Physicochemical and Pharmacological Properties of Sesquiterpene Esters - Cyclic

S.S. Azimova, A.I. Saidkhodzhaev (eds.), *Natural Compounds – Natural Sesquiterpene Esters*,
DOI 10.1007/978-1-4614-0539-9,

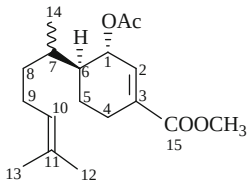
The Monocyclic Sesquiterpene Esters

Bisabolanes

Bisabolanes

Monoesters

1α-Acetoxy-6α(H)-bisabol-15-oic Acid Methyl Ester



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Monoesters

Biological sources: *Stevia salicifolia* var. *typica* B.L. Rob. [1]

$C_{18}H_{28}O_4$: 308.1988

Mp: colorless oil [1]

$[\alpha]_D$ + 95.0° (*c* 0.25, EtOH) [1]

UV (MeOH): 217 (ε 10358) [1]

IR (film): 1735, 1720, 1650 [1]

EI-MS: 308 $[M]^+$ (1.0), 248 (12.5), 181 (27), 163 (59), 109 (100), 82 (42.5), 69 (25) [1]

^{1}H NMR (90 MHz, $CDCl_3$, TMS): 0.80 (3H, d, J = 7, H-14), 1.57 (3H, br s, H-13), 1.65 (3H, br s, H-12), 2.10 (3H, s, OAc), 2.30 (2H, m, H-4), 3.73 (3H, s, OCH_3), 5.07 (1H, br t, J = 7; 1.5; 1.5, H-10), 5.40 (1H, m, J = 9; 1.2; 1.2, H-1), 6.67 (1H, dt, J = 1.2; 2.3, H-2) [1]

^{13}C NMR ($CDCl_3$, TMS): [1]

Table 1

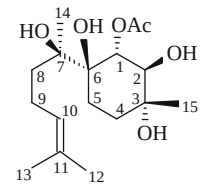
C-1	71.05 d	C-8	35.07 t	C-15	167.06 s
2	137.35 d	9	26.12 t	$COOCH_3$	51.61 q
3	133.42 s	10	124.66 d	OAc	170.45 s
4	24.66 t	11	131.37 s		20.93 q
5	20.93 t	12	25.62 q		
6	42.05 d	13	17.66 q		
7	31.34 d	14	14.60 q		

References

1. J.S. Calderon, E. Angeles, M. Salmon, G.A. Garcia de la Mora, Phytochemistry **23**(1), 186 (1984)

1α-Acetoxy-bisabol-10-ene-2β,3α,6β,7β-tetraol ((1*R**,2*R**,3*R**,6*R**,7*R**) 1,2,3,6,7-Pentahydroxy-1-acetoxy-bisabol-10(11)-ene)

CAS Registry Number: 243987-38-4



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Monoesters

Biological sources: *Matricaria aurea* (L.) Sch. Bip. [1]

$C_{17}H_{30}O_6$: 330.2042

$[\alpha]_D^{24}$ −24.1° (*c* 0.45, $CHCl_3$) [1]

IR ($CHCl_3$): 3590, 3570, 1710, 960 [1]

EI-MS: 330 $[M]^+$ (21.0), 312 $[M - H_2O]^+$ (2.4), 287 $[M - C_3H_7]^+$ (7.5), 68 (100) [1]

^{1}H NMR (400 MHz, $CDCl_3$): 1.14 (3H, s, H-15), 1.29 (3H, s, H-14), 1.58 (1H, H-4a), 2.03 (1H, H-4b), 1.61 (3H, s, H-13), 1.63 (3H, s, H-12), 1.70 (1H, H-5a), 2.11 (1H, H-5b), 1.70 (1H, H-8a), 2.11 (1H, H-8b), 2.10 (2H, m, H-9), 2.17 (3H, s, OAc), 3.60 (1H, H-2), 4.42 (1H, H-1), 5.13 (1H, H-10) [1]

^{13}C NMR (100.6 MHz, $CDCl_3$) [1]:

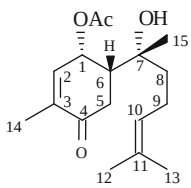
Table 1

C-1	87.2	C-7	71.9	C-13	17.6
2	79.3	8	27.9	14	22.4
3	72.2	9	21.1	15	23.0
4	39.1	10	124.9	OAc	
5	28.3	11	131.5	1′	172.6
6	76.5	12	25.7	2′	21.2

References

1. A.A. Ahmed, A. Maha, E. Abou, Phytochemistry **51**(4), 551 (1999)

1α-Acetoxy-7α-hydroxy-6β(H)-bisabola-2,10-dien-4-one (Acetoxydelobanone; 1α-Acetoxy-bisabolol-4-one)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Monoesters

Biological sources: *Lindera triloba* Sieb. et Zucc. [1]

$C_{17}H_{26}O_4$: 294.1831

Mp: colorless oil [1]

$[\alpha]_D^{23}$ +207° ± 1.7° (*c* 1.442, dioxane) [1]

UV: 229.5 (ε 9700) [1]

IR: 3600, 3525, 1742, 1688, 1227, 1214 [1]

MS: 294 $[M]^+$ [1]

TLC: $CHCl_3$ – EtOH (98:2), R_f 0.56 [1]

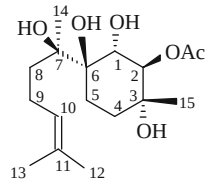
^{1}H NMR (60 MHz, C_6D_6, TMS): 1.20 (3H, s, H-15), 1.60 (3H, d, J = 1.5, H-12 or H-13), 1.67 (3H, d, J = 1.5, H-13 or H-12), 1.77 (3H, d, J = 1.5, H-14), 2.05 (3H, s, OAc), 5.07 (1H, br t, H-10), 5.25 (1H, dd, J = 3; 6, H-1), 6.72 (1H, dd, J = 1.5; 6, H-2) [1]

References

1. K. Takeda, K. Sakurawi, H. Ishii, Tetrahedron **27**, 6049 (1971)

2β-Acetoxy-bisabol-10-ene-1α,3α,6β,7β-tetraol ((1*R**,2*R**,3*R**,6*R**,7*R**)-1,2,3,6,7-Pentahydroxy-2-acetoxy-bisabol-10-ene)

CAS Registry Number: 23987-39-5



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Monoesters

Biological sources: *Matricaria aurea* (L.) Sch. Bip. [1]

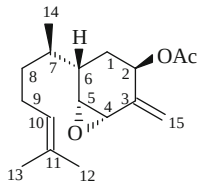
$C_{17}H_{30}O_6$: 330.2042

MS: 330 $[M]^+$, 312 $[M - H_2O]^+$, 287 $[M - C_3H_7]^+$ [1]
^{1}H NMR (400 MHz, $CDCl_3$): 1.23 (3H, s, H-14), 1.24 (3H, s, H-15), 1.33 (1H, H-8a), 1.82 (1H, H-8b), 1.62 (3H, s, H-13), 1.69 (3H, s, H-12), 1.72 (1H, H-5a), 2.05 (1H, H-5b), 2.05–2.00 (2H, m, H-9), 2.08 (3H, s, OAc), 2.18 (1H, H-4a), 2.05 (1H, H-4b), 3.50 (1H, br s, H-1), 5.25 (1H, H-2), 5.33 (1H, H-10) [1]

References

1. A.A. Ahmed, A. Maha, E. Abou, Phytochemistry **51**(4), 551 (1999)

2β-Acetoxy-4α,5α-epoxy-6β(H)-bisabola-3(15),10-diene

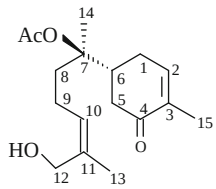


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Monoesters
Biological sources: *Helipterum roseum* (Hook.) Benth. [1]
$C_{17}H_{26}O_3$: 278.1882
Mp: colorless oil [1]
$[\alpha]_D^{24}$ −33° (*c* 1.1, $CHCl_3$) [1]
IR (CCl_4): 1740, 1245 [1]
MS: 278 $[M]^+$ (0.15), 218.167 $[M - HOAc]^+$ (2.5) (calc. for $C_{15}H_{22}O$: 218.167), 200 (3), 177 (6.5), 118 (100), 109 (64), 69 (93) [1]
TLC: Et_2O – petrol (3:1), R_f 0.62 [1]
^{1}H NMR (400 MHz, C_6D_6, TMS): 1.00 (3H, d, H-14), 1.29 (1H, m, H-8b), 1.45 (1H, dt, J = 3.5; 14; 4, H-1b), 1.51 (1H, m, H-8a), 1.62 (3H, br s, H-13), 1.64 (1H, m, H-1a), 1.70 (1H, m, H-7), 1.70 (3H, s, OAc), 1.74 (3H, br s, H-12), 2.01 (1H, br ddt, J = 7; 7, H-9b), 2.09 (1H, m, H-9a), 2.10 (1H, ddd, J = ∼0.5; 10; 4; 5, H-6), 3.10 (1H, dt, J = 4; ∼0.5; ∼0.5, H-5), 3.21 (1H, dd, J = 4, H-4), 5.23 (1H, tqq, J = 7; 1.5; 1.5, H-10), 5.32 (1H, br s, H-15b), 5.58 (1H, br s, H-15a), 5.65 (1H, t, J = ∼0.5; 3.5; 3.5, H-2) [1]

References

1. C. Zdero, F. Bohlmann, R.M. King, H. Robinson, Phytochemistry **28**(2), 517 (1989)

7β-Acetoxy-12-hydroxy-6β(H)-bisabola-2,10*E*-dien-4-one (7β-Acetoxy-12-hydroxy-4-oxo-bisabola-2,10*E*-diene)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Monoesters
Biological sources: *Achillea cretica* L. [1]
$C_{17}H_{26}O_4$: 294.1832
Mp: gum [1]
PCI-MS: 295 $[M + H]^+$ (63.1), 251 (16.4), 235 (100) [1]
^{1}H NMR (500 MHz, $CDCl_3$): 1.19 (3H, s, H-14), 1.54 (2H, dd, J = 9.5, 6.5, H-8a, H-8b), 1.66 (3H, br s, H-13), 1.77 (3H, br s, H-15), 2.07 (3H, s, OAc), 2.08 (1H, m, H-6), 2.09 (2H, m, H-9a, H-9b), 2.24 (1H, dddd, J = 18; 11; 2.5; 2.5, H-1_{ax}), 2.26 (1H, dd, J = 16; 14, H-5_{ax}), 2.38 (1H, dddd, J = 18; 5; 5; 1, H-1_{eq}), 2.60 (1H, ddd, J = 16; 3; 1.5, H-5_{eq}), 4.44 (2H, br s, H-12a, H-12b), 5.44 (1H, br t, J = 7, H-10), 6.74 (1H, ddq, J = 6; 2.5; 1, H-2) [1]

^{13}C NMR (67.89 MHz, $CDCl_3$) [1]:

Table 1

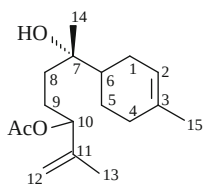
C-1	27.3 t	C-7	73.1 s	C-13	13.9 q
2	144.6 d	8	39.1 t*	14	24.4 q
3	135.4 s	9	25.3 t	15	15.5 q
4	199.1 s	10	128.8 d	OAc	170.8 s
5	39.2 t*	11	130.7 s		20.7 q
6	44.6 t	12	69.9 t		

*Assignments may be interchanged [1]

References

1. M. Bruno, M.L. Bondi, M.P. Paternostro, N.A. Arnold, J.G. Diaz, W. Herz, Phytochemistry **42**(3), 737 (1996)

10-Acetoxy-bisabola-2,11(12)-dien-7α-ol



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Monoesters

Biological sources: *Achillea odorata* L. [1]

$C_{17}H_{28}O_3$: 280.2038

Mp: oil [1]

$[\alpha]_D$ −43.0° (*c* 1.0, $CHCl_3$) [1]

IR (film): 3510 (OH), 3079, 1737 (C = O), 1678 (C = C), 1649 (C = C), 904 [1]

MS: 280 $[M]^+$ (0.1), 265 $[M - CH_3]^+$ (0.1), 262 $[M - H_2O]^+$ (0.7), 220 $[M - HOAc]^+$ (2), 205 [M – HOAc – H_2O] (2), 202 $[M - H_2O - HOAc]^+$ (6), 187 $[M - H_2O - HOAc - CH_3]^+$ (6), 107 (29), 67 (26), 43 (100) [1]

^{1}H NMR (300 MHz, $CDCl_3$, TMS): 1.07 (3H, s, H-14), 1.62 (3H, s, H-15), 1.69 (3H, s, H-13), 2.03 (3H, s, OAc), 4.86 (1H, dq, J = 1.5; 1.5, H-12a), 4.91 (1H, s, H-12b), 5.12 (1H, dt, J = 6.6; 2.1, H-10), 5.34 (1H, s, H-2) [1]

^{13}C NMR (75 MHz, $CDCl_3$) [1]:

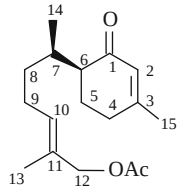
Table 1

C-1	26.9	C-7	73.9	C-13	18.1
2	120.5, 120.4	8	35.5, 35.6	14	23.4
3	134.2	9	26.3	15	23.4
4	31.0	10	77.7, 77.8	OAc	
5	23.4	11	143.0	1′	170.4
6	42.0, 43.0	12	112.9, 113.0	2′	21.3

References

1. A.F. Barerero, E.J. Alvarez-Manzaneda, R.R. Alvarez-Manzaneda, Phytochemistry **29**(10), 3213 (1990)

12-Acetoxy-6α(H)-bisabola-2,10-dien-1-one (12-Acetoxybisabolen-1-one)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Monoesters

Biological sources: *Senecio smithii* DC. [1]

$C_{17}H_{26}O_3$: 278.1882

$[\alpha]_D^{24}$ (λ, nm): −17.7° (589), −18.8° (578), −23.0° (546), −55.7° (436), −271.3° (365) (*c* 0.6, $CHCl_3$) [1]

IR (CCl_4): 1750, 1250, 1680 [1]

MS: 278 $[M]^+$ (0.1), 218.167 [M – AcOH]$^+$ (13) ($C_{15}H_{22}O$), 110 (100), 95 (18), 82 (9) [1]

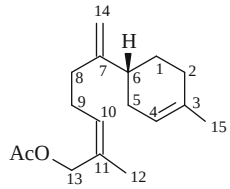
CI-MS: 279 $[M + 1]^+$ (18), 219 (100) [1]

^{1}H NMR (400, MHz, $CDCl_3$): 0.80 (3H, d, J = 14.5, H-14), 1.32 (2H, m, H-8), 1.32 (1H, m, J = 11; 15, H-5a), 1.64 (3H, br s, H-13), 1.78 (1H, dddd, J = 4.3; 15, H-5b), 1.93 (3H, br s, J = 1, H-15), 2.00 (2H, m, J = 7, H-9), 2.07 (3H, s, OAc), 2.14 (2H, ddd, J = 11; 4.3, H-6), 2.31 (2H, m, H-4), 2.31 (1H, m, J = 14.5, H-7), 4.43 (2H, br s, H-12), 5.46 (1H, br t, J = 7, H-10), 5.86 (1H, q, J = 1, H-2) [1]

References

1. F. Bohlmann, C. Zdero, R.M. King, H. Robinson, Phytochemistry **20**(10), 2389 (1981)

13-Acetoxy-6β(H)-bisabola-3,7(14),10-diene ((+)-(*Z*)-Lanceol Acetate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Monoesters

Biological sources: *Torilis arvensis* (Huds.) Link. [1]

$C_{17}H_{26}O_2$: 262.1933

Mp: faint yellow oil [1]

$[\alpha]_D^{22}$ +53.2° (*c* 1.41, MeOH) [1]

IR (CCl_4): 3080, 1740, 1645, 1235, 1040, 1020, 890 [1]

GC-EI-MS: 262 $[M]^+$ (0.04) (calc. for $C_{17}H_{26}O_2$: 262.1933), 220 (0.12), 202 (3), 187 (4), 174 (1), 173 (1), 159 (6), 134 (15), 119 (15), 107 (12), 105 (13), 93 (22), 91 (17), 79 (19), 67 (21), 55 (13), 43 (100), 41 (24) [1]

GC: 0.25 μ, capillary column (28 m × 0.25 mm i.d.), hexane solns (2.8 $\mu g \cdot \mu L^{-1}$), 50°/min from 50° to 270° at 4° min^{-1}, R_t 36.17 min [1]

^{1}H NMR (360 MHz, $CDCl_3$, TMS): 1.47–2.23 (*ca* 11H, complex ms, H-1, H-2, H-5 H-6, H-8, H-9), 1.65 (3H, s, H-15), 1.75 (3H, s, H-12), 2.06 (3H, br s, OAc), 4.58 (2H, s, H-13), 4.73 (1H, s, H-14b), 4.77 (1H, s, H-14a), 5.40 (2H, m, H-4, H-10) [1]

^{1}H NMR* (600 MHz, $CDCl_3$, TMS): 1.48 (1H, m, H-1a), 1.65 (3H, s, H-15), 1.75 (3H, s, H-12), 1.82 (1H, m, H-1b), 1.95 (1H, m, H-5a), 1.98 (2H, m, H-2), 2.06 (3H, br s, OAc), 2.08 (2H, m, H-8), 2.10 (1H, m, H-6), 2.12 (1H, m, H-5b), 2.21–2.23 (2H, m, H-9), 4.58 (2H, s, H-13), 4.73 (1H, br s, H-14b), 4.77 (1H, br s, H-14a), 5.40 (1H, m, H-4), 5.42 (1H, m, H-10), *-1D (^{1}H, ^{13}C) and 2D (HMQC, HMBC) NMR [1]

^{13}C DEPT (90 MHz, $CDCl_3$, 135°): 3 CH_3, 7 CH_2, 3 CH, 4C [1]

^{13}C NMR (150 MHz, $CDCl_3$, TMS) [1]:

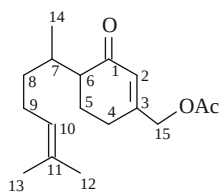
Table 1

C-1	28.3 t	C-7	153.5 s	C-13	63.2 t
2	30.8 s	8	34.8 t	14	107.6 t
3	133.7 s	9	26.5 t	15	23.4 q
4	120.7 d	10	130.4 d	OAc	20.9 q
5	31.4 t	11	129.9 s	1′	171.1 s
6	39.7 d	12	21.4 q	2′	

References

1. H.E.A. Saad, S.H. Ei-Sharkawy, J.P. Rosazza, A.F. Halim, Phytochemistry **37**(2), 473 (1994)

15-Acetoxy-bisabola-2,10-dien-1-one (15-Acetoxybisabolen-1-one)

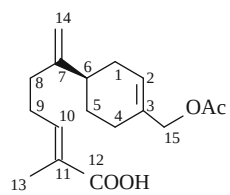


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters
Biological sources: *Stevia ovata* Willd. [1]
$C_{17}H_{26}O_3$: 278.1882
Mp: colorless oil [1]
IR (CCl_4): 1750, 1670 [1]
MS: 278.188 $[M]^+$ (8) (calc. for $C_{17}H_{26}O_3$: 278.188), 218 (11), 43 (100) [1]
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 0.82 (3H, d, J = 7, H-14), 1.60 (3H, br s, H-12), 1.69 (3H, br s, H-13), 2.13 (3H, s, OAc), 2.3 (4H, m, H-4, H-9), 4.67 (2H, br s, H-15), 5.12 (1H, br t, J = 7, H-10), 6.01 (1H, tq, J = 1; 1, H-2) [1]

References

1. F. Bohlmann, A. Suwita, A.A. Natu, H. Czerson, A. Suwita, Chem. Ber. **110**, 3572 (1977)

15-Acetoxy-6α(H)-bisabola-2,10-dien-12-oic Acid (15-Acetoxybrasilic Acid)

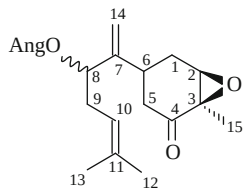


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Monoesters
Biological sources: *Brasilia sickii* Barrosa [1]
$C_{17}H_{24}O_4$: 292.1675
Mp: colorless gum, which was separated as its methyl ester [1]
$[\alpha]^{24}$ (its Me ester) (λ, nm): −55° (589), −58° (578), −66° (546), −114° (436) (*c* 0.87, $CHCl_3$) [1]
IR (CCl_4) (its Me ester): 1750, 1725, 1650, 1265 [1]
MS (its Me ester): 306 $[M]^+$ (0.5), 246.162 $[M - HOAc]^+$ (32) ($C_{16}H_{22}O_2$), 214 (17), 187 (44), 186 (44), 133 (100), 105 (68) [1]
^{1}H NMR (400 MHz, $CDCl_3$, TMS) (its Me ester): 1.51 (1H, dddd, J = 5; 11; 13, H-5a), 1.85 (3H, dt, J = 1.3, H-13), 1.89 (1H, m, H-5b), 1.98 (1H, m, H-1a), 2.15 (6H, m, H-6, H-1b, H-4a, H-8), 2.33 (2H, br dt, J = 7.5; 7.5, H-9), 3.74 (3H, s, OCH_3), 4.46 (2H, br s, H-15), 4.78 (1H, dt, J = 1; 1, H-14b), 4.82 (1H, br s, H-14a), 5.76 (1H, br d, J = 4; ∼1, H-2), 6.76 (1H, qt, J = 7.5; 1.3, H-10) [1]

References

1. F. Bohlmann, M. Grenz, J. Jakupovic, R.M. King, H. Robinson, Phytochemistry **22**(5), 1213 (1983)

8-Angeloyloxy-2β,3β-epoxy-bisabola-7(14),10-dien-4-one (8-*O*-Angeloyloxy-2,3-dihydro-2,3-epoxy-β-bisabolen-4-one)



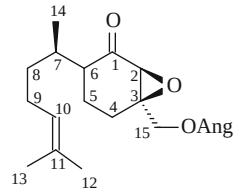
Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Monoesters
Biological sources: *Senecio oxydontus* DC. [1]
$C_{20}H_{28}O_4$: 332.1988
Mp: colorless oil [1]
IR (CCl_4): 1720, 1650 [1]
MS: 332.199 $[M]^+$ (2) (calc. for $C_{20}H_{28}O_4$: 332.199), 232 (42), 83 (100) [1]
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.41 (3H, s, H-15), 1.60 (3H, br s, H-12), 1.68 (3H, br s, H-13),

2.05 (2H, m, H-1), 2.36 (2H, m, H-9), 2.39 (1H, m, H-5α), 2.60 (1H, dddd, J = 6; 13; 2; 13, H-6), 2.87 (1H, dd, J = 13; 13, H-5β), 3.45 (1H, br d, J = 5, H-2), 4.99 (1H, br s, H-14b), 5.04 (1H, br t, J = 7, H-10), 5.17 (1H, br s, H-14a), 5.17 (1H, dd, J = 7; 7, H-8); OAng: 1.88 (3H, dq, J = 1.5; 1.5, H-5′), 1.92 (3H, dq, J = 7; 1.5, H-4′), 6.08 (1H, qq, J = 7; 1.5, H-3′) [1]

References

1. F. Bohlmann, C. Zdero, Phytochemistry **17**(9), 1591 (1978)

15-Angeloyloxy-2β,3β-epoxy-bisabol-10-en-1-one



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Monoesters

Biological sources: *Stevia amambayensis* B. L. Rob. [1]

$C_{20}H_{30}O_4$: 334.2144

Mp: colorless oil [1]

$[\alpha]_D^{24}$ +103° (*c* 0.24, $CHCl_3$) [1]

IR (CCl_4): 1715 [1]

MS: 334.214 $[M]^+$ (3), 234 $[M - C_4H_7COOH]^+$ (5), 109 (54), 83 $[C_4H_7CO]^+$ (100), 55 $[C_4H_7CO - CO]^+$ (47) [1]

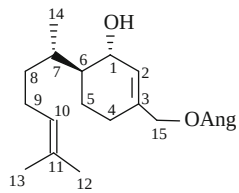
TLC: Et_2O – petrol (1:9), R_f 0.68 [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 0.80 (3H, d, J = 7, H-14), 1.59 (3H, br s, H-13), 1.68 (3H, br s, H-12), 2.27 (1H, m, H-7α), 3.28 (1H, s, H-2), 4.19 (1H, d, J = 12, H-15b), 4.41 (1H, d, J = 12, H-15a), 5.08 (1H, br t, J = 7, H-10); OAng: 1.90 (3H, dq, J = 7; 1.5, H-4′), 2.00 (3H, dq, J = 1.5; 1.5, H-5′), 6.14 (1H, qq, J = 7; 1.5, H-3′) [1]

References

1. G. Schmeda-Hirschmann, C. Zdero, F. Bohlmann, Phytochemistry **25**(7), 1755 (1986)

15-Angeloyloxy-1α-hydroxy-6α(H)-bisabola-2,10-diene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Monoesters

Biological sources: *Stevia myriadenia* Sch. Bip. ex Baker [1]

$C_{20}H_{32}O_3$: 320.2351

Mp: colorless oil, not free from 15-acetoxy-4α-hydroxygermacra-1*E*,5*E*-diene [1]

IR (CCl_4): 3600, 1720 [1]

MS: 320.235 $[M]^+$ (0.3), 302 (0.5), 220 (3), 202 (8), 187 (7), 108 (21), 83 (100), 69 (57) [1]

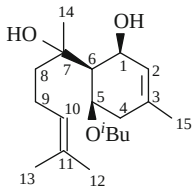
CI-MS: 321 $[M + 1]^+$ (0.5), 303 (4), 203 (100) [1]

^{1}H NMR (400 MHz, C_6D_6, TMS): 0.78 (3H, d, J = 7, H-14), 1.64 (3H, br s, H-13), 1.75 (3H, br s, H-12), 2.10 (2H, br dt, J = 7; 7, H-9), 3.90 (1H, br d, J = 9, H-1), 4.57 (2H, br s, H-15), 5.30 (1H, tqq, J = 7, H-10), 5.64 (1H, br s, H-2); OAng: 1.94 (3H, dq, H-5′), 2.06 (3H, dq, H-4′), 5.78 (1H, qq, H-3′) [1]

References

1. F. Bohlmann, C. Zdero, R.M. King, H. Robinson, Phytochemistry **21**(8), 2021 (1982)

5β-Isobutyroyloxy-1β,7-dihydroxy-6α(H)-bisabola-2,10-diene (5β-Isobutyryloxy-1β-hydroxy-bisabolol)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Monoesters

Biological sources: *Senecio pubigerus* L. [1]

$C_{19}H_{32}O_4$: 324.2301

Mp: colorless oil [1]

$[\alpha]_D^{24}$ (λ, nm): +7.8° (589), +8.1° (578), +9.5° (546), +19.1° (436) (*c* 0.74, $CHCl_3$) [1]

IR (CCl_4): 3590, 3530, 1740 [1]

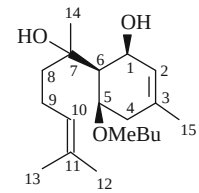
MS: 306.219 $[M - H_2O]^+$ (1), 291 (1), 288 (2), 218 (5), 203 (10), 200 (28), 132 (58), 93 (100), 92 (58), 71 (81), 69 (53) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.39 (3H, s, H-14), 1.60 (3H, br s, H-12), 1.64 (2H, m, H-8), 1.68 (3H, br s, H-13), 1.73 (3H, br s, H-15), 2.0 (2H, m, H-9), 2.23 (1H, br s, H-6), 2.34 (2H, m, H-4), 3.21 (1H, s, OH), 4.52 (1H, m, H-1), 5.14 (1H, br t, J = 7, H-10), 5.73 (1H, br s, H-5), 5.77 (1H, dq, J = ~1; 6; 1.3, H-2); O^{i}Bu: 1.14 (6H, d, H-3′, H-4′), 2.43 (1H, qq, H-2′) [1]

References

1. F. Bohlmann, C. Zdero, A.A. Natu, Phytochemistry **17**(10), 1757 (1978)

5β-(2′-Methylbutyroyloxy)-1β,7-dihydroxy-6α(H)-bisabola-2,10-diene (5β-[2-Methylbutyryloxy]-1β-hydroxy-bisabolol)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Monoesters

Biological sources: *Senecio pubigerus* L. [1]

$C_{20}H_{34}O_4$: 338.2457

Mp: colorless oil [1]

IR (CCl_4): 3590, 3530, 1740 [1]

MS: 320.235 $[M - H_2O]^+$ (1) ($C_{20}H_{32}O_3$), 305 (1), 302 (2), 218 (4), 200 (25), 132 (52), 93 (100), 92 (60), 85 (62), 69 (56) [1]

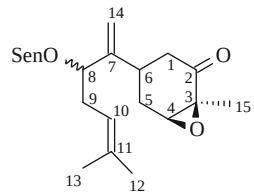
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.39 (3H, s, H-14), 1.60 (3H, br s, H-12), 1.62 (2H, m, H-8), 1.68 (3H, br s, H-13), 1.72 (3H, br s, H-15), 2.0 (2H, m, H-9), 2.24 (1H, br s, H-6), 2.35 (2H, m, H-4), 3.18 (1H, s, OH), 4.52 (1H, m, H-1), 5.14 (1H, br t, J = 7, H-10), 5.72 (1H, br s, H-5), 5.77 (1H, dq, J = ~1; 6; 1.3, H-2); OMeBu: 0.89 (3H, t, H-4′), 1.11 (3H, d, H-5′), 1.27 (1H, ddq, H-3′b), 1.45 (1H, ddq, H-3′a), 2.32 (1H, tq, H-2′) [1]

^{1}H NMR (270 MHz, C_6D_6, TMS): 1.30 (2H, m, H-8), 1.36 (3H, s, H-14), 1.46 (3H, br s, H-12), 1.60 (3H, br s, H-15), 1.66 (3H, br s, H-13), 1.82 (2H, m, H-9), 2.07 (1H, br s, H-6), 2.10 (2H, m, J = ~1.5; ~1, H-4), 3.22 (1H, s, OH), 4.40 (1H, m, H-1), 5.23 (1H, br t, J = 7, H-10), 5.65 (1H, dq, J = ~1; 6; 1.3, H-2), 5.89 (1H, br s, H-5); OMeBu: 0.78 (3H, t, H-4′), 0.96 (3H, d, H-5′), 1.30 (1H, ddq, H-3′b), 1.57 (1H, ddq, H-3′a), 2.03 (1H, tq, H-2′) [1]

References

1. F. Bohlmann, C. Zdero, A.A. Natu, Phytochemistry **17**(10), 1757 (1978)

8-Senecioyloxy-3β,4β-epoxy-bisabola-7(14),10-dien-2-one



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Monoesters

Biological sources: *Senecio macrospermus* DC. [1]

$C_{20}H_{28}O_4$: 332.1988

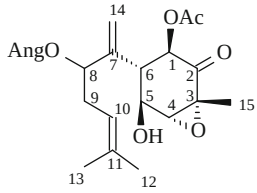
References

1. J. Jakupovic, V.P. Pathak, M. Grenz, S. Banerjee, C. Wolfrum, R.N. Baruah, F. Bohlmann, Phytochemistry **26**(4), 1049 (1987)

Bisabolanes

Diesters

(1*R*,3*R*,4*R*,5*S*,6*S*)-1β-Acetoxy-8-angeloyloxy-3α,4α-epoxy-5β-hydroxy-6β(H)-bisabola-7(14),10-dien-2-one



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Diesters

Biological sources: *Tussilago farfara* L. [1]

$C_{22}H_{30}O_7$: 406.1992

Mp: colorless oil [1]

$[\alpha]_D^{23}$ −32.0° (*c* 50.4, $CHCl_3$) [1]

UV (MeOH) : 217 (4.0) [1]

IR ($CHCl_3$): 3419, 1734, 1698, 1647 [1]

CD (nm): $\Delta\varepsilon_{296.0}$ +0.91°, $\Delta\varepsilon_{214.5}$ −4.69° (*c* 8.90 × 10^{-5}, MeOH) [1]

HR-MS: 406.1964 $[M]^+$ (calc. for $C_{22}H_{30}O_7$: 406.1991) [1]

^{1}H NMR (400 MHz, $CDCl_3$): 1.48 (3H, s, H-15), 1.64 (3H, s, H-12), 1.70 (3H, d, J = 1.0, H-13), 2.09 (3H, s, OAc), 2.18 (1H, m, H-9a), 2.52 (1H, m, H-9b), 2.56 (1H, d, J = 13.7; 8.5, H-6), 3.51 (1H, s, H-4), 4.25 (1H, d, J = 8.5, H-5), 4.72 (1H, dd, J = 8.8; 2.7, H-8), 5.08 (1H, s, H-14a), 5.13 (1H, tq, J = 7.1, 1.0, H-10), 5.20 (1H, d, J = 0.7, H-14b), 5.68 (1H, d, J = 13.7, H-1); OAng: 1.91 (3H, dq, J = 1.5; 1.5, H-5′), 2.00 (3H, dq, J = 7.3; 1.5, H-4′), 6.20 (1H, qq, J = 7.3; 1.5, H-3′) [1]

^{13}C NMR (100 MHz, $CDCl_3$) [1]:

Table 1

C-1	71.4	C-9	31.8	OAc	20.4[a]
2	200.3	10	119.1	OAng	169.5
3	61.4	11	134.8		168.9
4	68.2	12	18.0		127.2
5	73.7	13	25.8		140.6
6	54.0	14	110.8		15.9
7	148.2	15	14.7		20.4[a]
8	78.4				

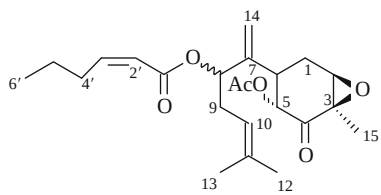
(*continued*)

[a]Signals overlapped [1]

References

1. Y. Yaoita, N. Suzuki, M. Kikuchi, Chem. Pharm. Bull. **49**, 645 (2001)

5-Acetoxy-8-(hex-2′*E*-enoyloxy)-2,3-epoxy-bisabola-7(14),10-dien-4-one (5-Acetoxy-8-(pent-2′*E*-enoyloxy)-2,3-epoxy-bisabola-7(14),10-dien-4-one)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Diesters

Biological sources: *Senecio erubescens* Aiton var. *crepidifolius* DC. [1]

$C_{23}H_{32}O_6$: 404.2199

Mp: 130°C, colorless crystals [1]

$[\alpha]_D$ −22° (*c* 0.23, $CHCl_3$) [1]

IR (CCl_4): 1740, 1730, 1720, 1640 [1]

MS: 404 $[M]^+$ (0.05), 344.199 $[M - HOAc]^+$ (1.5) (calc. for $C_{21}H_{28}O_4$: 344.199), 230 (10), 97 (100), 55 (43) [1]

TLC: C_6H_6 – CH_2Cl_2 – Et_2O (3:3:1) [1]

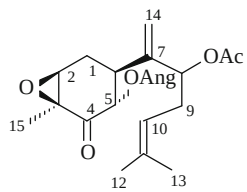
HPLC: MeOH – H_2O (4:1), R_t 5.2 min [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.45 (3H, s, H-15), 1.61 (3H, br s, H-13), 1.68 (3H, br s, H-12), 2.19 (1H, dd, J = 15.5; 11, H-1b), 2.29 (2H, m, H-9), 2.53 (1H, ddd, J = 4; 15.5; 7, H-1a), 2.78 (1H, ddd, J = 7; 11; 13, H-6), 3.43 (1H, d, J = 4, H-2), 5.00 (2H, br t, J = 6.5; 6.5, H-8, H-10), 5.09 (1H, s, H-14b), 5.22 (1H, s, H-14a), 5.76 (1H, d, J = 13, H-5); OCOCH = $CH(CH_2)_2CH_3$: 0.91 (3H, t, J = 7, H-6′), 1.5 (2H, m, H-5′), 2.61 (2H, ddt, J = 1.5; 7.5; 7, H-4′), 5.71 (1H, dt, J = 11; 1.5, H-2′), 6.21 (1H, dt, J = 11; 7.5, H-3′) [1]

References

1. F. Bohlmann, C. Zdero, J. Jakupovic, L.N. Misra, S. Banerjee, P. Singh, R.N. Baruah, M.A. Metwally, G. Schmeda-Hirschmann, L.P.D. Vincent, R.M. King, H. Robinson, Phytochemistry **24**(6), 1249 (1985)

8-Acetoxy-5α-angeloyloxy-2β,3β-epoxy-6α(H)-bisabola-7(14),10-dien-4-one



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Diesters

Biological sources: *Senecio lividus* L. [1]

$C_{22}H_{30}O_6$: 390.2042

Mp: colorless oil (mix. with 8-acetoxy-5α-senecioyloxy-2β,3β-epoxybisabola-7(14),10-dien-4-one) [1]

IR (CCl_4) (mix.): 1725 [1]

MS (mix.): 390.204 $[M]^+$ (0.6), (calc. for $C_{22}H_{30}O_6$: 390.204), 330 (5), 230 (18), 83 (100), 55 (38) [1]

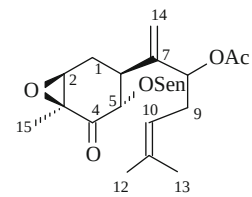
HPLC [1]

^{1}H NMR (400 MHz, $CDCl_3$): 1.47 (3H, s, H-15), 1.61 (3H, br s, H-13), 1.68 (3H, br s, H-12), 2.03 (3H, s, OAc), 2.18 (1H, dd, J = 10.5; 16, H-1β), 2.31 (2H, br dd, J = 6.5; 6.5, H-9), 2.56 (1H, ddd, J = 4; 16; 7.5, H-1α), 2.77 (1H, br ddd, J = 13.5; 7.5; 10.5, H-6), 3.43 (1H, d, J = 5, H-2), 5.02 (1H, br t, J = 6.5, H-10), 5.04 (1H, br t, J = 6.5, H-8), 5.10 (1H, br s, H-14b), 5.24 (1H, br s, H-14a), 5.85 (1H, d, J = 13.5, H-5); OAng: 1.88 (3H, dq, J = 1.5; 1.5, H-5′), 1.97 (3H, dq, J = 7; 1.5, H-4′), 6.06 (1H, qq, J = 7; 1.5, H-3′) [1]

References

1. J.M. Cardoso, J. Jakupovic, F. Bohlmann, Phytochemistry **26**(8), 2321 (1987)

8-Acetoxy-5α-senecioyloxy-2β,3β-epoxy-6α(H)-bisabola-7(14),10-dien-4-one



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Diesters

Biological sources: *Senecio lividus* L. [1]

$C_{22}H_{30}O_6$: 390.2042

Mp: colorless oil (mix. with 8-acetoxy-5α-angeloyloxy-2β,3β-epoxybisabola-7(14),10-dien-4-one) [1]

IR (CCl_4) (mix.): 1725 [1]

MS (mix.): 390.204 $[M]^+$ (0.6), (calc. for $C_{22}H_{30}O_6$: 390.204), 330 (5), 230 (18), 83 (100), 55 (38) [1]

HPLC [1]

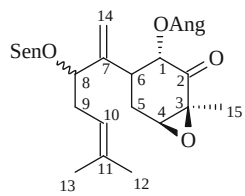
^{1}H NMR (400 MHz, $CDCl_3$): 1.46 (3, s, H-15), 1.63 (3, br s, H-13), 1.69 (3, br s, H-12), 2.05 (3, s, OAc),

2.18 (1, dd, J = 10.5; 16, H-1β), 2.31 (2H, br dd, J = 6.5; 6.5, H-9), 2.53 (1H, ddd, J = 4; 16; 7.5, H-1α), 2.75 (1H, br ddd, J = 13.5; 7.5; 10.5, H-6), 3.42 (1H, d, J = 5, H-2), 5.02 (1H, br t, J = 6.5, H-10), 5.04 (1H, br t, J = 6.5, H-8), 5.12 (1H, br s, H-14b), 5.24 (1H, br s, H-14a), 5.76 (1H, d, J = 13.5, H-5); OSen: 1.90 (3H, d, J = 1.5, H-4′), 2.15 (3H, d, J = 1.5, H-5′), 5.68 (1H, qq, J = 1.5; 1.5, H-2′) [1]

References

1. J.M. Cardoso, J. Jakupovic, F. Bohlmann, Phytochemistry **26**(8), 2321 (1987)

1α-Angeloyloxy-8-senecioyloxy-3β,4β-epoxy-bisabola-7(14),10-dien-2-one



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Diesters

Biological sources: *Senecio macrospermus* DC. [1]

$C_{25}H_{34}O_6$: 430.2355

Mp: colorless oil [1]

$[\alpha]_D^{24}$ −58° (*c* 0.37, $CHCl_3$) [1]

IR (CCl_4): 1730, 1660 [1]

MS: 430.236 $[M]^+$ (0.5) (calc. for $C_{25}H_{34}O_6$: 430.236), 361 (6), 330 (1), 230 (3), 83 (100) [1]

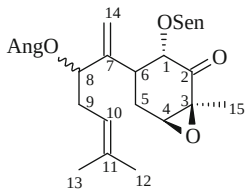
HPLC: MeOH – H_2O (4:1), R_t 5.0 min [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.44 (3H, s, H-15), 1.59 (3H, br s, H-13), 1.64 (3H, br s, H-12), 2.19 (1H, dd, J = 16; 11, H-5β), 2.32 (2H, m, H-9), 2.59 (1H, ddd, J = 4.5; 16; 7.5, H-5α), 2.76 (1H, ddd, J = 12; 7.5; 11, H-6), 3.43 (1H, d, J = 4.5, H-4), 5.04 (1H, br t, J = 7, H-10), 5.07 (1H, br s, H-14a), 5.09 (1H, m, H-8), 5.22 (1H, br s, H-14b), 5.85 (1H, d, J = 12, H-1); OAng: 1.87 (3H, dq, J = 1.5; 1.5, H-5′), 1.95 (3H, dq, J = 7; 1.5, H-4′), 6.04 (1H, qq, J = 7; 1.5, H-3′); OSen: 1.84 (3H, d, J = 1.3, H-4″), 2.14 (3H, d, J = 1.3, H-5″), 5.64 (1H, qq, J = 1.3; 1.3, H-2″) [1]

References

1. J. Jakupovic, V.P. Pathak, M. Grenz, S. Banerjee, C. Wolfrum, R.N. Baruah, F. Bohlmann, Phytochemistry **26**(4), 1049 (1987)

8-Angeloyloxy-1α-senecioyloxy-3β,4β-epoxy-bisabola-7(14),10-dien-2-one



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Diesters

Biological sources: *Senecio macrospermus* DC. [1]

$C_{25}H_{34}O_6$: 430.2355

Mp: colorless oil [1]

$[\alpha]_D^{24}$ −40° (*c* 0.81, $CHCl_3$) [1]

IR (CCl_4): 1730, 1660 [1]

MS: 430.236 $[M]^+$ (0.4) (calc. for $C_{25}H_{34}O_6$: 430.236), 361 (5), 330 (5), 230 (12), 83 (100) [1]

HPLC: MeOH – H_2O (4:1), R_t 4.5 min. [1]

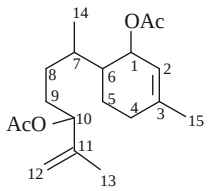
^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.42 (3H, s, H-15), 1.59 (3H, br s, H-13), 1.65 (3H, br s, H-12), 2.19 (1H, dd, J = 16; 11, H-5β), 2.34 (2H, m, H-9), 2.56 (1H, ddd, J = 4.5; 16; 7.5, H-5α), 2.77 (1H, ddd, J = 12; 7.5; 11, H-6), 3.42 (1H, d, J = 4.5, H-4), 5.03 (1H, br t, J = 7, H-10), 5.07 (1H, m, H-8),

5.10 (1H, br s, H-14a), 5.23 (1H, br s, H-14b), 5.75 (1H, d, J = 12, H-1); OAng: 1.87 (3H, dq, J = 1.5; 1.5, H-5′), 1.97 (3H, dq, J = 7; 1.5, H-4′), 6.09 (1H, qq, J = 7; 1.5, H-3′); OSen: 1.84 (3H, d, J = 1.3, H-4″), 2.12 (3H, d, J = 1.3, H-5″), 5.63 (1H, qq, J = 1.3; 1.3, H-2″) [1]

References

1. J. Jakupovic, V.P. Pathak, M. Grenz, S. Banerjee, C. Wolfrum, R.N. Baruah, F. Bohlmann, Phytochemistry **26**(4), 1049 (1987)

1,10-Diacetoxy-bisabola-2,11(12)-diene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Diesters

Biological sources: *Achillea odorata* L. [1]

$C_{19}H_{30}O_4$: 322.4275

Mp: oil [1]

$[\alpha]_D$ 53.2° (*c* 1.0, $CHCl_3$) [1]

IR (film): 1735, 1675, 1649, 905 [1]

MS: 262 $[M - HOAc]^+$ (1), 202 $[M - 2 \times HOAc]^+$ (3), 187 $[M - Me - 2 \times HOAc]^+$ (3), 132 (57), 119 (41), 93 (100), 92 (52), 91 (56), 68 (64), 43 (41) [1]

^{1}H NMR (300 MHz, $CDCl_3$, TMS): 0.79 (3H, d, J = 6.7, H-14), 1.66 (3H, s, H-15), 1.70 (3H, s, H-13), 2.05 (6H, s, 2 × OAc), 4.87 (1H, q, J = 1.5, H-12a), 4.92 (1H, s, H-12b), 5.13 (1H, t, J = 6.9, H-10), 5.26 (1H, m, H-1), 5.29 (1H, s, H-2) [1]

^{13}C NMR (75 MHz, $CDCl_3$) [1]:

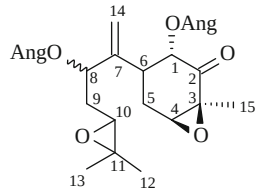
Table 1

C-1	72.1	C-7	31.4	C-13	18.0, 18.2
2	121.3, 121.43	8	21.10	14	14.7
3	139.4, 139.5	9	29.8, 30.0	15	23.2
4	30.4, 30.5	10	77.4, 77.6	2 × OAc	170.3, 171.3
5	20.9	11	143.1, 134.2	1′, 1″	21.3, 21.5
6	42.4	12	112.9, 113.1	2′, 2″	

References

1. A.F. Barerero, R.E.J. Alvarez-Manzaneda, R.R. Alvarez-Manzaneda, Phytochemistry **29**(10), 3213 (1990)

1α,8-Diangeloyloxy-3β,4β,10,11-diepoxy-bisabol-7(14)-en-2-one



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Diesters

Biological sources: *Senecio fulgens* G. Nicholson [1]

$C_{25}H_{34}O_7$: 446.2305

Mp: colorless oil [1]

$[\alpha]_D^{24}$ (λ, nm): −65.9° (589), −78.6° (578), −76.7° (546), −119.8° (436) (*c* 0.95) [1]

IR (CCl_4): 3100, 1730, 1655, 855 [1]

MS: 446.230 $[M]^+$ (22), 375 (15), 346 (8), 246 (8), 83 (100) [1]

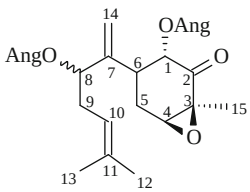
^{1}H NMR (270 MHz, C_6D_6, TMS): 1.16 (3H, s, H-12), 1.16 (3H, s, H-13), 1.24 (3H, s, H-15), 1.9 (2H, m, H-9), 2.45 (1H, br dd, J = 12; 7, H-6), 2.71 (1H, d, J = 4, H-4), 2.84 (1H, dd, J = 7; 5, H-10), 4.92 (1H, br s, H-14b), 5.16 (1H, br s, H-14a), 5.40 (1H, dd, J = 4; 8, H-8), 6.20 (1H, d, J = 12, H-1); 2 × OAng:

1.94 and 1.90 (each 3H, dq, J = 1.5; 1.5, H-5′, H-5″), 2.04 and 2.03 (each 3H, dq, J = 7; 1.5, H-4′, H-4″), 5.78 and 5.74 (each 1H, qq, J = 7; 1.5, H-3′, H-3″) [1]

