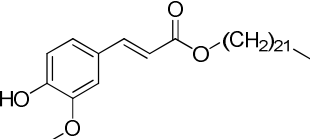
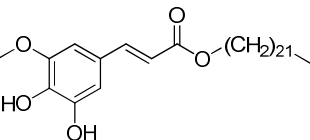
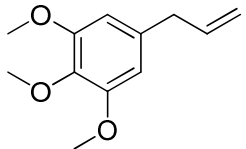
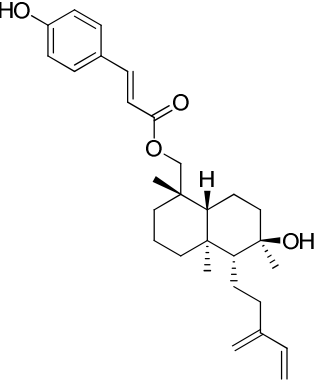
<i>Trivial name</i>	<i>CAS number</i>	<i>Sum formula</i>	<i>MW</i>	<i>Structure</i>	<i>Ref.</i>
Procyanidin B3	23567-23-9	C ₃₀ H ₂₆ O ₁₂	578.52		26
Putraflavone	23624-21-7	C ₃₂ H ₂₂ O ₁₀	566.51		19
Quercetin	117-39-5	C ₁₅ H ₁₀ O ₇	302.24		24, 25, 27, 30
Quercetin 7-O-rhamnoside	22007-72-3	C ₂₁ H ₂₀ O ₁₁	448.38		27
Quercitrin	522-12-3	C ₂₁ H ₂₀ O ₁₁	448.38		24
Rutin	153-18-4	C ₂₇ H ₃₀ O ₁₆	610.52		24, 30

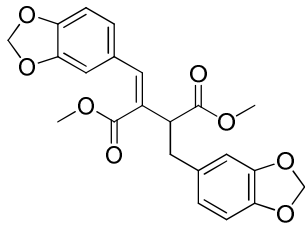
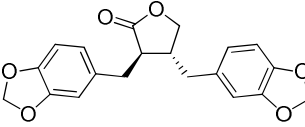
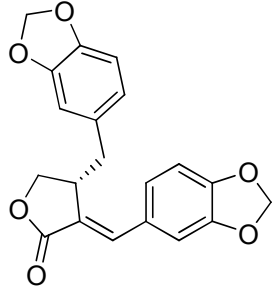
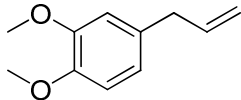
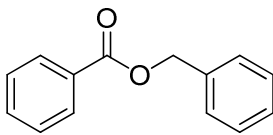
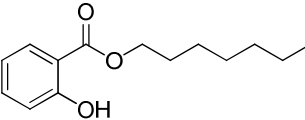
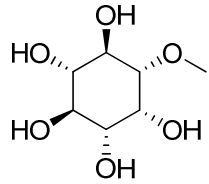
S15. Fatty acids isolated from *Biota orientalis*

Trivial name	CAS number	Sum formula	MW	Structure	Ref.
Decyl 11-hydroxytritracontanoate	444311-96-0	C ₄₃ H ₈₆ O ₃	651.14		21
Dodecane	112-40-3	C ₁₂ H ₂₆	170.33		12
5,11,14,17-Eicosatetraenoic acid, (5Z,11Z,14Z,17Z)-	18016-45-0	C ₂₀ H ₃₂ O ₂	304.47		31
11,14,17-Eicosatrienoic acid, (11Z,14Z,17Z)-	17046-59-2	C ₂₀ H ₃₄ O ₂	306.48		31
Ethyl tetradecanoate	124-06-1	C ₁₆ H ₃₂ O ₂	256.42		12
Ginnol	2606-50-0	C ₂₉ H ₆₀ O	424.79		4
Heptadecane	629-78-7	C ₁₇ H ₃₆	240.47		12
1-Hexacosanol	506-52-5	C ₂₆ H ₅₄ O	382.71		4
Hexadecanal	629-80-1	C ₁₆ H ₃₂ O	240.42		12
Hexadecane	544-76-3	C ₁₆ H ₃₄	226.44		12
8-Hexyltricosane	137280-60-5	C ₂₉ H ₆₀ O ₂	408.79		21
Linoleic acid	60-33-3	C ₁₈ H ₃₂ O ₂	280.45		31
Linolenic acid	463-40-1	C ₁₈ H ₃₀ O ₂	278.43		31
Nonacosane	630-03-5	C ₂₉ H ₆₀	408.79		30

<i>Trivial name</i>	<i>CAS number</i>	<i>Sum formula</i>	<i>MW</i>	<i>Structure</i>	<i>Ref.</i>
Octacosane-10-ol-21-ene	444311-95-9	C ₂₈ H ₅₆ O	408.74		21
Octadecane	593-45-3	C ₁₈ H ₃₈	254.49		12
Oleic acid	112-80-1	C ₁₈ H ₃₄ O ₂	282.46		31
Palmitic acid	57-10-3	C ₁₆ H ₃₂ O ₂	256.42		4, 31
Stearic acid	57-11-4	C ₁₈ H ₃₆ O ₂	284.48		31
Tetradecane	629-59-4	C ₁₄ H ₃₀	198.39		12
Triacontanoic acid	116044-06-5	C ₃₅ H ₇₀ O ₂	522.93		21
Tridecane	629-50-5	C ₁₃ H ₂₈	184.36		12
Tridecanoic acid	638-53-9	C ₁₃ H ₂₆ O ₂	214.34		12

S16. Miscellaneous compounds from *Biota orientalis*

Trivial name	CAS number	Sum formula	MW	Structure	Ref.
Coumarins					
Coumarin (Umbelliferon)	93-35-6	C ₉ H ₆ O ₃	162.14		19
Phenylpropanoids					
Cinnamyl valerate	10482-65-2	C ₁₄ H ₁₈ O ₂	218.29		12
Docosyl <i>cis</i> -ferulate	133882-81-2	C ₃₂ H ₅₄ O ₄	502.77		4
Docosyl <i>trans</i> -ferulate	101927-24-6	C ₃₂ H ₅₆ O ₄	502.77		4
Docosyl <i>trans</i> -3-hydroxy-ferulate	252366-72-6	C ₃₂ H ₅₄ O ₅	518.77		4
Elemicin	487-11-6	C ₁₂ H ₁₆ O ₃	208.25		12
8-Hydroxy-labda-13(16),14-dien-19-yl- <i>E</i> -coumarate	117254-98-5	C ₂₉ H ₄₀ O ₄	452.63		19

<i>Trivial name</i>	<i>CAS number</i>	<i>Sum formula</i>	<i>MW</i>	<i>Structure</i>	<i>Ref.</i>
Lignans					
Dehydrohelio- bupphthalmin	66547-92-0	C ₂₂ H ₂₀ O ₈	412.39		32
Hinokinin	26543-89-5	C ₂₀ H ₁₈ O ₆	354.35		32
Savinin	493-95-8	C ₂₀ H ₁₆ O ₆	352.34		32
Phenolic compounds					
Methyleugenol	93-15-2	C ₁₁ H ₁₄ O ₂	178.23		12
Benzylbenzoate	120-51-4	C ₁₄ H ₁₂ O ₂	212.24		12
Heptylsalicylate	6259-77-4	C ₁₄ H ₂₀ O ₃	236.31		12
Miscellaneous					
Bornesitol	484-71-9	C ₇ H ₁₄ O ₆	194.18		4

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