References

1. F. Bohlmann, J. Ziesche, Phytochemistry **20**(3), 469 (1981)

1α,8-Diangeloyloxy-3β,4β-epoxy-bisabola-7(14),10-dien-2-one



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Diesters

Biological sources: *Rugelia nudicaulis* Shuttlew. ex Chapm. [1]; *Senecio macrospermus* DC. [2]

$C_{25}H_{34}O_6$: 430.2355

Mp: colorless gum [1]

$[\alpha]^{24}$ (λ, nm): −28° (589), −29° (578), −33° (546), −43° (436) (*c* 2.4, $CHCl_3$) [1]

IR (CCl_4): 1725 [1]

MS: 430.234 $[M]^+$ (0.5) ($C_{25}H_{34}O_6$), 361 (1), 330 (15), 230 (3.5), 83 (100) [1]

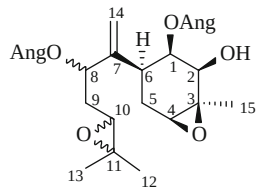
^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.46 (3H, s, H-15), 1.59 (1H, br s, H-13), 1.66 (3H, br s, H-12), 2.21 (1H, ddd, H-5b), 2.33 (2H, m, H-9), 2.62 (1H, ddd, H-5a), 2.78 (1H, br dd, J = 11; 3.5, H-6), 3.44 (1H, br d, H-4), 5.04 (1H, br t, J = 4.5, H-10), 5.08 (1H, br s, H-14b), 5.09 (1H, dd, H-8), 5.29 (1H, br s, H-14a), 5.86 (1H, d, J = 4.5, H-1); 2 × OAng: 1.91 and 1.89 (each 3H, dq, J = 1.5; 1.5, H-5′, H-5″), 2.01 and 1.98 (each 3H, dq, J = 7; 1.5, H-4′, H-4″), 6.11 and 6.06 (each 1H, qq, J = 7; 1.5, H-3′, H-3″) [1]

References

1. F. Bohlmann, R.K. Gupta, J. Jakupovic, R.M. King, H. Robinson, Phytochemistry **21**(7), 1665 (1982)
2. J. Jakupovic, V.P. Pathnak, M. Grenz, S. Banerjee, C. Wolfrum, R.N. Baruah, F. Bohlmann, Phytochemistry **26**(4), 1049 (1987)

1β,8-Diangeloyloxy-3β,4β,10,11-diepoxy-2β-hydroxy-bisabol-7(14)-ene

CAS Registry Number: 60263-02-7



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Diesters

Biological sources: *Senecio oxyriifolius* DC. [1]

$C_{25}H_{36}O_7$: 448.2461

Mp: colorless oil [1]

$[\alpha]^{24}$ (λ, nm): −17.5° (589), −18.2° (578), −21.3° (546), −37.7° (436) (*c* 0.88, $CHCl_3$) [1]

IR (CCl_4): 3590, 1720, 1650 [1]

MS: 448.246 $[M]^+$ (1), 430 (2), 377 (1), 348 (12), 83 (100), 71 (12), 55 (37) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.30 (6H, s, H-12, H-13), 1.46 (3H, s, H-15), 2.0 (2H, m, H-9), 2.00 (1H, m, H-5α), 2.08 (1H, dd, J = 17; 12, H-5β), 2.23 (1H, d, J = 8.5, OH), 2.42 (1H, br dd, J = 12, H-6α), 2.80 (1H, dd, J = 6.5; 5, H-10), 3.24 (1H, d, J = 5, H-4α), 4.01 (1H, dd, J = 4.5; 8.5, H-2α), 5.01 (1H, s, H-14b), 5.25 (1H, s, H-14a), 5.40 (1H, dd, J = 7.5; 6, H-8), 5.41 (1H, br d, J = >1, H-1α);

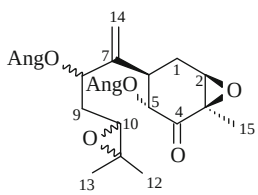
OAng-5: 1.91 (3H, dq, J = 1.6; 1.6, H-5′), 2.00 (3H, dq, J = 7; 1.6, H-4′), 6.12 (1H, qq, J = 7; 1.6, H-3′); OAng-8: 1.91 (3H, dq, J = 1.6; 1.6, H-5″), 2.00 (3H, dq, J = 7; 1.6, H-4″), 6.10 (1H, qq, J = 7; 1.6, H-3″) [1]

^{1}H NMR (270 MHz, C_6D_6, TMS): 1.16 (3H, s, H-15), 1.22 (3H, s, H-13), 1.24 (3H, s, H-12), 1.8 (2H, m, H-9), 1.90 (1H, m, H-5α), 2.03 (1H, dd, J = 17; 12, H-5β), 2.30 (1H, d, J = 6, OH), 2.32 (1H, br dd, J = 12, H-6α), 2.75 (1H, d, J = 5, H-4α), 2.82 (1H, dd, J = 6.5; 5, H-10), 3.65 (1H, dd, J = 4.5; 6, H-2α), 4.95 (1H, s, H-14b), 5.21 (1H, s, H-14a), 5.59 (1H, br d, J = >1, H-1α), 5.60 (1H, dd, J = 7.5; 6, H-8); OAng-5: 1.89 (3H, dq, J = 1.6; 1.6, H-5′), 1.98 (3H, dq, J = 7; 1.6, H-4′), 5.74 (1H, qq, J = 7; 1.6, H-3′); OAng-8: 1.89 (3H, dq, J = 1.6; 1.6, H-5″), 1.98 (3H, dq, J = 7; 1.6, H-4″), 5.72 (1H, qq, J = 7; 1.6, H-3″) [1]

References

1. F. Bohlmann, C. Zdero, Phytochemistry **17**(9), 1669 (1978)

5α,8-Diangeloyloxy-2,3;10,11-diepoxy-2,3,10,11-tetrahydro-β-bisabol-4-one (5α,8-Bisangeloyloxy-2,3;10,11-diepoxy-2,3,10,11-tetrahydro-β-bisabol-4-one)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Diesters

Biological sources: *Senecio abrotanifolius* L. [1]; *S. coccineiflorus* Rowley [2]

$C_{25}H_{34}O_7$: 446.2305

Mp: colorless oil [1]

$[\alpha]^{24}$ (λ, nm): −66° (589), −68° (578), −77° (546), −123° (436) (*c* 1.2, $CHCl_3$) [1]

IR (CCl_4): 1730, 1720, 1650 [1]

MS: 446.231 $[M]^+$ (2) (calc. for $C_{25}H_{34}O_7$: 446.230) [1]

^{1}H NMR (270 MHz, C_6D_6/$CDCl_3$, TMS): ∼1.8 (2H, m, H-9), 1.12 (3H, s, H-12), 1.15 (3H, s, H-13), 1.58 (3H, s, H-15), 2.02 (1H, br dd, J = 11; 16, H-1β), 2.30 (1H, ddd, J = 16; 4; 8, H-1α), 2.59 (1H, dd, J = 13; 8, H-6), 2.67 (1H, t, J = 6; 6, H-10), 3.00 (1H, br d, J = 4, H-2), 4.97 (1H, s, H-14a), 5.15 (1H, s, H-14b), 5.28 (1H, dd, J = 8; 6, H-8), 5.95 (1H, d, J = 13, H-5); 2 × OAng: 1.84 (3H, dq, J = 1; 1, H-5″), 1.86 (3H, dq, J = 1; 1, H-5′), 1.96 (6H, dq, J = 7; 1, H-4′, H-4″), 5.85 (1H, qq, J = 7; 1, H-3″), 5.91 (1H, qq, J = 7; 1, H-3′) [1]

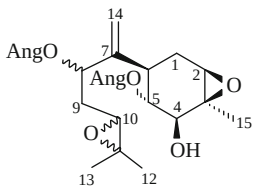
^{1}H NMR (270, C_6D_6, TMS): 1.09 (3, s, H-12), 1.12 (3, s, H-13), 1.20 (3H, s, H-15), ∼1.9 (2H, m, H-9), 1.97 (1H, br dd, J = 11; 16, H-1β), 2.12 (1H, ddd, J = 16; 4; 8, H-1α), 2.53 (1H, dd, J = 13; 8, H-6), 2.72 (1H, br d, J = 4, H-2), 2.72 (1H, t, J = 6; 6, H-10), 4.91 (1H, s, H-14a), 5.13 (1H, s, H-14b), 5.40 (1H, dd, J = 8; 6, H-8), 6.16 (1H, d, J = 13, H-5); 2 × OAng: 1.90 (3H, dq, J = 1; 1, H-5″), 1.91 (3H, dq, J = 1; 1, H-5′), 2.00 (6H, dq, J = 7; 1, H-4′, H-4″), 5.71 (1H, qq, J = 7; 1, H-3″), 5.76 (1H, qq, J = 7; 1, H-3′) [1]

^{1}H NMR (270 MHz, $(D_3C)_2CO$, TMS): ∼2.0 (2H, m, H-9), 1.22 (3H, s, H-12), 1.23 (3H, s, H-13), 1.38 (3H, s, H-15), 2.17 (1H, br dd, J = 11; 16, H-1β), 2.73 (1H, t, J = 6; 6, H-10), 2.74 (1H, ddd, J = 16; 4; 8, H-1α), 3.05 (1H, dd, J = 13; 8, H-6), 3.63 (1H, br d, J = 4, H-2), 5.15 (1H, s, H-14a), 5.31 (1H, s, H-14b), 5.45 (1H, dd, J = 8; 6, H-8), 5.81 (1H, d, J = 13, H-5); 2 × OAng: 1.86 (3H, dq, J = 1; 1, H-5″), 1.92 (3H, dq, J = 1; 1, H-5′), 1.98 (6H, dq, J = 7; 1, H-4′, H-4″), 6.08 (1H, qq, J = 7; 1, H-3″), 6.15 (1H, qq, J = 7; 1, H-3′) [1]

References

1. F. Bohlmann, A. Suwita, Chem. Ber. **109**, 2014 (1976)
2. F. Bohlmann, P.K. Mahanta, Phytochemistry **18**(4), 678 (1979)

5α,8-Diangeloyloxy-2β,3β;10,11-diepoxy-6α(H)-bisabol-7(14)-en-4β-ol (5α,8-bis-Angeloyloxy-2,3:10,11-diepoxy-2,3,10,11-tetrahydro-β-bisabol-4-ol)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Diesters

Biological sources: *Senecio abrotanifolius* L. [1]; *S. coccineiflorus* Rowley [2]

$C_{25}H_{36}O_7$: 448.2461

Mp: colorless oil [1]

IR (CCl_4): 3600, 1730, 1650 [1]

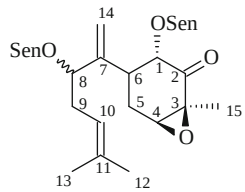
MS: 448.246 $[M]^+$ (1) (calc. for $C_{25}H_{36}O_7$: 448.246) [1]

^{1}H NMR (270 MHz, $(D_3C)_2CO$, TMS): ~2.0 (1H, m, H-1β), ~2.0 (2H, m, H-9), ~2.5 (1H, m, H-1α), ~2.5 (1H, m, H-6), 1.19 (3H, s, H-12), 1.21 (3H, s, H-13), 1.38 (3H, s, H-15), 2.68 (1H, t, J = 6; 6, H-10), 3.10 (1H, d, J = 4, H-2), 3.87 (1H, br d, J = 8, H-4), 5.02 (1H, s, H-14a), 5.15 (1H, s, H-14b), 5.22 (1H, dd, J = 11; 8, H-5), 5.35 (1H, dd, J = 8; 4.5, H-8); 2 × OAng: 1.78 (3H, dq, J = 1; 1, H-5″), 1.89 (3H, dq, J = 1; 1, H-5′), 1.97 (6H, dq, J = 7; 1, H-4′, H-4″), 5.94 (1H, qq, J = 7; 1, H-3″), 6.14 (1H, qq, J = 7; 1, H-3′) [1]

References

1. F. Bohlmann, A. Suwita, Chem. Ber. **109**, 2014 (1976)
2. F. Bohlmann, P.K. Mahanta, Phytochemistry **18**(4), 678 (1979)

1α,8-Disenecioyloxy-3β,4β-epoxy-bisabola-7(14),10-dien-2-one (1α,8-Bissenecioyloxy-3β,4β-epoxybisabola-7(14),10-dien-2-one)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Diesters

Biological sources: *Senecio macrospermus* DC. [1]

$C_{25}H_{34}O_6$: 430.2355

Mp: colorless oil [1]

$[\alpha]_D^{24}$ −75° (*c* 0.62, $CHCl_3$) [1]

IR (CCl_4): 1730, 1660 [1]

MS: 430.236 $[M]^+$ (0.5) (calc. for $C_{25}H_{34}O_6$: 430.236), 361 (6), 330 (4), 230 (6) [1]

PTLC: CH_2Cl_2 – C_6H_6 – Et_2O (4:4:1), R_f 0.65 [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.43 (3H, s, H-15), 1.59 (3H, br s, H-13), 1.65 (3H, br s, H-12), 2.18 (1H, dd, J = 16; 11, H-5β), 2.32 (2H, m, H-9), 2.54 (1H, ddd, J = 4.5; 16; 7.5, H-5α), 2.77 (1H, ddd, J = 12; 7.5; 11, H-6), 3.41 (1H, d, J = 4.5, H-4), 5.02 (1H, br t, J = 7, H-10), 5.05 (1H, m, H-8), 5.08 (1H, br s, H-14a), 5.22 (1H, br s, H-14b), 5.75 (1H, d, J = 12, H-1); 2 × OSen: 1.84 and 1.88 (each 3H, d, J = 1.3, H-4′, H-4″), 2.12 and 2.14 (each 3H, d, J = 1.3, H-5′, H-5″), 5.63 and 5.64 (each 1H, qq, J = 1.3; 1.3, H-2′, H-2″) [1]

References

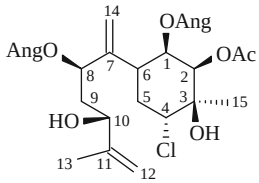
1. J. Jakupovic, V.P. Pathak, M. Grenz, S. Banerjee, C. Wolfrum, R.N. Baruah, F. Bohlmann, Phytochemistry **26**(4), 1049 (1987)

Bisabolanes

Triesters

2β-Acetoxy-1β,8-diangeloyloxy-4α-chloro-3β,10-dihydroxybisabola-7(14),11(12)-diene

CAS Registry Number: 250725-66-7



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Cremanthodium discoideum* Maxim. [1]

$C_{27}H_{39}O_8Cl$: 526.2333

Mp: colorless gum [1]

$[\alpha]_D^{20}$ −55.2°C (*c* 0.6, $CHCl_3$) [1]

IR: 3565, 3510, 1746, 1231, 1718, 1648, 846, 734 [1]

EI-MS: 526 $[M]^+$ (0.04), 508 $[M - 18]^+$ (0.3), 491 $[M - Cl]^+$ (0.2), 426 $[M - AngOH]^+$ (1), 390 $[M - HCl - AngOH]^+$ (0.1), 326 $[M - 2AngOH]^+$ (0.6), 290 $[M - HCl - 2AngOH]^+$ (0.1), 83 $[C_4H_7CO]^+$ (100), 55 $[83 - CO]^+$ (37), 43 $[CH_3CO]^+$ (25) [1]

FAB-MS: 533 $[M + Li]^+$, 549 $[M + Na]^+$ [1]

HR-FAB-MS: 527.241585 $[M + H]^+$ (calc. for $C_{27}H_{40}O_8Cl$: 527.241171) [1]

^{1}H NMR (400 MHz, $CDCl_3$): 1.34 (3H, s, H-15), 1.57 (1H, m, H-9b), 1.74 (1H, m, H-9a), 1.76 (3H, s, H-13), 1.89 (1H, m, H-5α), 2.06 (3H, s, OAc-2), 2.66 (1H, ddd, J = 15.3; 12.7; 2.6, H-5β), 3.20 (1H, br d, J = 12.7, H-6), 3.55 (1H, s, OH-3), 4.00 (1H, dd, J = 9.6; 2.2, H-10), 4.21 (1H, dd, J = 2.8; 2.6, H-4), 4.85 (1H, s, H-14b), 4.99 (1H, s, H-12b), 5.00 (1H, s, H-12a), 5.23 (1H, d, J = 3.2, H-2), 5.27 (1H, s, H-14a), 5.59 (1H, dd, J = 10.2; 2.9, H-8), 5.63 (1H, t, J = 3.2, H-1); OAng-1: 1.89 (3H, dq, J = 1.5; 1.3, H-5′), 1.95 (3H, dq, J = 7.3; 1.3, H-4′), 6.10 (1H, qq, J = 7.3; 1.5, H-3′); OAng-8: 1.95 (3H, dq, J = 1.5; 1.4, H-5″), 2.00 (3H, dq, J = 7.3; 1.4, H-4″), 6.13 (1H, qq, J = 7.3; 1.5, H-3″) [1]

^{13}C NMR [1]:

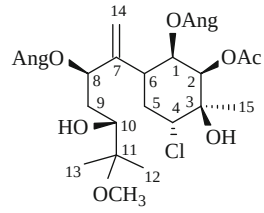
Table 1

C-1	70.5 d	C-11	145.7 s	OAng-1	165.6 s
2	70.7 d	12	111.0 t	OAng-8	126.5 s
3	74.2 s	13	18.1 q		139.3 d
4	64.3 d	14	115.4 t		15.7 q
5	29.8 t	15	23.8 q		20.5 q
6	35.1 d	OAc-2	169.7 s		167.7 s
7	146.6 s		20.6 q		127.4 s
8	73.5 d				139.9 d
9	40.0 t				15.8 q
10	71.5 d				20.5 q

References

1. Y. Zhu, L. Yang, Z.-J. Jia, J. Nat. Prod. **62**, 1479 (1999)

2β-Acetoxy-1β,8-diangeloyloxy-4α-chloro-3β,10-dihydroxy-11-methoxy-bisabol-7(14)-ene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Cremanthodium discoideum* Maxim. [1]

$C_{28}H_{43}O_9Cl$: 558.2596

Mp: colorless gum [1]

$[\alpha]_D^{20}$ −53.3° (*c* 1.0, $CHCl_3$) [1]

IR: 3562, 3519, 1746, 1230, 1718, 1648, 846, 753 [1]

EI-MS: 543 $[M - CH_3]^+$ (0.3), 485 $[M - C(OCH_3)Me_2]^+$ (0.4), 458 $[M - AngOH]^+$ (0.3), 427 $[M - OCH_3 - AngOH]^+$ (1), 385 $[M - AngOH - C(OCH_3)Me_2]^+$ (4), 358 $[M - 2AngOH]^+$ (1), 285 $[M - 2AngOH - C(OCH_3)Me_2]^+$ (2), 83 $[C_4H_7CO]^+$ (58), 73 $[C(OCH_3)Me_2]^+$ (100), 55 $[83 - CO]^+$ (27), 43 $[CH_3CO]^+$ (19) [1]

FAB-MS: 559 $[M + H]^+$, 565 $[M + Li]^+$, 581 $[M + Na]^+$ [1]

HR-FAB-MS: 559.272975 $[M + H]^+$ (calc. for $C_{28}H_{44}OCl$: 559.267386) [1]

^{1}H NMR (400 MHz, $CDCl_3$): 1.14 (3H, s, H-12), 1.14 (3H, s, H-13), 1.34 (3H, s, H-15), 1.61 (1H, m, H-9b), 1.89 (1H, m, H-5α), 1.98 (1H, m, H-9a), 2.06 (3H, s, OAc-2), 2.64 (1H, ddd, J = 15.5; 12.6; 2.9, H-5β), 2.73 (1H, br s, OH-10), 3.20 (1H, br dd, J = 12.5; 2.3, H-6), 3.22 (3H, s, OCH_3-11), 3.46 (1H, br d, J = 10.5, H-10), 3.56 (1H, s, OH-3), 4.21 (1H, dd, J = 2.9; 2.8, H-4), 4.99 (1H, s, H-14b), 5.23 (1H, d, J = 3.2, H-2), 5.28 (1H, s, H-14a), 5.59 (1H, dd, J = 10.4; 2.9, H-8), 5.63 (1H, t, J = 3.2, H-1); OAng-1: 1.89 (3H, dq, J = 1.4; 1.4, H-5′), 1.94 (3H, dq, J = 7.3; 1.4, H-4′), 6.10 (1H, qq, J = 7.3; 1.4, H-3′); OAng-8: 1.93 (3H, dq, J = 1.4; 1.5, H-5″), 2.00 (3H, dq, J = 7.3; 1.5, H-4″), 6.10 (1H, qq, J = 7.3; 1.4, H-3″) [1]

^{13}C NMR: [1]

Table 1

C-1	70.5 d	C-13	19.7 q	OAng-8	167.3 s
2	70.8 d	14	115.0 t		127.6 s
3	74.2 s	15	23.7 q		139.7 d
4	64.4 d	OCH_3-11	49.2 q		15.8 q
5	29.7 t	OAc-2	169.7 s		20.6 q
6	35.1 d	OAng-1	20.6 q		
7	146.0 s		165.5 s		
8	73.9 d		126.6 s		
9	35.9 t		138.7 d		
10	72.9 d		15.6 q		
11	76.9 s		20.5 q		
12	19.7 q				

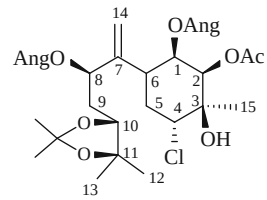
Pharm./Biol.: Antibacterial activity against *Bacillus acidilatici* and *B. subtilis* [1]

References

1. Y. Zhu, L. Yang, Z.-J. Jia, J. Nat. Prod. **62**, 1479 (1999)

2β-Acetoxy-1β,8-diangeloyloxy-4α-chloro-3β-hydroxy-10,11-isopropoxy-bisabol-7(14)-ene

CAS Registry Number: 250725-68-9



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Cremanthodium discoideum* Maxim. [1]

$C_{30}H_{45}O_9Cl$: 584.2752

Mp: colorless gum [1]

$[\alpha]_D^{20}$ −53.3° (*c* 1.0, $CHCl_3$) [1]

IR: 3576, 1748, 1231, 1719, 1650, 844, 743 [1]

EI-MS: 569 $[M - CH_3]^+$ (5), 484 $[M - C_4H_7COOH]^+$ (1), 384 $[M - 2C_4H_7COOH]^+$ (1), 129 $[C(CH_3)_2CHO_2C(CH_3)_2]^+$ (18), 83 $[C_4H_7CO]^+$ (100), 55 $[83 - CO]^+$ (37), 43 $[CH_3CO]^+$ (35) [1]

FAB-MS: 591 $[M + Li]^+$, 607 $[M + Na]^+$ [1]

HR-FAB-MS: 585.282951 $[M + H]^+$ (calc. for $C_{30}H_{46}O_9Cl$: 585.283067) [1]

^{1}H NMR (400 MHz, $CDCl_3$): 1.10 (3H, s, H-13), 1.25 (1H, s, H-10), 1.34 (3H, s, H-15), 1.42 (3H, s, H-17), 1.80 (1H, m, H-9a), 1.89 (1H, m, H-5α), 2.06 (3H, s, OAc), 2.64 (1H, ddd, J = 15.3; 12.6; 2.7, H-5β), 3.21 (1H, br d, J = 12.6, H-6), 3.69 (1H, dd, J = 9.0; 2.4, H-9b), 4.22 (1H, dd, J = 2.9; 2.7, H-4), 5.00 (1H, s, H-14b), 5.23 (1H, d, J = 3.2, H-2), 5.29 (1H, s, H-14a), 5.48 (1H, dd, J = 8.0, J = 5.5, H-8), 5.63 (1H, t, J = 3.2, H-1); 2 × OAng: 1.89 (3H, dq, J = 1.4; 1.5, H-5′), 1.93 (3H, dq, J = 7.6; 1.5, H-4′), 1.94 (3H, dq, J = 1.4; 1.4, H-5″), 2.00 (3H, dq, J = 7.6; 1.4, H-4″), 6.07 (1H, qq, J = 7.6; 1.4, H-3′), 6.10 (1H, qq, J = 7.6; 1.4, H-3″) [1]

^{13}C NMR: [1]

Table 1

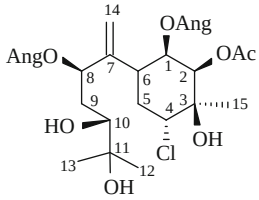
C-1	70.6 d	C-11	79.9 s	OAng-1	165.4 s
2	70.8 d	12	25.6 q	OAng-8	126.6 s
3	74.2 s	13	22.8 q		138.4 d
4	64.4 d	14	115.9 t		15.6 q
5	29.6 t	15	23.7 q		20.4 q
6	34.8 d	16	106.9 s		166.7 s
7	145.3 s	17	28.4 q		128.0 s
8	74.8 d	18	26.7 q		139.5 d
9	33.4 t	OAc-2	169.7 s		15.7 q
10	79.8 d		20.6 q		20.5 q

References

1. Y. Zhu, L. Yang, Z.-J. Jia, J. Nat. Prod. **62**, 1479 (1999)

2β-Acetoxy-1β,8-diangeloyloxy-4α-chloro-3β,10,11-trihydroxy-bisabol-7(14)-ene

CAS Registry Number: 250725-65-6



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Cremanthodium discoideum* Maxim. [1]

$C_{27}H_{41}O_9Cl$: 544.2439

Mp: colorless gum [1]

$[\alpha]_D^{20}$ −62.4° (*c* 2.0, $CHCl_3$) [1]

IR: 3564, 3499, 1733, 1230, 1720, 1647, 846, 734 [1]

EI-MS: 545 $[M + H]^+$ (0.06), 529 $[M - CH_3]^+$ (0.6), 526 $[M - H_2O]^+$ (0.1), 444 $[M - C_4H_7COOH]^+$ (0.1), 426 $[M - H_2O - C_4H_7COOH]^+$ (2), 408 $[M - HCl - C_4H_7COOH]^+$ (0.2), 385 $[M - CMe_2OH - C_4H_7COOH]^+$ (2), 344 $[M - 2 \times C_4H_7COOH]^+$ (0.03), 285 $[M - CMe_2OH - 2 \times C_4H_7COOH]^+$ (0.3), 83 $[C_4H_7CO]^+$ (100), 55 $[83 - CO]^+$ (46), 43 $[CH_3CO]^+$ (37) [1]

FAB-MS: 545 $[M + H]^+$ [1]

HR-FAB-MS: 545.243441 $[M + H]^+$ (calc. for $C_{27}H_{42}O_9Cl$: 545.251736) [1]

^{1}H NMR (400 MHz, $CDCl_3$): 1.34 (3H, s, H-15), 1.57 (3H, s, H-13), 1.58 (1H, s, H-10), 1.65 (1H, m, H-9b), 1.89 (1H, m, H-5β), 2.06 (3H, s, OAc-2), 2.12 (1H, m, H-9a), 2.65 (1H, ddd, J = 15.3; 12.3; 12.4; 2.8, H-5β), 2.82 (1H, br s, OH-10), 3.22 (1H, br d, J = 12.4, H-6), 3.53 (1H, br d, J = 10.5, H-10.5), 4.21 (1H, dd, J = 2.8; 2.6, H-4), 5.01 (1H, s, H-14b), 5.23 (1H, d, J = 3.2, H-2), 5.29 (1H, s, H-14a), 5.57 (1H, dd, J = 10.5; 2.4, H-8), 5.63 (1H, t, J = 3.2, H-1); OAng-1: 1.89 (3H, dq, J = 1.5; 1.4, H-5′), 1.95 (3H, dq, J = 7.3; 1.5, H-4′), 6.11 (1H, qq, J = 7.3; 1.5, H-3′); OAng-8: 1.93 (3H, dq, J = 1.4; 1.5, H-5″), 2.00 (3H, dq, J = 7.3; 1.4, H-4″), 6.13 (1H, qq, J = 7.3; 1.5, H-3″) [1]

^{13}C NMR [1]:

Table 1

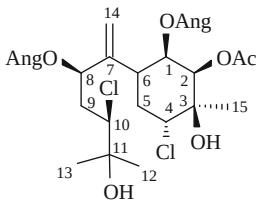
C-1	70.2 d	C-11	74.0 s	OAng-1	165.3 s
2	70.7 d	12	28.3 q	OAng-8	126.4 s
3	73.8 s	13	28.1 q		138.9 d
4	64.2 d	14	115.0 t		15.6 q
5	29.5 t	15	23.7 q		20.4 q
6	35.5 d	OAc-2	169.6 s		167.3 s
7	146.0 s		20.5 q		127.4 s
8	73.2 d				139.9 d
9	36.5 t				15.7 q
10	74.9 d				20.5 q

References

1. Y. Zhu, L. Yang, Z.-J. Jia, J. Nat. Prod. **62**, 1479 (1999)

2β-Acetoxy-1β,8-diangeloyloxy-4α,10-dichloro-3β,11-dihydroxy-bisabol-7(14)-ene

CAS Registry Number: 250725-67-8



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Cremanthodium discoideum* Maxim. [1]

$C_{27}H_{40}O_8Cl_2$: 562.2100

Mp: colorless gum [1]

$[\alpha]_D^{20}$ −67.8° (*c* 0.05, $CHCl_3$) [1]

IR: 3561, 3510, 1744, 1231, 1719, 1646, 846, 734 [1]

EI-MS: 562 $[M]^+$ (0.1), 527 $[M - Cl]^+$ (0.1), 467 (0.39), 465 (2), 463 (3), 462 $[M - C_4H_7COOH]^+$ (2), 427 $[M - Cl - C_4H_7COOH]^+$ (5), 404 $[M - C(OH)Me_2 - C_4H_7COO]^+$ (0.3), 362 $[M - 2 \times C_4H_7COOH]^+$ (0.4), 355 $[M - C(OH)Me_2CHCl - C_4H_7COOH]^+$ (0.1), 304 (2), 303 $[M - C(OH)Me_2 - 2 \times C_4H_7COOH]^+$ (2), 255 $[M - C(OH)Me_2CHCl - 2 \times AngOH]^+$ (0.4), 292 $[M - 2Cl - 2C_4H_7COOH]^+$ (0.1), 83 $[C_4H_7CO]^+$ (100), 59 $[C(OH)Me_2$ or $AcO]^+$ (15), 55 $[83 - CO]^+$ (34), 43 $[CH_3CO]^+$ (21) [1]

FAB-MS: 569 $[M + Li]^+$, 585 $[M + Na]^+$ [1]

HR-FAB-MS: 563.225090 $[M + H]^+$ (calc. for $C_{27}H_{41}O_8Cl_2$: 563.217849) [1]

^{1}H NMR (400 MHz, $CDCl_3$): 1.31 (3H, s, H-13), 1.32 (3H, s, H-12), 1.34 (3H, s, H-15), 1.74 (1H, ddd, J = 15.5; 2.7; 2.6, H-5α), 2.06 (3H, s, OAc-2), 2.09 (1H, m, H-9b), 2.24 (1H, m, H-9a), 2.74 (1H, ddd, J = 15.5; 12.8; 2.7, H-5β), 3.17 (1H, br d, J = 12.8, H-6), 3.57 (1H, dd, J = 11.5; 1.7, H-10), 4.22 (1H, dd, J = 2.7; 2.5, H-4), 5.15 (1H, s, H-14b), 5.21 (1H, d, J = 3.2, H-2), 5.42 (1H, s, H-14a), 5.61 (1H, t, J = 3.2, H-1), 5.68 (1H, dd, J = 10.1; 4.6, H-8); OAng-1: 1.90 (3H, dq, J = 1.6; 1.5, H-5′), 1.94 (3H, dq, J = 7.4; 1.5, H-4′), 6.10 (1H, qq, J = 7.4; 1.6, H-3′); OAng-8: 1.95 (3H, dq, J = 1.6; 1.6, H-5″), 2.00 (3H, dq, J = 7.4; 1.6, H-4″), 6.14 (1H, qq, J = 7.4; 1.6, H-3″) [1]

^{13}C NMR [1]:

Table 1

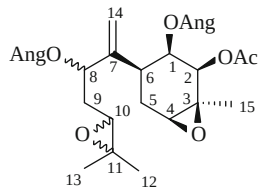
C-1	70.6 d	C-11	72.4 s	OAng-1	165.5 s
2	70.8 d	12	26.1 q	OAng-8	126.5 s
3	74.1 s	13	25.6 q		139.5 d
4	64.5 d	14	119.1 t		15.7 q
5	30.4 t	15	23.8 q		20.5 q
6	33.6 d	OAc-2	169.6 s		166.4 s
7	142.4 s		20.6 q		127.6 s
8	76.3 d				139.5 d
9	35.5 t				15.9 q
10	69.0 d				20.8 q

References

1. Y. Zhu, L. Yang, Z.-J. Jia, J. Nat. Prod. **62**, 1479 (1999)

2β-Acetoxy-1β,8-diangeloyloxy-3β,4β,10,11-diepoxy-6α(H)-bisabol-7(14)-ene

CAS Registry Number: 69940-48-3



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Senecio oxyriifolius* DC. [1]

$C_{27}H_{38}O_8$: 490.2567

Mp: colorless oil [1]

$[\alpha]_D^{25}$ −26.1° (*c* 0.62, $CHCl_3$) [1]

UV (EtOH) 214 [1]

IR (CCl_4): 1750, 1720, 1660, 1240 [1]

MS: 490.257 $[M]^+$ (0.5) ($C_{27}H_{38}O_8$), 430 (1), 390 (4), 290 (2), 83 (100) [1]

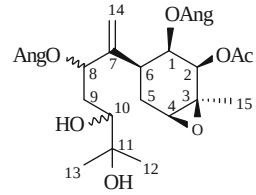
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.28 (6H, s, H-12, H-13), 1.32 (3H, s, H-15), 2.0 (2H, m, H-5), 2.0 (2H, m, H-9), 2.06 (3H, s, OAc), 2.48 (1H, br dd, J = 12, H-6α), 2.75 (1H, dd, J = 6.5; 5, H-10), 3.21 (1H, d, J = 5, H-4α), 5.04 (1H, s, H-14b), 5.24 (1H, s, H-14a), 5.27 (1H, d, J = 4.5, H-2α), 5.36 (1H, dd, J = 7.5; 6, H-8), 5.38 (1H, br d, J = 4.5, H-1α); OAng-5: 1.93 (3H, dq, J = 1.6; 1.6, H-5′), 1.99 (3H, dq, J = 7; 1.6, H-4′), 6.11 (1H, qq, J = 7; 1.6, H-3′); OAng-8: 1.92 (3H, dq, J = 1.6; 1.6, H-5″), 1.99 (3H, dq, J = 7; 1.6, H-4″), 6.05 (1H, qq, J = 7; 1.6, H-3″) [1]

^{1}H NMR (270 MHz, C_6D_6, TMS): 0.97 (3H, s, H-15), 1.11 (3H, s, H-13), 1.18 (3H, s, H-12), 1.77 (1H, s, OAc), 1.8 (2H, m, H-5), 2.0 (2H, m, H-9), 2.39 (1H, br dd, J = 12, H-6α), 2.65 (1H, dd, J = 6.5; 5, H-10), 2.68 (1H, d, J = 5, H-4α), 5.03 (1H, s, H-14b), 5.18 (1H, s, H-14a), 5.33 (1H, dd, J = 4.5; 6, H-2α), 5.55 (1H, dd, J = 7.5; 6, H-8), 5.72 (1H, br d, J = >1, H-1α); OAng-5: 2.02 (6H, br s, H-4′, H-5′), 5.78 (1H, qq, J = 7; 1.6, H-3′); OAng-8: 1.98 (3H, dq, J = 1.6; 1.6, H-5″), 2.02 (3H, dq, J = 7; 1.6, H-4″), 5.75 (1H, qq, J = 7; 1.6, H-3″) [1]

References

1. F. Bohlmann, C. Zdero, Phytochemistry **17**(9), 1669 (1978)

2β-Acetoxy-1β,8-diangeloyloxy-3β,4β-epoxy-10,11-dihydroxy-6α(H)-bisabol-7(14)-ene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Cremanthodium discoideum* Maxim. [1]

Mp: colorless gum [1]

$C_{27}H_{40}O_9$: 508.2672

$[\alpha]_D^{20}$ −69° (*c* 1.0, $CHCl_3$) [1]

IR: (KBr): 3497, 1746, 1231, 1717, 1648, 854 [1]

MS: 509.2671 $[M + H]^+$ ($C_{27}H_{41}O_9$ requires $[M + H]^+$, 509.2750) [1]

EI-MS: 508 $[M]^+$ (0.05), 490 (0.2), 449 (0.6), 408 (0.2), 390 (2), 349 (2), 308 (0.4), 249 (3), (100), 55 (44), 43 (30) [1]

^{1}H NMR (400 MHz, $CDCl_3$): 1.26 (3H, s, H-15), 1.51 (1H, m, H-9b), 1.53 (3H, s, H-13), 1.54 (3H, s, H-12), 2.05 (3H, s, OAc), 2.09 (1H, ddd, J = 14.8; 11.3; 3.4, H-9a), 2.12 (1H, m, H-5α), 2.14 (1H, m, H-5β), 2.60 (1H, br dd, J = 12; 1.2, H-6), 2.84 (1H, br s, OH-10), 3.19 (1H, br d, J = 3.4, H-4), 3.51 (1H, dd, J = 10.2; 3.4, H-10), 4.94 (1H, s, H-14b), 5.18 (1H, s, H-14a), 5.28 (1H, d, J = 4.2, H-2), 5.31 (1H, d, J = 10.2, H-8), 5.43 (1H, dd, J = 4.2; 1.2, H-1); OAng-1*: 1.87 (3H, dq, J = 1.2, H-5′), 1.97 (3H, dq, J = 7.0; 1.2, H-4′), 6.07 (1H, qq, J = 7.0; 1.2, H-3′); OAng-8*: 1.87 (3H, dq, J = 1.2, H-5″),

1.97 (3H, dq, J = 7.0; 1.2, H-4″), 6.08 (1H, qq, J = 7.0; 1.2, H-3″); * - Assignments bearing this superscript may be interchanged [1]

^{13}C NMR (100.6 MHz, $CDCl_3$) [1]:

Table 1

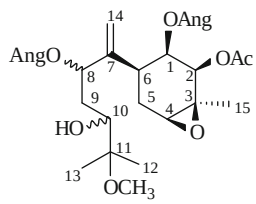
C-1	67.4	C-9	37.4	OAng-1	167.3
2	72.4	10	75.3	OAng-8	127.4
3	56.2	11	73.8		138.7
4	59.5	12	28.3		15.7
5	25.1	13	28.1		20.5
6	39.2	14	113.6		167.3
7	147.7	15	19.3		127.6
8	73.2	OAc	170.3		138.9
			20.6		15.7
					20.6

Pharm./Biol.: Antibacterial activity against *Bacillus aeruginosus* and *B. subtilis*; showed significant activity against two tumor cell lines: human promyelocytic leukemia cell HL-60 and human hapatoma cell SMMC-7721 [1]

References

1. Y. Zhu, Q.-X. Zhu, Z.-J. Jia, Aust. J. Chem. **53**, 831 (2000)

2β-Acetoxy-1β,8-diangeloyloxy-3β,4β-epoxy-10-hydroxy-11-methoxy-bisabol-7(14)-ene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Cremanthodium discoideum* Maxim. [1]

$C_{28}H_{42}O_9$: 522.2829

Mp: colorless gum [1]

$[\alpha]_D^{20}$ −84.3° (*c* 1.0, $CHCl_3$) [1]

IR (KBr): 3514, 1747, 1230, 1717, 1648, 860 [1]

MS: 545.2798 $[M + Na]^+$ ($C_{28}H_{42}O_9Na$, requires $[M + Na]^+$, 545.2727), 529 $[M + Li]^+$, 545 $[M + Na]^+$ [1]

EI-MS: 522 $[M]^+$ (0.02), 507 (0.3), 449 (1.6), 422 (1), 391(1.4), 349 (6), 322 (0.4), 249 (3), 83 (55), 73 (100), 55(29), 43 (20) [1]

^{1}H NMR (400 MHz, $CDCl_3$): 1.12 (3H, s, H-13), 1.13 (3H, s, H-12), 1.31 (3H, s, H-15), 1.54 (1H, ddd, J = 14.4; 10.4; 2.2, H-9a), 1.82 (1H, ddd, J = 14.4; 11.3; 2.5, H-9b), 2.01 (3H, s, OAc), 2.16 (1H, ddd, J = 14.4; 6.0; 3.1, H-5α), 2.17 (1H, ddd, J = 14.4; 11.6; 4.0, H-5β), 2.52 (1H, ddd, J = 1.6; 6.0; 1.2, H-6), 2.69 (1H, br s, OH-10), 3.20 (1H, dd, J = 4.0; 3.1, H-4), 3.21 (3H, s, OCH_3), 3.47 (1H, dd, J = 10.4; 2.5, H-10), 4.94 (1H, s, H-14b), 5.17 (1H, s, H-14a), 5.28 (1H, d, J = 4.4, H-2), 5.36 (1H, dd, J = 10.4; 2.2, H-8), 5.43 (1H, dd, J = 4.3;1.2, H-1); OAng-1*: 1.90 (3H, dq, J = 1.4, H-5′), 1.99 (3H, dq, J = 7.4; 1.4, H-4′), 6.07 (1H, qq, J = 7.4; 1.4, H-3′); OAng-8*: 1.90 (1H, dq, J = 1.4, H-5″), 1.99 (3H, dq, J = 7.4; 1.4, H-4″), 6.08 (1H, qq, J = 7.4; 1.4, H-3″); * - Assignments bearing this superscript may be interchanged [1]

^{13}C NMR (100.6 MHz, $CDCl_3$) [1]:

Table 1

C-1	67.8	C-9	36.7	OAng-1	167.3
2	72.5	10	73.7[a]	OAng-8	127.6
3	56.3	11	76.9		138.4
4	59.8	12	19.6		15.8
5	25.7	13	19.4		20.6
6	38.8	14	113.3		167.3
7	147.8	15	20.4		127.8

(*continued*)

Table 1 (continued)

8	73.2[a]	OAc	49.2	138.7
			170.4	15.8
			20.7	20.7

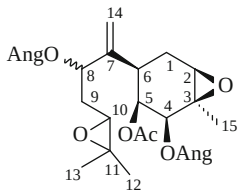
[a]Assignments bearing this superscript may be interchanged [1]

Pharm./Biol.: Antibacterial activity against *Bacillus aeruginosus* and *B. subtilis*; showed significant activity against two tumour cell lines: human promyelocytic leukemia cell HL-60 and human hapatoma cell SMMC-7721 [1]

References

1. Y. Zhu, Q.-X. Zhu, Z.-J. Jia, Aust. J. Chem. **53**, 831 (2000)

5β-Acetoxy-4β,8-diangeloyloxy-2β,3β;10,11-diepoxy-bisabol-7(14)-ene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Ligularia songarica* (Fisch.) Ling [1]

$C_{27}H_{38}O_8$: 490.2567

Mp: 90–90.5° C [1]

$[\alpha]_D^{25}$ −17.6° ($CHCl_3$, *c* 0.5) [1]

IR: 1744, 1717, 1650, 857 [1]

MS: 491 $[M + H]^+$ [1]

FAB-MS: 391 $[M + H - AngOH]^+$, 291 $[M + H - 2 \times AngOH]^+$, 231 $[291 - AcOH]^+$, 83 $[C_4H_7CO]^+$ [1]

^{1}H NMR (400 MHz, $CDCl_3$): 1.26 (3H, s, H-12), 1.26 (3H, s, H-13), 1.28 (3H, s, H-15), 1.83 (1H, m, H-9b), 1.98 (1H, m, H-1α), 2.01 (3H, s, OAc), 2.02 (1H, m, H-9a), 2.17 (1H, dd, J = 15.2; 12.5, H-1β), 2.45 (1H, dddd, J = 12.5; 4.0; 2.4, H-6), 2.71 (1H, dd, J = 6.6; 5.2, H-10), 3.17 (1H, brd, J = 5.2, H-2), 5.04 (1H, brs, H-14b), 5.23 (1H, br s, H-14a), 5.30 (1H, br dd, J = 4.8; 2.4, H-5), 5.35 (1H, d, J = 4.8, H-4), 5.38 (1H, dd, J = 11.6; 2.2, H-8); 2 × OAng: 1.95 and 1.83 (each 3H, dq, J = 1.5; 1.2, H-5′, H-5″), 1.98 and 1.88 (each 3H, dq, J = 7.6; 1.5, H-4′, H-4″), 6.10 and 6.06 (each 1H, qq, J = 7.6; 1. 2, H-3′, H-3″) [1]

^{13}C NMR (100 MHz, $CDCl_3$) [1]:

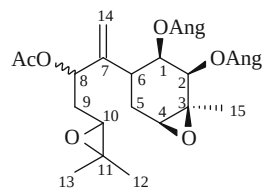
Table 1

C-1	25.7	10	60.7	2 × OAng	166.7
2	59.5	11	58.1		127.2
3	56.5	12	24.6		127.4
4	71.8	13	24.6		139.1
5	68.3	14	115.4		139.2
6	37.9	15	18.9		15.7
7	145.9	OAc	170.1		19.5
8	74.6	2 × OAng	20.4		20.5
9	33.4		166.6		20.8

References

1. B. Fu, X.-P. Yang, J. Wang, Z.-J. Jia, Chin. Chem. Lett. **10**, 29 (1999)

8-Acetoxy-1β,2β-diangeloyloxy-3β,4β;10,11-diepoxy-bisabol-7(14)-ene



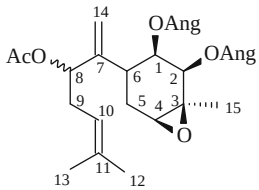
Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Senecio fulgens* G. Nicholson [1]
$C_{27}H_{38}O_8$: 490.2567

References

1. F. Bohlmann, J. Ziesche, Phytochemistry **20**(3), 469 (1981)

8-Acetoxy-1β,2β-diangeloyloxy-3β,4β-epoxy-bisabola-7(14),10-diene

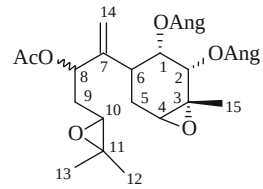


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters
Biological sources: *Senecio fulgens* G. Nicholson [1]
$C_{27}H_{38}O_7$: 474.2618
Mp: colorless oil [1]
$[\alpha]^{24}$ (λ, nm): −15.8° (589), −16.7° (578), −20.0° (546), −42.5° (436) (*c* 0.12, $CHCl_3$) [1]
IR (CCl_4): 1745, 1720, 1655, 1250 [1]
MS: 474.262 $[M]^+$ (7) ($C_{27}H_{38}O_7$), 405 (7), 374 (46), 314 (3), 214 (1), 83 (100) [1]
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.32 (3H, s, H-15), 1.64 (3H, br s, H-13), 1.70 (3H, br s, H-12), 2.0 (2H, m, H-9), 2.45 (1H, br dd, J = 12; 7, H-6), 3.19 (1H, d, J = 5, H-4), 5.02 (1H, br s, H-14b), 5.04 (1H, br t, J = 7, H-10), 5.16 (1H, dd, J = 6; 8, H-8), 5.20 (1H, br s, H-14a), 5.33 (1H, br dd, J = 4; 4, H-1), 5.36 (1H, d, J = 4, H-2); 2 × OAng: 1.91 and 1.89 (each 3H, dq, J = 1.5; 1.5, H-5′, H-5″), 2.01 and 1.98 (each 3H, dq, J = 7; 1.5, H-4′, H-4″), 6.11 and 6.06 (each 1H, qq, J = 7; 1.5, H-3′, H-3″) [1]

References

1. F. Bohlmann, J. Ziesche, Phytochemistry **20**(3), 469 (1981)

8-Acetoxy-1α,2α-diangeloyloxy-3α,4;10,11-diepoxy-bisabol-7(14)-ene

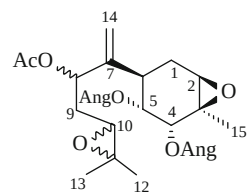


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters
Biological sources: *Notonia hildebrandtii* Vatke [1]; *Senecio fulgens* G. Nicholson [2]
$C_{27}H_{38}O_8$: 490.2567
The data of its compound may be analogous with the 8-acetoxy-4α,5α-diangeloyloxy-2β,3β:10,11-diepoxy-2,3,10,11-tetrahydro-β-bisabol-7(14)-ene from [3]
C-15 is α-position in [2]

References

1. F. Bohlmann, J. Ziesche, Phytochemistry **18**(9), 1489 (1979)
2. F. Bohlmann, J. Ziesche, Phytochemistry **20**(3), 469 (1981)
3. F. Bohlmann, P.K. Mahanta, Phytochemistry **18**(4), 678 (1979)

8-Acetoxy-4α,5α-diangeloyloxy-2β,3β:10,11-diepoxy-2,3,10,11-tetrahydro-β-bisabol-7(14)-ene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Senecio coccineiflorus* Rowley [1]

$C_{27}H_{38}O_8$: 490.2567

Mp: colorless oil [1]

$[\alpha]^{24}$ (λ, nm): −37.2° (589), −37.5° (578), −42.0° (546), −122.5° (436) (*c* 1.3, $CHCl_3$) [1]

IR (CCl_4): 1750, 1745, 1650 [1]

MS: 490.257 $[M]^+$ (0.2) (calc. for $C_{27}H_{38}O_8$: 490.257), 391 (1), 390 (0.5), 330 (0.5), 231 (5), 83 (100), 55 (95), 43 (90) [1]

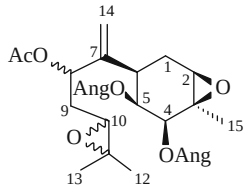
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.26 (6H, s, H-12, H-13), 1.29 (3H, s, H-15), 2.0 (1H, m, H-1α), 2.0 (2H, m, H-9), 2.01 (3H, s, OAc), 2.13 (1H, dd, J = 12; 14, H-1β), 2.48 (1H, dd, J = ∼1; 12, H-6), 2.75 (1H, dd, J = 6.5; 4.5, H-10), 3.19 (1H, d, J = 5, H-2), 5.07 (1H, s, H-14b), 5.26 (1H, s, H-14a), 5.34 (2H, m, H-4, H-5), 5.35 (1H, dd, J = 6.5; 7.5, H-8); 2 × OAng: 1.92 and 1.87 (each 3H, dq, J = 1.5; 1.5, H-5′, H-5″), 1.99 (6H, dq, J = 7; 4.5, H-4′, H-4″), 6.10 (2H, qq, J = 7; 1.5, H-3′, H-3″) [1]

^{1}H NMR (270 MHz, C_6D_6, TMS): 1.16 (3H, s, H-13), 1.17 (3H, s, H-12), 1.22 (3H, s, H-15), 1.84 (3H, s, OAc), 2.08 (1H, m, H-1α), 2.1−1.9 (2H, m, H-9), 2.20 (1H, dd, J = 12; 14, H-1β), 2.43 (1H, dd, J = ∼1; 12, H-6), 2.71 (1H, dd, J = 6.5; 4.5, H-10), 2.74 (1H, d, J = 5, H-2), 5.04 (1H, s, H-14b), 5.23 (1H, s, H-14a), 5.48 (1H, d, J = 4.5, H-4), 5.63 (1H, dd, J = 6.5; 7.5, H-8), 5.72 (1H, br d, J = 4.5, H-5); 2 × OAng: 2.08 and 1.95 (each 3H, dq, J = 1.5; 1.5, H-5′, H-5″), 2.08 (6H, dq, J = 7; 4.5, H-4′, H-4″), 5.82 and 5.79 (each 1H, qq, J = 7; 1.5, H-3′, H-3″) [1]

References

1. F. Bohlmann, P.K. Mahanta, Phytochemistry **18**(4), 678 (1979)

8-Acetoxy-4β,5β-diangeloyloxy-2β,3β:10,11-diepoxy-2,3,10,11-tetrahydro-β-bisabol-7(14)-ene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Senecio coccineiflorus* Rowley [1]

$C_{27}H_{38}O_8$: 490.2567

Mp: colorless oil [1]

$[\alpha]^{24}$ (λ, nm): −10° (589), −12.5° (578), −13° (546), −22.6° (436) (*c* 0.7, $CHCl_3$) [1]

IR (CCl_4): 1750, 1745, 1650 [1]

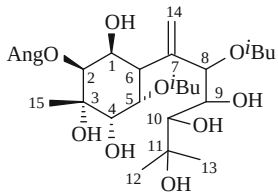
MS: 490.257 $[M]^+$ (1) (calc. for $C_{27}H_{38}O_8$: 490.257), 391 (7), 390 (1), 330 (2), 315 (2), 83 (100), 55 (61), 43 (31) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.26 (6H, s, H-12, H-13), 1.28 (3H, s, H-15), 2.0 (1H, m, H-1α), 2.0 (2H, m, H-9), 2.14 (3H, s, OAc), 2.18 (1H, dd, J = 12; 14, H-1β), 2.57 (1H, dd, J = 2.5; 12, H-6), 2.79 (1H, dd, J = 6.5; 4.5, H-10), 3.18 (1H, d, J = 5, H-2), 4.97 (1H, dd, J = 2.5; ∼1, H-5), 5.05 (1H, s, H-14b), 5.27 (1H, s, H-14a), 5.33 (1H, br d, J = 2.5, H-4), 5.49 (1H, dd, J = 8; 5, H-8); 2 × OAng: 1.90 and 1.88 (each 3H, dq, J = 1.5; 1.5, H-5′, H-5″), 2.00 (6H, dq, J = 7; 4.5, H-4′, H-4″), 6.11 and 6.08 (each 1H, qq, J = 7; 1.5, H-3′, H-3″) [1]

References

1. F. Bohlmann, P.K. Mahanta, Phytochemistry **18**(4), 678 (1979)

2β-Angeloyloxy-5α,8-diisobutyroyloxy-1β,3α,4α,9,10,11-hexahydroxy-bisabol-7(14)-ene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Cremanthodium ellisii* (Hook. f.) Kitam. [1]

$C_{28}H_{46}O_{12}$: 574.2989

Mp: white powder [1]

$[\alpha]_D^{25}$ −88° (*c* 0.08, $CHCl_3$) [1]

IR (KBr): 3479, 3076, 2976, 2936, 2878, 1716, 1645, 1463, 1385, 1359, 1229, 1201, 1153, 1087, 923, 847 [1]

EI-MS: 556 $[M - H_2O]^+$ (2), 538 (3), 468 (15), 246 (11), 205 (10), 179 (16), 151 (7), 137 (7), 123 (24), 83 (100), 71 (80), 55 (31), 43 (48) [1]

HR-EI-MS: 468.2343 $[M - H_2O$ − isobutyric acid$]^+$ ($C_{24}H_{36}O_9$, requires 468.2359) [1]

^{1}H NMR: 1.13 (3H, s, H-12), 1.14 (3H, s, H-13), 1.25 (3H, s, H-15), 2.84 (1H, dd, J = 2.8; 11.5, H-6), 4.12 (1H, d, J = 4.9, H-10), 4.12 (1H, d, J = 4.9, H-4), 4.70 (1H, dd, J = 3.0; 1.4, H-1), 4.80 (1H, t, J = 5.0, H-9), 4.95 (1H, d, J = 4.8, H-8), 5.07 (1H, s, H-14a), 5.27 (1H, s, H-14b), 5.36 (1H, d, J = 2.7, H-2), 5.36 (1H, dd, J = 2.8; 4.9, H-5); OAng: 1.94 (3H, br s, H-5′), 2.03 (3H, dq, J = 7.2; 1.3, H-4′), 6.14 (1H, qq, J = 7.2; 1.3, H-3′); 2 × O^{i}Bu: 1.20 (6H, d, J = 6.9, H-3″, H-4″) [1]

^{13}C NMR [1]:

Table 1

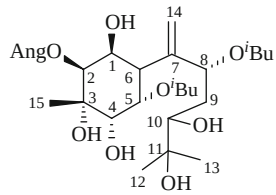
C-1	64.9	C-11	72.1	2 × O^{i}Bu	177.3
2	74.4	12	25.7		176.7
3	72.8	13	25.9		34.1
4	71.4	14	23.9		34.1
5	76.2	15	117.7		19.1
6	41.2	OAng	167.0		19.0
7	144.3		15.8		18.9
8	75.5		20.5		18.7
9	73.2		127.3		
10	71.9		138.9		

References

1. H. Chen, Y. Zhu, X.-M. Shen, Z.-J. Jia, J. Nat. Prod. **59**, 1117 (1996)

2β-Angeloyloxy-5α,8-diisobutyroyloxy-1β,3α,4α,10,11-pentahydroxy-bisabol-7(14)-ene

CAS Registry Number: 184650-18-8



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Cremanthodium ellisii* (Hook. f.) Kitam. [1]

$C_{28}H_{46}O_{11}$: 558.3040

Mp: 179–180°C (*n*-hexane – EtOAc) [1]

$[\alpha]_D^{25}$ −80° (*c* 0.20, $CHCl_3$) [1]

IR (KBr): 3463, 3076, 2976, 2936, 2878, 1716, 1649, 1463, 1385, 1359, 1229, 1201, 1153, 1087, 923, 847 [1]

EI-MS: 540 $[M - H_2O]^+$ (1), 525 (1), 452 (16), 434 (8), 367 (8), 334 (3), 246 (11), 205 (9), 179 (15), 151 (8), 137 (7), 123 (23), 83 (100), 71 (70), 55 (30), 43 (47) [1]

HR-EI-MS: 452.2453 $[M - H_2O$ – isobutyric acid$]^+$ ($C_{24}H_{36}O_8$, require 452.2410) [1]

^{1}H NMR: 1.11 (3H, s, H-12), 1.13 (3H, s, H-13), 1.28 (3H, s, H-15), 1.88 (1H, m, H-9a), 1.99 (1H, m, H-9b), 2.93 (1H, dd, J = 2.8; 11.7, H-6), 3.79 (1H, d, J = 4.7, H-4), 4.23 (2H, dd, J = 5.1; 9.7, H-10), 4.56 (1H, dd, J = 2.8; 11.7, H-1), 4.76 (1H, dd, J = 1.8; 9.4, H-8), 5.11 (1H, s, H-14a), 5.21 (1H, s, H-14b), 5.44 (1H, dd, J = 2.8; 4.7, H-5), 5.45 (1H, d, J = 2.8, H-2); OAng: 1.92 (3H, br s, H-5′), 2.00 (3H, dq, J = 7.3; 1.3, H-4′), 6.14 (1H, qq, J = 7.3; 1.3, H-3′); 2 × O^{i}Bu: 1.16 (3H, d, J = 7.0, H-3″), 1.19 (3H, d, J = 6.8, H-4″) [1]

^{13}C NMR [1]:

Table 1

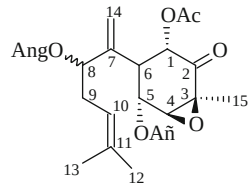
C-1	64.8	C-9	34.1	2 × O^{i}Bu	177.9 (C8-OCO)
2	74.7	10	75.4		175.2
3	74.3	11	72.0		34.4
4	70.3	12	24.7		34.4
5	76.4	13	26.1		19.1
6	39.9	14	23.3		19.1
7	143.9	15	117.2		19.0
8	75.9				18.8

X-ray [1]

References

1. H. Chen, Y. Zhu, X.-M. Shen, Z.-J. Jia, J. Nat. Prod. **59**, 1117 (1996)

1α,5α-Diacetoxy-8-angeloyloxy-3β,4β-epoxy-bisabola-7(14),10-dien-2-one



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Tussilago farfara* L. [1]

$C_{27}H_{36}O_8$: 488.2410

Mp: colorless oil [1]

$[\alpha]_D$ +4.64° (*c* 0.22, $CHCl_3$) [1]

UV (EtOH): 203.4 (4.20) [1]

IR ($CHCl_3$): 2624, 1736, 1650, 1228 [1]

CI-MS: 489 $[M + 1]^+$ [1]

EI-MS: 488 $[M]^+$ [1]

HR-CI-MS: 489.2169 $[M + 1]^+$ (calc. for $C_{24}H_{33}O_8$, 489.2175) [1]

^{1}H NMR (400 MHz, $CDCl_3$): 1.48 (3H, s, H-15), 1.62 (3H, br s, H-12), 1.68 (3H, br s, H-13), 2.06 (3H, s, OAc-1), 2.15 (3H, s, OAc-5), 2.33 (2H, m, H-9), 2.87 (1H, dd, J = 12.77; 8.67, H-6), 3.40 (1H, s, H-4), 5.04 (1H, br t, J = 7.22, H-10), 5.23 (1H, dd, J = 7.78; 4.32, H-8), 5.24 (1H, s, H-14b), 5.33 (1H, s, H-14a), 5.35 (1H, d, J = 8.67, H-5), 5.68 (1H, d, J = 12.77, H-1); OAng: 1.89 (3H, dq, J = 1.59; 1.49, H-5′), 1.97 (3H, dq, J = 7.11; 1.49, H-4′), 6.08 (1H, qq, J = 7.11; 1.59, H-3′) [1]

^{13}C NMR (100 MHz, $CDCl_3$) [1]:

Table 1

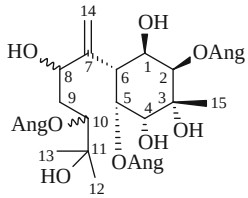
C-1	72.9 d	C-9	32.3 t	C-2′	128.2 s
2	199.9 s	10	119.4 d	3′	139.0 t
3	61.8 s	11	134.9 s	4′	21.0 q
4	66.1 d	12	26.1 q	5′	21.2 q
5	73.0 d	13	18.4 q	1-OAc: 1″	169.9 s
6	48.9 d	14	114.4 t	2″	16.1 q
7	146.1 s	15	14.8 q	5-OAc: 1‴	170.4 s
8	75.3 d	OAng: 1′	166.9 s	2‴	20.7 q

Pharm./Biol.: Showed inhibition of nitric oxide synthesis in lipopolysaccharide-activated macrophages [1]

References

1. J.-H. Ryu, Y.S. Jeong, D.H. Sohn, J. Nat. Prod. **62**, 1437 (1999)

2β,5α,10-Triangeloyloxy-6β(H)-bisabol-7(14)-ene-1β,3α,4α,8,11-pentaol ((6α,1β,2β,3*R**,4α,5α)-2,5,10-*Tris*[(angeloyl)oxy]-bisabol-7(14)-ene-1,3,4,8,11-pentol)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Ligularia lankongensis* (Franch.) Hand.-Mazz. [1]

$C_{30}H_{46}O_{11}$: 582.3040

Mp: 139.0–140.98°C, colorless crystals [1]

$[\alpha]_D^{20}$ −16.0° (*c* 0.16, MeOH) [1]

IR (KBr): 3470, 2980, 2956, 2930, 1719, 1696, 1647, 1239, 1162, 1046, 917, 851, 766 [1]

FAB-MS (+): 583 $[M + 1]^+$ (53) [1]

HR-ESI-MS: 605.2950 $[M + Na]^+$ ($[C_{30}H_{46}NaO_{11}]^+$ calc. 605.2938) [1]

^{1}H NMR (500 MHz, CD_3OD): 1.32 (3H, s, H-13), 1.32 (3H, s, H-12), 1.41 (3H, s, H-15), 2.20 (1H, m, H-9a), 2.13 (1H, m, H-9b), 3.19 (1H, dd, J = 11.8; 2.7, H-6), 3.95 (1H, d, J = 3.9, H-4), 4.36 (1H, dd, J = 8.6; 5.4, H-8), 4.75 (1H, dd, J = 11.8; 3.0, H-1), 5.16 (1H, dd, J = 9.7, 2.0, H-10), 5.32 (1H, s, H-14a), 5.21 (1H, s, H-14b), 5.55 (1H, d, J = 3.0, H-2), 5.72 (1H, dd, J = 3.9; 2.7, H-5); 3 × OAng: 2.16 (9H, H-5′, H-5″, H-5‴), 2.19 (9H, H-4′, H-4″, H-4‴), 6.30 (3H, H-3′, H-3″, H-3‴) [1]

^{13}C NMR (125 MHz, CD_3OD) [1]:

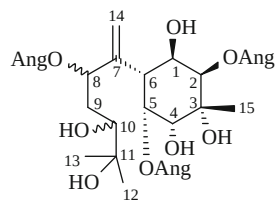
Table 1

C-1	66.5 d	C-11	73.0 s	C-1″	169.7 s
2	79.1 d	12	27.2 q	2″	138.9 s
3	75.5 s	13	25.6 q	3″	129.5 d
4	72.2 d	14	116.5 t	4″	16.3 q
5	76.1 d	15	24.3 q	5″	21.1 q
6	42.0 d	1′	168.7 s	1‴	169.5 s
7	146.9 s	2′	140.1 s	2‴	140.4 s
8	76.5 d	3′	129.8 d	3‴	129.4 d
9	36.3 t	4′	16.5 q	4‴	16.3 q
10	78.1 d	5′	21.4 q	5‴	21.2 q

References

1. A.-M. Tan, H.-P. He, M. Zhang, Z.-T. Wang, X.-J. Hao, Helv. Chim. Acta **90**, 101 (2007)

2β,5α,8-Triangeloyloxy-6β(H)-bisabol-7(14)-ene-1β,3α,4α,10,11-pentaol ((6α,1β,2β,3*R**,4α,5α)-2,5,8-*Tris*[(angeloyl)oxy]-bisabol-7(14)-ene-1,3,4,10,11-pentol)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Ligularia lankongensis* (Franch.) Hand.-Mazz. [1]

$C_{30}H_{46}O_{11}$: 582.3040

Mp: colorless gum [1]

$[\alpha]_D^{20}$ −18.37° (*c* 0.78, MeOH) [1]

IR (KBr): 3424, 2934, 1718, 1647, 1233, 1153, 1085, 931, 760 [1]

FAB-MS (+): 583 $[M + 1]^+$ (2) [1]

FAB-MS (−): 581 $[M - 1]^-$ [1]

HR-ESI-MS: 605.2924 $[M + Na]^+$ ($[C_{30}H_{46}NaO_{11}]^+$, calc. 605.2938) [1]

^{1}H NMR (500 MHz, CD_3OD): 1.31 (3H, s, H-12), 1.34 (3H, s, H-13), 1.39 (3H, s, H-15), 2.21 (1H, m, H-9a), 1.87 (1H, m, H-9b), 3.19 (1H, dd, J = 11.7; 2.6, H-6), 3.55 (1H, dd, J = 10.5; 1.4, H-10), 3.89 (1H, d, J = 3.9, H-4), 4.74 (1H, dd, J = 11.7; 2.9, H-1), 5.53 (1H, s, H-14a), 5.29 (1H, s, H-14b), 5.55 (1H, d, J = 2.9, H-2), 5.68 (1H, dd, J = 3.9; 2.6, H-5), 5.79 (1H, dd, J = 9.8; 3.7, H-8); 3 × OAng: 2.13 (9H, H-5′, H-5″, H-5‴), 2.21 (9H, H-4′, H-4″, H-4‴), 6.28 (1H, H-3‴), 6.36 (2H, H-3′, H-3″) [1]

^{13}C NMR (125 MHz, CD_3OD) [1]:

Table 1

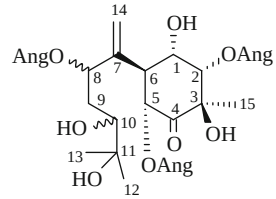
C-1	66.9 d	C-11	73.8 s	C-1″	168.5 s
2	78.8 d	12	25.4 q	2″	139.7 s
3	75.5 s	13	25.7 q	3″	129.4 d
4	72.4 d	14	117.0 t	4″	16.2 q
5	74.2 d	15	24.3 q	5″	21.2 q
6	43.6 d	1′	168.6 s	1‴	168.9 s
7	144.9 s	2′	139.8 s	2‴	139.9 s
8	77.5 d	3′	129.5 d	3‴	129.5 d
9	37.4 t	4′	16.5 q	4‴	16.5 q
10	76.0 d	5′	21.3 q	5‴	21.4 q

References

1. A.-M. Tan, H.-P. He, M. Zhang, Z.-T. Wang, X.-J. Hao, Helv. Chim. Acta **90**, 101 (2007)

2α,5α,8-Triangeloyloxy-1α,3β,10,11-tetrahydroxy-6α(H)-bisabol-7(14)-en-4-one

CAS Registry Number: 197577-26-7



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Ligularia dentata* (A. Gray) Hara [1]

$C_{30}H_{44}O_{11}$: 580.2884

Mp: colorless gum [1]

$[\alpha]_D^{20}$ +3.2° (*c* 0.51, $CHCl_3$) [1]

IR (film): 3410, 2930, 1720, 1646, 1442, 1382, 1220, 1145, 1042, 997, 849, 772 [1]

FAB-MS: 581 $[M + 1]^+$ (0.5), 563 $[M + 1 - H_2O]^+$ (0.8), 521 $[M + 1 - C_3H_7OH]^+$ (1.5), 463 [563 – $C_4H_7COOH]^+$ (2), 363 [563 – 2 × $C_4H_7COOH]^+$ (2), 263 [563 – 3 × $C_4H_7COOH]^+$ (6), 83 $[C_4H_7CO]^+$ (100) [1]

TLC: benzene – acetone (5:1), R_f 0.48 [1]

^{1}H NMR: 1.33 (3H, s, H-15), 1.52 (3H, s, H-12), 1.57 (3H, s, H-13), 1.81 (1H, m, H-9a), 1.84 (1H, m, H-9b), 2.81 (1H, dd, J = 12.4; 10.5, H-6), 3.66 (1H, dd, J = 10.1; 2.1, H-10), 4.69 (1H, dd, J = 10.5, 2.8, H-1), 5.16 (1H, br d, J = 9.4, H-8), 5.29 (1H, br s, H-14b), 5.33 (1H, br s, H-14a), 5.59 (1H, d, J = 2.8, H-2), 6.12 (1H, d, J = 12.4, H-5); 3 × OAng: 1.86 (3H, dq, J = 1.2; 1.0, H-5′), 1.90 (3H, dq, J = 1.2; 1.0, H-5″), 1.91 (3H, dq, J = 1.2; 1.0, H-5‴), 1.97 (3H, dq, J = 7.0; 1.0, H-4′), 1.98 (3H, dq, J = 7.0; 1.0, H-4″), 2.01 (3H, dq, J = 7.0; 1.0, H-4‴), 6.11 (1H, qq, J = 7.0; 1.2, H-3′), 6.13 (1H, qq, J = 7.0; 1.2, H-3″), 6.20 (1H, qq, J = 7.0; 1.2, H-3‴) [1]

^{13}C NMR [1]:

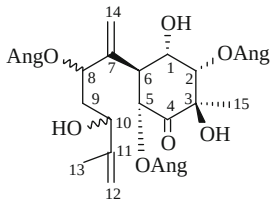
Table 1

C-1	71.6 d	C-12	27.3 q	C-3′	140.9 d
2	77.5 d	13	28.8 q	3″	139.3 d
3	76.0 s	14	111.0 t	3‴	139.2 d
4	202.4 s	15	19.8 q	4′	15.9 q
5	73.2 d	1′	168.0 s	4″	15.9 q
6	47.5 d	1″	167.1 s	4‴	15.8 q
7	147.3 s	1‴	166.5 s	5′	20.5 q
8	74.7 d	2′	127.3 s	5″	20.5 q
9	36.2 t	2″	127.0 s	5‴	20.4 q
10	75.1 d	2‴	126.9 s		
11	74.5 s				

References

1. K. Gao, L. Yang, Z. Jia, Planta Med. **63**, 461 (1997)

2α,5α,8-Triangeloyloxy-1α,3β,10-trihydroxy-6α(H)-bisabola-7(14),11(12)-dien-4-one



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Ligularia dentata* (A. Gray) Hara [1]

$C_{30}H_{42}O_{10}$: 562.2778

Mp: colorless gum [1]

$[\alpha]_D^{20}$ +289.1° (*c* 0.53, $CHCl_3$) [1]

IR (film): 3442, 2930, 1721, 1648, 1457, 1381, 1231, 1146, 1041, 905, 848, 755 [1]

FAB-MS: 563 $[M + 1]^+$ (0.5), 545 $[M + 1 - H_2O]^+$ (0.5), 463 $[M + 1 - C_4H_7COOH]^+$ (10), 445 [545 – $C_4H_7COOH]^+$ (0.5), 363 $[M + 1 - 2 \times C_4H_7COOH]^+$ (5), 345 [545 – 2 × $C_4H_7COOH]^+$ (8), 263 $[M + 1 - 3 \times C_4H_7COOH]^+$ (7), 245 [545 – 3 × $C_4H_7COOH]^+$ (13), 83 $[C_4H_7CO]^+$ (100) [1]

TLC: benzene – acetone (5:1), R_f 0.46 [1]

^{1}H NMR: 1.32 (3H, s, H-15), 1.56 (1H, m, H-9a), 1.71 (3H, s, H-13), 1.80 (1H, m, H-9b), 2.82 (1H, dd, J = 12.3; 10.5, H-6), 4.16 (1H, br d, J = 9.02, H-10), 4.77 (1H, dd, J = 10.5; 2.6, H-1), 4.82 (1H, br s, H-12′), 4.96 (1H, br s, H-12), 5.17 (1H, br d, J = 9.6, H-8), 5.28 (1H, br s, H-14b), 5.33 (1H, br s, H-14a), 5.59 (1H, d, J = 2.6, H-2), 6.10 (1H, d, J = 12.3, H-5); 3 × OAng: 1.86 (3H, dq, J = 1.2; 1.0, H-5′), 1.88 (3H, dq, J = 1.2 1.0, H-5″), 1.92 (3H, dq, J = 1.2; 1.0, H-5‴), 1.92 (3H, dq, J = 7.0; 1.0, H-4′), 1.95 (3H, dq, J = 7.0; 1.0, H-4″), 1.98 (3H, dq, J = 7.0; 1.0, H-4‴), 6.09 (1H, qq, J = 7.0; 1.2, H-3′), 6.09 (1H, qq, J = 7.0; 1.2, H-3″), 6.18 (1H, qq, J = 7.0; 1.2, H-3‴) [1]

^{13}C NMR [1]:

Table 1

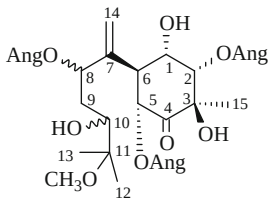
C-1	71.5 d	C-12	110.6 t	C-3′	140.6 d
2	77.5 d	13	18.0 q	3″	139.4 d
3	76.0 s	14	111.2 t	3‴	139.3 d
4	202.5 s	15	19.6 q	4′	15.9 q
5	73.5 d	1′	168.1 s	4″	15.9 q
6	47.6 d	1″	167.2 s	4‴	15.8 q
7	147.3 s	1‴	166.6 s	5′	20.5 q
8	74.6 d	2′	128.3 s	5″	20.5 q
9	39.5 t	2″	127.3 s	5‴	20.4 q
10	71.8 d	2‴	127.0 s		
11	147.2 s				

References

1. K. Gao, L. Yang, Z. Jia, Planta Med. **63**, 461 (1997)

2α,5α,8-Triangeloyloxy-1α,3β,10-trihydroxy-11-methoxy-6α(H)-bisabol-7(14)-en-4-one

CAS Registry Number: 197577-27-8



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Triesters

Biological sources: *Ligularia dentata* (A. Gray) Hara [1]

$C_{31}H_{46}O_{11}$: 594.3040

Mp: colorless gum [1]

$[\alpha]_D^{20}$ +178.5° (*c* 0.56, $CHCl_3$) [1]

IR (film): 3412, 2934, 1720, 1647, 1457, 1382, 1221, 1147, 1042, 997, 850, 772 [1]

FAB-MS: 595 $[M + 1]^+$ (0.8), 577 $[M + 1 - H_2O]^+$ (2.2), 563 $[M + 1 - MeOH]^+$ (2), 521 $[M + 1 - C_3H_7OMe]^+$ (1.5), 495 $[M + 1 - HOAng]^+$ (1.5), 463 $[563 - HOAng]^+$ (10), 395 $[M + 1 - 2 \times HOAng]^+$ (3), 363 $[563 - 2 \times HOAng]^+$ (6), 295 $[M + 1 - 3 \times HOAng]^+$ (2.8), 263 $[563 - 3 \times HOAng]^+$ (4), 83 $[C_4H_7CO]^+$ (100) [1]

TLC: benzene – acetone (5:1), R_f 0.43 [1]

^{1}H NMR: 1.05 (3H, s, H-12), 1.13 (3H, s, H-13), 1.32 (3H, s, H-15), 1.57 (1H, m, H-9a), 1.84 (1H, m, H-9b), 2.83 (1H, dd, J = 12.1; 10.4, H-6), 3.20 (3H, s, OCH_3), 3.56 (1H, br d, J = 10.3, H-10), 4.67 (1H, dd, J = 10.4; 2.8, H-1), 5.14 (1H, br d, J = 10.4, H-8), 5.26 (1H, br s, H-14b), 5.30 (1H, br s, H-14a), 5.59 (1H, d, J = 2.8, H-2), 6.10 (1H, d, J = 12.1, H-5); 3 × OAng: 1.86 (3H, dq, J = 1.3; 1.0, H-5′), 1.91 (3H, dq, J = 1.3; 1.0, H-5″), 1.91 (3H, dq, J = 1.3; 1.0, H-5‴), 1.96 (3H, dq, J = 7.0; 1.0, H-4′), 1.98 (3H, dq, J = 7.0; 1.0, H-4″), 2.00 (3H, dq, J = 7.0; 1.0, H-4‴), 6.08 (1H, qq, J = 7.0; 1.3, H-3′), 6.11 (1H, qq, J = 7.0; 1.3, H-3″), 6.17 (1H, qq, J = 7.0; 1.3, H-3‴) [1]

^{13}C NMR [1]:

Table 1

C-1	71.6 d	C-12	19.0 q	C-3′	140.5 d
2	77.4 d	13	20.4 q	3″	139.2 d
3	76.0 s	14	110.7 t	3‴	139.1 d
4	202.5 s	15	19.7 q	4′	15.9 q
5	73.1 d	1′	168.0 s	4″	15.9 q
6	47.5 d	1″	167.1 s	4‴	15.8 q
7	147.7 s	1‴	166.5 s	5′	20.7 q
8	75.0 d	2′	127.3 s	5″	20.7 q
9	35.8 t	2″	127.0 s	5‴	20.5 q
10	73.3 d	2‴	127.0 s	OCH_3	49.1 q
11	76.7 s				

References

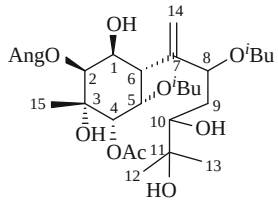
1. K. Gao, L. Yang, Z. Jia, Planta Med. **63**, 461 (1997)

Bisabolanes

Tetraesters

4α-Acetoxy-2β-angeloyloxy-5α,8-diisobutyroyloxy-6β(H)-bisabol-7(14)-ene-1β,3α,10,11-tetraol (4α-Acetyl-2β-angeloyl-5α,8-diisobutyryl-1β,3α,10,11-tetrahydroxy-bisabolene)

CAS Registry Number: 184650-20-2



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Tetraesters

Biological sources: *Cremanthodium ellisii* (Hook. f.) Kitam. [1, 2]

$C_{30}H_{48}O_{12}$: 600.3146

Mp: white powder [1]

$[\alpha]_D^{25}$ −45.5° (*c* 0.17, $CHCl_3$) [1]

IR (KBr): 3484, 3082, 2976, 2935, 2878, 1723, 1649, 1464, 1376, 1229, 1151, 1056, 917, 848 [1]

EI-MS: 582 $[M - H_2O]^+$ (1), 512 (2), 494 (20), 476 (4), 453 (4), 409 (10), 246 (10), 205 (10), 179 (14), 151 97), 123 (30), 83 (100), 71 (99), 55 (58) [1]

HR-EI-MS: 494.2488 $[M - H_2O$ – isobutyric acid$]^+$ ($C_{26}H_{38}O_9$, requires 494.2516) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.13–1.26 (3H, m, H-12), 1.13–1.26 (3H, m, H-13), 1.13–1.26 (3H, m, H-15), 1.65 (1H, m, H-9), 1.95 (1H, m, H-9′), 2.05 (3H, s, OAc), 3.03 (1H, br d, J = 11.6, H-6), 4.04 (1H, br d, J = 9.6, H-10), 4.56 (1H, dd, J = 11.6; 2.7, H-1), 4.93 (1H, dd, J = 9.2; 2.8, H-8), 5.08 (1H, d, J = 2.8, H-4), 5.09 (1H, s, H-14a), 5.26 (1H, s, H-14b), 5.47 (1H, d, J = 2.7, H-2), 5.53 (1H, m, H-5); OAng: 1.13–1.26 (6H, m, H-5′, H-4′), 6.14 (1H, dq, J = 7.2; 1.5, H-3′); 2 × O^{i}Bu: 1.13–1.26 (12H, m, H-3″, H-4″, H-3‴, H-4‴), 2.55–2.64 (2H, m, H-2″, H-2‴) [2]

^{13}C NMR (100 MHz, $CDCl_3$, TMS) [2]:

Table 1

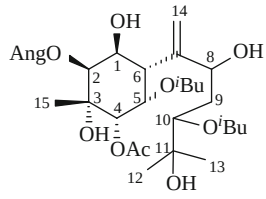
C-1	65.2	C-11	72.0	2 × O^{i}Bu	177.7
2	76.2	12	25.8		176.0
3	74.3	13	25.8		34.2
4	71.7	14	22.9		34.2
5	71.5	15	114.2		18.8
6	41.6	OAng	167.1		18.6
7	145.6		139.3		19.2
8	76.7		127.2		19.0
9	35.5		20.5		
10	71.4		15.9		

References

1. H. Chen, Y. Zhu, X.-M. Shen, Z.-J. Jia, J. Nat. Prod. **59**, 1117 (1996)
2. B.-N. Su, Q.-X. Zhu, Z.-J. Jia, Phytochemistry **53**(8), 1103 (2000)

4α-Acetoxy-2β-angeloyloxy-5α,10-diisobutyroyloxy-6β(H)-bisabol-7(14)-ene-1β,3α,8,11-tetraol (4α-Acetyl-2β-angeloyl-5α,10-diisobutyryl-1β,3α,8,11-tetrahydroxybisabolene)

CAS Registry Number: 184650-19-9



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Tetraesters

Biological sources: *Cremanthodium ellisii* (Hook. f.) Kitam. [1, 2]
$C_{30}H_{48}O_{12}$: 600.3146
Mp: white powder [1]
$[\alpha]_D^{25}$ −41.4° (*c* 0.15, $CHCl_3$) [1]
IR (KBr): 3478, 3089, 2976, 2928, 1728, 1649, 1466, 1376, 1229, 1151, 1059, 919, 848 [1]
EI-MS: 582 $[M - H_2O]^+$ (1), 567 (1), 541 (5), 523 (11), 494 (14), 453 (30), 436 (17), 408 (10), 365 (7), 353 (10), 264 (5), 247 (10), 205 (20), 177 (15), 141 (13), 123 (8), 83 (100), 71 (20), 71 (20), 55 (8) [1]
HR-EI-MS: 494.2491 $[M - H_2O$ – isobutyric acid$]^+$ ($C_{26}H_{38}O_9$, requires 494.2516) [1]
^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.10–1.20 (3H, m, H-12), 1.10–1.20 (3H, m, H-13), 1.10–1.20 (3H, m, H-15), 1.57–1.65 (1H, m, H-9a), 1.81–1.88 (1H, m, H-9b), 2.04 (3H, s, OAc), 3.01 (1H, br d, J = 11.6, H-6), 3.34 (1H, br d, J = 9.2, H-8), 4.65 (1H, dd, J = 11.6; 2.6, H-1), 4.98 (1H, d, J = 3.6, H-4), 5.23 (1H, s, H-14a), 5.37 (1H, t, J = 6.8, H-10), 5.46 (1H, s, H-14b), 5.49 (1H, d, J = 2.6, H-2), 5.54 (1H, m, H-5); OAng: 1.10–1.20 (6H, H-4′, H-5′), 6.13 (1H, dq, J = 7.2; 1.5, H-3′); 2 × O^{i}Bu: 1.10–1.20 (12H, m, H-3″, H-4″, H-3‴, H-4‴), 2.53–2.63 (2H, m, H-2″, H-2‴) [2]
^{13}C NMR (100 MHz, $CDCl_3$, TMS) [2]:

Table 1

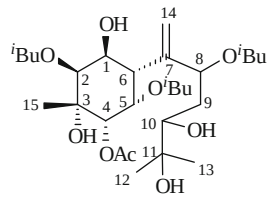
C-1	65.5	C-11	72.6	2 × O^{i}Bu	176.7
2	76.1	12	22.8		175.2
3	74.1	13	25.8		34.1
4	71.7	14	23.1		34.1
5	70.4	15	118.1		18.9
6	40.9	OAng	167.0		18.5
7	141.1		139.1		19.1
8	74.9		127.2		19.0
9	35.4		20.5		
10	77.3		15.8		

References

1. H. Chen, Y. Zhu, X.-M. Shen, Z.-J. Jia, J. Nat. Prod. **59**, 1117 (1996)
2. B.-N. Su, Q.-X. Zhu, Z.-J. Jia, Phytochemistry **53**(8), 1103 (2000)

4α-Acetoxy-2β,5α,8-triisobutyroyloxy-6β(H)-bisabol-7(14)-ene-1β,3α,10,11-tetraol (4α-Acetyl-2β,5α,8-triisobutyryl-1β,3α,10,11-tetrahydroxybisabolene)

CAS Registry Number: 280578-56-5



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Tetraesters
Biological sources: *Cremanthodium ellisii* (Hook. f.) Kitam. [1]
$C_{29}H_{48}O_{12}$: 588.3146
Mp: colorless gum [1]
$[\alpha]_D^{20}$ −47.4° (*c* 0.28, $CHCl_3$) [1]
IR (KBr): 3482, 3088, 2974, 2927, 1727, 1649, 1467, 1375, 1229, 1152, 1058 [1]
EI-MS: 570 $[M - H_2O]^+$ (1.2), 441 (4.7), 424 (2.9), 423 (2.1), 397 (2.0), 353 (4.8), 335 (2.1), 275 (1.4), 265 (4.0), 247 (4.5), 239 (3.0), 223 (4.9), 221 (3.7), 205 (16), 179 (11), 177 (13), 161 (10), 151 (6.3), 141 (13), 133 (5.8), 123 (13), 107 (5.8), 97 (18), 83 (53), 71 (100), 59 (22), 43 (67) [1]
^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.05–1.21 (3H, m, H-13), 1.05–1.21 (3H, m, H-15), 1.05–1.21 (3H, m, H-12), 1.63–1.65 (1H, m, H-9a), 1.85–1.89 (1H, m, H-9b), 2.05 (3H, s, OAc), 2.97 (1H, dd, J = 11.6; 3.5, H-6), 3.34 (1H, br d, J = 9.6, H-10), 4.60 (1H, dd, J = 11.6; 2.9, H-1), 4.98 (1H, d, J = 3.5, H-4), 5.24 (1H, s, H-14a), 5.34 (1H, t, J = 6.2, H-8), 5.36 (1H, d, J = 2.9, H-2), 5.45 (1H, s, H-14b), 5.56 (1H, t, J = 3.5, H-5); 3 × O^{i}Bu: 1.05–1.21 (18H, H-3′, H-4′, H-3″, H-4″, H-3‴, H-4‴) 2.54–2.69 (3H, m, H-2′, H-2″, H-2‴) [1]

^{13}C NMR (100 MHz, $CDCl_3$, TMS) [1]:

Table 1

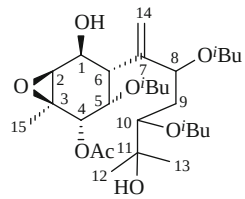
C-1	65.6	C-10	75.0	3 × O^{i}Bu	34.3
2	76.1	11	72.6		34.2
3	74.0	12	23.2		34.2
4	71.7	13	25.9		19.4
5	70.4	14	22.8		19.2
6	40.8	15	118.2		19.1
7	141.1	OAc	169.8		19.0
8	77.5	3 × O^{i}Bu	20.6		18.9
9	35.5		176.9		18.6
			176.4		
			175.2		

References

1. B.-N. Su, Q.-X. Zhu, Z.-J. Jia, Phytochemistry **53**(8), 1103 (2000)

4α-Acetoxy-5α,8,10-triisobutyroyloxy-2β,3β-epoxy-6β(H)-bisabol-7(14)-ene-1β,11-diol (2β,3β-Epoxy-4-acetyl-5α,8,10-triisobutyryl-1,11-dihydroxy-bisabolene)

CAS Registry Number: 280578-55-4



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Bisabolanes – Tetraesters

Biological sources: *Cremanthodium ellisii* (Hook. f.) Kitam. [1]

$C_{29}H_{46}O_{11}$: 570.3040

Mp: colorless gum [1]

$[\alpha]_D^{20}$ −68.4° (*c* 0.25, $CHCl_3$) [1]

IR (KBr): 3479, 3075, 2976, 2935, 2878, 1716, 1644, 1386, 1358, 1228, 1202 [1]

EI-MS: 552 $[M - H_2O]^+$ (1.9), 464 (1.5), 441 (1.8), 424 (1.2), 397 (1.5), 353 (1.5), 335 (1.3), 293 (1.2), 288 (1.0), 265 (2.3), 264 (2.3), 263 (1.3), 258 (1.4), 249 (1.9), 247 (3.8), 246 (5.5), 239 (1.7), 231 (2.8), 223 (2.0), 221 (3.0), 195 (2.0), 188 (6.5), 178 (6.8), 161 (7.0), 149 (5.3), 141 (4.4), 135 (5.4), 123 (20), 97 (6.1), 86 (28), 84 (36), 71 (80), 59 (17), 43 (100) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.09–1.22 (3H, m, H-12), 1.09–1.22 (3H, m, H-13), 1.09–1.22 (3H, m, H-15), 1.67 (1H, m, H-9a), 1.83–1.89 (1H, m, H-9b), 2.05 (3H, s, OAc), 2.05 (3H, s, OAc), 2.97 (1H, d, J = 4.0, H-2), 3.00 (1H, dd, J = 11.6; 2.7, H-6), 4.57 (1H, dd, J = 11.6; 4.0, H-1), 4.72 (1H, d, J = 9.2, H-8), 4.96 (1H, d, J = 3.5, H-4), 5.10 (1H, s, H-14a), 5.22 (1H, dd, J = 3.5; 2.7, H-5), 5.31 (1H, s, H-14b), 5.48 (1H, t, 3.6, H-10); 3 × O^{i}Bu: 1.09–1.22 (18H, H-3′, H-4′, H-3″, H-4″, H-3‴, H-4‴), 2.53–2.66 (3H, m, H-2′, H-2″, H-2‴) [1]

^{13}C NMR (100 MHz, $CDCl_3$, TMS) [1]:

Table 1

C-1	66.7	C-10	74.9	3 × O^{i}Bu	34.1
2	62.6	11	72.4		33.9
3	57.2	12	25.9		33.8
4	71.5	13	26.1		19.2
5	70.0	14	23.9		19.0
6	43.6	15	116.2		18.9
7	141.9	OAc	170.0		18.8
8	73.5	3 × O^{i}Bu	20.4		18.7
9	34.6		176.4		18.6
			176.2		
			175.0		

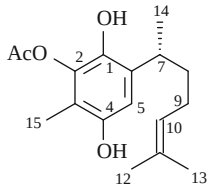
References

1. B.-N. Su, Q.-X. Zhu, Z.-J. Jia, Phytochemistry **53**(8), 1103 (2000)

Curcumenes

Monoesters

2-Acetoxycurcuquinol



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters

Biological sources: *Coreopsis senaria* S. F. Blake et Sherff [1]

$C_{17}H_{24}O_4$: 292.1675

Mp: colorless oil [1]

IR (CCl_4): 3500, 1770 [1]

MS: 292.167 $[M]^+$ (24) (calc. for $C_{17}H_{24}O_4$: 292.167), 250 (65), 167 (100), 166 (50) [1]

TLC: Et_2O – petrol (3:7), R_f 0.4 [1]

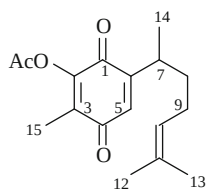
^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.12 (3H, d, J = 7, H-14), 1.52 (3H, br s, H-12), 1.66 (3H, br s, H-13), 2.11 (3H, s, H-15), 2.34 (3H, s, OAc), 3.18 (1H, m, H-7), 5.15 (1H, br t, J = 7, H-10), 6.28 (1H, s, H-5) [1]

References

1. F. Bohlmann, S. Banerjee, J. Jakupovic, R.M. King, H. Robinson, Phytochemistry **24**(6), 1295 (1985)

2-Acetoxycurcuquinone (2-Acetoxy-5-desoxyperezone)

CAS Registry Number: 89913-50-8



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters

Biological sources: *Coreopsis fasciculata* Wedd. [1]

$C_{17}H_{22}O_4$: 290.1518

Mp: yellow oil [1]

IR (CCl_4): 1785, 1670, 1655, 1610 [1]

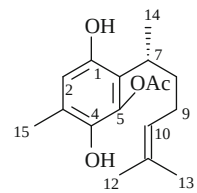
MS: 290.152 $[M]^+$ (2.5) ($C_{17}H_{22}O_4$), 248 (17), 209 (44), 166 (100) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.10 (3H, d, J = 7, H-14), 1.55 (3H, br s, H-13), 1.65 (3H, dt, J = ~1, H-12), 1.93 (3H, s, H-15), 1.96 (2H, m, H-9), 2.35 (3H, s, OAc), 2.92 (1H, br tq, J = 1; 7; 7, H-7), 5.04 (1H, tqq, J = 7; ~1; ~1, H-10), 6.52 (1H, d, J = 1, H-5) [1]

References

1. F. Bohlmann, M. Ahmed, M. Grenz, R.M. King, H. Robinson, Phytochemistry **22**(12), 2858 (1983)

5-Acetoxycurcuquinol



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters

Biological sources: *Coreopsis senaria* S. F. Blake et Sherff [1]

$C_{17}H_{24}O_4$: 292.1675

Mp: colorless oil [1]

IR (CCl_4): 3500, 1770 [1]

MS: 292.167 $[M]^+$ (20) (calc. for $C_{17}H_{24}O_4$: 292.167), 250 (60), 167 (100), 166 (54) [1]

TLC: Et_2O – petrol (3:7), R_f 0.55 [1]

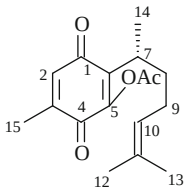
^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.30 (3H, d, J = 7, H-14), 1.51 (3H, br s, H-12), 1.65 (3H, br s, H-13),

2.03 (3H, s, H-15), 2.31 (3H, s, OAc), 3.19 (1H, m, H-7), 5.10 (1H, br t, J = 7, H-10), 6.16 (1H, s, H-2) [1]

References

1. F. Bohlmann, S. Banerjee, J. Jakupovic, R.M. King, H. Robinson, Phytochemistry **24**(6), 1295 (1985)

5-Acetoxy-7β(H)-curcuquinone (Perezone Acetate; 5-Acetoxy-perezone)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters

Biological sources: *Coreopsis senaria* S. F. Blake et Sherff [1]

$C_{17}H_{22}O_4$: 290.1518

Mp: yellow oil [1]

IR ($CHCl_3$): 1785, 1670, 1655, 1610 [1]

MS: 290.152 $[M]^+$ (10) (calc. for $C_{17}H_{22}O_4$: 290.152), 248 (40), 166 (100) [1]

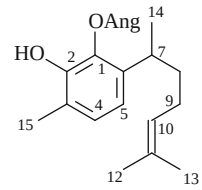
TLC: Et_2O – petrol (3:7), R_f 0.7 [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.17 (3H, d, J = 7, H-14), 1.52 (3H, br s, H-12), 1.64 (3H, br s, H-13), 2.05 (3H, s, H-15), 2.34 (3H, s, OAc), 2.97 (1H, m, H-7), 5.03 (1H, br t, J = 7, H-10), 6.55 (1H, q, H-2) [1]

References

1. F. Bohlmann, S. Banerjee, J. Jakupovic, R.M. King, H. Robinson, Phytochemistry **24**(6), 1295 (1985)

1-Angeloyloxy-2-hydroxy-α-curcumene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters

Biological sources: *Wedelia regis* H. Rob. [1]

$C_{20}H_{28}O_3$: 316.2038

Mp: inseparable colorless oil (mix. with 2-angeloyloxy-1-hydroxy-α-curcumene) [1]

IR (CCl_4): 3580, 1735 [1]

MS: 316.204 $[M]^+$ (21) (calc. for $C_{20}H_{28}O_3$: 316.204), 149 (61), 83 $[C_4H_7CO]^+$ (100), 55 $[83 - CO]^+$ (95) [1]

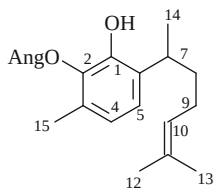
TLC: Et_2O – petrol (1:2) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.21 (3H, d, J = 7, H-14), 1.54 (3H, br s, H-12), 1.66 (3H, br s, H-13), 2.25 (3H, s, H-15), 3.09 (1H, dq, J = 7; 7, H-7), 5.11 (1H, tqq, H-10), 6.76 (1H, d, J = 8, H-5), 6.99 (1H, d, J = 8, H-4); OAng: 2.10 (6H, br s, H-4′, H-5′), 6.33 (1H, br q, H-3′) [1]

References

1. F. Bohlmann, T. Gerke, J. Jakupovic, N. Borthakur, R.M. King, H. Robinson, Phytochemistry **23**(8), 1673 (1984)

2-Angeloyloxy-1-hydroxy-α-curcumene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters

Biological sources: *Wedelia regis* H. Rob. [1]

$C_{20}H_{28}O_3$: 316.2038

Mp: inseparable colorless oil (mix. with 1-angeloyloxy-2-hydroxy-α-curcumene) [1]

IR (CCl_4) (mix.): 3580, 1735 [1]

MS (mix.): 316.204 $[M]^+$ (21) (calc. for $C_{20}H_{28}O_3$: 316.204), 149 (61), 83 $[C_4H_7CO]^+$ (100), 55 [83 − $CO]^+$ (95) [1]

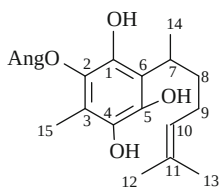
TLC (mix.): Et_2O – petrol (1:2) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS) (mix.): 1.15 (3H, d, J = 7, H-14), 1.50 (3H, br s, H-12), 1.53 (3H, br s, H-13), 2.14 (3H, s, H-15), 2.78 (1H, dq, J = 7; 7, H-7), 5.04 (1H, tqq, H-10), 6.74 (1H, d, J = 8, H-4), 6.94 (1H, d, J = 8, H-5); OAng: 2.10 (6H, br s, H-4′, H-5′), 6.33 (1H, br q, H-3′) [1]

References

1. F. Bohlmann, T. Gerke, J. Jakupovic, N. Borthakur, R.M. King, H. Robinson, Phytochemistry **23**(8), 1673 (1984)

2-Angeloyloxy-5-hydroxy-curcuquinol (1-Hydroxy-2-angeloyloxy-dihydroperezone; 1-Hydroxy-dihydroperezon-2-*O*-angelate; 2-Angeloyloxy-5-hydroxy-curcuhydroquinone)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters

Biological sources: *Acourtia thurberi* (A. Gray) J. Reveal et R. M. King [1]

$C_{20}H_{28}O_4$: 332.1988

Mp: oily mixture, which could not be separated

Mp (its triAc): colorless oil (mix. with 2-hydroxy-dihydroperezon-5-*O*-angelate) [1]

IR (triAc) (CCl_4): 1785, 1775, 1750, 1645 [1]

MS (triAc): 474.225 $[M]^+$ (1) (calc. for $C_{26}H_{34}O_8$: 474.225), 390 (7), 348 (5), 308 (14), 266 (15), 83 (100), 43 (41) [1];

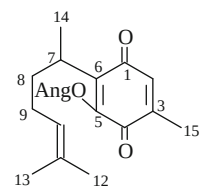
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.21 (3H, d, J = 7, H-14), 1.52 (3H, br s, H-12), 1.63 (3H, br s, H-13), 1.96 (3H, s, H-15), 3.02 (1H, tq, J = 7; 7, H-7), 5.04 (1H, tqq, J = 7, H-10); OAng: 2.03 (3H, br s, H-5′), 2.06 (3H, br d, J = 7; 1.5, H-4′), 6.34 (1H, br q, J = 7; 1.5, H-3′) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS) (triAc): 1.20 (3H, d, J = 7, H-14), 1.53 (3H, br s, H-12), 1.64 (3H, br s, H-13), 1.98 (3H, s, H-15), 2.22 (3H, s, OAc), 2.29 (3H, s, OAc), 2.89 (1H, tq, J = 7; 7, H-7), 3.28 (3H, s, OAc), 5.02 (1H, br t, J = 7, H-10); OAng: 2.04 (3H, br s, H-5′), 2.07 (3H, dq, J = 7; 1.5, H-4′), 6.31 (1H, qq, J = 7; 1.5, H-3′) [1]

References

1. F. Bohlmann, C. Zdero, R.M. King, H. Robinson, Phytochemistry **18**(11), 1894 (1979)

5-Angeloyloxy-curcuquinone (Perezone Angelicate)



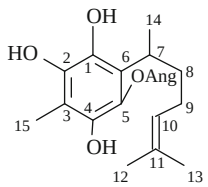
Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters

Biological sources: *Acourtia thurberi* (A. Gray) J. Reveal et R. M. King [1]
$C_{20}H_{26}O_4$: 330.1831
Mp: yellow not separated oil [1]
IR (CCl_4): 1745, 1675, 1670, 1625 [1]
MS: 330.188 $[M]^+$ (1) (calc. for $C_{20}H_{26}O_4$: 330.188), 248 $[M - O = C = C(Me)CH = CH_2]^+$ (8), 83 $[C_4H_7CO]^+$ (100) [1]
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.20 (3H, d, J = 1, H-14), 1.53 (3H, br s, H-12), 1.64 (3H, br s, H-13), 2.05 (3H, br s, H-15), 3.02 (1H, tq, J = 7; 7, H-7), 5.04 (1H, tqq, J = 7, H-10), 6.58 (1H, q, J = 1, H-2); OAng: 2.05 (6H, m, H-4′, H-5′), 6.34 (1H, br q, J = 7; 1.5, H-3′) [1]

References

1. F. Bohlmann, C. Zdero, R.M. King, H. Robinson, Phytochemistry **18**(11), 1894 (1979)

5-Angeloyloxy-2-hydroxy-curcuquinol (2-Hydroxy-5-angeloyloxy-dihydroperezone; 2-Hydroxy-dihydroperezon-5-*O*-angelate; 5-Angeloyloxy-2-hydroxy-curcuhydroquinone)

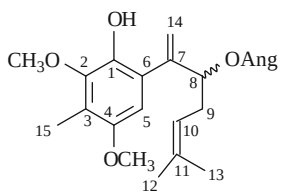


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters
Biological sources: *Acourtia thurberi* (A. Gray) J. Reveal et R. M. King [1]
$C_{20}H_{28}O_4$: 332.1988
Mp: oily mixture, which could not be separated
Mp (its triOAc): colorless oil (mix. with 2-hydroxy-dihydroperezon-2-*O*-angelate) [1]
IR (CCl_4) (triOAc): 1775, 1750, 1645 [1]
MS (triOAc): 474.225 $[M]^+$ (1) (calc. for $C_{26}H_{34}O_8$: 474.225), 390 (6), 348 (5), 308 (12), 266 (13), 83 (100), 43 (35) [1]
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.21 (3H, d, J = 7, H-14), 1.54 (3H, br s, H-12), 1.64 (3H, br s, H-13), 1.94 (3H, s, H-15), 3.08 (1H, tq, J = 7; 7, H-7), 5.04 (1H, tqq, J = 7, H-10); OAng: 2.03 (3H, br s, H-5′), 2.06 (3H, br d, J = 7; 1.5, H-4′), 6.34 (1H, br q, J = 7; 1.5, H-3′) [1]
^{1}H NMR (270 MHz, $CDCl_3$, TMS) (triOAc): 1.21 (3H, d, J = 7, H-14), 1.55 (3H, br s, H-12), 1.67 (3H, br s, H-13), 1.97 (3H, s, H-15), 2.23 (3H, s, OAc), 2.28 (3H, s, OAc), 2.29 (3H, s, OAc), 2.87 (1H, tq, J = 7; 7, H-7), 5.04 (1H, br t, J = 7, H-10); OAng: 2.03 (3H, dq, J = 1.5; 1.5, H-5′), 2.07 (3H, dq, J = 7; 1.5, H-4′), 6.30 (1H, qq, J = 7; 1.5, H-3′) [1]

References

1. F. Bohlmann, C. Zdero, R.M. King, H. Robinson, Phytochemistry **18**(11), 1894 (1979)

8-Angeloyloxy-2,4-dimethoxy-7(14)-en-curcuquinol (2,4-Di-*O*-methyl-senecioodontol; 2,4-Dimethoxy-8-angeloyloxy-7(14)-en-curcuhydroquinone)

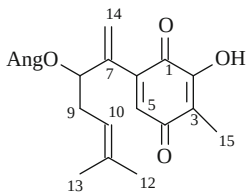


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters
Biological sources: *Senecio oxydontus* DC. [1]
$C_{22}H_{30}O_5$: 374.2093
Mp: colorless oil [1]
IR (CCl_4): 3540, 1720, 1700, 1650 [1]
MS: 374.209 $[M]^+$ (2) (calc. for $C_{22}H_{30}O_5$: 374.209), 274 (12), 259 (8), 232.146 (3) (calc. for $C_{15}H_{20}O_2$: 232.146), 205 (40), 83 (100), 55 (47) [1]
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.57 (3H, br s, H-12), 1.68 (3H, br s, H-13), 2.18 (3H, s, H-15), 2.40 (2H, m, H-9), 3.77* (3H, s, OCH_3), 3.84* (3H, s, OCH_3), 5.13 (1H, br t, J = 7, H-10), 5.22 (1H, br s, H-14b), 5.38 (1H, br s, H-14a), 5.40 (1H, dd, J = 7; 5, H-8), 6.37 (1H, s, H-5), 7.30 (1H, s, OH); OAng: 1.96 (3H, dq, J = 1.5; 1.5, H-5′), 2.04 (3H, dq, J = 7; 1.5, H-4′), 6.18 (1H, qq, J = 7; 1.5, H-3′); * - Assignments may be interchanged [1]

References

1. F. Bohlmann, C. Zdero, Phytochemistry **17**(9), 1591 (1978)

8-Angeloyloxy-2-hydroxy-7(14)-en-curcuquinone (8-Angeloyloxy-2-hydroxy-5-desoxy-7,14-dehydroperezone)

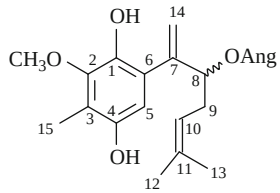


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters
Biological sources: *Senecio longifolius* L. [1]
$C_{20}H_{24}O_5$: 344.1624
Mp: 73°C, orange crystals [1]
$[\alpha]_D$ +40° (*c* 0.72, $CHCl_3$) [1]
IR (CCl_4): 3420, 1720, 1665, 1640 [1]
MS: 344.162 $[M]^+$ (0.2) (calc. for $C_{20}H_{24}O_5$: 344.162), 244 (30), 229 (14), 83 (100), 55 (70) [1]
TLC: Et_2O – petrol (1:3), R_f 0.57 [1]
^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.52 (3H, br s, H-13), 1.61 (3H, br s, H-12), 1.94 (3H, s, H-15), 2.42 (2H, br t, J = 6.5; 7.5, H-9), 5.02 (1H, tqq, J = 7.5; 1; 1, H-10), 5.51 (1H, s, H-14b), 5.52 (1H, br s, H-14a), 5.66 (1H, br t, J = 6.5, H-8), 6.67 (1H, s, H-5); OAng: 1.85 (3H, dq, J = 1.5; 1.5, H-5′), 1.95 (3H, dq, J = 7.5; 1.5, H-4′), 6.08 (1H, qq, J = 7.5; 1.5, H-3′) [1]

References

1. F. Bohlmann, C. Zdero, J. Jakupovic, L.N. Misra, S. Banerjee, P. Singh, R.N. Baruah, M.A. Metwally, G. Schmeda-Hirschmann, L.P.D. Vincent, R.M. King, H. Robinson, Phytochemistry **24**(6), 1249 (1985)

8-Angeloyloxy-2-methoxy-7(14)-en-curcuquinol (2-*O*-Methyl-senecioodontol; 2-Methoxy-8-angeloyloxy-7(14)-en-curcuhydroquinone)



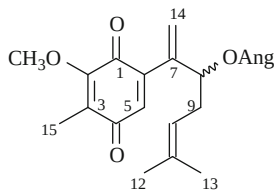
Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters
Biological sources: *Senecio oxydontus* DC. [1]; *S. longifolius* L. [2]
$C_{21}H_{28}O_5$: 360.1937
Mp: colorless oil [1]

IR (CCl_4): 3620, 3320, 1720, 1700, 1650 [1]
MS: 360.194 $[M]^+$ (5) (calc. for $C_{21}H_{28}O_5$: 360.194), 260.141 $[M - HOAng]^+$ (calc. for $C_{16}H_{20}O_3$: 260.141) (42), 245 (26), 191 (100), 83 (55), 55 (58) [1]
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.56 (3H, br s, H-12), 1.67 (3H, br s, H-13), 2.19 (3H, s, H-15), 2.28 (2H, m, H-9), 3.84 (3H, s, OCH_3), 5.11 (1H, br t, J = 7, H-10), 5.18 (1H, m, H-14b), 5.33 (1H, br s, H-14a), 5.36 (1H, dd, J = 7; 5, H-8), 6.38 (1H, dd, J = 7; 5, H-5), 7.27 (1H, s, OH); OAng: 1.95 (3H, dq, J = 1.5; 1.5, H-5′), 2.03 (3H, dq, J = 7; 1.5, H-4′), 6.17 (1H, qq, J = 7; 1.5, H-3′) [1]

References

1. F. Bohlmann, C. Zdero, Phytochemistry **17**(9), 1591 (1978)
2. F. Bohlmann, C. Zdero, A.A. Natu, Phytochemistry **17**(10), 1757 (1978)

8-Angeloyloxy-2-methoxy-7(14)-en-curcuquinone (2-*O*-Methyl-1,4-dehydrosenecioodontol)

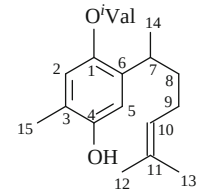


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters
Biological sources: *Senecio oxydontus* DC. [1]
$C_{21}H_{26}O_5$: 358.1780
Mp: yellow colored oil [1]
$[\alpha]^{24}$ (λ, nm): +12.4° (589), +13.7° (578), +16.8° (546) (*c* 0.6, $CHCl_3$) [1]
IR (CCl_4): 1710, 1660, 1635 [1]
MS: 358.178 $[M]^+$ (1) (calc. for $C_{21}H_{26}O_5$: 358.178), 258 (9), 243 (11), 83 (100), 55 (61) [1]
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.58 (3H, br s, H-12), 1.67 (3H, br s, H-13), 1.95 (3H, s, H-15), 2.46 (2H, t, J = 7; 7, H-9), 5.08 (1H, br t, J = 7, H-10), 5.43 (1H, br s, H-14b), 5.55 (1H, br s, H-14a), 5.66 (1H, dd, J = 7; 7, H-8), 6.64 (1H, s, H-5); OAng: 1.88 (3H, dq, J = 1.5; 1.5, H-5′), 1.96 (3H, dq, J = 7; 1.5, H-4′), 6.07 (1H, qq, J = 7; 1.5, H-3′) [1]

References

1. F. Bohlmann, C. Zdero, Phytochemistry **17**(9), 1591 (1978)

1-Isovaleroyloxy-curcuquinol (Curcuquinol Monoisovalerate; 1-Isovaleryloxy-curcuhydroquinone)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters
Biological sources: *Perezia carpholepis* (A. Gray) [1]
$C_{20}H_{30}O_3$: 318.2195
Mp: pale yellow oil [1]
$[\alpha]_D$ −10° (*c* 1, $CHCl_3$) [1]
UV (95% EOH): 209 (ε 14000), 220 (ε 8000), 283 (ε 2500) [1]
IR ($CHCl_4$): 3600, 1760, 1630 [1]
MS: 318 $[M]^+$, 234, 218, 136, 85 [1]
^{1}H NMR (60 MHz, $CDCl_3$, TMS): 1.55 (3H, br s, H-12 or H-13), 1.68 (3H, br s, H-13 or H-12), 2.08 (3H, s, H-15), 5.12 (1H, t, J = 7, H-10), 5.58 (1H, s, H-5), 6.70 (1H, br s, H-2); O^{i}Val: 0.93 (6H, d, J = 7, H-4′, H-5′), 2.36 (2H, br s, H-2′) [1]

^{13}C NMR (50 MHz, DMSO-d_6, TMS) [1]:

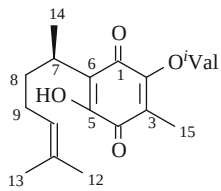
Table 1

C-1	141.0	C-8	31.9	C-15	25.8
2	137.1	9	21.1	O^{i}Val	172.2
3	113.0 d	10	37.5		43.3
4	152.2	11	26.1		31.9
5	122.4	12	124.3		22.5
6	123.8 d	13	131.2		22.5
7	15.5	14	17.6		

References

1. F. Bohlmann, C. Zdero, Phytochemistry **15**(6), 1075 (1976)

2-Isovaleroyloxy-5-hydroxy-curcuquinone (2-Isovaleroyloxy-5-hydroxyperezone; 5-Hydroxyperezon-monoisovalerate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters

Biological sources: *Jungia spectabilis* D. Don [1]; *J. stuebelii* (Hieron.) Crisci [2]; *Perezia runcinata* Lag. ex D. Don [3]

$C_{20}H_{28}O_5$: 348.1937

Mp: yellow oil, not be could separated (mix. with the 5-isovaleroyloxy-2-hydroxyperezone) [1]; red oil (mix. with the 5-isovaleroyloxy-2-hydroxyperezone) [3]

UV (95% EtOH) (mix.): 201 (ε 23200), 274 (ε 13200) [3]

IR (CCl_4) (mix.): 3415, 1780, 1660 [1]; ($CHCl_3$): 3400, 1770, 1650 [3]

MS: 348.194 $[M]^+$ (2) (calc. for $C_{20}H_{28}O_5$: 348.194), 264 (75), 85 (71), 57 (100) [1]

MS (mix.): 348 $[M]^+$, 264, 248, 85 [3]

MS (Me ether): 362 $[M]^+$ [3]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.21 (3H, d, J = 7, H-14), 1.54 (3H, br s, H-12), 1.65 (2H, m, H-8), 1.65 (3H, br s, H-13), 1.91 (2H, dt, J = 7; 6.5, H-9), 1.94 (3H, s, H-15), 2.97 (1H, tq, J = 7, H-7), 5.02 (1H, br t, J = 6.5, H-10); O^{i}Val: 1.09 (6H, d, H-4′, H-5′), 2.24 (1H, m, H-3′), 2.50 (2H, dd, H-2′) [1]

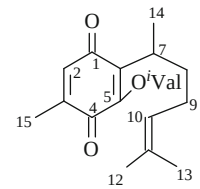
^{1}H NMR ($CDCl_3$) (mix.): 1.19 (3H, d, J = 7, H-14), 1.53 (3H, br s, H-13 or H-12), 1.63 (3H, br s, H-12 or H-13), 1.91 (3H, s, H-15), 2.97 (1H, m, H-7), 5.00 (1H, m, H-10), O^{i}Val: 1.08 (6H, d, J = 7, H-4′, H-5′), 2.41 (2H, br s, H-2′) [3]

^{1}H NMR ($CDCl_3$) (its Me ether): 1.18 (3H, d, J = 7, H-14), 1.53 (3H, br s, H-13 or H-12), 1.67 (3H, br s, H-12 or H-13), 1.93 (3H, s, H-15), 2.97 (1H, m, H-7), 5.0 (1H, m, H-10), 4.02 (3H, s, OCH_3); O^{i}Val: 1.07 (6H, d, J = 7, H-4′, H-5′), 2.41 (2H, br s, H-2′) [3]

References

1. F. Bohlmann, C. Zdero, Phytochemistry **16**(2), 239 (1977)
2. F. Bohlmann, C. Zdero, R.M. King, H. Robinson, Phytochemistry **22**(5), 1201 (1983)
3. P. Joseph-Nathan, E. Garcia, V. Mendoza, Phytochemistry **16**(7), 1086 (1977)

5-Isovaleroyloxy-curcuquinone (Isovaleryloxyperezone)



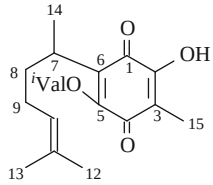
Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters

Biological sources: *Perezia runcinata* Lag. ex D. Don [1]; *Coreopsis mutica* DC. [2]
$C_{20}H_{28}O_4$: 332.1988
Mp: yellow oil [1]
UV (95% EtOH): 204 (ε 25200), 259 (ε 9600) [1]
IR ($CHCl_3$): 1780, 1670, 1630 [1]
MS: 332 $[M]^+$, 248, 192, 166, 85 [1]
^{1}H NMR ($CDCl_3$ or CCl_4, TMS): 1.16 (3H, d, J = 7, H-14), 1.53 (3H, br s, H-13 or H-12), 1.66 (3H, br s, H-12 or H-13), 2.01 (3H, d, J = 1.6, H-15), 2.84 (1H, m, H-7), 5.01 (1H, m, H-10), 6.50 (1H, q, J = 1.6, H-2); O^{i}Val: 1.08 (6H, d, J = 7, H-4′, H-5′), 2.41 (2H, br s, H-2′) [1]

References

1. P. Joseph-Nathan, E. Garcia, V. Mendoza, Phytochemistry **16**(7), 1086 (1977)
2. F. Bohlmann, M. Ahmed, M. Grenz, R.M. King, H. Robinson, Phytochemistry **22**(12), 2858 (1983)

5-Isovaleroyloxy-2-hydroxy-curcuquinone (5-Isovaleroyloxy-2-hydroxyperezone; 2-Hydroxyperezon-monoisovalerate)

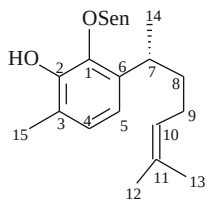


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters
Biological sources: *Jungia spectabilis* D. Don [1]; *J. stuebelii* (Hieron.) Crisci [2]; *Perezia runcinata* Lag. ex D. Don [3]
$C_{20}H_{28}O_5$: 348.1937
Mp: yellow oil, not be could separated (mix. with the 5-hydroxy-perezon-monoisovalerate) [1]; red oil (mix. with the 5-hydroxy-perezon-monoisovalerate) [3]
UV (95% EtOH) (mix.): 201 (ε 23200), 274 (ε 13200) [3]
IR (CCl_4) (mix.): 3415, 1780, 1660 [1]; ($CHCl_3$): 3400, 1770, 1650 [3]
MS (mix.): 348.194 $[M]^+$ (2) (calc. for $C_{20}H_{28}O_5$: 348.194), 264 (75), 85 (71), 57 (100) [1]
MS (mix.): 348 $[M]^+$, 264, 248, 85 [3]
MS (Me ether): 362 $[M]^+$ [3]
^{1}H NMR (270 MHz, $CDCl_3$, TMS) (mix.): 1.21 (3H, d, J = 7, H-14), 1.54 (3H, br s, H-12), 1.65 (2H, m, H-8), 1.65 (3H, br s, H-13), 1.92 (2H, dt, J = 7; 6.5, H-9), 1.95 (3H, s, H-15), 3.06 (1H, tq, J = 7, H-7), 5.07 (1H, br t, J = 6.5, H-10); O^{i}Val: 1.09 (6H, d, H-5′, H-6′), 2.24 (1H, m, H-1′), 2.50 (2H, dd, H-2′) [1]
^{1}H NMR ($CDCl_3$) (mix.): 1.19 (3H, d, J = 7, H-14), 1.53 (3H, br s, H-13 or H-12), 1.63 (3H, br s, H-12 or H-13), 1.91 (3H, s, H-15), 2.97 (1H, m, H-7), 5.00 (1H, m, H-10); O^{i}Val: 1.08 (6H, d, J = 7, H-4′, H-5′), 2.41 (2H, br s, H-2′) [3]
^{1}H NMR ($CDCl_3$) (its Me ether): 1.18 (3H, d, J = 7, H-14), 1.53 (3H, br s, H-13 or H-12), 1.67 (3H, br s, H-12 or H-13), 1.88 (3H, s, H-15), 2.97 (1H, m, H-7), 5.0 (1H, m, H-10); O^{i}Val: 1.07 (6H, d, J = 7, H-4′, H-5′), 2.41 (2H, br s, H-2′) [3]

References

1. F. Bohlmann, C. Zdero, Phytochemistry **16**(2), 239 (1977)
2. F. Bohlmann, C. Zdero, R.M. King, H. Robinson, Phytochemistry **22**(5), 1201 (1983)
3. P. Joseph-Nathan, E. Garcia, V. Mendoza, Phytochemistry **16**(7), 1086 (1977)

1-Senecioyloxy-2-hydroxy-α-curcumene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters

Biological sources: *Rutidosis murchisonii* F. Muell. [1]

$C_{20}H_{28}O_3$: 316.2038

Mp: colorless oil (mix. with the 1-hydroxy-2-senecioyloxy-α-curcumene) [1]

IR (CCl_4) (its OAc): 1775, 1745 [1]

MS (mix.): 316.204 $[M]^+$ (5) (calc. for $C_{20}H_{28}O_3$: 316.204), 234 (1), 83 (100), 55 (16) [1]

MS (its Ac): 358.214 $[M]^+$ (2) (calc. for $C_{22}H_{30}O_4$: 358.214), 316 (1), 275 (1), 193 (1.5), 83 (100) [1]

PTLC: Et_2O – petrol (1:10), R_f 0.40 [1]

HPLC: MeOH – H_2O (17:3), R_t 6.5 min [1]

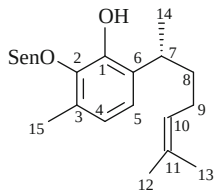
^{1}H NMR (400 MHz, $CDCl_3$, TMS) (mix.): 1.16 (3H, d, J = 8, H-14), 1.48 (1H, ddt, J = 8; 14; 7, H-8b), 1.51 (3H, br s, H-13), 1.58 (1H, ddt, J = 8; 14; 7, H-8a), 1.64 (3H, br s, H-12), 1.87 (2H, br q, J = 7; 7, H-9), 2.24 (3H, s, H-15), 2.77 (1H, tq, J = 8; 8, H-7), 5.05 (1H, tqq, J = 7, H-10), 6.73 (1H, d, J = 8, H-5), 6.97 (1H, d, J = 8, H-4); OSen: 2.02 (3H, d, H-4′), 2.25 (3H, d, H-5′), 6.01 (1H, qq, H-2′) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS) (its OAc): 1.15 (3H, d, J = 8, H-14), 1.50 (1H, ddt, J = 8; 14; 7, H-8b), 1.51 (3H, br s, H-13), 1.60 (1H, ddt, J = 8; 14; 7, H-8a), 1.63 (3H, br s, H-12), 1.88 (2H, br q, J = 7; 7, H-9), 2.14 (3H, s, OAc), 2.23 (3H, s, H-15), 2.80 (1H, tq, J = 8; 8, H-7), 5.05 (1H, tqq, J = 7, H-10), 7.05 (2H, ABq, J = 8, H-4, H-5); OSen: 1.99 (3H, d, H-4′), 2.21 (3H, d, H-5′), 5.94 (1H, br s, H-2′) [1]

References

1. C. Zdero, F. Bohlmann, R.M. King, H. Robinson, Phytochemistry **26**(6), 1759 (1987)

2-Senecioyloxy-1-hydroxy-α-curcumene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters

Biological sources: *Rutidosis murchisonii* F. Muell. [1]

$C_{20}H_{28}O_3$: 316.2038

Mp: colorless oil (mix. with the 1-senecioyloxy-2-hydroxy-α-curcumene) [1]

IR (CCl_4) (its OAc): 1775, 1745, 1650 [1]

MS (mix.): 316.204 $[M]^+$ (5) (calc. for $C_{20}H_{28}O_3$: 316.204), 234 (1), 83 (100), 55 (16) [1]

MS (its Ac): 358.214 $[M]^+$ (2) (calc. for $C_{22}H_{30}O_4$: 358.214), 316 (1), 275 (1), 193 (1.5), 83 (100) [1]

PTLC: Et_2O – petrol (1:10), R_f 0.40 [1]

HPLC: MeOH – H_2O (17:3), R_t 6.5 min [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS) (mix.): 1.21 (3H, d, J = 8, H-14), 1.49 (1H, ddt, J = 8; 14; 7, H-8b), 1.53 (3H, br s, H-13), 1.58 (1H, ddt, J = 8; 14; 7, H-8a), 1.66 (3H, br s, H-12), 1.95 (2H, br q, J = 7; 7, H-9), 2.12 (3H, s, H-15), 3.09 (1H, tq, J = 8; 8, H-7), 5.10 (1H, tqq, J = 7, H-10), 6.74 (1H, d, J = 8, H-4), 6.93 (1H, d, J = 8, H-5); OSen: 2.02 (3H, d, H-4′), 2.25 (3H, d, H-5′), 6.01 (1H, qq, H-2′) [1]

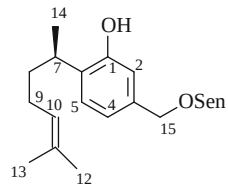
^{1}H NMR (400 MHz, $CDCl_3$, TMS) (its OAc): 1.17 (3H, d, J = 8, H-14), 1.50 (1H, m, H-8b), 1.54 (3H, br s, H-13), 1.60 (1H, m, H-8a), 1.66 (3H, br s, H-12), 1.90 (2H, br q, J = 7; 7, H-9), 2.14 (3H, s, OAc), 2.24 (3H, s, H-15), 2.78 (1H, tq, J = 8; 8,

H-7), 5.06 (1H, br t, H-10), 7.03 (1H, d, J = 8, H-4), 7.08 (1H, d, J = 8, H-5); OSen: 1.99 (3H, d, H-4′), 2.22 (3H, d, H-5′), 5.94 (1H, br s, H-2′) [1]

References

1. C. Zdero, F. Bohlmann, R.M. King, H. Robinson, Phytochemistry **26**(6), 1759 (1987)

15-Senecioyloxy-1-hydroxy-α-curcumene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Monoesters

Biological sources: *Elephantopus mollis* H.B.K. [1]

$C_{20}H_{28}O_3$: 316.2038

Mp: oil [1]

IR: 3603 (OH), 1720, 1650, 1615, 1585, 1420, 1340, 1070 [1]

MS: 316.2032 $[M]^+$ (9) (calc. for $C_{20}H_{28}O_3$: 316.2038), 233 (19), 216 $[M - SenOH]^+$ (51), 201 $[216 - CH_3]^+$ (6), 83 $[C_4H_7CO]^+$ (100) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.22 (3H, d, J = 7, H-14), 1.53 (3H, br s, H-13), 1.62 (2H, dt, J = 7; 7; H-8), 1.68 (3H, br s, H-12), 1.84 (2H, dt, J = 7, H-9), 3.01 (1H, tq, J = 7; 7, H-7), 4.94 (1H, br s, OH), 5.05 (2H, br s, H-15), 5.12 (1H, tqq, J = 1; 1, H-10), 6.78 (1H, d, J = 1.5, H-2), 6.89 (1H, dd, J = 1.5; 8, H-4), 7.13 (1H, d, J = 8, H-5); OSen: 1.89 (3H, d, J = 1, H-4′), 2.18 (3H, d, J = 1, H-5′), 5.73 (1H, qq, J = 1, H-2′) [1]

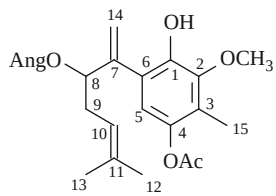
References

1. F. Bohlmann, C. Zdero, Chem. Ber. **109**, 3956 (1976)

Curcumenes

Diesters

4-Acetoxy-8-angeloyloxy-2-methoxy-7(14)-en-curcuquinol (1,3,5,7(14),10-Bisabolapentaene-8-angeloyloxy-4-acetoxy-2-methoxy-1-ol; Senecioodontol-4-*O*-acetate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Diesters

Biological sources: *Senecio longifolius* L. [1]

$C_{23}H_{30}O_6$: 402.2042

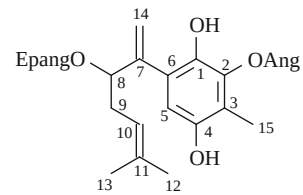
Mp: colorless oil [1]

IR (CCl_4): 3480, 1770, 1725, 1655 [1]

MS: 402.204 $[M]^+$ (3) ($C_{23}H_{30}O_6$), 302 (74), 260 (88), 83 (100) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.57 (3H, br s, H-12), 1.67 (3H, br s, H-13), 2.11 (3H, s, H-15), 2.28 (2H, br dd, J = 7; 7, H-9), 2.32 (3H, s, OAc), 3.77 (3H, s, OCH_3), 5.08 (1H, br t, J = 7, H-10), 5.14 (1H, br s, H-14b), 5.32 (1H, br s, H-14a), 5.62 (1H, br t, J = 7, H-8), 6.80 (1H, s, H-5); OAng: 1.95 (3H, dq, J = 1.5; 1.5, H-5′), 2.03 (3H, dq, J = 7; 1.5, H-4′), 6.20 (1H, qq, J = 7; 1.5, H-3′) [1]

2-Angeloyloxy-8-(2″,3″-epoxy-angeloyloxy)-7(14)-en-curcuquinol (2-Desmethoxy-2-angeloyloxy-8-[2-methyl-2,3-epoxybutyryloxy]-senecioodontol)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Diesters

Biological sources: *Senecio longifolius* L. [1]

$C_{25}H_{32}O_6$: 428.2199

Isolated as its oxygenated deriv.: 4-*O*-angeloyl-8-desangeloyloxy-8-[2-methyl-2,3-epoxybutyryloxy]-dehydrosenecioodontol [1]

Mp: yellow oil (mix. with senecioodontol-2-desmethoxy-2-angeloyloxy-8-angeloyloxy (7:1)) [1]

$[\alpha]^{24}$ (λ, nm) (its oxygenated deriv.): +54.6° (589), +58.9° (578), +69.4° (546) (*c* 1.5, $CHCl_3$) [1]

IR (CCl_4) (its oxygenated deriv.): 1750, 1725, 1670 [1]

MS (its oxygenated deriv.): 442.199 $[M]^+$ (2) ($C_{25}H_{30}O_7$), 326 (25), 244 (58) 83 (100) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS) (its oxygenated deriv.): 1.58 (3H, br s, H-12), 1.67 (3H, br s, H-13), 2.06 (3H, s, H-15), 2.43 (2H, br dd, J = 7; 7, H-9), 5.03 (1H, br t, J = 7, H-10), 5.53 (1H, br s, H-14a), 5.64 (1H, br s, H-14b), 5.70 (1H, t, J = 7, H-8), 6.78 (1H, s, H-5), OAng: 2.04 (3H, dq, J = 1.5; 1.5, H-5′), 2.06 (3H, dq, J = 7; 1.5, H-4′), 6.35 (1H, qq, J = 7; 1.5, H-3′); OEpang: 1.30 (3H, d, J = 5, H-4″), 1.55 (3H, s, H-5″), 3.05 (1H, q, J = 5, H-3″) [1]

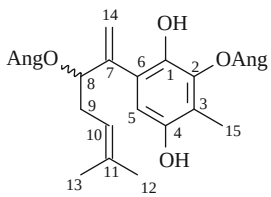
References

1. F. Bohlmann, C. Zdero, A.A. Natu, Phytochemistry **17**(10), 1757 (1978)

References

1. F. Bohlmann, C. Zdero, A.A. Natu, Phytochemistry **17**(10), 1757 (1978)

2,8-Diangeloyloxy-7(14)-encurcuquinol (2-*O*-Angeloylsenecioodontol; 2,8-Diangeloyloxy-7(14)-encurcuhydroquinone)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Diesters

Biological sources: *Senecio oxydontus* DC. [1]; *S. longifolius* L. [2]

$C_{25}H_{32}O_6$: 428.2199

Mp: colorless oil [1]

IR (CCl_4): 3600, 3420, 1715, 1640 [1]

MS: 428.220 $[M]^+$ (2) (calc. for $C_{25}H_{32}O_6$: 428.220), 328 (16), 246 (40), 231 (14), 83 (100), 55 (35) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.52 (3H, br s, H-12), 1.63 (3H, br s, H-13), 2.03 (3H, s, H-15), 2.37 (2H, m, H-9), 5.08 (1H, br t, J = 7, H-10), 5.17 (1H, br s, H-14b), 5.34 (1H, br s, H-14a), 5.55 (1H, dd, J = 7; 5, H-8), 6.48 (1H, s, H-5), 7.28 (1H, s, OH), 7.92 (1H, s, OH); OAng-3: 1.89 (3H, dq, J = 1.5; 1.5, H-5′), 1.97 (3H, dq, J = 7; 1.5, H-4′), 6.06 (1H, qq, J = 7; 1.5, H-3′); OAng-8: 2.03 (3H, dq, J = 1.5; 1.5, H-5″), 2.05 (3H, dq, J = 7; 1.5, H-4″), 6.25 (1H, qq, J = 7; 1.5, H-3″) [1]

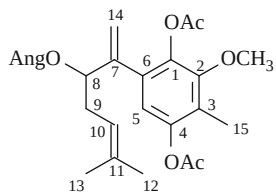
References

1. F. Bohlmann, C. Zdero, Phytochemistry **17**(9), 1591 (1978)
2. F. Bohlmann, C. Zdero, A.A. Natu, Phytochemistry **17**(10), 1757 (1978)

Curcumenes

Triester

1,4-Diacetoxy-8-angeloyloxy-2-methoxy-7(14)-en-curcuquinol (Senecioodontol-1,4-*O*-diacetat; 1,3,5,7(14),10-Bisabolapentaene-8-angeloyloxy-1,4-diacetoxy-2-methoxy)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Bisabolanes – Curcumenes – Triester

Biological sources: *Senecio longifolius* L. [1]

$C_{25}H_{32}O_7$: 444.2148

Mp: colorless oil [1]

$[\alpha]^{24}$ (λ, nm): +18.3° (589), +21.6° (578), +24.2° (546) (*c* 0.4, $CHCl_3$) [1]

IR (CCl_4): 1770, 1725, 1655, 912 [1]

MS: 444.215 $[M]^+$ (2) ($C_{25}H_{32}O_7$), 344 (65), 302 (68), 260 (91), 83 (100) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.56 (3H, br s, H-12), 1.65 (3H, br s, H-13), 2.10 (3H, s, H-15), 2.28 (3H, s, OAc), 2.39 (2H, br dd, J = 7; 7, H-9), 3.88 (3H, s, OCH_3), 5.10 (1H, br t, J = 7, H-10), 5.21 (1H, br s, H-14b), 5.27 (1H, br t, J = 7, H-8), 5.36 (1H, br s, H-14a), 6.55 (1H, s, H-5); OAng: 1.91 (3H, dq, J = 1.5; 1.5, H-5′), 1.99 (3H, dq, J = 7; 1.5, H-4′), 6.08 (1H, qq, J = 7; 1.5, H-3′) [1]

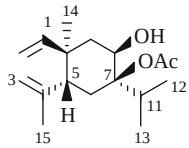
References

1. F. Bohlmann, C. Zdero, A.A. Natu, Phytochemistry **17**(10), 1757 (1978)

Elemanes

Monoesters

7β-Acetoxy-8β-hydroxy-7βH-elema-1(2),3(4)-diene ((+)-(1*R*,2*R*,4*R*,5*R*)-4-Ethenyl-2-hydroxy-4-methyl-5-(1-methylethenyl)-1-(1-methylethyl)-Cyclohexylacetate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Elemanes – Monoesters

Biological sources: *Lepidozia fauriana* Steph. [1]

$C_{17}H_{28}O_3$: 280.2038

Mp: colorless oil [1]

RI$_{CPSil5}$: 1793; sense of optical rotation (benzene): + [1]

EI-MS: 280 $[M]^+$ (0), 237 (3), 177 (74), 159 (50), 139 (45), 109 (29), 107 (20), 93 (22), 81 (29), 71 (32), 69 (22), 43 (100), 41 (27) [1]

^{1}H NMR (500.1 MHz, C_6D_6): 0.55 (1H, s, OH-8), 0.73 and 0.74 (each 3H, d, J = 9, H-12, H-13), 1.07 (3H, s, H-14), 1.59 (1H, br d, J = 14, H-6a), 1.68 (3H, s, OAc), 1.69–1.72 (2H, m, H-9a, H-11), 1.73 (3H, s, H-15), 1.81 (1H, dd, J = 2× ~14, H-6b), 2.03 (1H, dd, J =3; 15, H-9b), 2.50 (1H, dd, J = 3; 13, H-5), 4.73 (1H, s, H-3a), 4.90 (1H, d, J = 18, H-2a), 4.91 (1H, d, J = 10, H-2b), 4.94 (1H, dd, J = 2; 5, H-8), 4.95 (1H, m, H-3b), 5.77 (1H, dd, J = 10; 18, H-1) [1]

^{13}C NMR [125.77 MHz, C_6D_6 and data taken from HMBC (500.13 MHz)] [1]:

Table 1

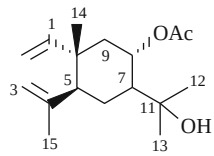
C-1	150.3 d	C-7	73.5 s	C-13	16.0 q
2	110.7 t	8	72.2 d	14	18.8 q
3	113.0 t	9	38.7 t	15	25.2 q
4	147.2 s	10	38.7 s	OO<u>C</u>CH$_3$	169.3 s
5	46.0 d	11	33.8 d	OOC<u>C</u>H$_3$	20.9 q
6	34.5 t	12	16.0 q		

(*continued*)

References

1. C. Paul, W.A. Konig, C.-L. Wu, Phytochemistry **58**(5), 789 (2001)

8α-Acetoxy-11-hydroxy-elema-1(2),3(4)-diene (8-Acetoxy Elemol)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Elemanes – Monoesters

Biological sources: *Juniperus recurva* Buch.-Ham. ex D. Don var. *squamata* (Buch.-Ham. ex Don) Parl. [1]; *J. thurifera* L. [2, 3]; *Parabenzoin praecox* (Sieb. et Zucc.) [4]

$C_{17}H_{28}O_3$: 280.2039

$[\alpha]_D^{20}$ +30° (*c* 1.7, EtOH) [1]

$[\alpha]_D$ +32° (*c* 0.8, $CHCl_3$) [3]

$[\alpha]_D$ −3.5° [4]

IR: 3350, 1730, 1240, 910, 890

MS: 280 $[M]^+$ (0.05), 220 [M – CH_3COOH], 202 [M – CH_3COOH – $H_2O]^+$ (0.9), 162 (22), 147 (23), 119 (60), 117 (71), 108 (47), 59 $[C_3H_7O]^+$ (42), 43 $[C_3H_7]^+$ (100) [4]

^{1}H NMR: 1.07, 1.19, 1.20 (each 3H, 3 × s, 3 × CH_3), 1.48 (1H, dd, J = 12; 11, H_{ax}-9), 1.71 (br s, CH_3), 1.75 (m, 2H), 1.77 (1H, dd, J = 12; 4, H_{eq}-9), 2.03 (1H, dd, J = 13; 3, H_{ax}-5), 2.06 (3H, s, OAc), 4.61 (br s), 4.86 (2H, q, J = 1, H_2C=), 4.91 (dd, J = 17; 1), 4.93 (dd, J = 11; 1), 5.07 (1H, ddd, J = 11; 11; 4, H_{ax}-8), 5.76 (1H, dd, J = 17; 11, C<u>H</u> = CH_2) [1]

^{13}C NMR [1]:

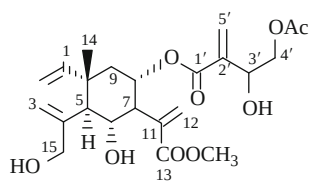
Table 1

C-1	148.2 d	C-7	52.1 q	Other	17.5
2	112.8 t	8	72.7 d	signals	21.7
3	110.8 t	9	44.7 t		24.6
4	146.2 s	10	41.1 s		26.1
5	52.0 q	CO	169.9 s		
6	29.0 t	C-OH	72.9 s		

References

1. P. Weyerstahl, H. Marschall-Weyerstahl, E. Manteuffel, V.K. Kaul, Planta Med. **54**, 259 (1988)
2. J. de Pascual Teresa, A. San Feliciano, T. Egido, A.F. Barrero, An. Quim **73**, 151 (1977). *C.A.* **87**, 152411u (1977)
3. J. de Pascual Teresa, A.F. Barrero, A. San Feliciano, M.C. Caballero, Riv. Ital. EPPOS **62**, 116 (1980). *C.A.*, **93**, 245243e (1980)
4. K. Ohara, Y. Ohta, Y. Hirose, Bull. Chem. Soc. Jpn. **46**, 641 (1973)

8α-(4′-Acetoxy-3′-hydroxy-2′-methylenebutanoyloxy)-6α,15-dihydroxy-elema-1(2),3(4),11(12)-triene-13-methyl Ester (Methyl-8α-(4-acetoxy-3-hydroxy-2-methylene-butanoyloxy)-6α,15-dihydroxy-elema-1,3,11(13)-trien-12-oate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Elemanes – Monoesters

Biological sources: *Centaurea deusta* Ten. (=*Centaurea* alba subsp. deusta (Ten.) Nyman)

$C_{23}H_{32}O_9$: 452.2046

Mp: oil [1]

$[\alpha]_D^{20}$ +11.58° (*c* 0.10, $CHCl_3$) [1]

IR (KBr): 3600–3300 (OH), 1773, 1764 (C = O, ester), 1719, 1712 (C = O, acetate) [1]

CI-MS: 452.2067 $[M]^+$ (19) ($C_{23}H_{32}O_9$ requires 452.2046), 420 $[M - MeOH]^+$ (5), 374 $[M - AcOH - H_2O]^+$ (8), 360 $[M - AcOH - MeOH]^+$ (6), 342 $[360 - H_2O]^+$ (5), 241 (100) [1]

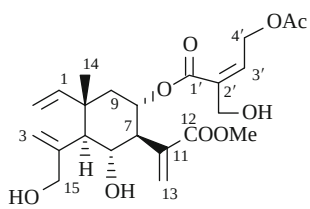
^{1}H NMR (400 MHz, $CDCl_3$): 1.15 (3H, s, H-14), 1.57 (1H, t, J = 12.4, H-9b), 1.87 (1H, dd, J = 4.4; 12.4, H-9a), 2.04 (3H, s, OAc), 2.13 (1H, d, J = 10.0, H-5), 2.73 (1H, t, J = 10.8, H-7), 3.76 (3H, s, CH_3O), 3.93 (1H, d, J = 12.8, H-15b), 4.04 (1H, d, J = 12.8, H-15a), 4.07 (1H, dd, J = 6.9; 11.9, H-4′b), 4.18 (1H, dd, J = 3.7; 11.8, H-4′a), 4.18 (1H, t, J = 10.6, H-6), 4.63 (1H, dd, J = 3.6; 6.6, H-3′), 4.89 (1H, d, J = 17.2, H-2b), 4.93 (1H, d, J = 10.8, H-2a), 4.98 (1H, br s, H-3b), 5.35 (1H, br s, H-3a), 5.43 (1H, dt, J = 4.4; 11.0, H-8), 5.64 (1H, dd, J = 10.8; 17.2, H-1), 5.72 (1H, s, H-12b), 5.90 (1H, br s, H-5′b), 6.27 (1H, br s, H-5′a), 6.27 (1H, s, H-12a) [1]

Pharm./Biol.: antifungal activity [1]

References

1. A. Karioti, H. Skaltsa, D. Lazari, M. Sokovic, B. Garcia, C. Harvala, Z. Naturforsch. **57C**, 75 (2002)

8α-[(*Z*)-4-Acetoxy-5-hydroxy-2-methylbut-2-enoyloxy]-6α,15-dihydroxy-elema-1(2),3(4),11(13)-triene-12-methyl Ester



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Elemanes – Monoesters

Biological sources: *Centaurea aspera* L. subsp. *aspera* [1]

$C_{23}H_{32}O_9$: 452.2046

Mp: colorless oil [1]

$[\alpha]_D$ +11.5 (*c* 1.2, $CHCl_3$) [1]

IR: 3400, 1745, 1710 (br), 1650, 1625, 1440, 1370, 1325, 1225, 1155, 1050, 910, 815 [1]

EI-MS: 278 $[M - C_7H_{10}O_5]^+$ (18), 260 (24), 246 (15), 229(14), 119 (69), 115 (100) [1]

TLC: $CHCl_3$ – EtOAc (1:5), R_f 0.3 [1]

^{1}H NMR (200 MHz, $CDCl_3$): 1.17 (3H, s, H-14), 1.60 (1H, dd, J = 12.5, 11.5, H-9α), 1.95 (1H, dd, J = 12.5, 4.5, H-9β), 2.07 (3H, s, AcO), 2.11 (1H, d, J = 10.5, H-5), 2.70 (1H, dd, J = 10.8, 10.8, H-7), 3.76 (3H, s, OCH_3), 4.05 and 3.93 (2H, d, J = 13, H-15), 4.20 (br s, H-5′), 4.20* (1H, dd, J = 10.8, 10.5, H-6), 4.91 (1H, br d, J = 17.3, H-2β), 4.94 (1H, br d, J = 10.7, H-2α), 5.02* (1H, br s, H-3β), 5.02* (2H, br s, H-4′), 5.37 (1H, br s, H-3α), 5.45 (1H, ddd, J = 11.5; 10.8; 4.5, H-8), 5.68 (1H, dd, J = 17.3; 10.7, H-1), 6.25 (1H, br t, J = 5, H-3′), 6.30 and 5.76 (2H, br s, H-13); * - Overlapped signals [1]

^{13}C NMR (50 MHz, $CDCl_3$): [1]

Table 1

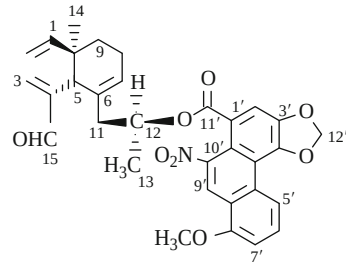
C-1	146.2	C-9	43.6	C-1′	164.9
2	112.1	10	40.3	2′	131.4
3	115.0	11	138.0	3′	140.8
4	146.3	12	167.2	4′	63.9
5	55.3	13	128.7	5′	62.9
6	71.0	14	18.3	OAc	52.1
7	54.8	15	67.8		170.8
8	71.4				20.9

References

1. J.A. Marco, J.F. Sanz-Cervera, A. Yuste, F. Sancenon, M. Carda, Phytochemistry **66**(14), 1644 (2005)

Aristophyllide A

CAS Registry Number: 221148-60-3



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Elemanes – Monoesters

Biological sources: *Aristolochia heterophylla* Hemsl. [1]; *Aristolochia mollissima* Hance [2]

$C_{32}H_{31}NO_8$: 557.2050

Mp: 226–228°C (yellow needles) [1]

$[\alpha]_D$ +120° (*c* 0.0245, $CHCl_3$) [1]

UV: 224 (4.34), 251 (4.16), 266 (4.07), 283 (3.86), 320 (3.82), 390 (3.59) [1]

IR: 2855, 1705, 1693, 1536, 1324 [1]

EI-MS: 557 $[M]^+$ (6), 341 (49), 295 (100) [1]

HR-FAB-MS: 558.2128 $[M + H]^+$ (calc. for $C_{32}H_{32}NO_8$, found 558.2123) [1]

CD (4.65×10^{-5} M, $CHCl_3$): $\Delta\varepsilon_{206}$ 8.62, $\Delta\varepsilon_{221}$ 2.28, $\Delta\varepsilon_{236}$ 0.54, $\Delta\varepsilon_{240}$ 0, $\Delta\varepsilon_{250}$ –1.18, $\Delta\varepsilon_{266}$ –1.78, $\Delta\varepsilon_{286}$ 0, $\Delta\varepsilon_{317}$ 244, $\Delta\varepsilon_{379}$ 0 [1]

^{1}H NMR (400 MHz, $CDCl_3$): 0.71 (3H, s, H-14), 1.36 (2H, m, H-9), 1.38 (3H, d, J = 6.0, H-13), 1.95 (1H, br d, J = 14.4, H-11b), 2.11 (2H, br s, H-8), 2.33 (1H, dd, J = 14.4, 8.0, H-11a), 3.42 (1H, s, H-5), 4.05 (3H, s, 8′-OMe), 4.79 (1H, d, J = 10.8, H-2b), 4.98 (1H, d, J = 17.6, H-2a), 5.17 (1H, m, H-12), 5.77 (1H, m, H-7′), 5.81 (1H, dd, J = 17.6, 10.8 Hz, H-1), 6.19 (1H, s, H-3b), 6.24 (1H, s, H-3a), 6.35 (1H, d, J = 1.2, H-12′), 6.36 (1H, d, J = 1.2, H-12′), 7.07 (1H, d, J = 8.0, H-7′), 7.68 (1H, t, J = 8.0, H-6′), 7.72 (1H, s, H-2′), 8.64 (1H,

d, J = 8.0, H-5′), 8.79 (1H, s, H-9′), 9.63 (1H, s, H-15) [1]

^{13}C NMR (100 MHz, $CDCl_3$): [1]

Table 1

C-1	145.5 d	C-12	71.1 d	C-5′	119.1 d
2	111.9 t	13	20.1 q	6′	130.7 d
3	137.4	14	25.9 q	7′	107.8 d
4	150.6 s	15	194.2 d	8′	156.8 s
5	43.5 d	1′	124.1 s	8′a	120.1 s
6	133.4 s	2′	112.7 d	9′	120.8 d
7	126.0 d	3′	145.9 s	10′	145.7 s
8	22.8 t	4′	146.3 s	10′a	118.3 s
9	27.9 t	4′a	118.4 s	11′	166.3 s
10	38.3 s	4′b	130.7 s	12′	102.3 t
11	42.3 t			8′-OMe	55.9 q

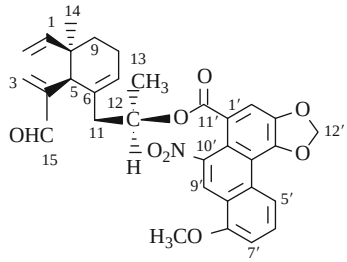
HMBC ($CDCl_3$) [1]
ROESY ($CDCl_3$) [1]

References

1. T.-S. Wu, Y.-Y. Chan, Y.-L. Leu, W. Pei-Lin, C.-Y. Li, Y. Mori, J. Nat. Prod. **62**, 348 (1999)
2. T.-S. Wu, Y.-Y. Chan, Y.-L. Leu, J. Nat. Prod. **64**, 71 (2001)

Aristophyllide B

CAS Registry Number: 221148-61-4



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Elemanes – Monoesters

Biological sources: *Aristolochia heterophylla* Hemsl. [1]

$C_{32}H_{31}NO_8$: 557.2050

Mp: 229–231°C (yellow needles) [1]

$[\alpha]_D$ −79° (*c* 0.0218, $CHCl_3$) [1]

UV: 224 (4.55), 249 (4.40), 268 (4.28), 283 (4.04), 318 (4.04), 390 (3.79) [1]

IR: 2856, 1707, 1693, 1536, 1342 [1]

EI-MS: 557 $[M]^+$ (1), 341 (17), 293 (100) [1]

HR-FAB-MS: 558.2128 $[M + H]^+$ (calc. for $C_{32}H_{32}NO_8$, found 558.2130) [1]

CD (4.69×10^{-5} M, $CHCl_3$): $\Delta\varepsilon_{211}$ −3.96, $\Delta\varepsilon_{227}$ −1.22, $\Delta\varepsilon_{244}$ 0, $\Delta\varepsilon_{244}$ 0, $\Delta\varepsilon_{261}$ 0.33, $\Delta\varepsilon_{272}$ 0, $\Delta\varepsilon_{336}$ −1.32, $\Delta\varepsilon_{384}$ 0 [1]

^{1}H NMR (400 MHz, $CDCl_3$): 0.75 (3H, s, H-14), 1.34 (3H, d, J = 6.5, H-13), 1.42 (2H, m, H-9), 2.09 (1H, m, H-11), 2.09 (2H, m, H-8), 2.30 (1H, dd, J = 14.0; 5.3, H-11), 3.43 (1H, s, H-5), 4.05 (3H, s, 8′-OMe), 4.94 (1H, d, J = 10.8, H-2a), 5.00 (1H, d, J = 17.5, H-2b), 5.09 (1H, q, J = 6.5, H-12), 5.71 (1H, m, H-7), 5.86 (1H, dd, J = 17.5; 10.8, H-1), 6.23 (2H, s, H-3), 6.36 (1H, d, J = 1.5, H-12′), 6.37 (1H, d, J = 1.5, H-12′), 7.10 (1H, d, J = 8.2, H-7′), 7.70 (1H, t, J = 8.2, H-6′), 7.76 (1H, s, H-2′), 8.68 (1H, d, J = 8.2, H-5′), 8.81 (1H, s, H-9′), 9.66 (1H, s, H-15) [1]

^{13}C NMR (100 MHz, $CDCl_3$) [1]:

Table 1

C-1	145.6 d	C-12	71.7 d	C-5′	119.1 d
2	111.9 t	13	19.7 q	6′	130.8 d
3	137.3 t	14	25.4 q	7′	107.8 d
4	150.5	15	194.2 d	8′	156.8 s
5	43.4 d	1′	124.0 s	8′a	120.2 s
6	133.6 s	2′	112.8 d	9′	120.9 d
7	125.7 d	3′	145.9 s	10′	145.9
8	22.9 t	4′	146.4 s	10′a	118.4 s
9	28.0 t	4′a	118.4 s	11′	166.2 s
10	38.3 s	4′b	130.8 s	12′	102.3 t
11	42.5 t			8-OMe	55.9 q

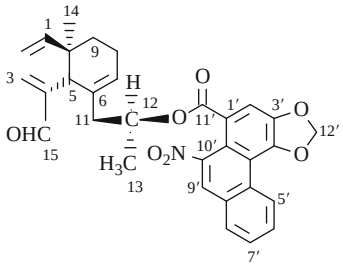
HMBC ($CDCl_3$) [1]
ROESY ($CDCl_3$) [1]

References

1. T.-S. Wu, Y.-Y. Chan, Y.-L. Leu, P.-L. Wu, C.-Y. Li, Y. Mori, J. Nat. Prod. **62**, 348 (1999)

Aristophyllide C

CAS Registry Number: 221148-62-5



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Elemanes – Monoesters

Biological sources: *Aristolochia heterophylla* Hemsl. [1]

$C_{31}H_{29}NO_7$: 527.1944

Mp: 217–219°C (yellow needles) [1]

$[\alpha]_D$ +113° (*c* 0.0656, $CHCl_3$) [1]

UV: 218 (4.33), 243 (4.32), 252 (4.37), 266 (4.20), 298 (3.98), 377 (3.48) [1]

IR: 2860, 1695, 1691, 1525, 1335 [1]

EI-MS: 527 $[M]^+$ (4), 311 (47), 265 (100)

HR-FAB-MS: 528.2022 $[M + H]^+$ (calc. for $C_{31}H_{30}NO_7$, found 528.2016) [1]

CD (3.54×10^{-5} M, $CHCl_3$): $\Delta\varepsilon_{205}$ 11.83, $\Delta\varepsilon_{218}$ 3.57, $\Delta\varepsilon_{231}$ 0.76, $\Delta\varepsilon_{235}$ 0, $\Delta\varepsilon_{247}$ −2.09, $\Delta\varepsilon_{255}$ −1.89, $\Delta\varepsilon_{278}$ 0, $\Delta\varepsilon_{301}$ 3.20, $\Delta\varepsilon_{381}$ 0 [1]

^{1}H NMR (400 MHz, $CDCl_3$): 0.66 (3H, s, H-14), 1.36 (2H, m, H-9), 1.38 (3H, d, J = 6.4, H-13), 1.95 (1H, br d, J = 15.0, H-11a), 2.12 (2H, br s, H-8), 2.33 (1H, dd, J = 15.0; 8.8, H-11b), 3.43 (1H, s, H-5), 4.79 (1H, d, J = 11.2, H-2a), 4.99 (1H, d, J = 17.6, H-2b), 5.17 (1H, q, J = 6.5, H-12), 5.78 (1H, m, H-7), 5.80 (1H, dd, J = 17.6; 11.2, H-1), 6.20 (1H, s, H-3a), 6.25 (1H, s, H-3b), 6.38 (1H, s, H-12′b), 6.40 (1H, 8, H-12′b), 7.70 (1H, t, J = 8.0, H-7′), 7.73 (1H, s, H-2′), 7.79 (1H, t, J = 8.0, H-6′), 7.97 (1H, d, J = 8.0, H-8′), 8.31 (1H, s, H-9′), 9.12 (1H, d, J = 8.0, H-5′), 9.64 (1H, 8, H-15) [1]

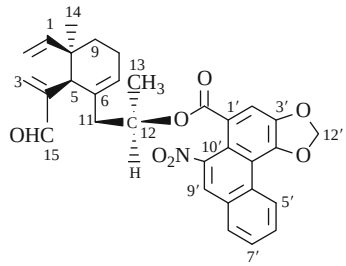
ROESY ($CDCl_3$) [1]

References

1. T.-S. Wu, Y.-Y. Chan, Y.-L. Leu, P.-L. Wu, C.-Y. Li, Y. Mori, J. Nat. Prod. **62**, 348 (1999)

Aristophyllide D

CAS Registry Number: 221148-63-6



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Elemanes – Monoesters

Biological sources: *Aristolochia heterophylla* Hemsl. [1]

$C_{31}H_{29}NO_7$: 527.1944

Mp: 220–222°C (yellow needles [1]

$[\alpha]_D$ −100° (*c* 0.0098, $CHCl_3$) [1]

UV: 219 (4.60), 242 (4.55), 252 (4.61), 266 (4.47), 297 (4.19), 355 (3.76), 373 (3.73) [1]

IR: 2858, 1699, 1649, 1521, 1342 [1]

EI-MS: 527 $[M]^+$ (10), 311 (23), 265 (56) [1]

HR-FAB-MS: 528.2022 $[M + H]^+$ (calc. for $C_{31}H_{30}NO_7$), found 528.2015 [1]

CD (4.65×10^{-5} M, $CHCl_3$): $\Delta\varepsilon_{209}$ −7.65, $\Delta\varepsilon_{225}$ −2.18, $\Delta\varepsilon_{244}$ 3.37, $\Delta\varepsilon_{284}$ 0, $\Delta\varepsilon_{310}$ −1.79, $\Delta\varepsilon_{338}$ −1.94, $\Delta\varepsilon_{384}$ 0 [1]

^{1}H NMR (400 MHz, $CDCl_3$): 0.72 (3H, s, H-14), 1.35 (3H, d, J = 6.4, H-13), 1.44 (2H, m, H-9), 2.10 (1H, m, H-11), 2.10 (2H, т, H-8), 2.32 (1H, dd, J = 14.2, 6.4, H-11), 3.42 (1H, s, H-5), 4.91 (1H, dd, J = 10.8; 0.8, H-2b), 5.00 (1H, dd, J = 17.6; 0.8, H-2a),

5.10 (1H, q, J = 6.4, H-12), 5.72 (1H, m, H-7), 5.85 (1H, dd, J = 17.6; 10.8, H-1), 6.24 (2H, s, H-3), 6.39 (1H, d, J = 1.4, H-12′b), 6.40 (1H, d, J = 1.4, H-12′a), 7.73 (1H, t, J = 8.3, H-7′), 7.77 (1H, s, H-2′), 7.79 (1H, t, J = 8.3, H-6′), 7.98 (1H, d, J = 8.3, H-8′), 8.33 (1H, s, H-9′), 9.13 (1H, d, J = 8.3, H-5′), 9.67 (1H, s, H-15) [1]

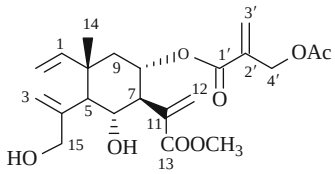
ROESY ($CDCl_3$) [1]

References

1. T.-S. Wu, Y.-Y. Chan, Y.-L. Leu, P.-L. Wu, C.-Y. Li, Y. Mori, J. Nat. Prod. **62**, 348 (1999)

8α-(4′-Acetoxy-2′-methylacryloyloxy)-6α,15-dihydroxy-elema-1(2),3(4),11(12)-triene-13-methyl Ester (4′-Acetylelemacarmanin)

CAS Registry Number: 248243-52-9



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Elemanes – Monoesters

Biological sources: *Onopordum illyricum* L. [1]

$C_{22}H_{30}O_8$: 422.1941

Mp: white yellow oil [1]

$[\alpha]_D^{25}$ +28° (*c* 0.05, MeOH) [1]

EI-MS: 409 (calc. for $C_{21}H_{29}O_8$) [1]

^{1}H NMR (600 MHz, CD_3OD): 1.22 (3H, s, H-14), 1.67 (1H, dd, J = 10.0; 12.5, H-9b), 1.75 (1H, dd, J = 4.0; 12.5, H-9a), 1.95 (1H, d, J = 11.5, H-5), 1.98 (3H, s, OAc), 2.68 (1H, m, H-7), 3.93 (1H, br s, H-15b), 4.03 (1H, br s, H-15a), 4.22 (1H, d, J = 11.0, H-4′b), 4.28 (1H, dd, J = 11.5; 12.0, H-6), 4.41 (1H, d, J = 11.0, H-4′a), 4.95 (1H, d, J = 17.5, H-2), 4.99 (1H, d, J = 11.0, H-2), 5.02 (1H, br s, H-3a), 5.38 (1H, m, H-8), 5.39 (1H, br s, H-3b), 5.77 (1H, br s, H-3′b), 5.81 (IH, dd, J = 11.0; 17.5, H-1), 5.85 (1H, br s, H-12b), 6.10 (1H, br s, H-12a), 6.30 (1H, br s, H-3′a) [1]

^{13}C NMR (600 MHz, CD_3OD) [1]:

Table 1

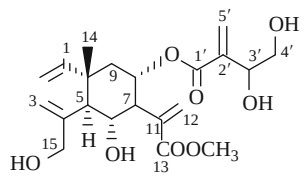
C-1	147.0	C-7	58.0	C-13	121.3
2	113.0	8	72.3	14	15.0
3	111.0	9	44.2	1′	167.0
4	140.5	10	40.0	OAc	175.0
5	52.0	11	138.0		21.0
6	72.6	12	169.0		

References

1. A. Braca, N. De Tommasi, I. Morelli, C. Pizza, J. Nat. Prod. **62**, 1371 (1999)

8α-(3′,4′-Dihydroxy-2′-methylenebutanoyloxy)-6α,15-dihydroxy-elema-1(2),3(4),11(12)-triene-13-methyl Ester (Methyl-8α-(3,4-dihydroxy-2-methylene-butanoyloxy)-6α,15-dihydroxyelema-1,3,11(12)-trien-13-oate)

CAS Registry Number: 189458-61-5



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Elemanes – Monoesters

Biological sources: *Centaurea paui* Loscos ex Willk. [1]; *C. attica* subsp. *attica* [2]; *Centaurea deusta* Ten. (=*Centaurea* alba subsp. deusta (Ten.) Nyman) [3]

$C_{21}H_{30}O_8$: 410.1941

Mp: colorless oil [1]

$[\alpha]_D^{22}$ −8.7° (*c* 0.3, $CHCl_3$) [1]

$[\alpha]_D$ +8.5° (*c* 0.3, $CHCl_3$) [2]

IR (NaCl): 3600–3300, 1710, 1650, 1180, 1090, 760 [1]

MS: 411 $[M + 1]^+$ (22), 280 $[M + 1 - C_4H_5(OH)_2COO]^+$ (22), 279 $[M - C_4H_5(OH)_2COO]^+$ (100), 263 [280 – OH]$^+$ (14), 262 [280 – $H_2O]^+$ (13), 261 [279 – $H_2O]^+$ (5) [1]

HR-MS: 411.2011 $[M + 1]^+$ (411.2010 calc. for $C_{21}H_{31}O_8$) [1]

^{1}H NMR (400 MHz, $CDCl_3$): 1.19 (3H, s, H-14), 1.61 (1H, dd, J = 11.6; 12.4, H-9α), 1.91 (1H, dd, J = 4.4; 12.4, H-9β), 2.11 (1H, d, J = 10.8, H-5), 2.71 (1H, t, J = 10.8, H-7), 3.50 (1H, dd, J = 6.8; 11.2, H-4′b), 3.71 (1H, dd, J = 3.2; 11.2, H-4′a), 3.77 (3H, s, MeO), 3.95 (1H, d, J = 13.2, H-15b), 4.08 (1H, d, J = 13.2, H-15a), 4.22 (1H, t, J = 10.8, H-6), 4.51 (1H, br dd, J = 3.2; 6.8, H-3′), 4.93 (d, J = 17.6, H-2b), 4.97 (d, J = 10.6, H-2a), 5.05 (s, H-3b), 5.40 (s, H-3a), 5.44 (ddd, J = 4.4; 10.8; 11.6, H-8β), 5.68 (dd, J = 10.6; 17.6, H-1), 5.74 (s, H-12b), 5.89 (s, H-5′b), 6.26 (s, H-5′a), 6.31 (s, H-12a) [1]

^{13}C NMR (50.32 MHz, $CDCl_3$) [1]:

Table 1

C-1	146.2[a]	C-8	71.1	C-15	67.8
2	112.1	9	43.5	1′	165.2
3	114.9	10	40.2	2′	139.1
4	146.2[a]	11	138.0[b]	3′	71.6
5	55.3	12	167.1	4′	65.7
6	70.9	13	128.4	5′	126.8
7	54.7	14	18.3	$COOCH_3$	52.0

[a]Overlapped signals

[b]The signals may be interchanged

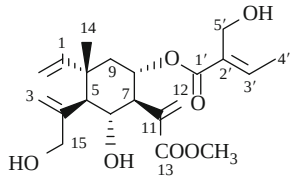
Pharm./Biol.: Antifungal activity [3]

References

1. L. Cardona, B. Garcia, M.C. Munoz, F.I. Navarro, J.R. Pedro, Liebigs Ann./Recl. **1997**, 527, (1997)
2. H. Skaltsa, D. Lazari, E. Georgiadou, S. Kakavas, T. Constantinidis, Planta Med. **65**, 393 (1999)
3. A. Karioti, H. Skaltsa, D. Lazari, M. Sokovic, B. Garcia, C. Harvala, Z. Naturforsch. **57C**, 75 (2002)

8α-(2′-Hydroxymethyl-2′-butenoyloxy)-6α,15-dihydroxy-elema-1(2),3(4),11(12)-triene-13-methyl Ester

CAS Registry Number: 174231-80-2



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Elemanes – Monoesters

Biological sources: *Onopordon myriacanthum* Boiss. [1]

$C_{21}H_{30}O_7$: 394.1992

Mp: oil [1]

$[\alpha]_D^{24}$ +21.2° (*c* 0.6, $CHCl_3$) [1]

IR (NaCl): 3500–3300, 1700, 1640 [1]

CI-MS: 395.2061 $[M + H]^+$ (8) ($C_{21}H_{31}O_7$, requires 395.2069), 280 (17), 279 (100), 261 (62) [1]

^{1}H NMR (400 MHz, $CDCl_3$): 1.18 (3H, s, H-14), 1.60 (1H, dd, J = 11.2; 12.8, H-9a), 1.79 (1H, dd, J = 4.4; 12.8, H-9b), 1.86 (3H, d, J = 7.2, H-4′), 2.10 (1H, d, J = 10.8, H-5), 2.71 (1H, t, J = 10.8, H-7), 3.76 (3H, s, MeO), 3.93 (1H, d, J = 13.2, H-15b), 4.06 (1H, d, J = 13.2, H-15a), 4.20 (1H, t, J = 10.8, H-6), 4.27 (2H, br s, H-5′), 4.91 (1H, d, J = 17.6,

H-2b), 4.95 (1H, d, J = 10.8, H-2a), 5.03 (1H, br s, H-3b), 5.38 (1H, br s, H-3a), 5.38 (1H, ddd, J = 4.4; 10.8; 11.2, H-8), 5.68 (1H, dd, J = 10.8; 17.6, H-1), 5.74 (1H, s, H-12b), 6.29 (1H, s, H-12a), 6.87 (1H, q, J = 7.2, H-3′) [1]

^{13}C NMR (75.43 MHz, $CDCl_3$) [1]:

Table 1

C-1	146.3	C-9	43.5	C-1′	166.4[a]
2	111.9	10	40.1	2′	131.7
3	114.8	11	138.0	3′	140.7
5	55.2	12	167.2[b]	4′	14.1
6	70.9	13	128.1	5′	56.7
7	54.4	14	18.3	CH_3O	51.9
8	70.7	15	67.7		

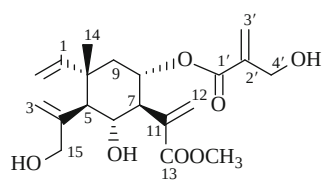
[a]Signals may be interchanged within each column
[b]Assignment by heteronuclear ^{1}H – ^{13}C correlation (HMQC)

References

1. B. Garcia, H. Skaltsa, F.I. Navarro, J.R. Pedro, D. Lazari, Phytochemistry **41**(4), 1113 (1996)

8α-(4′-Hydroxy-2′-methylacryloyloxy)-6α,15-dihydroxy-elema-1(2),3(4),11(12)-triene-13-methyl Ester (Elemacarmanin; (8-*O*-(2-Hydroxymethyl-propenoyl), Methyl Ester)

CAS Registry Number: 105242-48-6



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Elemanes – Monoesters

Biological sources: *Onopordon carmanicum* (Bornm.) Bornm. [1]; *O. corymbosum* Boiss. [2]; *O. ambiguum* Fresen. [3]; *O. anatolicum* Boiss. et Heldr. ex Boiss. [4]; *O. myriacanthum* Boiss. [5]; *O. acaulon* L. [6]; *Centaurea paui* Loscos ex Willk. [7]; *C. aspera* L. subsp. *aspera* [8]

$C_{20}H_{28}O_7$: 380.1835

Mp: colorless oil [1, 2]

$[\alpha]_D$ +29° (*c* 0.26, $CHCl_3$) [1]

IR ($CHCl_3$): 3605, 1715, 1630 [1]; 3550–3150, 1715, 1630 [2]

MS: 380 (0.1) $[M]^+$, 278.152 (3), 260 (4), 85 (100) [1]

MS: 278 $[M - (HO)MeacrOH]^+$ (4.9), 85 (57) [2]

HPLC [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.16 (3H, s, H-14), 1.60 (1H, t, J = 11; 13, H-9b), 1.90 (1H, dd, J = 4; 13, H-9a), 2.10 (1H, d, J = 10, H-5), 2.70 (1H, t, J = ~3; 11, H-7), 3.75 (3H, s, OCH_3), 3.90 (1H, d, J = 13, H-15b), 4.03 (1H, d, J = 13, H-15a), 4.18 (1H, t, J = 10; 10, H-6), 4.21 (2H, br s, H-3′), 4.91 (1H, br d, J = 17, H-2b), 4.95 (1H, br d, J = 11, H-2a), 5.01 (1H, br s, H-3b), 5.37 (1H, br s, H-3a), 5.41 (1H, ddd, J = 11; 11; 4, H-8), 5.68 (1H, dd, J = 11; 17, H-1), 5.72 (1H, br s, H-12b), 5.78 (1H, br s, H-4′b), 6.15 (1H, br s, H-4′a), 6.28 (1H, br s, H-12a) [1]

^{1}H NMR (400 MHz, $CDCl_3$) [6]

^{13}C NMR (50.32 MHz, $CDCl_3$): [2]

Table 1

C-1	146.31	C-8	70.92[a]	C-15	67.84
2	112.03	9	43.53	1′	165.42[b]
3	114.95	10	40.24	3′	126.01
4	139.33	11	137.97	4′	62.47
5	55.37[a]	12	128.35	OCH_3	52.03
6	70.92*	13	167.13		
7	54.66[a]	14	18.36		

*Overlapped signals
[a,b]Chemical shifts denoted by the same letter in each column may be interchanged [2]

References

1. A. Rustaiyan, B. Ahmadi, J. Jakupovic, F. Bohlmann, Phytochemistry **25**(7), 1659 (1986)
2. M.L. Cardona, B. Garcia, J.R. Pedro, J.F. Sinisterra, Phytochemistry. **28**(4), 1264 (1989)
3. F. Eid, S. El-Dahmy, Pharmazie **42**, 710 (1987)
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5. B. Garcia, H. Skaltsa, F.I. Navarro, J.R. Pedro, D. Lazari, Phytochemistry **41**(4), 1113 (1996)
6. L. Cardona, R.A. Aleman, B. Garcia, J.R. Pedro, Phytochemistry **31**(10), 3630 (1992)
7. L. Cardona, B. Garcia, M. C. Munoz, F. I. Navarro, J. R. Pedro, Liebigs Ann./Recl. **1997**, 527, (1997)
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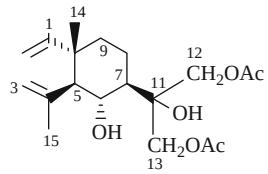
Elemanes

Diesters

12,13-Diacetoxy-6α,11-dihydroxy-elema-1(2),3(4)-diene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Elemanes – Diesters

Biological sources: *Magnolia grandiflora* L. [1]

$C_{19}H_{30}O_6$: 354.2042

Mp: 80–82.8°C (Me_2CO, colorless needles) [1]

$[\alpha]_D^{22}$ +14.88° (*c* 0.61, $CHCl_3$)[1]

IR (KBr): 3553, 3427, 2958, 1745, 1731, 1642, 1438, 1386, 1298, 1252, 1223, 1172, 1128, 1085, 1048, 976, 938, 913, 857 [1]

EI-MS: 354 $[M]^+$ (1), 337 $[M - OH]^+$ (4), 336 $[M - H_2O]^+$ (3), 318 $[M - 2H_2O]^+$ (1), 294 $[M - HOAc]^+$ (3), 281 $[M - CH_2COOCH_3]^+$ (30), 263 $[281 - H_2O]^+$ (20), 221 $[281 - HOAc]^+$ (50), 203 $[221 - H_2O]^+$ (40), 175 (30), 161 (49), 147 (33), 133(43), 121 (40), 109 (78), 93 (58), 81 (100), 67 (47), 55 (80) [1]

HR-FAB-MS (+): 355.2073 $[M + H]^+$ (calc. for $C_{19}H_{31}O_6$, 355.2120)

^{1}H NMR (400 MHz, $CDCl_3$): 0.91 (3H, s, H-14), 1.39 (2H, m, H-9), 1.56 (2H, m, H-8), 1.69 (3H, s, H-15), 1.86 (1H, ddd, J = 10.4; 10.2; 2.6, H-7), 1.95 (1H, dd, J = 10.4; 1.6, H-5), 2.02 (3H, s, OAc), 2.08 (3H, s, OAc), 2.82 (1H, br s, OH), 3.97 (1H, t, J = 10.4, H-6), 4.10 (2H, dt, J = 2.4; 12.0, H-13), 4.20 (2H, dt, J = 2.4; 12.0, H-12), 4.70 (1H, br s, H-3a), 4.82 (1H, d, J = 17.4, H-2a), 4.86 (1H, d, J = 10.4, H-2b), 5.06 (1H, br s, H-3b), 5.65 (1H, ddd, J = 17.4; 10.4; 1.8, H-1) [1]

^{13}C NMR (100 MHz, $CDCl_3$) [1]:

Table 1

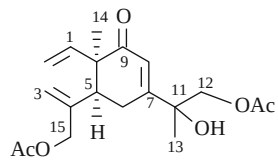
C-1	147.9 d	C-8	21.7 t	C-14	17.5 q
2	110.8 t	9	38.8 t	15	25.6 q
3	114.4 t	10	40.6 s	$CH_3\underline{C}OO$	170.5 s
4	143.4 s	11	74.4 s	$\underline{C}H_3COO$	170.8 s
5	60.8 d	12	65.5 t		20.7 q
6	70.3 d	13	66.6 t		20.7 q
7	48.5				

References

1. X.-D. Luo, S.-H. Wu, Y.-B. Ma, D.-G. Wu, J. Zhou, Planta Med. **67**, 354 (2001)

12,15-Diacetoxy-11-hydroxy-elema-1(2),3(4),7(8)-trien-9-one (Sipaucin B)

CAS Registry Number: 603110-57-2



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Elemanes – Diesters

Biological sources: *Siparuna pauciflora* (Beurl.) A. DC. (=*Citrosma paucifora* Beurl.)

$C_{19}H_{26}O_6$: 350.1729

Mp: yellow oil [1]

$[\alpha]_D^{20}$ +8° (*c* 0.25, $CHCl_3$) [1]

EI-MS: 350 $[M]^+$ (11), 332 (7), 290 (16), 277 (21), 272 (15), 233 (44), 184 (68), 142 (100), 124 (63), 106 (76), 91 (77) [1]

HR-EI-MS: 350.1728 (calc. for $C_{19}H_{26}O_6$, 350.1729), 332.1622 (calc. for $C_{19}H_{24}O_5$ 332.1624), 290.1514 (calc. for $C_{17}H_{22}O_4$ 290.1518) [1]

^{1}H NMR (400 MHz, $CDCl_3$): 1.17 (3H, s, H-14), 1.37 (3H, s, H-13), 2.05 (3H, s, OAc), 2.08 (3H, s, OAc), 2.44 (1H, dd, J = 5.5; 18.0, H-6a), 2.59 (1H, ddd, J = 5.5; 18.0, J = 1.5, H-6b), 2.73 (1H, t, J = 5.5,

H-5), 4.05 (1H, d, J = 12.0, H-12a), 4.27 (1H d, J = 12.0, H-12b), 4.41 (1H, d, J = 14.0, H-15a), 4.45 (1H, d, J = 14.0, H-15b), 5.02 (1H, br s, H-3a), 5.02 (1H, d, J = 17.0, H-2a), 5.15 (1H, d, J = 11.0, H-2b), 5.19 (1H, br s, H-3b), 5.83 (1H, dd, J = 11.0; 17.0, H-1), 6.30 (1H, br s, H-8) [1]

^{13}C NMR (125 MHz, $CDCl_3$): [1]

Table 1

C-1	140.6	C-9	201.1	C-1′	170.6
2	115.2	10	50.8	2′	20.9
3	115.8	11	74.0	1″	170.8
4	143.2	12	69.4	2″	20.7
5	47.0	13	23.6		
6	29.1	14	17.8		
7	162.5	15	67.2		
8	124.1				

(*continued*)

References

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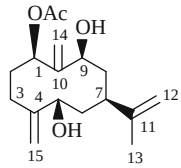
1β-Acetoxy-5α,7αH-germacra-4(15),10(14),11-triene-5β,9β-diol (1-*O*-Acetylageratriol)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Achillea ageratum* L. [1]

$C_{17}H_{26}O_4$: 294.1831

$[\alpha]_D^{20}$ +31° (*c* 0.16, $CHCl_3$)

IR (film): 3600–3200, 3077, 3069, 2930, 2874, 2856, 1730, 1644, 1463, 1454, 1445, 1433, 1373, 1241, 1077, 1024, 960, 924, 895, 803 [1]

PCI-MS: 295 $[M + H]^+$ (63), 277 (38), 235 (46), 217 (32), 199 (23) [1]

^{1}H NMR (300 MHz, $CDCl_3$): 1.51 (1H, ddd, J = 13; 10.5; 9, H-8β), 1.55–1.7 (3H, c, H-6α, 6β, H-7α), 1.69 (3H, s, H-13), 1.95 (1H, ddd, J = 13; 5; 1, H-8α), 2.05–2.3 (4H, c, H-2α, 2β, H-3α, 3β), 2.05 (3H, s, OAc), 3.96 (1H, dd, J = 11; 4, H-5α), 4.05 (1H, dd, J = 11.5; 5.5, H-9α), 4.68 (2H, br s, H-12), 5.19 (1H, s, H-15b), 5.21 (1H, s, H-15a), 5.30 (1H, m, H-1α), 5.51 (1H, s, H-14b), 5.74 (1H, s, H-14a) [1]

^{13}C NMR (75 MHz, $CDCl_3$) [1]:

Table 1

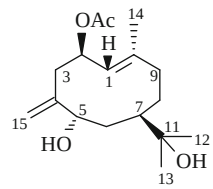
C-1	73.5 d	C-7	38.3 d	C-12	110.7 t
2	28.4 t	8	43.2 t	13	18.2 q
3	22.2 t	9	73.8 d	14	116.8 t
4	148.0 s	10	150.2 s	15	115.6 t
5	76.3 d	11	147.5 s	OAc	170.9 s
6	36.6 t				21.3 q

References

1. A. Kijjoa, L.M. Vieira, J.A. Pereira, A.M.S. Silva, W. Herz, Phytochemistry **51**(4), 555 (1999)

2β-Acetoxy-1(10),4(15)-germacradiene-5α,11-diol (Tanacetol B)

CAS Registry Number: 86787-28-2



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Tanacetum vulgare* L. [1]

$C_{17}H_{28}O_4$: 296.1988

Mp: 163°C (Et_2O), shining needles [1]

$[\alpha]_D^{25}$ −65.4° (*c* 1.5, MeOH) [1]

IR (KBr): 3200, 1735, 1670, 1240, 1030 [1]

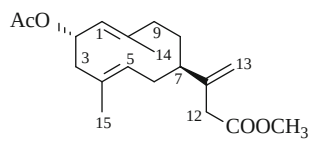
EI-MS: 296 $[M]^+$ (0.16), 236 (4.16), 160 (36), 145 (70), 59 (70), 43 (100) [1]

^{1}H NMR (200 MHz, $CDCl_3$, TMS): 1.11* (3H, s, H-12), 1.21* (3H, s, H-13), 1.70 (3H, br s, H-14), 1.80 (1H, m, H-7), 2.00 (3H, s, OAc), 2.53 (1H, ddd, J = 4, H-6a), 2.75 (1H, q, J = 10; 5.0; 13, H-3a), 3.80 (1H, br s, OH), 4.00 (1H, t, J = 4; 4, H-5), 5.06 (1H, br d, J = 11, H-1), 5.08 (1H, br s, H-15b), 5.19 (1H, br s, H-15a), 5.37 (1H, dq, J = 10; 5.0, H-2), H-3b, H-6b, H-8a,b, H-9a,b signals could not be observed because of overlapping; *Assignments are interchangeable [1]

References

1. G. Appendino, P. Gariboldi, G.M. Nano, Phytochemistry **22**(2), 509 (1983)

2α-Acetoxy-germacra-1(10) *E*,4*E*,11(13)-trien-12-oic Acid Methyl Ester (Methyl-2α-acetoxy-germacra-1(10) *E*,4*E*,11(13)-trien-12-oate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Cratystylis conocephala* (F. Muell.) S. Moore [1]

$C_{18}H_{26}O_4$: 306.1831

Mp: colorless oil [1]

$[\alpha]_D^{24}$ +82° (*c* 0.17, $CHCl_3$) [1]

IR (CCl_4): 1740, 1725, 1250 [1]

MS: 306.183 $[M]^+$ (0.2) (calc. for $C_{18}H_{26}O_4$: 306.183), 264 (2), 246 (14), 214 (6), 199 (10), 171 (12), 97 (100) [1]

HPLC [1]

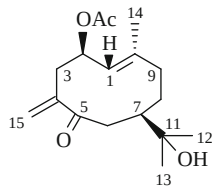
^{1}H NMR (400 MHz, $CDCl_3$): 1.57 (3H, br s, H-14), 1.60 (3H, br s, H-15), 2.07 (3H, s, OAc), 3.76 (3H, s, OCH_3), 4.30 (1H, br d, J = 10, H-5), 4.42 (1H, br d, J = 10, H-1), 5.53 (1H, br s, H-13b), 5.61 (1H, ddd, J = 10; 10; 5, H-2), 6.12 (1H, br s, H-13a) [1]

References

1. C. Zdero, F. Bohlmann, L. Haegi, R.M. King, Phytochemistry **27**(3), 865 (1988)

2β-Acetoxy-11-hydroxy-1(10),4(15)-germacradien-5-one (Tanacetol A; 5-Ketone-2β-acetoxy-1(10),4(15)-germacradiene-11-ol)

CAS Registry Number: 86778-06-5



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Tanacetum vulgare* L. [1]

$C_{17}H_{26}O_4$: 294.1831

Mp: 98°C (C_6H_6 – EtOAc), needles [1]

$[\alpha]_D^{25}$ −99° (*c* 1.0, $CHCl_3$) [1]

UV (EtOH): 218 (3.8) [1]

IR (KBr): 3200, 1735, 1670, 1240, 1030 [1]

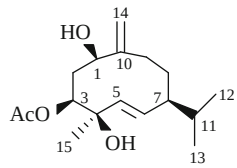
EI-MS: 294 $[M]^+$ (4.73), 279 (2.3), 276 (4.7), 234 (89), 97 (100) [1]

^{1}H NMR (200 MHz, $CDCl_3$, TMS): 1.15* (3H, s, H-12), 1.24* (3H, s, H-13), 1.60 (1H, m, H-7), 1.72 (3H, br s, H-14), 2.02 (3H, s, OAc), 2.27 (1H, br s, OH), 2.34 (1H, dd, J = 14; 3, H-6b), 2.65 (1H, dd, J = 6; 12, H-3b), 2.94 (1H, dd, J = 9; 12, H-3a), 3.12 (1H, dd, J = 14; 10, H-6a), 5.06 (1H, br d, J = 9, H-1), 5.40 (1H, td, J = 9; 9; 6, H-2), 5.58 (1H, br s, H-15b), 5.67 (1H, br s, H-15a); H-8a,b, H-9a,b signals could not be observed because of overlapping; * – Assignments are interchangeable [1]

References

1. G. Appendino, P. Gariboldi, G.M. Nano, Phytochemistry **22**(2), 509 (1983)

3β-Acetoxy-germacra-5*E*,10(14)-diene-1β,4β-diol



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Senecio adenophyllus* Walp. [1]

$C_{17}H_{28}O_4$: 296.1988

Mp: gum [1]

$[\alpha]_D^{24}$ −54° (*c* 0.8, $CHCl_3$) [1]

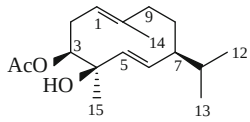
IR ($CHCl_3$): 3600, 1735 [1]

MS: 296.199 $[M]^+$ (1) (calc. for $C_{17}H_{28}O_4$: 296.199), 236 $[M - HOAc]^+$ (32), 218 $[236 - H_2O]^+$ (14), 193 $[236 - C_3H_7]^+$ (55), 175 $[193 - H_2O]^+$ (58), 139 (80), 109 (88), 97 (80), 81 (75), 71 (100) [1]

HPLC: MeOH – H_2O (3:1), R_t 7.1 min [1]

^{1}H NMR (400 MHz, $CDCl_3$): 0.84 (3H, d, J = 7, H-13), 0.89 (3H, d, J = 7, H-12), 1.24 (3H, s, H-15), 1.50 (1H, m, H-11), 1.85 (1H, m, J = 10, H-7), 1.90 (1H, m, J = 3; 15; 1, H-2a), 2.12 (3H, s, OAc), 2.63 (1H, ddd, J = 10; 15; 7, H-2b), 4.30 (1H, dd, J = 10; 3, H-1), 4.43 (1H, dd, J = 7; 1, H-3), 4.85 (1H, br s, H-14b), 4.96 (1H, d, J = 15, H-5), 5.18 (1H, br s, H-14a), 5.45 (1H, dd, J = 15; 10, H-6) [1]

3β-Acetoxy-7α(H)-germacra-[3 *S**,4*R**, 7 *S**]-1(10)*E*,5*E*-dien-4β-ol



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Pallenis spinosa* (L.) Cass. [1, 2]; *Senecio adenophyllus* Walp. [3]

$C_{17}H_{28}O_3$: 280.2038

Mp: 113°C (hexane), colorless needles [1]

$[\alpha]_D^{25}$ −145° (*c* 0.80, CH_2Cl_2) [1]

IR (KBr): 3500, 1710, 1675, 1375, 1270, 1200, 1030, 975 [1]

EI-MS: 280 $[M]^+$ (11), 220 (14), 81 (95), 71 (22), 43 (100) [1]

^{1}H NMR (300 MHz, $CDCl_3$, TMS): 0.78 (3H, d, J = 6.1, H-13), 0.82 (3H, d, J = 6.1, H-12), 1.16 (3H, s, H-15), 1.54 (3H, br s, H-14), 2.10 (3H, s, OAc), 2.70 (2H, dt, J = 14.3; 12.3; 12.3, H-2), 4.76 (1H, dd, J = 12.3; 4.2, H-3), 5.02 (1H, br d, J = 12.3, H-1), 5.16 (1H, d, J = 15.6, H-5), 5.35 (1H, dd, J = 15.6; 10.7, H-6) [1]

^{13}C NMR (75.1 MHz, $CDCl_3$, TMS): [1]

Table 1

C-1	125.14 d	C-7	52.81 d	C-13	18.97 q[a]
2	30.05 t	8	23.74 t	14	16.90 q
3	76.67 d	9	41.03 t	15	26.2 q
4	74.64 s	10	133.93 s	OAc	170.32 s
5	135.19 d	11	33.03 d		21.16 s
6	127.31 d	12	20.56 q[a]		

[a]Assignment may be interchanged [1]

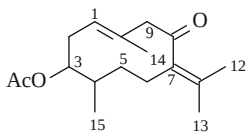
References

1. S. Dupre, M. Grenz, J. Jakupovic, F. Bohlmann, H.M. Niemeyer, Phytochemistry **30**(4), 1211 (1991)

References

1. G. Appendino, G. Cravotto, P. Gariboldi, F. Claudi, V. Picci, Phytochemistry **28**(3), 849 (1989)
2. G. Appendino, J. Jakupovic, S. Jakupovic, Phytochemistry **46**(6), 1039 (1997)
3. S. Dupre, M. Grenz, J. Jakupovic, F. Bohlmann, H.M. Niemeyer, Phytochemistry **30**(4), 1211 (1991)

3-Acetoxy-germacra-1(10),7(11)-dien-8-one



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Eugenia uniflora* L. (= *E. michelii* Lam., *Stenocalyx michelii* Berg, *S. brasiliensis* Berg) [1]

$C_{17}H_{26}O_3$: 278.1881

Mp: oil [1]

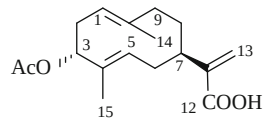
GC-MS: 278.1881 $[M]^+$ (calc. for $C_{17}H_{26}O_3$: 278.1882) (2), 236 (8), 218 (18). 203 (10), 175 (18), 139 (22), 123 (40), 109 (40), 107 (40), 95 (46), 81 (64), 69 (68), 67 (100), 55 (55) [1]

^{1}H NMR (57°C): 0.96 (3H, d, J = 7, H-15), 1.69, 1.72, 1.78 (each 3H, s, H-12, H-13, H-14), 2.03 (3H, s, OAc), 2.26 (1H, dd, AB, J = 14; 10; 2.5, H-2a), 2.61 (1H, AB, J = 14, dd, J = 7; 6.5, H-2b), 2.37 (2H, ddd, J = 14; 4; 4, H-6), 3.09 (1H, d, J = 11.5, H-9a), 3.41 (1H, d, J = 11.5, H-9b), 5.06 (1H, ddd, 7 = 6.5; 6.5; 2.5, H-3), 5.35 (1H, br dd, J = 10; 7, H-1) [1]

References

1. P. Weyerstahl, H. Marschall-Weyerstahl, C. Christiansen, B.O. Oguntimein, A.O. Adeoye, Planta Med. **54**, 546 (1988)

3α-Acetoxy-germacr-1(10)*E*,4*E*,11(13)-en-12-oic Acid



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Haeckeria punctulata* (F. Muell.) J. H. Willis [1]

$C_{17}H_{24}O_4$: 292.1675

Mp: isolated as its methyl ester [1]

IR (CCl_4) (its methyl ester): 3600, 1740, 1725, 1250 [1]

MS (its methyl ester): 246.162 $[M - HOAc]^+$ (18) (calc. for $C_{16}H_{22}O_2$: 246.162) [1]

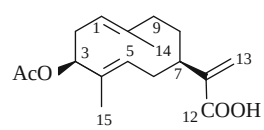
HPLC (its methyl ester): MeOH – H_2O (4:1), R_t 9.3 min [1]

^{1}H NMR ($CDCl_3$) (its methyl ester): 1.56 (3H, br s, H-14), 1.62 (3H, br s, H-15), 2.07 (3H, s, OAc), 2.81 (1H, m, H-7), 3.77 (3H, s, OCH_3), 5.18 (1H, m, H-5), 5.31 (1H, m, H-1), 5.39 (1H, m, H-3), 5.55 (1H, br s, H-13b), 6.14 (1H, br s, H-13a) [1]

References

1. C. Zdero, F. Bohlmann, A. Anderberg, R.M. King, Phytochemistry **30**(8), 2643 (1991)

3β-Acetoxy-germacr-1(10)*E*,4*E*,11(13)-en-12-oic Acid



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Haeckeria punctulata* (F. Muell.) J. H. Willis [1]

$C_{17}H_{24}O_4$: 292.1675

Mp: isolated as its methyl ester [1]

IR (CCl_4) (its methyl ester): 3600, 1740, 1725, 1250 [1]

MS (its methyl ester): 306.183 $[M]^+$ (3) (calc. for $C_{18}H_{26}O_4$: 306.183) [1]

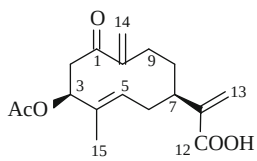
HPLC (its methyl ester): MeOH – H_2O (4:1), R_t 9.7 min [1]

^{1}H NMR ($CDCl_3$) (its methyl ester): 1.45 (3H, br s, H-14), 1.52 (3H, br s, H-15), 2.08 (3H, s, OAc), 3.76 (3H, s, OCH_3), 4.82 (1H, br t, J = ~7, H-5), 4.93 (1H, dd, J = 12; 4, H-1), 5.12 (1H, br dd, J = 10; 5, H-3), 5.56 (1H, br s, H-13b), 6.10 (1H, br s, H-13a) [1]

References

1. C. Zdero, F. Bohlmann, A. Anderberg, R.M. King, Phytochemistry **30**(8), 2643 (1991)

3β-Acetoxy-1-oxo-7α(H)-germacra-4(5)*E*,10(14),11(13)-trien-12-oic Acid



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Haeckeria punctulata* (F. Muell.) J. H. Willis [1]

$C_{17}H_{22}O_5$: 306.1467

Mp: isolated as its methyl ester [1]

IR (CCl_4) (its methyl ester): 1750, 1730, 1680 [1]

MS (its methyl ester): 320.162 $[M]^+$ (1) (calc. for $C_{18}H_{24}O_5$: 320.162), 278 (6), 260 (25), 246 (57), 231 (20), 119 (56), 105 (66), 91 (88), 55 (100) [1]

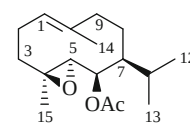
HPLC (its methyl ester): MeOH – H_2O (4:1), R_t 3.4 min [1]

^{1}H NMR ($CDCl_3/C_6D_6$) (its methyl ester): 1.40 (1H, m, H-8b), 1.52 (1H, m, H-8a), 1.77 (1H, m, H-6a), 1.86 (3H, s, OAc), 2.02 (1H, m, H-6b), 2.02 (1H, m, H-9b), 2.48 (1H, m, H-7), 2.58 (1H, dd, J = 11; 5.5, H-2α), 2.63 (1H, br dt, J = 4; 4; 14, H-9a), 3.18 (1H, t, J = 11; 11, H-2β), 3.55 (3H, s, OCH_3), 5.32 (1H, dd, J = 11; 5.5, H-3), 5.34 (1H, br s, H-13b), 5.40 (1H, br t, J = 7.5; 7.5, H-5), 5.56 (1H, br s, H-14b), 5.62 (1H, br s, H-14a), 6.03 (1H, br s, H-13a) [1]

References

1. C. Zdero, F. Bohlmann, A. Anderberg, R.M. King, Phytochemistry **30**(8), 2643 (1991)

6β-Acetoxy-4β,5α-epoxy-*trans*-germacr-1(10)-ene (Shiromool Acetate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Sideritis varoi* subsp. *cuatrecasasii* [1]; *S. varoi* subsp. *nijarensis* [2]

$C_{17}H_{28}O_3$: 280.2038

Mp: 45–47°C [1]

$[\alpha]_D^{20}$ +48.4° (*c* 1, $CHCl_3$) [1]

IR (KBr): 3110, 2980, 1745, 1230, 860 [1]

MS: 280 $[M]^+$ (3), 262 (3), 251 (3), 237 (8), 220 (10), 205 (13), 202 (10), 195 (10), 191 (15), 187 (10), 177 (55), 162 (30), 159 (45), 149 (38), 147 (38), 135 (50), 122 (55), 107 (100) [1]

Found: C, 72.85; H, 10.09; calc. for $C_{17}H_{28}O_3$: C, 72.82; H, 10.06% [1]

^{1}H NMR (80 MHz, $CDCl_3$): 0.85 (3H, d, J = 6.5, H-13), 0.96 (3H, d, J = 6.5, H-12), 1.25 (3H, s, H-15), 1.67 (3H, br s, H-14), 2.05 (3H, s, OAc), 2.62 (1H, d, J = 8, H-5), 4.97 (1H, dd, J = 8; 1.5, H-6), 5.27 (1H, br t, J = 7, H-1) [1]

^{13}C NMR (20.13 MHz, $CDCl_3$) [1]:

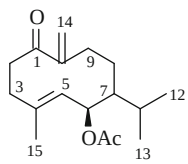
Table 1

C-1	123.59 d	C-7	45.97 d	C-13	20.66 q
2	22.97 t	8	26.61 t	14	16.45 q
3	37.17 t	9	38.25 t	15	18.61 q
4	59.60 s	10	136.75 s	OAc	170.00 s
5	66.06 d	11	31.43 d		20.98 q
6	74.13 d	12	20.66 q		

References

1. A. Garcia-Granados, A. Molina, E. Cabrera, Tetrahedron **42**, 81 (1986)
2. E. Cabrera, A. Garcia-Granados, M.A. Quecuty, Phytochemistry **27**(1), 183 (1988)

6β-Acetoxy-germacra-4*E*,10(14)-dien-1-one



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Liabum floribundum* Less. [1]

$C_{17}H_{26}O_3$: 278.1882

Mp: 100°C [1]

$[\alpha]^{24}$ (λ, nm): −113° (589), −118° (578), −138° (546), −258° (436) (*c* 0.18, $CHCl_3$) [1]

IR ($CHCl_3$): 1735, 1684, 1640 [1]

MS: 278.188 $[M]^+$ (5) (calc. for $C_{17}H_{26}O_3$: 278.188), 236 (12), 218 (38), 190 (21), 175 (69), 109 (100) [1]

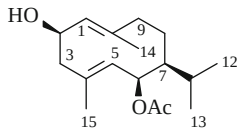
TLC: C_6H_6 – CH_2Cl_2 – Et_2O (6:6:1), R_f 0.64 [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 0.84 (1H, m, H-7), 0.92 (3H, d, J = 7, H-12), 1.29 (1H, dddd, J = 4; 14, H-8b), 1.55 (1H, m, H-11), 1.61 (3H, s, H-15), 1.81 (1H, ddd, J = 16.5; 14, H-9b), 1.87 (3H, d, J = 7, H-13), 1.89 (1H, dddd, J = 3; 14; 14, H-8a), 1.96 (3H, s, OAc), 2.15 (1H, m, H-2b), 2.15 (1H, m, H-3b), 2.47 (1H, ddd, J = 6; 13; 13, H-3a), 2.92 (1H, br d, J = 16.5, H-9a), 3.23 (1H, ddd, J = 13; 13; 6, H-2a), 5.01 (1H, br d, J = 7, H-5), 5.44 (1H, br dd, J = 7; 2.5, H-6), 5.54 (1H, br s, H-14b), 5.75 (1H, s, H-14a) [1]

References

1. F. Bohlmann, K. Umemoto, J. Jakupovic, R.M. King, H. Robinson, Phytochemistry **23**(8), 1800 (1984)

6β-Acetoxy-7α(H)-germacra-1(10),4*E*-dien-2β-ol



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Santolina chamaecyparissus* ssp. *squarrosa* (DC.) Nyman [1]

$C_{17}H_{28}O_3$: 280.2038

Mp: colorless syrup [1]

$[\alpha]_D^{20}$ −15.9° (*c* 1, $CHCl_3$) [1]

IR (film): 3421, 2933, 1736, 1632, 1437, 1368, 1241, 1138, 1101, 1020, 974, 865, 802 [1]

EI-MS: 280 $[M]^+$ (1), 265 (1), 220 (7), 205 (6), 176 (47), 161 (12), 149 (9), 133 (36), 123 (28), 107 (42), 93 (38), 81 (19), 69 (16), 55 (23), 43 (100) [1]

^{1}H NMR (400 MHz): 0.92 (3H, d, J = 7.6, H-12), 0.96 (3H, d, J = 7.8, H-13), 1.55 (3H, s, H-15), 1.71 (3H, s, H-14), 2.02 (3H, s, OAc), 2.55 (1H, dd, J = 11.1; 5.5, H-3α), 4.66 (1H, dt, J = 10.0; 5.5, H-2), 5.04 (1H, d, J = 10.0, H-1), 5.07 (1H, d, J = 7.1, H-5), 5.55 (1H, dd, J = 7.1; 1.8, H-6) [1]

^{13}C NMR [1]:

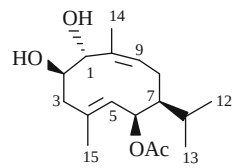
Table 1

C-1	131.7	C-7	47.6	C-13	22.2
2	72.1	8	29.9	14	17.3
3	47.8	9	35.2	15	17.2
4	137.3	10	137.3	$OCOCH_3$	170.4
5	131.8	11	31.1	$OCOCH_3$	20.7
6	66.5	12	20.4		

References

1. A.F. Barrero, R. Alvarez-Manzaneda, J.F. Quilez, M.M. Herrador, Phytochemistry **48**(5), 807 (1998)

6β-Acetoxy-7αH-germacra-4*E*,9*Z*-diene-1α,2β-diol ((4*E*,9*Z*)-6β-Acetoxy-7αH-germacra-4,9-diene-1α,2β-diol)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Santolina chamaecyparissus* ssp. *squarrosa* (DC.) Nyman [1]

$C_{17}H_{28}O_4$: 296.1988

$C_{23}H_{42}O_4Si$: 410.2852 (isolated as 2-TBDMS derivative: (4*E*,9*Z*)-6β-Acetoxy-2β-(*tert*-butyldimethylsilyloxy)-7αH-germacra-4,9-dien-1α-ol)

Mp (2-TBDMS derivative): colorless syrup [1]

$[\alpha]_D^{20}$ (2-TBDMS derivative): +24.3° (*c* 1, $CHCl_3$) [1]

IR (film) (2-TBDMS derivative): 3406, 2958, 2930, 1736, 1460, 1368, 1259, 1023, 836, 801 [1]

EI-MS (2-TBDMS derivative): 392 $[M - 18]^+$ (1), 307 (5), 293 (18), 279 (7), 253 (7), 219 (6), 198 (94), 175 (16), 159 (22), 141 (85), 119 (26), 105 (20), 75 (100), 43 (62) [1]

^{1}H NMR (400 MHz, 25°C) (2-TBDMS derivative): 0.03 (3H, s, MeSiMe), 0.10 (3H, s, MeSiMe), 0.89 (3H, d, J = 6.7, H-12), 0.90 (3H, s, $(Me)_3$ C), 0.98 (3H, d, J = 6.7, H-13), 1.57 (3H, s, H-15), 1.63 (3H, br s, H-14), 2.07 (3H, s, OAc), 2.43 (2H, ddd, J = 14; 12.5; 7.7, H-8), 3.67 (1H, br dt, J = 8.2; 5.2, H-2), 4.36 (1H, d, J = 7.8, H-1), 5.12 (1H, dd, J = 12.7; 4.7, H-9), 5.23 (1H, br s, H-5), 5.52 (1H, br t, J = 6.3, H-6) [1]

^{13}C NMR (2-TBDMS derivative) [1]:

Table 1

C-1	73.4	C-9	129.8	OCOMe	189.4
2	67.9	10	[a]	$OCOCH_3$	21.3[b]
3	47.5	11	30.1[b]	CH_3SiCH_3	−4.6
4	[a]	12	20.1[b]	CH_3SiCH_3	−4.9
5	126.6	13	20.7[b]	$(CH_3)_3$ C	[a]
6	72.9	14	18.2	$(CH_3)_3$ C	25.8
7	29.7[b]	15	17.4		
8	26.8				

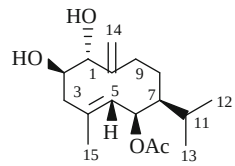
[a]Not observable

[b]Assignments with the same symbol may be interchanged

References

1. A.F. Barrero, R. Alvarez-Manzaneda, J.F. Quilez, M.M. Herrador, Phytochemistry **48**(5), 807 (1998)

6β-Acetoxy-7αH-germacra-4*E*,10(14)-diene-1α,2β-diol



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Santolina chamaecyparissus* ssp. *squarrosa* (DC.) Nyman [1]

$C_{17}H_{28}O_4$: 296.1988

$C_{20}H_{32}O_4$: 336.2301 (isolated as acetonide derivative: 6β-acetoxy-1α,2β-isopropoxy-5β,7αH-germacra-4*E*,10(14)-diene)

Mp: colorless syrup [1]

Mp (acetonide derivative): colorless syrup [1]

$[\alpha]_D^{20}$ −37.5° (*c* 1, $CHCl_3$) [1]

$[\alpha]_D^{20}$ (acetonide derivative): −53.0° (*c* 1, $CHCl_3$) [1]

IR (film): 3402, 2959, 2925, 1737, 1441, 1368, 1259, 1241, 1023, 801 [1]

IR (film) (acetonide derivative): 3070, 2958, 2937, 1728, 1647, 1449, 1368, 1241, 1167, 1108, 1030, 980, 891, 818 [1]

EI-MS: 236 $[M - AcOH]^+$ (24), 218 (21), 203 (12), 193 (21), 189 (7), 175 (45), 157 (17), 147 (21), 119 (16), 109 (16), 91 (21), 79 (14), 69 (20), 55 (19), 43 (100) [1]

EI-MS (acetonide derivative): 336 $[M]^+$ (4), 276 (2), 261 (1), 218 (9), 201 (8), 175 (25), 163 (7), 147 (15), 140 (16), 121 (15), 109 (26), 95 (23), 81 (21), 69 (20), 55 (17), 43 (100) [1]

^{1}H NMR (400 MHz, $CDCl_3$) (acetonide derivative): 0.91 (3H, d, J = 6.6, H-12), 0.95 (3H, d, J = 6.7, H-13), 1.25 (1H, m, H-7α), 1.40 (3H, s, H-17), 1.44 (3H, s, H-18), 1.51 (1H, m, H-8α), 1.53 (1H, m, H-11), 1.59 (3H, br s, H-15), 1.87 (1H, m, H-8β), 2.04 (3H, s, OAc), 2.07 (1H, ddd, J = 14.5; 10.4; 3.0, H-9α), 2.16 (1H, t, J = 11.3, H-3β), 2.40 (1H, ddd, J = 14.8; 7.5; 4.5, H-9β), 2.58 (1H, dd, J = 11.8; 4.3, H-3α), 3.95 (1H, d, J = 8.7, H-1), 4.06 (1H, ddd, J = 10.8; 8.8; 4.4, H-2), 5.10 (1H, s, H-14a), 5.31 (1H, s, H-14b), 5.32 (1H, br d, J = 5.7, H-5β), 5.54 (1H, br d, J = 5.7, H-6α) [1]

^{13}C NMR (100 MHz, $(CD_3)_2CO$) [1]:

Table 1

C-1	77.8	C-7	43.7	C-13	21.2
2	73.1	8	24.3	14	113.1
3	47.1	9	36.3	15	17.9
4	130.1	10	150.1	$OCOCH_3$	170.5
5	131.9	11	31.7	$OCOCH_3$	21.0
6	72.8	12	21.1		

^{13}C NMR (75 MHz) (acetonide derivative): [1]

Table 2

C-1	81.6	C-8	24.2	C-15	18.0
2	79.3	9	36.8	16	108.7
3	43.7	10	144.5	17	27.2
4	130.1	11	31.3	18	27.3
5	130.8	12	20.9	$OCOCH_3$	107.8
6	72.8	13	21.0	$OCOCH_3$	21.2
7	44.4	14	116.3		

COSY (acetonide derivative) [1]

HETCOR (acetonide derivative) [1]

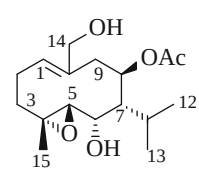
HMBC (acetonide derivative) [1]

References

1. A.F. Barrero, R. Alvarez-Manzaneda, J.F. Quilez, M.M. Herrador, Phytochemistry **48**(5), 807 (1998)

8β-Acetoxy-4α,5β-epoxy-7βH-germacr-1(*E*)-ene-6α,14-diol (Pulicanol)

CAS Registry Number: 851595-68-1



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Pulicaria canariensis* Bolle subsp. *canariensis* [1]

$C_{17}H_{28}O_5$: 312.1937

Mp: colorless oil [1]

IR (KBr): 3404, 2929, 1736, 1647, 1470, 1375, 1243, 1088, 1023, 963, 897 [1]

EI-MS: 312 $[M]^+$ (2), 279 (11), 252 (4), 234 (5), 216 (4), 173 (14), 171 (16), 167 (37), 149 (87), 133 (32), 129 (33), 123 (46), 121 (50), 111 (56), 105 (48), 97 (87), 95 (91), 91 (57), 85 (70), 83 (100), 57 (89), 55 (96) [1]

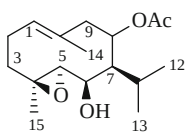
^{1}H NMR ($CDCl_3$, 400 MHz): 0.95 (3H, d, J = 6.4, H-13), 1.12 (3H, d, J = 6.4, H-12), 1.16 (3H, s, H-15), 1.59 (1H, m, H-7), 1.80 (1H, m, H-11), 2.10 (1H, m, H-3b), 2.15 (3H, s, OAc), 2.34 (1H, m, H-3a), 2.53 (2H, d, J = 12.4, H-9), 2.82 (1H, d, J = 7.7, H-5), 3.51 (1H, m, H-6), 4.12 (1H, d, J = 11.6, H-14b), 4.29 (1H, d, J = 11.8, H-14a), 5.18 (1H, dd, J = 5.2, 12.0, H-8), 5.45 (1H, t, J = 6.8, H-1) [1]

References

1. J. Triana, M. Lopez, F.J. Perez, J. Gonzalez-Platas, J. Quintana, F. Estevez, F. Leon, J. Bermejo, J. Nat. Prod. **68**, 523 (2005)

8-Acetoxy-4,5-epoxy-5β,6α,7α(H)-germacr-1(10)-en-6-ol (Shiromodiol 8-Monoacetate)

CAS Registry Number: 20071-59-4



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Parabenzoin trilobum* Nakai (=*Lindera triloba* (Siebold & Zucc.) Blume) [1, 2]

$C_{17}H_{28}O_4$: 296.1988

Mp: 80°C [1]; 78–80°C [3]

$[\alpha]_D^{25}$ −44.8° (*c* 0.34, $CHCl_3$) [1, 3]

IR (KBr): 3460, 1700, 1250 [1]

MS: 296 $[M]^+$ [3]

^{1}H NMR (100 MHz, $CDCl_3$, TMS) (its 6,8-diOAc) [1]

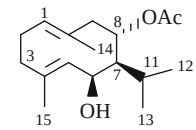
Chemistry of shiromodiol 8-monoacetate [3]

Parm./Biol.: Showed 100% antifeeding activity against *Prodenia litura* at 0.5% concentration; on entomological test against an Oligophagous insect, *Trimeresia miranda* Butler, the former showed 100% antifeeding activity at 0.13% concentration, while the latter showed only weak activity even at 0.25% [1]; inhibitors against a polyphagous insect, *Spodoptera littoralis* Boisd, and an oligophagous insect, *Trimeresia miranda* Butler [2]

References

1. K. Wada, Y. Enomoto, K. Matsui, K. Munakata, Tetrahedron Lett. **9**, 4673 (1968)
2. K. Wada, K. Matsui, Y. Enomoto, O. Ogiso, K. Munakata, Agr. Biol. Chem. **34**, 941 (1970)
3. K. Wada, Y. Enomoto, K. Munakata, Agr. Biol. Chem. **34**, 946 (1970)

8α-Acetoxy-6α,7α(H)-germacra-1(10),4-dien-6β-ol (8-Acetyltovarol)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Pallenis spinosa* (L.) Cass. [1]

$C_{17}H_{28}O_3$: 280.2038

Mp: colorless oil [1]
IR (liquid film): 3400 (OH), 1735, 1240 (OAc) [1]
MS: 280 $[M]^+$ (2), 220 $[M - AcOH]^+$ (56), 205 $[220 - CH_3]^+$ (20), 177 $[220 - (CH_3)_2CH]^+$ (82), 159 $[177 - H_2O]^+$ (70), 136 (85), 109 (52), 93 (75), 81 (100), 43 (99) [1]
^{1}H NMR (400 MHz, $CHCl_3$): 1.03 (3H, d, J = 7.0, H-12), 1.05 (3H, d, J = 7.0, H-13), 1.20 (1H, ddd, J = 11.0; 2.5; 2.0, H-7), 1.42 (3H, br s, H-15), 1.60 (1H, dqq, J = 11.0; 7.0; 7.0, H-11), 1.64 (3H, br s, H-14), 2.00 (1H, dd, J = 13.5; 12.0, H-9b), 2.07 (3H, s, OAc), 2.12 (1H, m, H-2b), 2.12 (1H, m, H-3a), 2.12 (1H, m, H-3b), 2.33 (1H, m, H-2a), 2.55 (1H, br dd, J = 13.5; 6.0, H-9a), 4.44 (1H, br dd, J = 8.0; 2.5, H-6), 5.00 (1H, br d, J = 12.0, H-1), 5.10 (1H, ddd, J = 12.0; 6.0; 2.0, H-8), 5.18 (1H, br d, J = 8.0, H-5) [1]
^{13}C NMR (75 MHz, $CDCl_3$) [1]:

Table 1

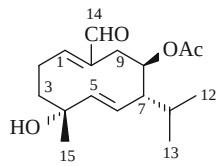
C-1	131.9 d	C-7	54.4 d	C-13	23.3 q
2	24.6 t	8	74.7 d	14	21.1 q
3	38.7 t	9	42.0 t	15	16.1 q
4	129.3 s	10	133.1 s	OAc	172.7 s
5	133.2 d	11	26.6 d		21.2 q
6	67.4 d	12	21.4 q		

References

1. G. Appendino, J. Jakupovic, S. Jakupovic, Phytochemistry **46**(6), 1039 (1997)

8β-Acetoxy-4α-hydroxy-7β(H)-germacra-1(10)*E*,5*E*-dien-14-al (Pulicanadienal B)

CAS Registry Number: 851595-73-8



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters
Biological sources: *Pulicaria canariensis* Bolle subsp. *canariensis* [1]
$C_{17}H_{26}O_4$: 294.1831
Mp: amorphous solid [1]
$[\alpha]_D^{25}$ 49.1° (*c* 0.059, $CHCl_3$) [1]
UV (EtOH): 214 (3.0), 251 (2.1) [1]
IR (KBr): 3459, 2922, 1732, 1684, 1630, 1375, 1256, 1026, 880, 803 [1]
EI-MS: 317 $[M + Na]^+$ (2), 165 (1), 154 (8), 136 (13), 109 (12), 97 (17), 95 (31), 81 (35), 71 (31), 69 (66), 57 (81), 55 (100) [1]
HR-FAB-MS: 317.1718 $[M + Na]^+$ (calc. for $C_{17}H_{26}O_4Na$ 317.1729) [1]
^{1}H NMR: 0.79 (3H, d, J = 6.8, H-13), 0.80 (3H, d, J = 6.8, H-12), 1.34 (3H, s, H-15), 1.6 (1H, m, H-7), 1.74 and 1.98 (each 1H, m, H-3), 2.04 and 2.53 (each 1H, m, H-2), 2.12 (3H, s, OAc), 2.16 (1H, m, H-11), 2.51 (1H, dd, J = 3.4; 15.0, H-9b), 2.79 (1H, dd, J = 3.4; 15.0, H-9a), 5.00 (1H, m, H-8), 5.20 (1H, dd, J = 10.0; 15.4, H-6), 6.41 (1H, dd, J = 5.8; 10.5, H-1), 9.42 (1H, s, H-14) [1]
^{13}C NMR [1]:

Table 1

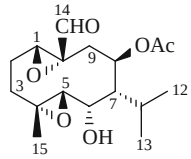
C-1	161.6	C-7	52.8	C-13	16.8
2	25.2	8	70.3	14	194.8
3	39.9	9	31.9	15	29.6
4	73.6	10	157.6	OAc	171.2
5	138.6	11	27.5		21.2
6	121.4	12	21.4		

References

1. J. Triana, M. Lopez, F.J. Perez, J. Gonzalez-Platas, J. Quintana, F. Estevez, F. Leon, J. Bermejo, J. Nat. Prod. **68**, 523 (2005)

8β-Acetoxy-6α-hydroxy-1β,10α;4α5β-diepoxy-7βH-germacr-14-al (Pulicanaral C)

CAS Registry Number: 851595-71-6



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Pulicaria canariensis* Bolle subsp. *canariensis* [1]

$C_{17}H_{26}O_6$: 326.1729

Mp: colorless oil [1]

IR (KBr): 3462, 2964, 2925, 2856, 1719, 1597, 1455, 1382, 1255, 1074 [1]

EI-MS: 326 $[M]^+$ (0.2), 279 (15), 251 (6), 237 (6), 223 (8), 219 (10), 205 (7), 195 (5), 191 (13), 177 (13), 167 (27), 163 (19), 149 (90), 139 (28), 137 (31), 123 (42), 111 (41), 109 (68), 97 (100), 95 (79), 83 (72), 81 (66), 69 (61), 55 (77) [1]

^{1}H NMR: 0.99 (3H, d, J = 6.6, H-13), 1.13 (3H, s, H-15), 1.3 (1H, m, H-3a), 1.31 (3H, d, J = 6.6, H-12), 1.54 (1H, m, H-7β), 1.54 (1H, m, H-9b), 1.75 (2H, m, H-2), 1.90 (1H, m, H-11), 2.12 (3H, s, OAc), 2.20 (1H, ddd, J = 3.5, 7.0, 13.5, H-3b), 3.01 (1H, t, J = 12.6, H-9a), 3.03 (1H, d, J = 6.7, H-5α), 3.45 (1H, d, J = 11.5, H-1), 3.51 (1H, dd, J = 1.2; 6.7, H-6β), 5.20 (1H, dd, J = 4.6; 12.6, H-8α), 9.40 (1H, s, H-14) [1]

^{13}C NMR [1]:

Table 1

C-1	62.5	C-7	49.7	C-13	21.1
2	23.0	8	70.0	14	199.3
3	35.8	9	34.5	15	16.1
4	58.0	10	61.5	OAc	173.0
5	67.7	11	26.3		21.0
6	70.2	12	22.1		

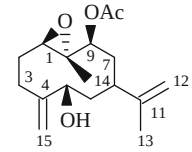
(*continued*)

Table 1 (continued)

References

1. J. Triana, M. Lopez, F.J. Perez, J. Gonzalez-Platas, J. Quintana, F. Estevez, F. Leon, J. Bermejo, J. Nat. Prod. **68**, 523 (2005)

9β-Acetoxy-1β,10α-epoxy-5α,7α(H)-germacra-4(15),11-dien-5β-ol ((1*R**,5*R**,7*S**,9*S**,10*S**)-9-Acetoxy-1(10)-epoxy-5-hydroxygermacra-4(15),11-diene)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Achillea ageratum* L. [1]

$C_{17}H_{26}O_4$: 294.1831

Mp: viscous liquid [1]

$[\alpha]_D$ −46° (*c* 0.0041, $CHCl_3$) [1]

IR (film): 3600–3200, 3070, 2940, 2870, 1740, 1645, 1460, 1375, 1240, 1080, 1030, 995, 905, 855 [1]

PCI-MS: 295 $[M + H]^+$ (18.9), 277 (100), 253 (32.8), 235 (66.1), 217 (42.8) [1]

^{1}H NMR (500 MHz, $CDCl_3$): 1.37 (3H, s, H-14), 1.68 (3H, br s, H-13), 2.06 (3H, s, OAc), 3.11 (1H, dd,

J = 10; 4.5, H-1), 3.96 (1H, dd, J = 12; 3, H-5), 4.24 (1H, dd, J = 12; 5, H-9), 4.65 (1H, br s, H-12b), 4.68 (1H, br s, H-12a), 5.16 (1H, br s, H-15b), 5.17 (1H, br s, H-15a) [1]

^{13}C NMR (75 MHz, DMSO-d_6) [1]:

Table 1

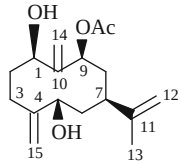
C-1	59.9 d	C-7	38.4d	C-13	18.2 q
2	25.7 t	8	36.0 t	14	111.5 q
3	21.1 t	9	80.9 d	15	115.9 t
4	147.3 s[a]	10	59.4 s	OAc	170.0 s
5	75.6 d	11	146.4 s[a]		21.2q
6	35.9 t	12	111.2 t		

[a]In the same interchangeable signals

References

1. L.M. Vieira, A. Kijjoa, J.A. Pereira, T.E. Gedris, W. Herz, Phytochemistry **45**(1), 111 (1997)

9β-Acetoxy-5α,7αH-germacra-4(15),10(14),11-triene-1β,5β-diol ((1*R**,5*R**,7*S**,9*S**)-9-Acetoxy-1,5-dihydroxy-germacra-4(15),10(14),11-triene; 9-*O*-Acetylageratriol)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Achillea ageratum* L. [1]

$C_{17}H_{26}O_4$: 294.1831

Mp: viscous liquid [1]

$[\alpha]_D$ −18° (*c* 0.0006, $CHCl_3$) [1]

PCI-MS: 295 $[M + H]^+$ (8.7), 277 (23.5), 235 (53.4), 233 (27.3), 217 (100), 199 (25.3), 197 (68.0) [1]

^{1}H NMR (500 MHz, $CDCl_3$): 1.68 (3H, br s, H-13), 2.01 (3H, s, OAc), 3.90 (1H, dd, J = 12; 3.5, H-5), 4.21 (1H, dd, J = 11; 5, H-1), 4.65 (1H, br s, H-12b), 4.67 (1H, br s, H-12a), 4.70 (1H, dd, J = 12; 5.5, H-9), 5.12 (1H, br, H-15b), 5.16 (1H, br s, H-15a), 5.36 (1H, br s, H-14b), 5.42 (1H, br s, H-14a) [1]

^{1}H NMR (300 MHz, DMSO-d_6) [2]

^{13}C NMR (75 MHz, DMSO-d_6) [1]:

Table 1

C-1	74.1 a[a]	C-7	37.6 d	C-13	18.2 q
2	31.6 t	8	39.8 t	14	113.6 t
3	21.7 t	9	74.5 a[a]	15	113.2 t
4	150.7 s	10	149.5 s	OAc	169.5 s
5	69.4 d	11	148.0 s		21.0 q
6	36.5 t	12	110.1 t		

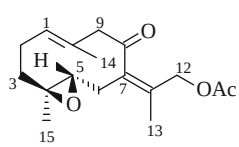
[a]In the same interchangeable signals

^{13}C NMR (75 MHz, $CDCl_3$) [2]

References

1. L.M. Vieira, A. Kijjoa, J.A. Pereira, T.E. Gedris, W. Herz, Phytochemistry **45**(1), 111 (1997)
2. A. Kijjoa, L.M. Vieira, J.A. Pereira, A.M.S. Silva, W. Herz, Phytochemistry **51**(4), 555 (1999)

12-Acetoxy-4β,5β-epoxy-4*S*,5*S*-germacra-1(10),7(11)-dien-8-one ((4*S*,5*S*)-12-Acetoxygermacrone-4,5-epoxide)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters
Biological sources: *Curcuma aromatica* Salisb. [1]
$C_{17}H_{24}O_4$: 292.1675
Mp: viscous oil [1]
$[\alpha]_D$ +118.4° (*c* 0.05, MeOH) [1]
CD: $[\theta]_{306}$ +6837°, $[\theta]_{249}$ +3874°, $[\theta]_{224}$ −8660° (*c* 0.01, MeOH) [1]
MS: 292.1712 $[M]^+$ (calc. for $C_{17}H_{24}O_4$: 292.1675) [1]
^{1}H NMR ($CDCl_3$): 1.06 (3H, s, H-14), 1.73 (3H, s, H-15), 1.86 (3H, s, H-13), 2.10 (3H, s, OAc), 4.57 (2H, s, H-12), 5.23 (1H, t, J = 7.5, H-1) [1]
^{13}C NMR [1]:

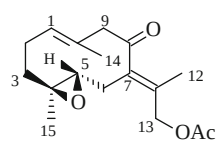
Table 1

C-1	130.0	C-7	126.4	C-13	16.3
2	24.6	8	202.9	14	15.9
3	37.5	9	55.6	15	17.0
4	60.6	10	132.5	OAc	171.0
5	63.9	11	138.0		20.7
6	30.0	12	65.1		

References

1. M. Kuroyanagi, A. Ueno, K. Koyama, Sh. Natori, Chem. Pharm. Bull. **38**, 55 (1990)

13-Acetoxy-4β,5β-epoxy-4*S*,5*S*-germacra-1(10),7(11)-dien-8-one ((4*S*,5*S*)-13-Acetoxygermacrone-4,5-epoxide)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters
Biological sources: *Curcuma aromatica* Salisb. [1]
$C_{17}H_{24}O_4$: 292.1675
$[\alpha]_D$ +171.8° (*c* 0.22, MeOH) [1]
MS: 292.1676 $[M]^+$ (calc. for $C_{17}H_{24}O_4$: 292.1675) [1]
^{1}H NMR ($CDCl_3$): 1.05 (3H, s, H-14), 1.73 (3H, s, H-15), 1.83 (3H, s, H-12), 2.10 (3H, s, OAc), 4.69 (2H, s, H-13), 5.23 (1H, t, J = 7.5, H-1) [1]
^{13}C NMR [1]:

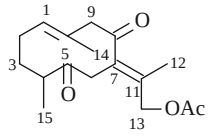
Table 1

C-1	130.3	C-7	126.3	C-13	64.1
2	24.5	8	203.3	14	15.8
3	37.7	9	55.1	15	17.6
4	60.6	10	131.9	OAc	170.6
5	64.1	11	138.3		20.6
6	29.4	12	18.4		

References

1. M. Kuroyanagi, A. Ueno, K. Koyama, Sh. Natori, Chem. Pharm. Bull. **38**, 55 (1990)

13-Acetoxy-germacra-1(10),7(11)-diene-5,8-dione ((4*S*)-13-Acetoxydehydrocurdione)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters
Biological sources: *Curcuma aromatica* Salisb. [1]
$C_{17}H_{24}O_4$: 292.1675
Mp: 77–78°C (hexane); colorless needles [1]

IR (KBr): 1740, 1715, 1695, 1230 [1]
$[\alpha]_D$ +313.5° (*c* 0.3, MeOH) [1]
CD: $[\theta]_{317}$ +24718° (*c* 0.01, MeOH) [1]
MS: 292.166 $[M]^+$ (calc. for $C_{17}H_{24}O_4$, 292.166) [1]
^{1}H NMR ($CDCl_3$): 1.03 (3H, d, J = 6.9, H-15), 1.67 (3H, s, H-14), 1.77 (3H, s, H-12), 2.05 (3H, s, OAc), 3.04 (1H, d, J = 11.0, H-6), 3.23 (1H, d, J = 16.2, H-10), 3.26 (1H, d, J = 11.0, H-6), 3.49 (1H, d, J = 16.2, H-10), 4.47 (1H, d, J = 12.9, H-13a), 4.76 (1H, d, J = 12.9, H-13b), 5.11 (1H, dd, J = 6.0; 9.1, H-1) [1]
^{13}C NMR [1]:

Table 1

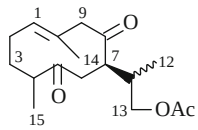
C-1	133.1	C-7	128.8	C-13	64.5
2	26.7	8	206.0	14	18.2
3	34.2	9	56.7	15	16.2
4	47.3	10	132.6[a]	OAc	170.6
5	210.3	11	133.6[a]		20.8
6	34.2	12	17.2		

[a]Assigments may be interchangeable within the same column [1]

References

1. M. Kuroyanagi, A. Ueno, K. Koyama, Sh. Natori, Chem. Pharm. Bull. **38**, 55 (1990)

13-Acetoxy-7α(H)-germacr-1(10)-ene-5,8-dione (Acetoxyneocurdione)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters
Biological sources: *Curcuma aromatica* Salisb. [1]
$C_{17}H_{26}O_4$: 294.1831
Mp: colorless oil [1]
IR (KBr): 1740, 1704, 1460, 1378 [1]
CD: $[\theta]_{298}$ −24806° (*c* 0.02, MeOH) [1]
MS: 294.1869 $[M]^+$ (calc. for $C_{17}H_{26}O_4$: 294.1831) [1]
^{1}H NMR (400 MHz, $CDCl_3$): 0.99 (3H, d, J = 6.8, H-12), 1.06 (3H, d, J = 7.0, H-14), 1.67 (3H, s, H-15), 2.06 (3H, s, OAc), 3.82 (2H, d, J = 5.7, H-13), 5.12 (1H, br t, J = 7.0, H-1) [1]
^{13}C NMR [1]:

Table 1

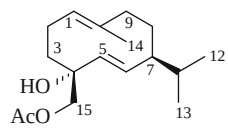
C-1	131.1	C-7	47.8	C-13	67.4
2	25.5	8	211.9[a]	14	17.8
3	33.1	9	54.9	15	17.9
4	46.2	10	129.4	OAc	170.6
5	209.1[a]	11	35.0		20.7
6	40.9	12	14.5		

[a]Assigments may be interchangeable within the same column [1]

References

1. M. Kuroyanagi, A. Ueno, K. Koyama, Sh. Natori, Chem. Pharm. Bull. **38**, 55 (1990)

15-Acetoxy-germacra-1*E*,5*E*-dien-4α-ol



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters
Biological sources: *Stevia myriadenia* Sch. Bip. ex Baker [1]
$C_{17}H_{28}O_3$: 280.2038
Mp: colorless oil, not free from 15-angeloyloxy-2α-hydroxy-bisabol-2,10-diene [1]
IR (CCl_4): 3600, 1740 [1]
MS: 280.203 $[M]^+$ (0.5), 262 (0.5), 207 (10), 81 (100) [1]
CI-MS: 281 $[M + 1]^+$ (0.5), 263 (100) [1]

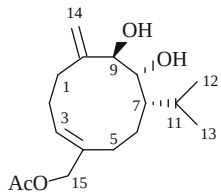
^{1}H NMR (400 MHz, C_6D_6, TMS): 0.85 (3H, d, J = 7, H-13), 0.92 (3H, d, J = 7, H-12), 1.63 (3H, br s, H-14), 1.70 (3H, s, OAc), 2.05 (1H, m, H-2b), 2.05 (3H, m, H-7, H-9), 2.41 (1H, dddd, J = 12; 13; 11; 3, H-2a), 3.76 (1H, d, J = 11, H-15b), 4.04 (1H, d, J = 11, H-15a), 4.91 (1H, d, J = 15, H-5), 4.96 (1H, br d, J = 12, H-1), 5.40 (1H, dd, J = 15; 10, H-6) [1]

References

1. F. Bohlmann, C. Zdero, R.M. King, H. Robinson, Phytochemistry **21**(8), 2021 (1982)

15-Acetoxy-7β(H)-germacra-3*E*,10(14)-diene-8α,9β-diol (Kikkanol D Monoacetate)

CAS Registry Number: 242136-56-7



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Chrysanthemum indicum* L. [1]

$C_{17}H_{28}O_4$: 296.1988

Mp: colorless oil [1]

$[\alpha]_D^{24}$ −138.1° (*c* 0.1, $CHCl_3$) [1]

IR (film): 3436, 2957, 1717, 1648, 909 [1]

FAB-MS: 319.1886 $[M + Na]^+$ (calc. for $C_{17}H_{28}O_4Na$, found: 319.1895) [1]

^{1}H NMR (500 MHz, $CDCl_3$): 0.96, 0.98 (each 3H, both d, J = 7.1, H-12 and H-13), 1.40 (1H, m, H-6β), 1.51 (IH, br ddd, J = ca. 2; 6; 10, H-7), 1.68 (1H, dq, J = 2.4; 7.1, H-11), 1.97 (1H, dddd, J = 2.7; 5.2; 9.8; 15.3, H-6α), 2.06 (1H, m, H-5), 2.06 (3H, s, OAc), 2.10 (1H, m, H-2), 2.21 (1H, m, H-1β), 2.46 (1H, ddd, J = 5.2; 12.5; 16.6, H-5), 2.61 (1H, m, H-6), 2.63 (1H, m, H-1α), 3.95 (1H, br d, J = ca. 10, H-8), 4.10 (1H, d, J = 10.0, H-9), 4.33, 4.52 (2, ABq, J = 12.3, H-15), 4.94 (1H, brs, H-14a), 5.01 (1H, d, J = 1.2, H-14b), 5.50 (1H, dd, J = 8.8; 13.0, H-3) [1]

^{13}C NMR (125 MHz, $CDCl_3$) [1]:

Table 1

C-1	35.9	C-7	40.3	C-13	20.8[a]
2	24.6	8	75.5	14	115.0
3	129.6	9	72.1	15	67.6
4	134.5	10	148.7	$\underline{C}H_3$–CO–	21.0
5	26.0	11	34.2	CH_3–$\underline{C}O$–	170.9
6	21.9	12	20.5[a]		

[a]Assigments may be interchangeable within the same column

^{1}H – ^{1}H COSY [1]

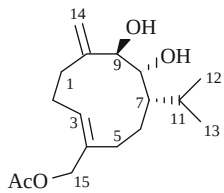
HMBC [1]

References

1. M. Yoshikawa, T. Morikawa, I. Toguchida, S. Haima, H. Matsuda, Chem. Pharm. Bull. **48**, 651 (2000)

15-Acetoxy-7β(H)-germacra-3*Z*,10(14)-diene-8α,9β-diol (Kikkanol F Monoacetate)

CAS Registry Number: 281655-20-7



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Chrysanthemum indicum* L. [1]

$C_{17}H_{28}O_4$: 296.1987

Mp: colorless oil [1]

$[\alpha]$ −59.6° (*c* 0.8, $CHCl_3$) [1]

IR (film): 3436, 2977, 1738, 1651, 903 [1]

EI-MS: 296 $[M]^+$ (1) (calc. for $C_{17}H_{28}O_4$ 296.1987; found: 296.1993), 278 $[M - H_2O]^+$ (3), 95 (100) [1]

^{1}H NMR (500 MHz, $CDCl_3$): 1.00, 1.00 (each 3H, both d, J = 6.8, H-12, H-13), 1.27 (1H, m, H-7), 1.41 (1H, dddd, J = 3.7; 4.1; 8.6; 15.0, H-6β), 1.66 (1H, dddd, J = 2.1; 4.1; 4.1; 15.0, H-6α), 1.78 (1H, dq, J = 1.8; 6.8, H-11), 1.81 (1H, ddd, J = 4.1; 4.1; 13.9, H-5), 2.06 (3H, s, OAc), 2.23 (1H, m, H-1α), 2.37 (1H, m, H-5), 2.43, 2.46 (1H each, both m, H-2), 2.50 (1H, m, H-1β), 3.50 (1H, d, J = 9.8, H-9), 3.94 (1H, br d, J = ∼10, H-8), 4.49, 4.59 (each 1H, ABq, J = 12.2, H-15), 4.99, 5.04 (each 1H, both s, H-14), 5.51 (1H, dd, J = 6.7; 10.4, H-3) [1]

^{13}C NMR (125 MHz, $CDCl_3$) [1]:

Table 1

C-1	35.1	C-7	42.7	C-13	21.3[a]
2	27.6	8	72.7	14	113.9
3	130.9	9	77.0	15	63.6
4	135.1	10	149.5	CH_3–CO–	21.0
5	32.6	11	32.2	CH_3–CO–	171.2
6	27.1	12	21.0[a]		

[a]Assigments may be interchangeable within the same column

^{1}H-^{1}H COSY [1]

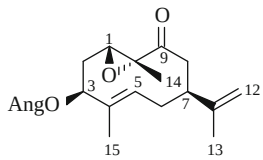
HMBC [1]

References

1. M. Yoshikawa, T. Morikawa, I. Toguchida, S. Haima, H. Matsuda, Chem. Pharm. Bull. **48**, 651 (2000)

3β-Angeloyloxy-1β,2α-epoxy-7α(H)-germacra-4,11-dien-9-one (Ligularinone B)

CAS Registry Number: 64185-22-4



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Ligularia hodgsonii* Hook. f. [1]

$C_{20}H_{28}O_4$: 332.1988

Mp: colorless oil [1]

IR (CCl_4): 1715, 1650, 850 [1]

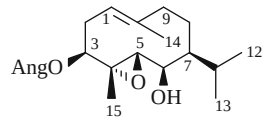
MS: 332.199 $[M]^+$ (0.5) (calc. for $C_{20}H_{28}O_4$: 392.199), 232 (5), 83 (100) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.42 (3H, s, H-15), 1.62 (3H, s, H-13), 1.69 (3H, br s, H-14), 2.15 (1H, br d, J = 14, H-8α), 2.30 (2H, m, H-2), 2.30 (2H, m, H-6), 2.6 (1H, m, H-7), 2.87 (1H, dd, J = 2; 14; 12, H-8β), 3.45 (1H, d, J = 4, H-1), 4.99 (1H, br s, H-12b), 5.04 (1H, br tq, J = 7, H-5), 5.13 (1H, br s, H-12a), 5.16 (1H, dd, J = 3.5; 8.5, H-3); OAng: 1.90 (3H, dq, J = 1; 1, H-5′), 1.98 (3H, dq, J = 7; 1, H-4′), 6.08 (1H, qq, J = 7; 1, H-3′) [1]

References

1. F. Bohlmann, D. Ehlers, C. Zdero, M. Crenz, Chem. Ber. **110**, 2640 (1977)

3β-Angeloyloxy-4α,5β-epoxy-5α,6α,7α(H)-germacr-1(10)-en-6β-ol



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Senecio cylindricus* (A. Berger) Jacobsen [1]; *S. vitalis* N.E.Br [2]; *S. crassissimus* Humbert [3]

$C_{20}H_{32}O_4$: 336.2301

Mp: colorless oil (mix. with 3β-senecioyloxy-6β-hydroxy-4,5,6,7αH-4α,5β-epoxy-germacrene C) [1]

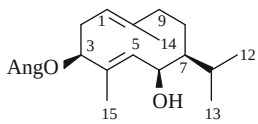
$[\alpha]^{24}$ (λ, nm): −33.7° (589), −34.9° (578), −40.4° (546), −74.7° (436) (*c* 2.2, $CHCl_3$) [3]

IR (CCl_4) (mix.): 3460, 1710, 1650, 850 [1]
MS (mix.): 336.230 $[M]^+$ (2) (calc. for $C_{20}H_{32}O_4$: 336.230), 236 (5), 218 (5), 203 (3), 83 (100) [1]
^{1}H NMR (270 MHz, C_6D_6, 75°, TMS) (mix.): 0.88 (3H, d, J = 7, H-13), 0.89 (3H, d, J = 7, H-12), 1.01 (3H, s, H-14), 1.70 (3H, br s, H-15), 1.8−2.1 (5H, m, H-8, H-9, H-11), 2.55 (2H, dd, J = 5; 12, H-2), 2.81 (1H, d, J = 8, H-5), 3.64 (1H, dd, J = 8, 2, H-6), 5.04 (1H, m, H-1), 5.40 (1H, ddd, J = 5; 12, H-3); OAng: 1.85 (3H, dq, J = 1.5; 1.5, H-5′), 1.97 (3H, dq, J = 7; 1.5, H-4′), 5.79 (1H, qq, J = 7; 1.5, H-3′) [1]

References

1. F. Bohlmann, J. Ziesche, Phytochemistry **18**(9), 1489 (1979)
2. F. Bohlmann, J. Ziesche, Phytochemistry **19**(8), 1851 (1980)
3. F. Bohlmann, J. Ziesche, Phytochemistry **20**(3), 469 (1981)

3β-Angeloyloxy-6α,7α(H)-germacra-1(10),4-dien-6β-ol (3β-Angeloyloxy-6β-hydroxy-6,7-H-germacrene C)



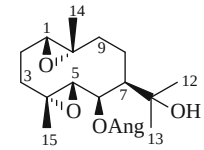
Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters
Biological sources: *Senecio cylindricus* (A. Berger) Jacobsen [1]; *S. crassissimus* Humbert [2]
$C_{20}H_{32}O_3$: 320.2351
Mp: colorless oil, which could not be separated (mix. with 3β-senecioyloxy-6β-hydroxy-6,7-H-germacrene C) [1]
$[\alpha]^{24}$ (λ, nm) (mix.): −111.4° (589), −116.7° (578), −134.7° (546), −247.0° (436) (*c* 2.84, $CHCl_3$) [1]
IR (CCl_4) (mix.): 3460, 1720, 1650 [1]
MS (mix.): 320.235 $[M]^+$ (1) (calc. for $C_{20}H_{32}O_3$: 320.235), 220 (25), 202 (10), 83 (100) [1]
^{1}H NMR (270 MHz, $CDCl_3$, TMS) (mix.): 1.05 (3H, d, J = 7, H-13), 1.09 (3H, d, J = 7, H-12), 1.47 (3H, s, H-15), 1.6 (2H, m, H-8), 1.69 (3H, br s, H-14), 2.0 (1H, m, H-11), 2.1 (1H, m, H-9α), 2.62 (1H, m, H-9β), 2.63 (2H, br d, J = 12, H-2), 3.55 (1H, d, J = 10, OH), 4.48 (1H, br t, J = 8, 10; 2, H-6), 5.07 (1H, br d, J = 12, H-1), 5.23 (1H, dd, J = 5; 12, H-3), 5.28 (1H, d, J = 8, H-5); OAng: 1.89 (3H, d, J = 1.5; 1.5, H-5′), 2.03 (3H, dq, J = 7; 1.5, H-4′), 6.16 (1H, qq, J = 7; 1.5, H-3′) [1]

References

1. F. Bohlmann, J. Ziesche, Phytochemistry **18**(9), 1489 (1979)
2. F. Bohlmann, J. Ziesche, Phytochemistry **20**(3), 469 (1981)

6β-Angeloyloxy-1β,10α;4α,5β-diepoxy-7α(H)-germacr-11-ol ((1*R*,4*R*,5*R*,6*R*,10*R*)-1,10;4,5-Diepoxy-11-hydroxygermacran-6-yl (*Z*)-2-methylbut-2-enoate)

CAS Registry Number: 114176-07-7



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters
Biological sources: *Nanothamnus sericeous* Thomson [1]
$C_{20}H_{32}O_5$: 352.2250
Mp: 129–130°C [1]
$[\alpha]_D$ −88° (*c* 0.5, $CHCl_3$) [1]
IR (nujol): 3840, 1700, 1650 [1]

MS: 352.255 $[M]^+$ (0.01), 334 (0.3), 234 (0.3), 219 (0.5), 205, 83 (100), 55 (78) [1]

Found: C, 68.4; H, 9.4. $C_{20}H_{32}O_5$ requires C, 68.15; H, 9.15% [1]

^{1}H NMR (90 MHz, $CDCl_3$, TMS): 1.26 (3H, s, H-12), 1.29 (3H, s, H-13), 1.39 (3H, s, H-14), 1.52 (3H, s, H-15), 2.98 (1H, br d, J = 10, H-1), 3.07 (1H, d, J = 6.5, H-5), 5.23 (1H, dd, J = 6.5; 1, H-6); OAng: 1.91 (3H, dq, H-4′), 2.04 (3H, dq, H-5′), 6.16 (1H, qq, J = 7; 1.5, H-3′) [1]

^{13}C NMR (23.63 MHz, $CDCl_3$, TMS) [1]:

Table 1

C-1	61.40 d	C-8	22.54 t[a]	C-15	22.80 q
2	36.97 t[a]	9	36.54 t[a]	OAng: 1′	167.08 s
3	23.64[a]	10	61.40 s[a]	2′	127.50 s
4	58.74 s[a]	11	73.10 s	3′	139.26 d
5	66.54 d	12	27.80 q	4′	20.20 q
6	73.10 d	13	28.45 q	5′	15.64 q
7	46.91 d	14	16.56 q		

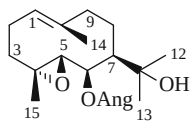
[a]Assignments may be interchanged [1]

X-ray [1]

References

1. U.G. Bhat, V.G. Puranik, N.N. Dhaneshwar, S.S. Tavale, T. N. Guru Row, B.A. Nagasampagi, J. Chem. Soc., Perkin Trans. **1**, 657 (1988)

6β-Angeloyloxy-4α,5β-epoxy-7α(H)-germacr-1(10)-en-11-ol ((4*R*,5*R*,6*R*)-4,5-Epoxy-11-hydroxygermacr-1(10)-en-6-yl (*Z*)-2-Methylbut-2-enoate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Nanothamnus sericeous* Thomson [1]

$C_{20}H_{32}O_4$: 336.2301

Mp: 116–117°C [1]

$[\alpha]_D$ +113.5° (*c* 0.2, $CHCl_3$) [1]

IR (nujol): 3520, 1700, 1640, 880 [1]

MS: 336 $[M]^+$, 318, 218, 83 (100), 55 [1]

Found: C, 71.5; H, 9.8. $C_{20}H_{32}O_4$ requires C, 71.39; H, 9.59% [1]

^{1}H NMR (90 MHz, $CDCl_3$, TMS): 1.20 (3H, s, H-12), 1.26 (3H, s, H-13), 1.33 (3H, s, H-15), 1.69 (3H, br s, H-14), 2.68 (1H, d, J = 6.5, H-5), 5.29 (1H, dd, J = 6.5; 1, H-6), 5.33 (1H, d, J = 8, H-1); OAng: 1.91 (3H, dq, J = 7; 1.5, H-4′), 6.13 (1H, qq, J = 7; 1.5, H-3′) [1]

^{13}C NMR (23.63 MHz, $CDCl_3$, TMS) [1]:

Table 1

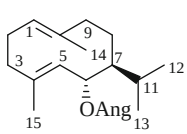
C-1	123.73 d	C-8	22.80 t[a]	C-15	18.15 q[a]
2	39.44 t	9	36.90 t	OAng: 1′	167.61 s
3	23.51 t[a]	10	137.18 s	2′	128.61 s
4	59.84 s	11	73.43 s	3′	138.61 d
5	66.41 d	12	27.41 q	4′	20.33 q
6	73.23 d	13	28.71 q	5′	15.71 q
7	49.31 d	14	16.50 q[a]		

[a]Assignments may be interchanged [1]

References

1. U.G. Bhat, V.G. Puranik, N.N. Dhaneshwar, S.S. Tavale, T. N. Guru Row, B.A. Nagasampagi, J. Chem. Soc., Perkin Trans. **1**, 657 (1988)

6α-Angeloyloxy-6β,7α(H)-germacra-1(10),4-diene (6α-Angeloyloxy-6.7H-germacrene C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

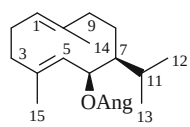
Biological sources: *Senecio archeri* (Compton) Jacobsen [1]

$C_{20}H_{32}O_2$: 304.2402

References

1. F. Bohlmann, C. Zdero, D. Berger, A. Suwita, P. Mahanta, C. Jeffrey, Phytochemistry **18**(1), 79 (1979)

6β-Angeloyloxy-6α,7α(H)-germacra-1(10),4-diene (6β-Angeloyloxy-6.7H-germacrene C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Senecio crassulifolius* (DC.) Sch. Bip. [1]; *S. cylindricus* (A. Berger) Jacobsen [2]

$C_{20}H_{32}O_2$: 304.2402

Mp: colorless oil [1]

$[\alpha]^{24}$ (λ, nm): −31.2° (589), −32.0° (578), −38.4° (546), −81.4° (436) (*c* 0.5, $CHCl_3$) [2]

IR (CCl_4): 1715, 1655, 855 [1]

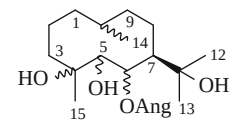
MS: 304.241 $[M]^+$ (1) (calc. for $C_{20}H_{32}O_2$: 304.240), 204 $[M - C_4H_7COOH]^+$ (50), 161 $[204 - C_3H_7]^+$ (68), 83 $[C_4H_7CO]^+$ (100) [1]

^{1}H NMR (270 MHz, CCl_4, TMS): 0.95 (3H, d, J = 7, H-13), 0.96 (3H, d, J = 7, H-12), 1.57 (3H, s, H-15), 1.60 (3H, s, H-14), 4.91 (1H, br d, J = 7, H-5), 4.95 (1H, m, H-1), 5.69 (1H, br d, J = 7, H-6); OAng: 1.89 (3H, dq, H-5′), 2.04 (3H, dq, H-4′), 5.79 (1H, qq, H-3′) [1]

References

1. F. Bohlmann, K.-H. Knoll, C. Zdero, P.K. Mahanta, M. Grenz, A. Suwita, D. Ehlers, N. Le Van, W.-R. Abraham, A.A. Natu, Phytochemistry **16**(7), 965 (1977)
2. F. Bohlmann, J. Ziesche, Phytochemistry **18**(9), 1489 (1979)

6-Angeloyloxy-7α(H)-germacra-4,5,11-triol (4ξ,5ξ,11-Trihydroxygermacran-6-yl (*Z*)-2-Methylbut-2-enoate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Nanothamnus sericeous* Thomson [1]

$C_{20}H_{36}O_5$: 356.2563

Mp: gum [1]; (its 5-OAc) 161–163°C (acetone – light petroleum, 3:7) [1]

IR (nujol): 3460, 1710, 1640 [1]

IR (its 5-OAc): 3430, 1725, 1715, 1650 [1]

MS: 356 $[M]^+$, 338, 238, 83 (100), 55 [1]

MS (its 5-OAc): 430 $[M]^+$, 370, 352, 252, 83 (100), 55, 43 [1]

^{1}H NMR (90 MHz, $CDCl_3$, TMS): 1.03 (3H, d, J = 7, H-14), 1.19 (3H, s, H-12), 1.25 (3H, s, H-13), 1.29 (3H, s, H-15), 3.69 (1H, d, J = 6, H-5), 5.15 (1H, dd, J = 8; 6, H-6); OAng: 1.98 (3H, dq, J = 7; 1.5, H-4′), 6.11 (1H, qq, J = 7; 1.5, H-3′) [1]

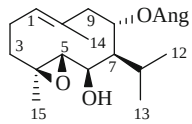
^{1}H NMR (90 MHz, $CDCl_3$, TMS) (its 5-Ac): 1.08 (3H, d, J = 7, H-14), 1.24 (3H, s, H-12), 1.31 (3H, s, H-13), 1.31 (3H, s, H-15), 2.02 (3H, s, OAc), 5.45 (1H, d, J = 5, H-5), 5.45 (1H, dd, J = 5; 9, H-6); OAng: 1.95 (3H, dq, J = 7; 1.5, H-4′), 6.11 (1H, qq, J = 7; 1.5, H-3′) [1]

References

1. U.G. Bhat, V.G. Puranik, N.N. Dhaneshwar, S.S. Tavale, T. N. Guru Row, B.A. Nagasampagi, J. Chem. Soc., Perkin Trans. **1**, 657 (1988)

8α-Angeloyloxy-4β,5-epoxy-1(10)-germacren-6β-ol (8α-*O*-Angeloylepoxytovarol; 8-*O*-Angeloylshiromodiol; Shiromodiol-8-*O*-angelate; Leucoferin)

CAS Registry Number: 98941-63-0



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Thapsia villosa* var. *minor* (Hoff. et Link) Cout. [1]; *Laserpitium halleri* subsp. *halleri* Crantz [2]; *Ferula leucographa* Korov. [3]

$C_{20}H_{32}O_4$: 336.2301

Mp: 113–114°C ($CHCl_3$/light petroleum) [2]; 79–80°C [3]

$[\alpha]_D$ −47.7°C (*c* 3.6, $CHCl_3$) [1]; $[\alpha]_D^{25}$ −57° (*c* 1.04, $CHCl_3$) [2]; $[\alpha]_D$ −66° (*c* 1.0, $CHCl_3$) [3]

UV: 218 (3.8) [2]

IR: 3400, 2950, 1710, 1650, 1460, 1400, 1250, 1170, 1080, 1050, 780 [1]; (KBr): 3420, 1720 [2]; (KBr): 3500–3300 (OH), 1700 (C = O), 1660 (C = C) [3]

MS: 336.230200 $[M]^+$ (1) (calc for $C_{20}H_{32}O_4$: 336.230045), 83 (100) [2]

MS: 236 $[M - 100]^+$ (5), 218 $[M - 100 - 18]^+$ (5), 193 $[M - 100 - 43]^+$ (6), 175 $[M - 100 - 43 - 18]^+$ (10), 136 (20), 83 $[C_5H_7O]^+$ (100) [3]

EI-MS: 236 $[M - AngOH]^+$ (20), 218 $[M - AngOH - H_2O]^+$ (15), 175 (40), 149 (100) [1]

^{1}H NMR (60 MHz, $CDCl_3$, TMS): 0.90* (3H, d, J = 6, H-13), 1.05* (3H, d, J = 6, H-12), 1.10 (3H, s, H-15), 1.71 (3H, s, H-14), 2.70 (1H, d, J = 8, H-5), 3.40 (1H, d, J = 8, H-6), 5.15 (2H, m, H-1, H-8); OAng: 1.90 (3H, s, H-5′), 2.00 (3H, d, J = 7, H-4′), 5.97 (1H, q, J = 7, H-3′), * – Assignment may be interchanged [1]

^{1}H NMR (200 MHz, $CDCl_3$, 25°C, TMS): 0.94 (3H, d, J = 7.0, H-12), 1.10 (3H, d, J = 7.0, H-13), 1.14 (3H, s, H-15), 1.78 (3H, br s, H-14), 2.03 (3H, s, OAc), 2.60 (1H, br s, H-9a), 2.82 (1H, br d, J = 8.0, H-5), 3.48 (1H, dt, J = 8.0; 8.0; 1.8, H-6), 5.20 (1H, br dd, J = 12; 5.0, H-8), 5.32 (1H, br t, J = 8.0, H-1); OAng: 1.88 (3H, quint, J = 1.5; 1.5, H-5′), 2.00 (3H, dq, J = 7.0; 1.5; H-4′), 6.10 (1H, qq, J = 7.0; 1.5, H-3′) [2]

^{1}H NMR (200 MHz, C_6D_6, 25°C, TMS): 0.93 (3H, d, J = 7.0, H-12), 0.97 (3H, s, H-15), 1.06 (3H, d, J = 7.0, H-13), 1.42 (3H, br s, H-14), 1.70 (3H, s, OAc), 2.50 (1H, br dd, J = 14; 4.0, H-9a), 2.87 (1H, br d, J = 8.0, H-5), 3.62 (1H, br d, J = 8.0, H-6), 4.90 (1H, br t, J = 8.0, H-1), 5.34 (1H, dq, J = 12; 5.0; 1.5, H-8); OAng: 1.86 (3H, q, J = 1.5; 1.5, H-5′), 1.98 (3H, dq, J = 7.0; 1.5; 1.5, H-4′), 5.78 (1H, qq, J = 7.0; 1.5, H-3′) [2]

^{1}H NMR (100 MHz, $CDCl_3$, TMS): 0.96 and 1.12 (6H, d, J = 6.5, H-12, H-13), 1.18 (3H, s, H-15), 1.79 (3H, w.s, H-14), 2.83 (1H, d, J = 8.0, H-5), 3.51 (1H, dd, J = 1.5; 8.0, H-6), 5.26 (2H, m, H-1, H-8); OAng: 1.91 (3H, m, J = 1.5, H-5′), 2.03 (3H, dd, J = 1.5; 7.2, H-4′), 6.2 (1H, q, J = 1.5; 7.5, H-3′) [3]

^{13}C NMR (50.30 MHz, $CDCl_3$, 25°C, TMS) [2]:

Table 1

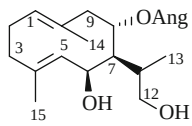
C-1	128.77 d	C-8	72.14 d	C-15	16.32 q
2	24.29 t	9	42.74 t	OAng: 1′	168.58 s
3	38.37 t	10	129.98 s	2′	127.15 s
4	59.64 s	11	26.16 d	3′	140.26 d
5	68.52 d	12	23.59 q[a]	4′	15.90 q
6	71.21 d	13	21.37 q[a]	5′	20.70 q
7	50.58 d	14	20.42 q		

[a]Assignment may be interchanged [2]

References

1. J. de Pascual Teresa, J.R. Moran, J.M. Hernandez, M. Grande, Phytochemistry **24**(8), 1779 (1985)
2. G. Appendino, M.G. Valle, P. Gariboldi, J. Chem. Soc., Perkin Trans. **1**, 1363 (1986)
3. M.N. Kobilov, A.I. Saidkhodzhaev, N.D. Abdullaev, Chem. Nat. Comp. **31**, 530 (1995)

8α-Angeloyloxy-(*E*)-1(10),4-germacradiene-6β,12-diol (12-Hydroxy-8-*O*-angeloyltovarol)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Thapsia villosa* var. *minor* (Hoff. et Link) Cout. [1]

$C_{20}H_{30}O_4$: 334.2144

Mp: oil [1]

IR (film): 3400, 1710, 1650, 1450, 1390, 1240, 1160, 1080, 1050, 1000, 850 [1]

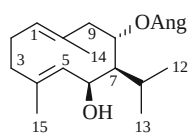
^{1}H NMR (60 MHz, CCl_4): 1.10 (3H, d, J = 6.5, H-13), 1.48 (3H, s, H-15), 1.68 (3H, s, H-14), 2.15 (4H, br s, H-2 and H-3), 3.50 (2H, m, H-12), 4.50 (1H, br t, J = 7, H-8), 5.10 (m, H-1, H-5, H-6); OAng: 1.90 (3H, br s, H-5′), 1.96 (3H, br d, J = 6, H-4′), 6.00 (1H, br q, J = 6, H-3′) [1]

References

1. J. de Pascual Teresa, J.R. Moran, J.M. Hernandez, M. Grande, Phytochemistry **25**(5), 1167 (1986)

8α-Angeloyloxy-1(10),4-germacradien-6β-ol (8-*O*-Angeloyltovarol)

CAS Registry Number: 98941-67-4



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Thapsia villosa* var. *minor* (Hoff. et Link) Cout., *T. villosa* L. var. *villosa* [1]

$C_{20}H_{32}O_3$: 320.2351

Mp: oil [1]

$[\alpha]_D$ −130.4° (*c* 4.6, $CHCl_3$) [1]

IR (film): 3400, 2954, 1700, 1654, 1450, 1380, 1250, 1170, 1100, 1000, 970, 850, 750 [1]

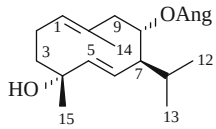
EI-MS: 220 $[M - AngOH]^+$ (5), 202 $[M - AngOH - H_2O]^+$ (10), 177 (10), 159 (30) [1]

^{1}H NMR (60 MHz, $CDCl_3$, TMS): 1.00* (3H, d, J = 6, H-13), 1.05* (3H, d, J = 6, H-12), 1.40 (3H, s, H-15), 1.70 (3H, s, H-14), 2.25 (4H, br s, H-2, H-3), 4.47 (1H, m, H-8), 5.10 (2H, m, H-1, H-6), 5.27 (1H, d, J = 7, H-5); OAng: 1.90 (3H, s, H-5′), 2.05 (3H, d, J = 7, H-4′), 6.15 (1H, q, J = 7, H-3′); * – Assignment may be interchanged [1]

References

1. J. de Pascual Teresa, J.R. Moran, J.M. Hernandez, M. Grande, Phytochemistry **24**(8), 1779 (1985)

8α-Angeloyloxy-1(10),5-germacradien-4α-ol (8α-Angeloyloxy-4α-hydroxy-4,14H-germacrene D)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

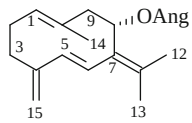
Biological sources: *Senecio cylindricus* (A. Berger) Jacobsen [1]

$C_{20}H_{32}O_3$: 320.2351
Mp: colorless oil [1]
$[\alpha]^{24}$ (λ, nm): −75.5° (589), −78.8° (578), −92.7° (546), −190.4° (436) (*c* 1.0, $CHCl_3$) [1]
IR (CCl_4): 3610, 1710, 1650, 850 [1]
MS: 320.235 $[M]^+$ (1) (calc. for $C_{20}H_{32}O_3$: 320.235), 220 (7), 205 (27), 202 (12), 159 (55), 83 (100) [1]
^{1}H NMR (270 MHz, C_6D_6, TMS): 0.88 (3H, d, J = 7, H-13), 0.89 (3H, d, J = 7, H-12), 1.01 (3H, s, H-14), 1.70 (3H, br s, H-15), 1.82 (1H, dd, J = 10.5; 12, H-9α), 2.10 (1H, dqq, J = 3; 7, H-11), 2.68 (1H, dd, J = 4; 12, H-9β), 4.86 (1H, dd, J = 12, H-1), 5.00 (1H, d, J = 15.5, H-5), 5.32 (1H, ddd, J = 10.5; 10.5; 4, H-8), 5.36 (1H, dd, J = 15.5, 10.5, H-6); OAng: 1.90 (3H, dq, J = 1.5; 1.5, H-5′), 2.01 (3H, dq, J = 7; 1.5, H-4′), 5.75 (1H, qq, J = 7; 1.5, H-3′) [1]

References

1. F. Bohlmann, J. Ziesche, Phytochemistry **18**(9), 1489 (1979)

8α-Angeloyloxy-germacra-1(10),4(15),5,7(11)-tetraene (8α-Angeloyloxy-germacrene D)

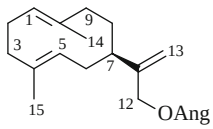


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters
Biological sources: *Senecio cylindricus* (A. Berger) Jacobsen [1]
$C_{20}H_{30}O_2$: 302.2246
Mp: colorless oil [1]
IR (CCl_4): 1715, 1655, 900, 850 [1]
MS: 302 $[M]^+$ (0.4), 202.172 $[M - C_4H_7COOH]^+$ (34) (calc. for $C_{15}H_{22}O_2$: 202.172), 159 (84), 83 (93), 55 (100) [1]
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 0.78 (3H, d, J = 7, H-13), 0.83 (3H, d, J = 7, H-12), 1.68 (3H, br s, H-14), 1.9 (1H, m, H-11), 2.1 (1H, m, H-9α), 2.48 (1H, m, H-9β), 2.48 (4H, m, H-2, H-3), 4.85 (2H, s, H-15), 5.12 (1H, ddd, J = 10; 10; 4, H-8), 5.20 (1H, m, H-1), 5.27 (1H, dd, J = 16, 10, H-6), 5.92 (1H, d, J = 16, H-5); OAng: 1.89 (3H, dq, J = 1.5; 1.5, H-5′), 1.99 (3H, dq, J = 7; 1.5, H-4′), 6.05 (1H, qq, J = 7; 1.5, H-3′) [1]

References

1. F. Bohlmann, J. Ziesche, Phytochemistry **18**(9), 1489 (1979)

12-Angeloyloxy-germacra-1(10)*E*,4*E*,11(13)-triene

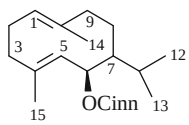


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters
Biological sources: *Perezia multiflora* (Humb. et Bonpl.) Less. [1]
$C_{20}H_{30}O_2$: 302.2246
IR: 1715 [1]
MS: 302.225 $[M]^+$ (2), 202 (41), 187 (53), 83 (100) [1]
HPLC [1]
^{1}H NMR (400 MHz, $CDCl_3$): 1.41 or 1.49 (3H, br s, H-14), 1.54 or 1.56 (3H, br s, H-15), 2.25 (2H, m, H-3), 4.50 (1H, br d, J = 10, H-5), 4.67 (2H, br s, H-12), 4.78 (1H, br d, J = 11, H-1), 4.94 (1H, br s, H-13b), 4.97 (1H, br s, H-13a); OAng: 1.94 (3H, br s, H-5′), 2.02 (3H, br d, J = 7; 1.5, H-4′), 6.10 (1H, br q, J = 7; 1.5, H-3′) [1]

References

1. C. Zdero, F. Bohlmann, J. Solomon, X.A. Dominguez, Phytochemistry **27**(3), 849 (1988)
2. F. Bohlmann, M. Grenz, R.K. Gupta, A.K. Dhar, M. Ahmed, R.M. King, H. Robinson, Phytochemistry **19**(11), 2391 (1980)

6β-Cinnamoyloxy-6α,7α(H)-germacra-1(10),4-diene (6β-Cinnamoyloxy-6,7-dihydrogermacrene C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Verbesina eggersii* Hieron. [1]; *V. luetzelburgii* Mattf. [2]

$C_{24}H_{32}O_2$: 352.2402

Mp: colorless oil [1]

$[\alpha]^{24}$ (λ, nm): −82° (589), −86° (578), −101° (546), −213 (436) (*c* 0.8, $CHCl_3$) [1]

IR (CCl_4): 1710, 1640, 1170 [1]

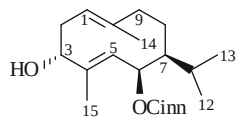
MS: 352.240 $[M]^+$ (1) (calc. for $C_{24}H_{32}O_2$; 352.240), 221 $[M - PhCH = CHCO]^+$ (24), 204 $[M - PhCH = CHCOOH]^+$ (34), 189 $[204 - \cdot CH_3]^+$ (15), 161 $[204 - \cdot C_3H_7]^+$ (44), 131 $[PhCH = CHCO]^+$ (100) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 4.93 (1H, br t, J = 0.5, H-1), 2.10 (2H, m, H-2), 2.40 (2H, m, H-3), 5.14 (1H, br d, J = 8, H-5), 6.11 (1H, br d, J = 6, H-6), 1.09 (3H, d, J = 7, H-12), 1.01 (3H, d, J = 7, H-13), 1.53 (3H, br s, H-15), 1.49 (3H, br s, H-14); OCinn: 6.51 (1H, d, J = 16, H-8′), 7.01 (5H, m, protons of Ph), 7.81 (1H, d, J = 16, H-7′) [1]

References

1. F. Bohlmann, M. Lonitz, Chem. Ber. **111**, 254 (1978)

6β-Cinnamoyloxy-7α(H)-germacra-1(10),4-dien-3α-ol (3α-Hydroxy-6β-cinnamoyloxy-6,7-dihydrogermacrene C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Verbesina eggersii* Hieron. [1]

$C_{24}H_{32}O_3$: 368.2351

Isolated as its 3-OAc [1]

Mp (its 3-OAc): colorless oil [1]

$[\alpha]^{24}$ (λ, nm) (its 3-OAc): −74° (589), −77° (578), −91° (546), −194° (436) (*c* 0.37, $CHCl_3$) [1]

IR (CCl_4) (its 3-OAc):1740, 1715, 1640, 1240, 1170 [1]

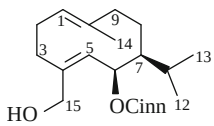
MS: (its 3-OAc): 410.246 $[M]^+$ (2) (calc. for $C_{26}H_{34}O_4$: 410.246), 350 $[M - AcOH]^+$ (1.5), 202 $[350 - PhCH = CHCOOH]^+$ (32), 159 $[202 - \cdot C_3H_7]^+$ (60), 131 $[PhCH = CHCO]^+$ (100) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS) (its 3-OAc): 0.86 (3H, d, J = 7, H-13), 1.04 (3H, d, J = 7, H-12), 1.52 (3H, br s, H-14), 1.60 (3H, br s, H-15), 1.75 (3H, s, OAc), 2.0−2.3 (2H, m, H-2), 4.88 (1H, br t, J = 0.5, H-1), 5.31 (1H, br d, J = 8, H-5), 5.49 (1H, br dd, J = 7; 8, H-3), 6.11 (1H, br d, J = 8, H-6); OCinn: 6.47 (1H, d, J = 16, H-8′), 7.02 (5H, m, Ph), 7.79 (1H, d, J = 16, H-7′) [1]

References

1. F. Bohlmann, M. Lonitz, Chem. Ber. **111**, 254 (1978)

6β-Cinnamoyloxy-7α(H)-germacra-1(10),4-dien-15-ol (15-Hydroxy-6β-cinnamoyloxy-6,7-dihydrogermacrane C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Verbesina eggersii* Hieron. [1]

$C_{24}H_{32}O_3$: 368.2351

Isolated as its 15-OAc [1]

Mp (its 15-OAc): colorless oil [1]

$[\alpha]^{24}$ (λ, nm) (its 15-OAc): −74° (589), −77° (578), −91° (546), −189° (436) (*c* 0.42, $CHCl_3$) [1]

IR (CCl_4) (its 15-OAc): 1740, 1715, 1640, 1240, 1170 [1]

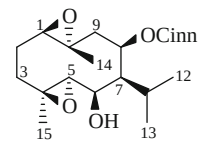
MS: (its 15-OAc): 410.246 $[M]^+$ (3) (calc. for $C_{26}H_{34}O_4$: 410.246), 350 $[M - AcOH]^+$ (2), 262 $[M - PhCH = CHCOOH]^+$ (4), 220 $[262 - H_2C = C = O]^+$ (7), 202 $[262 - AcOH]^+$ (30), 159 $[202 - \cdot C_3H_7]^+$ (41), 131 $[PhCH = CHCO]^+$ (100) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS) (its 15-OAc): 0.98 (3H, d, J = 7, H-13), 1.05 (3H, d, J = 7, H-12), 1.50 (3H, s, H-14), 1.79 (3H, s, OAc), 2.1–2.4 (4H, m, H-2, H-3), 4.19 (1H, br dd, J = 7.5; 7.5, H-1), 4.63 (1H, br d, J = 13, H-15b), 4.75 (1H, br d, J = 13, H-15a), 5.26 (1H, br d, J = 8, H-5), 6.22 (1H, br d, J = 8, H-6); OCinn: 6.48 (1H, d, J = 16, H-8′), 7.01 (5H, m, protons of Ph), 7.80 (1H, d, J = 16, H-7′) [1]

References

1. F. Bohlmann, M. Lonitz, Chem. Ber. **111**, 254 (1978)

8β-Cinnamoyloxy-1β,10α;4β,5α-diepoxy-6α,7α(H)-germacran-6β-ol (8β-Cinnamoyl-epoxy-echinadiol; 4,5:8,9-Diepoxy-3-hydroxy-2-isopropyl-5,9-dimetyl-cyclodecyl Cinnamate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Echinacea purpurea* (L.) Moench [1]

$C_{24}H_{32}O_5$: 400.2250

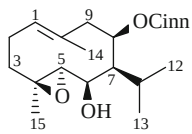
X-ray (epoxyechinadiol (=4,5:8,9-diepoxy-2-isopropyl-5,9-dimethyl-5-cyclodecane-1,3-diol)) [1]

Pharm./Biol.: Immunological activity tests showed that it enhances granulocyte phagocytosis in vitro up to 30%. It is likely that these esters contribute to the immunostimulating activity of the *Echinacea purpurea* drug [1]

References

1. R.F.X. Bauer, I.A. Khan, H. Lotter, H. Wagner, V. Wray, Helv. Chim. Acta **68**, 2355 (1985)

8β-Cinnamoyloxy-4β,5α-epoxy-6α,7α(H)-germacr-1(10)-en-6β-ol (8β-Cinnamoyl-echinadiol; 7,8-Epoxy-9-hydroxy-10-isopropyl-3,7-dimetyl-3-cyclodecen-1-yl Cinnamate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Echinacea purpurea* (L.) Moench [1]

$C_{24}H_{32}O_4$: 384.2301

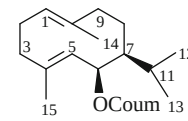
X-ray (echinadiol (=9,10-epoxy-2-isopropyl-5,9-dimethyl-5-cyclodecene-1,3-diol)): [1]

Pharm./Biol: Immunological activity tests showed that it enhances granulocyte phagocytosis in vitro up to 30%; in particular, showed significant activity in lymphocyte transformation test. It is likely that these esters contribute to the immunostimulating activity of the *Echinacea purpurea* drug [1]

References

1. R.F.X. Bauer, I.A. Khan, H. Lotter, H. Wagner, V. Wray, Helv. Chim. Acta **68**, 2355 (1985)

6β-Coumaroyloxy-germacra-1(10),4-diene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Verbesina macrophylla* (Cass.) Blake, *V. pentantha* Blake [1]

$C_{24}H_{32}O_3$: 368.2351

Mp: colorless gum [1]

$[\alpha]^{24}$ (λ, nm): −64.2° (589), −67.2° (578), −79.5° (546), −175.0° (436) (*c* 1.4, $CHCl_3$) [1]

IR (CCl_4): 3620, 1715, 1640, 1610 [1]

MS: 204.188 $[C_{15}H_{24}]^+$ (44), 189 [204 − ·Me] (15), 147 $[HOC_6H_4CH = CHCO]^+$ (100) [1]

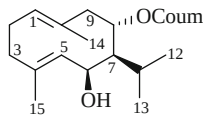
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 0.98 (6H, d, J = 6.5, H-12, H-13), 1.57 (6H, br s, H-14, H-15), 4.97 (2H, m, H-1, H-5), 5.72 (1H, br d, J = 8, H-6); OCoum: 6.44 (1H, d, J = 15.5, H-8′), 7.38 (2H, m, H-3′, H-5′), 7.59 (2H, m, H-2′, H-6′), 7.65 (1H, d, J = 15.5, H-7′) [1]

References

1. F. Bohlmann, M. Grenz, R.K. Gupta, A.K. Dhar, M. Ahmed, R.M. King, H. Robinson, Phytochemistry **19**(11), 2391 (1980)

8α-Coumaroyloxy-(*E*)-1(10),4-germacradien-6-ol (8-*O*-Coumaroyltovarol; 8-(4-Hydroxycinnamoyl)-(*E*)-1(10),4-germacradiene-6-ol)

CAS Registry Number: 98941-69-6



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Thapsia villosa* L. var. *minor* (Hoff. et Link) Cout. [1]

$C_{24}H_{32}O_4$: 384.2301

Mp: 177–179°C (Me_2CO) [1]

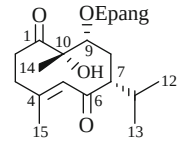
$[\alpha]_D$ −55.1° (*c* 1.6, EtOH) [1]

IR (film): 3300, 3150, 2900, 1670, 1620, 1600, 1500, 1450, 1370, 1320, 1270, 1200, 1180, 1160, 960 [1]

EI-MS: 384 $[M]^+$ (1), 366 $[M - H_2O]^+$ (1), 220 [M − (OH)PhCH = CHCOO]$^+$ (1), 202 [M − (OH) PhCH = CHCOO − H_2O]$^+$ (25), 192 (10), 187 (10), 177 (10), 164 (30), 159 (55), 147 (85), 119 (75), 107 (30), 91 (100), 81 (55), 69 (55) [1]

^{1}H NMR (60 MHz, C_5D_5N, TMS): 1.25* (3H, d, J = 6, H-13), 1.35* (3H, d, J = 6, H-12), 1.50 (3H, s, H-15), 1.70 (3H, s, H-14), 2.15 (4H, br s, H-2, H-3), 4.90 (1H, d, J = 7, H-6), 5.20 (1H, m, H-8), 5.70 (1H, d, J = 7, H-5), 5.80 (1H, m, H-1); OCoum: 6.70 (1H, d, J = 16, H-8′), 7.20 (2H, d, J = 8, H-3′, H-5′), 7.70 (2H, d, J = 8, H-2′, H-6′), 7.90 (1H, d, J = 16, H-7′); * – Assignment may be interchanged [1]

9α-(2′,3′-Epoxy-angeloyloxy)-10α-hydroxy-7β(H)-germacr-4-ene-1,6-dione



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Blumea balsamifera* DC. [1]

$C_{20}H_{30}O_6$: 366.2018

Mp: amorphous solid [1]

$[\alpha]_D^{24}$ +32° (*c* 0.08, $CHCl_3$) [1]

UV (EtOH): 234 (ε 30 000) [1]

CD (EtOH): ε_{310} +10.5°, ε_{235} +24.9° [1]

IR (ATR): 3487, 1733, 1712, 1686 [1]

FAB-MS: 367 $[M + H]^+$, 349 $[M - H_2O + H]^+$ [1]

HR-FAB-MS: 367.2097 $[M + H]^+$ (calc. for $C_{20}H_{31}O_6$ 367.2121) [1]

^{1}H NMR ($CDCl_3$): 0.88 (3H, d, J = 6.6, H-12), 0.88 (3H, d, J = 6.6, H-13), 1.31 (3H, s, H-14), 1.56 (1H, m, H-8β), 1.80 (1H, dd, J = 15.6, 13.1, H-8α), 1.88 (1H, m, H-11), 1.88 (1H, m, H-7), 1.97 (3H, d, J = 1.2, H-15), 2.15 (1H, ddd, J = 14.8, 5.5, 2.8, H-2β), 2.24 (1H, ddd, J = 11.9, 5.5, 2.4, H-3α), 2.69 (1H, ddd, J = 13.4, 11.9, 2.8, H-3β), 3.58 (1H, ddd, J = 14.8, 13.4, 2.4, H-2α), 4.77 (1H, d, J = 7.9, H-9), 5.85 (1H, br s, H-5); OEpang: 1.32 (3H, d, J = 5.4, H-4′), 1.56 (3H, s, H-5′), 3.06 (1H, q, J = 5.4, H-3′) [1]

^{13}C NMR [1]:

Table 1

C-1	213.5	C-8	28.8	C-15	17.8
2	34.4	9	74.0	OEpang	
3	36.7	10	82.5	1′	171.1
4	149.2	11	31.0	2′	60.0
5	127.5	12	20.5	3′	59.9
6	204.6	13	19.5	4′	14.0
7	55.3	14	17.0	5′	19.2

^{1}H-^{1}H COSY [1]

References

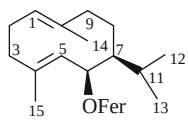
1. J. de Pascual Teresa, J.R. Moran, J.M. Hernandez, M. Grande, Phytochemistry **24**(8), 1779 (1985)

Pharm./Biol.: Weakly cytotoxic against Jurkat human T-cell leukemia cells [1]

References

1. N. Osaki, T. Koyano, T. Kowithayakorn, M. Hayashi, K. Komiyama, M. Ishibashi, J. Nat. Prod. **68**, 447 (2005)

6β-Feruloyloxy-germacra-1(10),4-diene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Verbesina macrophylla* (Cass.) Blake [1]

$C_{25}H_{34}O_4$: 398.2457

Mp: colorless gum [1]

$[\alpha]^{24}$ (λ, nm): −81.2° (589), −83.4° (578), −102.1° (546), −230.0° (436) (*c* 3.0, $CHCl_3$) [1]

IR (CCl_4): 3540, 1700, 1650 [1]

MS: 204.288 $[M - FerOH]^+$ (13) ($C_{15}H_{24}$), 161 $[204 - \cdot C_3H_7]^+$ (35), 177 $[HO(MeO)C_6H_3CH = CHCO]^+$ (100) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 0.96 (6H, d, J = 6.5, H-12, H-13), 1.57 (6H, br s, H-14, H-15), 4.95 (2H, m, H-1, H-5), 5.72 (1H, br d, J = 8, H-6); OFer: 3.93 (3H, s, OCH_3), 6.28 (1H, d, J = 15.5, H-8′), 6.91 (1H, d, J = 8.5, H-5′), 7.06 (1H, m, H-2′), 7.57 (1H, m, H-6′), 7.86 (1H, d, J = 15.5, H-7′) [1]

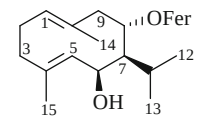
^{1}H NMR (270 MHz, C_6D_6, 75°C, TMS): 0.98 (6H, d, J = 6.5, H-12, H-13), 1.00 (3H, br s, H-14), 1.60 (3H, br s, H-15), 4.95 (2H, m, H-1, H-5), 5.73 (1H, br d, J = 8, H-6); OFer: 3.88 (3H, s, OCH_3), 6.38 (1H, d, J = 15.5, H-8′), 7.05 (1H, d, J = 8.5, H-5′), 7.11 (2H, m, H-2′, H-6′), 7.60 (1H, d, J = 15.5, H-7′) [1]

References

1. F. Bohlmann, M. Grenz, R.K. Gupta, A.K. Dhar, M. Ahmed, R.M. King, H. Robinson, Phytochemistry **19**(11), 2391 (1980)

8α-Feruloyloxy-(*E*)-1(10),4-germacradien-6-ol (8-*O*-Feruloyltovarol; 8-(7-Hydroxy-6-methoxycinnamoyl)-(*E*)-1(10),4-germacradiene-6-ol)

CAS Registry Number: 98941-70-9



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Thapsia villosa* L. var. *minor* (Hoff. et Link) Cout. [1]

$C_{25}H_{34}O_5$: 414.2406

Mp: 160–163°C (hexane–Et_2O) [1]

$[\alpha]_D$ −117.0° (*c* 1.4, $CHCl_3$) [1]

IR (film): 3500, 3400, 2900, 1680, 1630, 1600, 1500, 1450, 1420, 1370, 1250, 1170, 1100, 1040, 1020, 1000, 970 [1]

EI-MS: 414 $[M]^+$ (1), 220 $[M - FerOH]^+$ (2), 193 (100), 177 (80), 159 (20), 142 (50), 117 (25), 93 (25), 81 (35), 69 (20), 55 (20) [1]

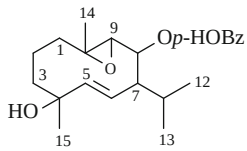
^{1}H NMR (60 MHz, $CDCl_3$, TMS): 1.05* (3H, d, J = 6, H-13), 1.15* (3H, d, J = 6, H-12), 1.50 (3H, s, H-15), 1.70 (3H, s, H-14), 2.20 (4H, br s, H-2, H-3), 4.60 (1H, d, J = 8, H-6), 5.30 (1H, m, H-5), 5.30 (2H, m, H-1, H-8); OFer: 3.90 (3H, s, OCH_3), 6.30 (1H, d, J = 16, H-8′), 7.00 (3H, m, H-2′, H-5′, H-6′), 7.70 (1H, d, J = 16, H-7′); * – Assignment may be interchanged [1]

References

1. J. de Pascual Teresa, J.R. Moran, J.M. Hernandez, M. Grande, Phytochemistry **24**(8), 1779 (1985)

8-(4′-Hydroxy-benzoyloxy)-9(10)-epoxy-germacr-5-en-4-ol (Fertenin)

CAS Registry Number: 72172-61-3



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Ferula tenuisecta* Korov. [1]

$C_{22}H_{30}O_5$: 374.2093

Mp: 209–211°C [1]

$[\alpha]_D$ +125° (*c* 0.8, EtOH) [1]

UV 260 (3.80) [1]

IR: 3600–3200, 1685, 1610, 1590, 1520, 1290, 1070, 856 [1]

MS: 331, 236, 218, 203, 193, 175, 138 [1]

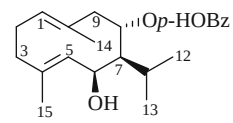
^{1}H NMR: 0.81 and 0.89 (each 3H, d, J = 5, H-12, H-13), 1.24 and 1.31(each 3H, s, H-15, H-14), 2.91 (1H, d, J = 7, H-9), 5.39 and 5.61 (each 1H, d, J = 10, H-5, H-6), 5.86 (1H, m, H-8); O*p*-HOBz: 6.83 (2H, d, J = 10, H-3′, H-5′), 7.82 (2H, d, J = 10, H-2′, H-6′) [1]

References

1. G.V. Sagitdinova, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **15**, 135 (1979)

8α-(4′-Hydroxy-benzoyloxy)-1(10),4-germacradien-6β-ol (Ferolin; 8α-[4-Hydroxy-benzoyloxy]-6β-hydroxy-6,7-H-germacrene C)

CAS Registry Number: 39380-12-6



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Ferula pallida* Korov. [1]; *F. rubroarenosa* Korov. [2]; *F. calcarea* M. Pimen. [3]; *F. tenuisecta* Korov. [4]; *F. karakalensis* Korov. [5]; *F. angreni* Korov. [6]; *F. kopetdagensis* Korov. [7]; *F. lapidosa* Korov. [4, 8]; *F. tschimganica* Lipsky ex Korov. [9]; *F. fedtschenkoana* K.-Pol. [10]; *F. karategina* Lipsky ex Korov. [11]; *F. kyzylkumica* Korov. [11]; *F. ferganensis* Lipsky ex Korov. [12]; *F. nuratavica* M. Pimen. [13]

$C_{22}H_{30}O_4$: 358.2144

Mp: 189–190°C [1]

$[\alpha]_D^{23}$ −91.6° (*c* 1.2, $CHCl_3$) [1]

UV (EtOH) 262 (4.18) [1]

IR (KBr): 3100–3420, 1680, 1615, 1595, 1520, 1240, 1105 [1]

TLC: petrol – EtOAc (3:1), R_f 0.49 [3]

^{1}H NMR (100 MHz, $CDCl_3$, HMDS): 0.99 and 1.10 (6H, d, J = 6, H-12, H-13), 1.42(3H, s, H-15), 1.66 (3H, s, H-14), 4.60 (1H, q, J = 11.4; 5.3, H-6), 5.24 (2H, m, H-1, H-8), 5.05 (1H, d, J = 6, H-5); O*p*-HOBz: 6.84 (2H, d, J = 10, H-3′, H-5′), 7.80 (2H, d, J = 10, H-2′, H-6′) [1]

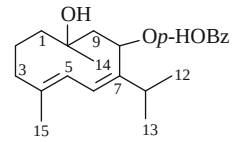
References

1. T.Kh. Khasanov, A.I. Saidkhodzjaev, G.K. Nikonov, Chem. Nat. Comp. **8**, 794 (1972)
2. L.I. Golovina, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **14**, 606 (1978)

3. S.Sh. Kerimov, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **23**, 641 (1987)
4. A.I. Saidkhodzjaev, L.A. Golovina, V.M. Malikov, S. Melibaev, U. Rakhmankulov, Chem. Nat. Comp. **21**, 388 (1985)
5. A.I. Saidkhodzjaev, V.M. Malikov, M.G. Pimenov, Chem. Nat. Comp. **29**, 187 (1993)
6. G.V. Sagitdinova, A.I. Saidkhodzjaev, V.M. Malikov, S. Melibaev, Chem. Nat. Comp. **14**, 692 (1978)
7. A.I. Saidkhodzhaev, Kh.M. Kamilov, M.A. Pimenov, Chem. Nat. Comp. **23**, 640 (1987)
8. G.V. Sagitdinova, A.I. Saidkhodzjaev, G.K. Nikonov, U. Rakhmankulov, Chem. Nat. Comp. **11**, 137 (1975)
9. A.Sh. Kadyrov, T.Kh. Khasanov, A.I. Saidkhodzjaev, G.K. Nikonov, Chem. Nat. Comp. **8**, 796 (1972)
10. Kh.M. Kamilov, G.K. Nikonov, N.N. Sharakhimov, Chem. Nat. Comp. **10**, 540 (1974)
11. A.I. Saidkhodzhaev, V.M. Malikov, M.G. Pimenov, S. Melibaev, Chem. Nat. Comp. **29**, 253 (1993)
12. A.Sh. Kadyrov, A.I. Saidkhodzjaev, G.K. Nikonov, S. Melibaev, Chem. Nat. Comp. **13**, 587 (1977)
13. M.N. Kobilov, A.I. Saidkhodzhaev, N.D. Abdullaev, Chem. Nat. Comp. **31**, 273 (1995)

8-(4′-Hydroxy-benzoyloxy)-4,6-germacradien-10-ol (Fertenicin)

CAS Registry Number: 74285-97-5



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Ferula tenuisecta* Korov. [1]

$C_{22}H_{30}O_4$: 358.2144

UV (EtOH) 260 (4.76) [1]

IR (KBr): 3600–3200, 1690, 1615, 1590, 1520 [1]

MS: 236 [M − $C_7H_6O_2$]$^+$, 218 [M − $C_7H_6O_2$ − H_2O]$^+$, 193 [M − $C_7H_6O_2$ − C_3H_7]$^+$, 175 [M − $C_7H_6O_2$ − C_3H_7 − H_2O]$^+$, 138 [M − 220]$^+$, 121 [M − 220 − OH]$^+$ [1]

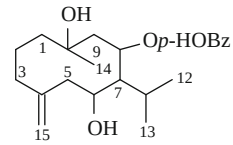
^{1}H NMR (100 MHz, $CDCl_3$, HMDS): 0.94 (6H, t, J = 7.0, H-12, H-13), 1.25 (3H, s, H-15), 1.76 (3H, s, H-14), 5.45 and 5.76 (2H, d, J = 10, H-5, H-6), 6.15 (1H, m, H-8); O*p*-HOBz: 7.03 (2H, d, J = 9.5, H-3′, H-5′), 8.05 (2H, d, J = 9.5, H-2′, H-6′) [1]

References

1. G.V. Sagitdinova, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **16**, 34 (1980)

8-(4′-Hydroxy-benzoyloxy)-4(15)-germacrene-6,10-diol (Fertenidin)

CAS Registry Number: 74285-98-6



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Ferula tenuisecta* Korov. [1]

$C_{22}H_{32}O_5$: 376.2250

Mp: 236–238°C [1]

$[\alpha]_D$ +145° (*c* 0.5, EtOH) [1]

UV (EtOH) 260 (3.0) [1]

IR (KBr): 3600–3200, 1680, 1610, 1590, 1520, 1280, 1050, 855 [1]

MS: 333 [M – C_3H_7]$^+$, 238 [M – $C_7H_6O_3$]$^+$, 220 [M – $C_7H_6O_3$ – H_2O]$^+$, 195 [M – C_3H_7 – $C_7H_6O_3$]$^+$, 138 [$C_7H_6O_3$]$^+$ [1]

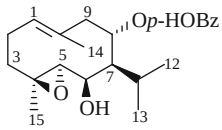
^{1}H NMR (100 MHz, $CDCl_3$, HMDS): 0.81 (6H, t, J = 6; 6, H-12, H-13), 1.15 (3H, s, H-14), 2.56 (2H, d, J = 5, H-9), 4.86 and 5.18 (each 1H, s, H-15), 4.15 (1H, q, J = 10; 5, H-6), 5.35 (1H, m, H-8); O*p*-HOBz: 6.84 (2H, d, J = 9, H-3′, H-5′), 7.88 (2H, d, J = 9, H-2′, H-6′) [1]

References

1. G.V. Sagitdinova, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **16**, 34 (1980)

8α-(4′-Hydroxy-benzoyloxy)-4β,5α-epoxy-6α,7α(H)-germacr-1(10)-en-6β-ol (Rubaferidin)

CAS Registry Number: 70476-17-4



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Ferula rubroarenosa* Korov. [1]; *F. tenuisecta* Korov. [2]; *F. calcarea* M. Pimen. [3]; *F. kopetdagensis* Korov. [4]

$C_{22}H_{30}O_5$: 374.2093

Mp: 162–164°C (hexane – ether 9:1) [1]

$[\alpha]_D$ −40.0° (*c* 1.1, $CHCl_3$) [1]

UV (EtOH) 261 (4.19) [1]

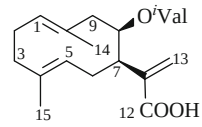
IR (KBr): 3200–3400, 1710–1675, 1515–1620 [1]

^{1}H NMR (100 MHz, $CDCl_3$, HMDS): 0.92 (3H, d, J = 6, H-12 or H-13), 1.15 (3H, d, J = 6, H-13 or H-12), 1.15 (3H, s, H-15), 1.77 (3H, s, H-14), 2.8 (1H, d, J = 7, H-5), 3.84 (1H, d, J = 7, H-6), 5.3 (2H, m, H-1, H-8); O*p*-HOBz: signals of *p*-hydroxybenzoic acid [1]

References

1. L.I. Golovina, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **14**, 606 (1978)
2. A.I. Saidkhodzjaev, L.A. Golovina, V.M. Malikov, S. Melibaev, U. Rakhmankulov, Chem. Nat. Comp. **21**, 388 (1985)
3. S.Sh. Kerimov, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **23**, 641 (1987)
4. A.I. Saidkhodzhaev, Kh.M. Kamilov, M.A. Pimenov, Chem. Nat. Comp. **23**, 640 (1987)

8β-Isovaleroyloxy-germacra-1(10)*Z*,4*Z*,11-trien-12-oic Acid



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Pegolettia senegalensis* Cass. [1]

$C_{20}H_{30}O_4$: 334.2144

Mp: colorless gum which, by addition of CH_2N_2 in Et_2O, afforded the corresponding esters (mix. with 8β-(2-methylbutyroyloxy and tigloyloxy)-germacra-1(10)*Z*,4*Z*,11-trien-12-oic acids) [1]

IR (CCl_4) (mix.): 3500−2700, 1730, 1690 [1]

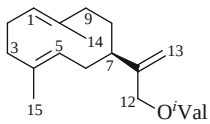
MS (mix.): 334.214 $[M]^+$ (0.3) ($C_{20}H_{30}O_4$), 232 (18), 85 (31), 83 (28) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS) (heating of the mixture in C_6H_6 for 2 hr at 200° afforded, after TLC mixture 8β-(its ethers)-5α-H,10β-methylelema-1,3,11-trien-12-oic acid methyl esters again could not be separated completely, only 8β-tiloyloxy-5α-H,10β-methylelema-1,3,11-trien-12-oic acid methyl ester was enriched): 1.10 (3H, s, H-14), 1.43 (1H, br d, J = 13; ∼3, H-6b), 1.77 (2H, m, J = ∼3, H-9), 1.77 (3H, br s, H-15), 2.10 (1H, ddd, J = ∼10; 13; ∼10, H-6a), 2.18 (1H, br d, J = ∼10, H-5), 2.92 (1H, br d, J = ∼10; ∼3, H-7), 4.68 (1H, br s, H-3b), 4.88 (1H, br s, H-3a), 4.89 (1H, d, J = 17, H-2-*trans*), 4.92 (1H, d, J = 10, H-2-*cis*), 5.30 (1H, br s, H-8), 5.60 (1H, br s, H-13b), 5.80 (1H, dd, J = 10; 17, H-1), 6.27 (1H, br s, H-13a); O^{i}Val: 0.90 (6H, d, H-4′, H-5′), 2.18 (2H, d, H-2′) [1]

References

1. F. Bohlmann, J. Jakupovic, A. Schuster, Phytochemistry **22**(7), 1637 (1983)

12-Isovaleroyloxy-germacra-1(10)*E*,4*E*,11(13)-triene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Perezia multiflora* (Humb. et Bonpl.) Less. [1]

$C_{20}H_{32}O_2$: 304.2402

Mp: (mix. with 12-(2′-methylbutyroyloxy)-germacra-1(10)*E*,4*E*,11(13)-triene) [1]

IR: 1735 [1]

MS: 304.240 $[M]^+$ (2), 202 (29), 187 (50), 145 (53), 57 (100) [1]

HPLC [1]

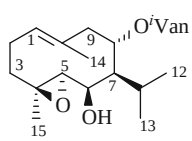
^{1}H NMR (400 MHz, $CDCl_3$): 1.40 or 1.49 (3H, br s, H-14), 1.54 or 1.56 (3H, br s, H-15), 2.15 (2H, m, H-3), 4.50 (1H, br d, J = 10, H-5), 4.60 (2H, br s, H-12), 4.79 (1H, br d, J = 11, H-1), 4.93 (1H, br s, H-13b), 4.94 (1H, br s, H-13a); O^{i}Val: 0.99 (6H, d, J = 7, H-4′, H-5′), 2.14 (1H, m, H-3′), 2.23 (2H, m, H-2′) [1]

References

1. C. Zdero, F. Bohlmann, J. Solomon, X.A. Dominguez, Phytochemistry **27**(3), 849 (1988)

8α-Isovanilloyloxy-4β,5α-epoxy-1(10)-germacren-6β-ol (Rubaferin)

CAS Registry Number: 70476-16-3



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Ferula rubroarenosa* Korov. [1]

$C_{18}H_{24}O_4$: 304.1675

Mp: 106–107°C (hexane – ether 9:1) [1]

$[\alpha]_D$ −45.08° (*c* 0.66, $CHCl_3$) [1]

UV (EtOH): 263 (3.94), 298 (3.68) [1]

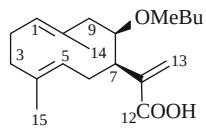
IR (KBr): 3200–3400, 1710–1675, 1620–1515 [1]

^{1}H NMR (100 MHz, $CDCl_3$, HMDS): 0.92 (3H, d, J = 6, H-12 or H-13), 1.15 (3H, d, J = 6, H-13 or H-12), 1.15 (3H, s, H-15), 1.77 (3H, s, H-14), 2.8 (1H, d, J = 7, H-5), 3.84 (1H, d, J = 7, H-6), 5.3 (2H, m, H-1, H-8); O^{i}Van: signals of isovanillic acid, 3.88 (3H, s, OCH_3) [1]

References

1. L.I. Golovina, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **14**, 606 (1978)

8β-(2′-Methylbutyroyloxy)-germacra-1(10)*Z*,4*Z*,11-trien-12-oic Acid



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Pegolettia senegalensis* Cass. [1]

$C_{20}H_{30}O_4$: 334.2144

Mp: colorless gum which, by addition of CH_2N_2 in Et_2O, afforded the corresponding esters (mix. with 8β-(tigloyloxy and isovaleryloxy)−germacra-1(10)*Z*,4*Z*,11-trien-12-oic acids) [1]

IR (CCl_4) (mix.): 3500−2700, 1730, 1690 [1]

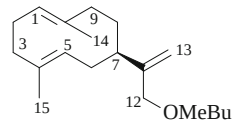
MS (mix.): 334.214 $[M]^+$ (0.3) ($C_{20}H_{30}O_4$), 232 (18), 85 (31), 83 (28) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS) (heating of the mixture in C_6H_6 for 2 hr at 200° afforded, after TLC mixture 8β-(its ethers)-5α-H,10β-methylelema-1,3,11-trien-12-oic acid methyl esters again could not be separated completely, only 8β-tiloyloxy-5α-H,10β-methylelema-1,3,11-trien-12-oic acid methyl ester was enriched): 1.10 (3H, s, H-14), 1.43 (1H, br d, J = 13; ~3, H-6b), 1.77 (2H, m, J = ~3, H-9), 1.77 (3H, br s, H-15), 2.10 (1H, ddd, J = ~10; 13; ~10, H-6a), 2.18 (1H, br d, J = ~10, H-5), 2.92 (1H, br d, J = ~10; ~3, H-7), 4.68 (1H, br s, H-3b), 4.88 (1H, br s, H-3a), 4.89 (1H, d, J = 17, H-2*t*), 4.92 (1H, d, J = 10, H-2*c*), 5.30 (1H, br s, H-8), 5.60 (1H, br s, H-13′), 5.80 (1H, dd, J = 10; 17, H-1), 6.27 (1H, br s, H-13); OMeBu: 0.86 (3H, t, H-4′), 1.08 (3H, d, H-5′), 2.30 (3H, tq, H-2′, H-3′) [1]

References

1. F. Bohlmann, J. Jakupovic, A. Schuster, Phytochemistry **22**(7), 1637 (1983)

12-(2′-Methylbutyroyloxy)-germacra-1(10)*E*,4*E*,11(13)-triene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Perezia multiflora* (Humb. et Bonpl.) Less. [1]

$C_{20}H_{32}O_2$: 304.2402

Mp: (mix. with 12-isovaleroyloxy-germacra-1(10)*E*,4*E*,11(13)-triene) [1]

IR (mix.): 1735 [1]

MS (mix.): 304.240 $[M]^+$ (2), 202 (29), 187 (50), 145 (53), 57 (100) [1]

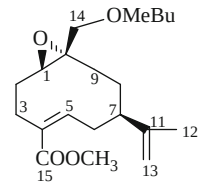
HPLC [1]

^{1}H NMR (400 MHz, $CDCl_3$) (mix.): 1.40 or 1.49 (3H, br s, H-14), 1.54 or 1.56 (3H, br s, H-15), 2.15 (2H, m, H-3), 4.50 (1H, br d, J = 10, H-5), 4.60 (2H, br s, H-12), 4.79 (1H, br d, J = 11, H-1), 4.93 (1H, br s, H-13b), 4.94 (1H, br s, H-13a); OMeBu: 0.94 (3H, t, J = 7, H-4′), 1.19 (3H, d, J = 7, H-5′), 2.42 (3H, m, H-2′, H-3′) [1]

References

1. C. Zdero, F. Bohlmann, J. Solomon, X.A. Dominguez, Phytochemistry **27**(3), 849 (1988)

14-(2′-Methylbutyroyloxy)-1β,10α-epoxy-4,11-germacradien-15-oic Acid Methyl Ester (Methyl-14-*O*-[2-methylbutyryl]-oxyphylloate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Oxyphyllum ulicinum* Phil. [1]

$C_{21}H_{32}O_5$: 364.2250

Mp: colorless oil [1]

$[\alpha]_D^{24}$ −46° (*c* 0.32, $CHCl_3$) [1]

IR (CCl_4): 1735, 1715 [1]

MS: 364.225 $[M]^+$ (1), 332 (0.5), 262 (1.5), 245 (1), 230 (1.5), 85 (41), 57 (100) [1]

HPLC [1]

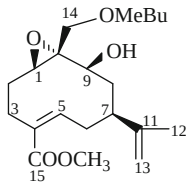
^{1}H NMR (400 MHz, $CDCl_3$): 0.96 (1H, br dd, J = 1; 9, H-9β), 1.38 (1H, m, H-8α), 1.61 (1H, dddd, J = 11; 13; 12; 5, H-2β), 1.73 (3H, br s, H-12), 1.79 (1H, br dd, J = 12; 14; 9, H-8β), 2.01 (1H, br t, J = 12; 12,

H-7), 2.16 (1H, dddd, J = 2.5; 13; 2; 2, H-2α), 2.26 (1H, m, J = 2; 12; 13.5, H-3α), 2.39 (1H, br d, J = 4, H-6α), 2.59 (1H, br dd, J = 1; 9, H-9α), 2.75 (1H, br d, J = 2; 5; 13.5, H-3β), 2.92 (1H, dd, J = 2.5; 11, H-1), 3.15 (1H, br q, J = 11; 14; 12, H-6β), 3.62 (1H, d, J = 12, H-14′), 3.80 (3H, s, OCH_3), 4.32 (1H, d, J = 12, H-14), 4.67 (1H, dq, J = 1; 1, H-13a), 4.73 (1H, br s, H-13b), 5.97 (1H, dd, J = 4; 11, H-5); OMeBu: 0.90 (3H, t, J = 7, H-4′), 1.13 (3H, d, J = 7, H-5′), 1.49 (1H, ddq, J = 7, H-3′a), 1.66 (1H, ddq, J = 7, H-3′b), 2.44 (1H, tq, J = 7, H-2′) [1]

References

1. C. Zdero, F. Bohlmann, H.M. Niemeyer, Phytochemistry **27**(7), 2165 (1988)

14-(2′-Methylbutyroyloxy)-9β-hydroxy-1β,10α-epoxy-4,11-germacradien-15-oic Acid Methyl Ester (Methyl-14-*O*-[2-methylbutyryl]-9β-hydroxy-oxyphylloate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Oxyphyllum ulicinum* Phil. [1]

$C_{21}H_{32}O_6$: 380.2199

Mp: colorless oil [1]

IR (CCl_4): 3580, 1735, 1720 [1]

MS: 380.220 $[M]^+$ (1.7), 362 (0.2), 348 (0.4), 278 (1.5), 247 (1.1), 85 (58), 57 (100) [1]

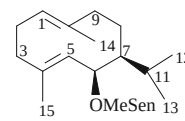
HPLC [1]

^{1}H NMR (400 MHz, $CDCl_3$): 1.61 (1H, dddd, J = 11; 13; 12; 5, H-2β), 1.68 (1H, br d, J = 14; 1, H-8α), 1.73 (3H, br s, H-12), 1.98 (1H, ddd, J = 12; 14; 9, H-8β), 2.16 (1H, dddd, J = 2.5; 13; 2; 2, H-2α), 2.26 (1H, m, J = 12; 12, H-7), 2.26 (1H, m, J = 2; 12; 13.5, H-3α), 2.39 (1H, br d, J = 4, H-6α), 2.75 (1H, br d, J = 2; 5; 13.5, H-3β), 2.92 (1H, dd, J = 2.5; 11, H-1), 3.15 (1H, br q, J = 11; 14; 12, H-6β), 3.26 (1H, br d, J = 9, H-9), 3.80 (3H, s, OCH_3), 3.84 (1H, d, J = 12, H-14a), 4.52 (1H, d, J = 12, H-14b), 4.67 (1H, dq, J = 1; 1, H-13′), 4.73 (1H, br s, H-13), 5.97 (1H, dd, J = 4; 11, H-5); OMeBu: 0.91 (3H, t, J = 7, H-4′), 1.14 (3H, d, J = 7, H-5′), 2.40 (3H, tq, J = 7, H-2′, H-3′) [1]

References

1. C. Zdero, F. Bohlmann, H.M. Niemeyer, Phytochemistry **27**(7), 2165 (1988)

6β-(4′-Methylsenecioyloxy)-6α,7α(H)-germacra-1(10),4-diene (6β-[3-Methylpent-2-enoyloxy]-6.7H-germacrene C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Senecio phonolithicus* Dinter [1]

$C_{21}H_{34}O_2$: 318.2559

Mp: colorless oil [1]

$[\alpha]^{24}$ (λ, nm) (its 6β-hydroxy deriv.): −5.7° (589), −5.7° (578), −6.6° (546), −15.0° (436) (*c* 0.33, $CHCl_3$) [1]

IR (CCl_4): 1715, 1650, 855 [1]

MS: 318 $[M]^+$ (1), 204 $[M - C_5H_9COOH]^+$ (42), 97 $[C_5H_9CO]^+$ (100) [1]

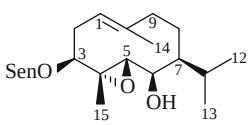
MS (its 6β-hydroxy deriv.): 222.198 $[M]^+$ (34) (calc. for $C_{15}H_{26}O$: 222.198), 207 $[M - CH_3]^+$ (7), 204 $[M - H_2O]^+$ (15), 189 $[204 - CH_3]^+$ (7), 161 $[204 - C_3H_7]^+$ (36), 81 $[C_6H_9]^+$ (100) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 0.93 (6H, d, J = 7, H-12, H-13), 1.54 (6H, s, H-14, H-15), 4.86 (2H, m, H-1, H-5), 5.58 (1H, br d, J = 7, H-6); OMeSen: 2.11 (3H, d, H-6′), 5.53 (1H, br q, H-2′) [1]

References

1. F. Bohlmann, K.-H. Knoll, C. Zdero, P.K. Mahanta, M. Grenz, A. Suwita, D. Ehlers, N.L. Van, W.-R. Abraham, A. A. Natu, Phytochemistry **16**(7), 965 (1977)

3β-Senecioyloxy-4α,5β-epoxy-5α,6α,7α(H)-germacr-1(10)-en-6β-ol (3β-Senecioyloxy-6β-hydroxy-4,5,6,7H-4α,5β-epoxygermacrene C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Senecio cylindricus* (A. Berger) Jacobsen [1]; *S. vitalis* N.E.Br [2]; *S. crassissimus* Humbert [3]

$C_{20}H_{32}O_4$: 336.2301

Mp: colorless oil [1]; mix. with 3β-angeloyloxy-6β-hydroxy-4,5,6,7H-4α,5β-epoxygermacrene C [3]

$[\alpha]^{24}$ (λ, nm): −33.7° (589), −34.9° (578), −40.4° (546), −74.7° (436) (*c* 2.2, $CHCl_3$) [1]

IR (CCl_4): 3460, 1710, 1650, 850 [1]

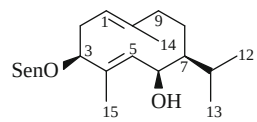
MS: 336.230 $[M]^+$ (2) (calc. for $C_{20}H_{32}O_4$: 336.230), 236 (5), 218 (5), 203 (3), 83 (100) [1]

^{1}H NMR (270 MHz, C_6D_6, 75°, TMS): 0.88 (3H, d, J = 7, H-13), 0.89 (3H, d, J = 7, H-12), 1.01 (3H, s, H-14), 1.70 (3H, br s, H-15), 1.8–2.1 (5H, m, H-8, H-9, H-11), 2.55 (2H, dd, J = 5; 12, H-2), 2.82 (1H, d, J = 8, H-5), 3.64 (1H, dd, J = 8, 2, H-6), 5.04 (1H, m, H-1), 5.40 (1H, ddd, J = 5; 12, H-3); OSen: 1.51 (3H, d, J = 1.5, H-5′), 2.07 (3H, d, J = 1.5, H-4′), 5.69 (1H, qq, J = 1.5; 1.5, H-2′) [1]

References

1. F. Bohlmann, J. Ziesche, Phytochemistry **18**(9), 1489 (1979)
2. F. Bohlmann, J. Ziesche, Phytochemistry **19**(8), 1851 (1980)
3. F. Bohlmann, J. Ziesche, Phytochemistry **20**(3), 469 (1981)

3β-Senecioyloxy-6α,7α(H)-germacra-1(10),4-dien-6β-ol (3β-Senecioyloxy-6β-hydroxy-6,7(H)-germacrene C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Senecio cylindricus* (A. Berger) Jacobsen [1]

$C_{20}H_{32}O_3$: 320.2351

Mp: colorless oil, which could not be separated (mix. with 3β-angeloyloxy-6β-hydroxy-6,7H-germacrene C) [1]

$[\alpha]^{24}$ (λ, nm) (mix.): −111.4° (589), −116.7° (578), −134.7° (546), −247.0° (436) (*c* 2.84, $CHCl_3$) [1]

IR (CCl_4) (mix.): 3460, 1720, 1650 [1]

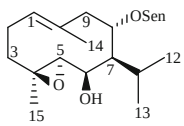
MS (mix.): 320.235 $[M]^+$ (1) (calc. for $C_{20}H_{32}O_3$: 320.235), 220 (25), 202 (10), 83 (100) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS) (mix.): 1.05 (3H, d, J = 7, H-13), 1.09 (3H, d, J = 7, H-12), 1.47 (3H, s, H-15), 1.6 (2H, m, H-8), 1.69 (3H, br s, H-14), 2.0 (1H, m, H-11), 2.1 (1H, m, H-9α), 2.62 (1H, m, H-9β), 2.63 (2H, br d, J = 12, H-2), 3.55 (1H, d, J = 10, OH), 4.48 (1H, br t, J = 8, 10; 2, H-6), 5.07 (1H, br d, J = 12, H-1), 5.23 (1H, dd, J = 5; 12, H-3), 5.28 (1H, d, J = 8, H-5); OSen: 1.92 (3H, d, J = 1.5, H-4′), 2.19 (3H, d, J = 1.5, H-5′), 5.70 (1H, qq, J = 1.5; 1.5, H-2′) [1]

References

1. F. Bohlmann, J. Ziesche, Phytochemistry **18**(9), 1489 (1979)

8α-Senecioyloxy-4β,5α-epoxy-1(10)-germacren-6-ol (8-*O*-Senecioylshiromodiol; 8-*O*-(3-Methyl-2-butenoyl)-4,5-epoxy-1(10)-germacrene-6-ol)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Ligularia persica* Boiss. [1]

$C_{20}H_{32}O_4$: 336.2301

Mp: oil [1]

$[\alpha]_D$ −66° (*c* 0.5, $CHCl_3$) [1]

IR (film): 3450, 1690, 1640, 1230, 1150, 1070 [1]

EI-MS: 336.2308 $[M]^+$ (14) (calc. for $C_{20}H_{32}O_4$ 336.2300), 236 (22), 193 (9), 177 (15), 136 (42), 121 (28), 93 (38), 83 (100), 55 (48) [1]

HPLC [1]

^{1}H NMR (400 MHz, $CDCl_3$, 57°C): 0.98 (3H, d, J = 6.5, H-12 or H-13), 1.12 (3H, d, J = 6.5, H-12 or H-13), 1.17 (3H, s, H-15), 1.45 (1H, br d, J = 1.5, H-7), 1.78 (3H, br s, H-14), 1.81 (1H, m, overlapped by other signals, H-11), 2.12 (2H, ddd, J = 6; 2; 13, H-3), 2.16 (1H, m, overlapped by other signals, H-9b), 2.30 (2H, m, H-2), 2.59 (1H, br dd, J = 5; 13, H-9a), 2.80 (1H, d, J = 8, H-5), 3.30 (1H, br s, OH), 3.50 (1H, dd, J = 8; 1.5, H-6), 5.20 (1H, ddd, J = 1.5; 5; 12, H-8), 5.31 (1H, ddq, J = 8; 1.5; 8, H-1); OSen: 1.93 (3H, d, J = 1.5, H-4′), 2.20 (3H, d, J = 1.5, H-5′), 5.70 (1H, qq, J = 1.5; 1.5, H-2′) [1]

^{13}C NMR (50.32 MHz, $CDCl_3$) [1]:

Table 1

C-1	128.81	C-8	71.41[a]	C-15	16.33
2	24.25	9	43.26	OSen	167.68
3	38.48	10	130.45		158.60
4	59.51	11	26.29		115.84
5	68.71	12	23.61[a]		27.41
6	71.55[a]	13	21.33[a]		20.42
7	50.88	14	26.29[b]		

[a]Signals may be interchanged within the same column

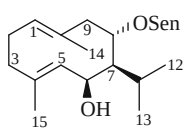
[b]The signal of C-14 is coincident with either that of C-11 (as in this Table) or with one of the other methyl signals. The proposed assignment is only tentative

References

1. J.A. Marco, J.F. Sanz, A. Garcia-Sarrion, A. Rustaiyan, Phytochemistry **30**(7), 2325 (1991)

8α-Senecioyloxy-1(10),4-germacradien-6β-ol (8-*O*-Senecioyltovarol; 8-(3-Methyl-2-butenoyl)-1(10),4-germacradiene)

CAS Registry Number: 98941-68-5



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Thapsia villosa* var. *minor* (Hoff. et Link) Cout. [1]; *Ligularia persica* Boiss. [2]

$C_{20}H_{32}O_3$: 320.2351

Mp: oily [1]

$[\alpha]_D$ −144.0° (*c* 1.2, $CHCl_3$) [1]

IR (film): 3400, 1690, 1630, 1210, 1140, 750 [1]

EI-MS: 220 $[M - SenOH]^+$ (5), 202 $[M - SenOH - H_2O]^+$ (5), 177 (30), 123 (85), 109 (80), 83 (100), 81 (60), 69 (25), 55 (20), 43 (10), 41 (10) [1]

HPLC [1]

^{1}H NMR (60 MHz, $CDCl_3$, TMS): 1.10 (6H, d, J = 6, H-12, H-13), 1.50 (3H, s, H-15), 1.70 (3H, s, H-14), 2.25 (4H, br s, H-2, H-3), 4.47 (1H, m, H-8), 5.10 (2H, m, H-1, H-6), 5.27 (1H, d, J = 7, H-5); OSen: 1.90 (3H, br s), 2.20 (3H, br s), 5.70 (1H, br s, H-2′) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.03 (3H, d, J = 6.5, H-12 or H-13), 1.07 (3H, d, J = 6.5, H-12 or H-13), 1.30 (1H, br d, J = 11, H-7), 1.46 (3H, br s, H-15), 1.64 (1H, m, overlapped by other signals, H-11), 1.67 (3H, br s, H-14), 2.05 (1H, dd, J = 12; 13, H-9b), 2.20–2.10 (2H, m, H-3), 2.36 (2H, br ddd, J = 12; 12; 5, H-2), 2.57 (1H, br dd, J = 5.5; 13, H-9a), 3.70 (1H, br d, J = 1.5, OH), 4.47 (1H, br dd, J = 8; 9, H-6), 5.05 (1H, br d, J = 12, H-1), 5.16 (1H, br dd, J = 5.5; 12, H-8), 5.27 (1H, br d, J = 8, H-5); OSen: 1.92 (3H, d, J = 1.5, H-4′), 2.20 (3H, d, J = 1.5, H-5′), 5.70 (1H, qq, J = 1.5; 1.5, H-2′) [2]

^{13}C NMR (50.32 MHz, $CDCl_3$) [2]:

Table 1

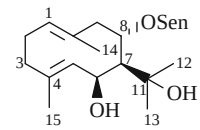
C-1	131.99	C-8	73.85	C-15	16.17
2	24.77	9	42.37	OSen	168.21
3	38.88	10	132.85[a]		158.95
4	129.67[a]	11	26.64		115.72
5	133.66	12	23.50[a]		27.65
6	67.59	13	21.49[a]		20.46
7	54.76	14	21.16		

[a]Signals may be interchanged within the same column [1]

References

1. J. de Pascual Teresa, J.R. Moran, J.M. Hernandez, M. Grande, Phytochemistry **24**(8), 1779 (1985)
2. J.A. Marco, J.F. Sanz, A. Garcia-Sarrion, A. Rustaiyan, Phytochemistry **30**(7), 2325 (1991)

8α-Senecioyloxy-6α,7α(H)-germacra-1(10)*E*,4*E*-diene-6β,8α,11-triol (8-*O*-Senecioyl-6β,8α-11-trihydroxygermacra-1(10)*E*,4*E*-diene)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Anisotome pilifera* (Hook. f.) Cockayne et Laing [1]

$C_{20}H_{32}O_4$: 336.2301

Mp: colorless oil [1]

$[\alpha]_D^{26.5}$ −72.0° (*c* 0.113, $CHCl_3$) [1]

UV (MeOH) 214 (4.38) [1]

IR (film): 3500 (br), 2924, 1718, 1379, 1229, 1144 [1]

EI-MS: 335 $[M - H]^+$ (1), 318 $[M - H_2O]^+$ (3), 235 $[M - C_4H_7COOH - H]^+$ (18), 218 $[M - C_4H_7COOH - H_2O]^+$ (100) [1]

HR-EI-MS: 318.21871 $[M - H_2O]^+$ (calc. for $C_{20}H_{30}O_3$, 318.21950) [1]

^{1}H NMR (500 MHz, $CDCl_3$): 1.41 (3H, s, H-13), 1.44 (3H, s, H-15), 1.48* (1H, m, H-7), 1.49 (3H, s, H-12), 1.63 (3H, s, H-14), 2.01 (1H, dd, J = 13.5; 12.0, H-9b), 2.13* (1H, m, H-2b), 2.13* (1H, m, H-3b), 2.17 (1H, m, H-3a), 2.35 (1H, dd, J = 13.0; 5.5, H-2a), 2.71 (1H, dd, J = 13.5; 5.0, H-9a), 3.25 (1H, s, 11-OH), 3.98 (1H, d, J = 6.0, 6-OH), 4.91 (1H, J = dd, J = 7.0; 6.0, H-6), 5.13 (1H, br d, J = 12.0, H-1), 5.26 (1H, d, J = 7.0, H-5), 5.40 (1H, br dd, J = 12.0; 5.0, H-8); OSen: 1.90 (3H, d, J = 1.0, H-4′), 2.18 (3H, d, J = 1.0, H-5′), 5.65 (1H, br s, H-2′); * - Unresolved signals [1]

^{13}C NMR (125 MHz, $CDCl_3$) [1]:

Table 1

C-1	132.1	C-8	74.1	C-15	16.4
2	24.7	9	41.7	OSen:	166.6
3	38.7	10	129.3	1′	115.8

(*continued*)

Table 1 (continued)

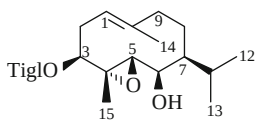
4	134.1	11	74.7	2′	158.7
5	132.3	12	29.8	3′	27.5
6	68.8	13	30.6	4′	20.4
7	52.5	14	20.8	5′	

HMBC [1]

References

1. C. Zidorn, N.B. Perry, Biochem. Syst. Ecol. **30**, 1055 (2002)

3β-Tigloyloxy-4α,5β-epoxy-5α,6α,7α(H)-germacr-1(10)-en-6β-ol (6β-Hydroxy-3β-tiglinoyloxy-4.5.6.7H-4.5-epoxygermacrene C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Senecio ficoides* Harv. [1]; *S. vitalis* [2]; *S. crassissimus* Humbert [3]

$C_{20}H_{32}O_4$: 336.2301

Mp: colorless oil [1]

$[\alpha]^{24}$ (λ, nm): −10.8° (589), −10.8° (578), −12.3° (546), −25.0° (436) (*c* 1.0, $CHCl_3$) [2]

IR (CCl_4): 3480, 1655 [1]

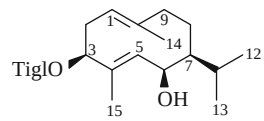
MS: 336.225 $[M]^+$ (1.5) (calc. for $C_{20}H_{32}O_4$: 336.230), 236 $[M - C_4H_7COOH]^+$ (2), 218 $[236 - H_2O]^+$ (2), 203 $[218 - CH_3]^+$ (3), 83 $[C_4H_7CO]^+$ (100) [1]

^{1}H NMR (270 MHz, C_6D_6, 76°C, TMS): 1.00 (3H, d, J = 7, H-13), 1.04 (3H, s, H-14), 1.16 (3H, d, J = 7, H-12), 1.56 (3H, s, H-15), 2.85 (1H, d, J = 7, H-5), 3.68 (1H, dd, J = 7; 1.5, H-6), 5.09 (1H, m, H-1), 5.45 (1H, ddd, J = 5; 12, H-3); OTigl: 1.48 (3H, dq), 1.81 (3H, dq), 6.95 (1H, qq, H-3′) [1]

References

1. F. Bohlmann, K.-H. Knoll, C. Zdero, P.K. Mahanta, M. Grenz, A. Suwita, D. Ehlers, N.L. Van, W.-R. Abraham, A. A. Natu, Phytochemistry **16**(7), 965 (1977)
2. F. Bohlmann, J. Ziesche, Phytochemistry **19**(8), 1851 (1980)
3. F. Bohlmann, J. Ziesche, Phytochemistry **20**(3), 469 (1981)

3β-Tigloyloxy-6α,7α(H)-germacra-1(10),4-dien-6β-ol (3β-Tiglinoyloxy-6β-hydroxy-6,7-H-germacrene C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Senecio cylindricus* (A. Berger) Jacobsen [1]

$C_{20}H_{32}O_3$: 320.2351

Mp: colorless oil [1]

$[\alpha]^{24}$ (λ, nm): −78.2° (589), −81.9° (578), −94.8° (546), −174.1° (436) (*c* 0.3, $CHCl_3$) [1]

IR (CCl_4): 3470, 1715, 1660, 860 [1]

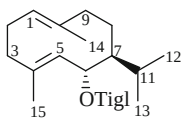
MS: 320 $[M]^+$ (0.4), 220.183 $[M - C_4H_7COOH]^+$ (8) (calc. for $C_{15}H_{24}O$: 220.183), 202 (7), 83 (100) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.05 (3H, d, J = 7, H-13), 1.10 (3H, d, J = 7, H-12), 1.47 (3H, br s, H-14), 1.6 (2H, m, H-8), 1.69 (3H, s, H-15), 2.0 (1H, m, H-11), 2.1 (1H, m, H-9α), 2.62 (1H, m, H-9β), 2.62 (2H, dd, J = 12; 13, H-2), 3.55 (1H, d, J = 10, OH), 4.48 (1H, br t, J = 8; 10; 2, H-6), 5.06 (1H, br d, J = 12, H-1), 5.22 (1H, dd, J = 5; 12, H-3), 5.27 (1H, d, J = 8, H-5); OTigl: 1.83 (3H, dq, J = 1.5; 1.5, H-5′), 1.85 (3H, dq, J = 7; 1.5, H-4′), 6.93 (1H, qq, J = 7; 1.5, H-3′) [1]

References

1. F. Bohlmann, J. Ziesche, Phytochemistry **18**(9), 1489 (1979)

6α-Tigloyloxy-6α,7α(H)-germacra-1(10),4-diene (6α-Tiglinoyloxy-6.7(H)-germacrene C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

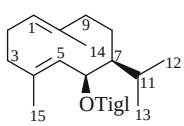
Biological sources: *Senecio archeri* (Compton) Jacobsen [1]

$C_{20}H_{32}O_2$: 304.2402

References

1. F. Bohlmann, C. Zdero, D. Berger, A. Suwita, P. Mahanta, C. Jeffrey, Phytochemistry **18**(1), 79 (1979)

6β-Tigloyloxy-6α,7α(H)-germacra-1(10),4-diene (6β-Tiglinoyloxy-6.7(H)-Germacrene C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Senecio crassulifolius* (DC.) Sch. Bip. [1]

$C_{20}H_{32}O_2$: 304.2402

Mp: colorless oil [1]

$[\alpha]^{24}$ (λ, nm): −43.5° (589), −45.7° (578), −53.8° (546), −110.3° (436) (*c* 2.0, $CHCl_3$) [1]

IR (CCl_4): 1715, 1658, 855 [1]

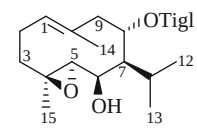
MS: 304.242 $[M]^+$ (7) (calc. for $C_{20}H_{32}O_2$: 304.240), 204 $[M - C_4H_7COOH]^+$ (100), 161 $[204 - C_3H_7]^+$ (82), 83 $[C_4H_7CO]^+$ (67) [1]

^{1}H NMR (270 MHz, C_6D_6, TMS): 0.99 (3H, d, J = 7, H-13), 1.07 (3H, d, J = 7, H-12), 1.45 (3H, s, H-15), 1.46 (3H, s, H-14), 4.92 (1H, m, H-1), 5.11 (1H, br d, J = 7, H-5), 6.06 (1H, br d, J = 7, H-6); OTigl: 1.52 (3H, dq), 1.88 (3H, dq), 6.96 (1H, qq, H-3′) [1]

References

1. F. Bohlmann, K.-H. Knoll, C. Zdero, P.K. Mahanta, M. Grenz, A. Suwita, D. Ehlers, N.L. Van, W.-R. Abraham, A. A. Natu, Phytochemistry **16**(7), 965 (1977)

8α-Tigloyloxy-4β,5α-epoxy-1(10)-germacren-6β-ol (8-*O*-Tigloyl-shiromodiol)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Ligularia persica* Boiss. [1]

$C_{20}H_{32}O_4$: 336.2301

Mp: oil [1]

$[\alpha]_D$ −27° (*c* 0.6, $CHCl_3$) [1]

IR (film): 3450, 1690, 1645, 1270, 1150, 1070 [1]

EI-MS: 336.2309 $[M]^+$ (4), 236 (15), 218 (8), 193 (9), 177 (25), 136 (50), 121 (32), 93 (43), 83 (100), 55 (60) [1]

HPLC [1]

^{1}H NMR (400 MHz, $CDCl_3$, 57°C): 0.98 (3H, d, J = 6.5, H-12 or H-13), 1.14 (3H, d, J = 6.5, H-12 or

H-13), 1.17 (3H, s, H-15), 1.46 (1H, br d, J = 1.5, H-7), 1.79 (3H, br s, H-14), 1.83 (1H, m, overlapped by other signals, H-11), 2.11 (2H, ddd, J = 6; 2; 13, H-3), 2.19 (1H, dd, J = 12; 13, H-9b), 2.30 (2H, m, H-2), 2.60 (1H, br dd, J = 5; 13, H-9a), 2.79 (1H, d, J = 8, H-5), 3.20 (1H, br s, OH), 3.51 (1H, dd, J = 8; 1.5, H-6), 5.25 (1H, ddd, J = 1.5; 5; 12, H-8), 5.32 (1H, ddq, J = 8; 1.5; 8, H-1); OTigl: 1.82 (3H, dq, J = 1.5; 7.5, H-4′), 1.87 (3H, dq, J = 1.5; 1.5, H-5′), 6.92 (1H, qq, J = 1.5; 7.5, H-3′) [1]

^{13}C NMR (50.32 MHz, $CDCl_3$) [1]:

Table 1

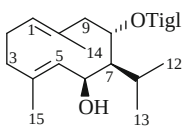
C-1	128.88	C-8	70.88[a]	C-15	16.38
2	24.28	9	43.82	OTigl	168.92
3	38.49	10	130.45		138.26
4	59.59	11	26.30		128.88
5	68.68	12	23.64[a]		14.37
6	71.46[a]	13	21.37		11.88
7	50.96	14	26.30[b]		

[a]Signals may be interchanged within the same column
[b]The signal of C-14 is coincident with either that of C-11 (as in this Table) or with one of the other methyl signals. The proposed assignment is only tentative

References

1. J.A. Marco, J.F. Sanz, A. Garcia-Sarrion, A. Rustaiyan, Phytochemistry **30**(7), 2325 (1991)

8α-Tigloyloxy-1(10),4-germacradien-6-ol (8-*O*-Tigloyl-tovarol; 8α-Tigloyloxy-6β-hydroxy-6,7(H)-germacrene C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Ligularia persica* Boiss.[1]

$C_{20}H_{32}O_3$: 320.2351

Mp: oil [1]

$[\alpha]_D$ −108° (*c* 1.2, $CHCl_3$) [1]

IR (film): 3450, 1690, 1645, 1270, 1150, 1070 [1]

EI-MS: 320.2351 $[M]^+$ (1), 220 (12), 205 (8), 177 (18), 159 (20), 136 (39), 93 (40), 83 (100), 55 (72) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.04 (3H, d, J = 6.5, H-12 or H-13), 1.09 (3H, d, J = 6.5, H-12 or H-13), 1.32 (1H, br d, J = 11, H-7), 1.46 (3H, br s, H-15), 1.65 (1H, m, overlapped by other signals, H-11), 1.68 (3H, br s, H-14), 2.06 (1H, dd, J = 12; 13, H-9b), 2.20–2.10 (2H, m, H-3), 2.36 (2H, br ddd, J = 12; 12; 5, H-2), 2.60 (1H, br dd, J = 5.5; 13, H-9a), 3.67 (1H, br d, J = 1.5, OH), 4.47 (1H, br dd, J = 8; 9, H-6), 5.05 (1H, br d, J = 12, H-1), 5.20 (1H, br dd, J = 5.5; 12, H-8), 5.26 (1H, br d, J = 8, H-5); OTigl: 1.81 (3H, dq, J = 1.5; 7.5, H-4′), 1.84 (3H, dq, J = 1.5; 1.5, H-5′), 6.92 (1H, qq, J = 1.5; 7.5, H-3′) [1]

^{13}C NMR (50.32 MHz, $CDCl_3$) [1]:

Table 1

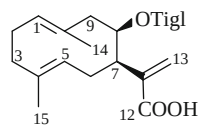
C-1	131.99	C-8	74.72	C-15	16.20
2	24.78	9	42.28	OTigl	169.37
3	38.88	10	133.00[a]		138.48
4	129.54[a]	11	26.61		128.46
5	133.56	12	23.47[a]		14.54
6	67.57	13	21.45[a]		11.96
7	54.76	14	21.17		

[a]Signals my be interchanged within the same column [1]

References

1. J.A. Marco, J.F. Sanz, A. Garcia-Sarrion, A. Rustaiyan, Phytochemistry **30**(7), 2325 (1991)

8β-Tigloyloxy-germacra-*trans*,*trans*-1(10),4,11-trien-12-oic Acid



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Pegolettia senegalensis* Cass. [1]

$C_{20}H_{30}O_4$: 334.2144

Mp: colorless gum which, by addition of CH_2N_2 in Et_2O, afforded the corresponding esters (mix. with 8β-(2-methylbutyroyloxy and isovaleryloxy)-germacra-*trans,trans*-1(10),4,11-trien-12-oic acid) [1]

IR (CCl_4) (mix.): 3500−2700, 1730, 1690 [1]

MS (mix.): 334.214 $[M]^+$ (0.3) ($C_{20}H_{30}O_4$), 232 (18), 85 (31), 83 (28) [1]

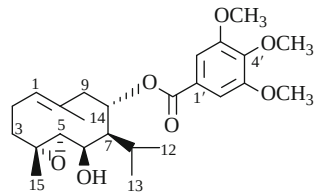
^{1}H NMR (400 MHz, $CDCl_3$, TMS) (heating of the mixture in C_6H_6 for 2 hr at 200° afforded, after TLC mixture 8β-(its ethers)-5α-H,10β-methylelema-1,3,11-trien-12-oic acid methyl esters again could not be separated completely, only 8β-tiloyloxy-5α-H,10β-methylelema-1,3,11-trien-12-oic acid methyl ester was enriched): 1.10 (3H, s, H-14), 1.43 (1H, br d, J = 13; ∼3, H-6b), 1.77 (2H, m, J = ∼3, H-9), 1.77 (3H, br s, H-15), 2.10 (1H, ddd, J = ∼10; 13; ∼10, H-6a), 2.18 (1H, br d, J = ∼10, H-5), 2.92 (1H, br d, J = ∼10; ∼3, H-7), 4.68 (1H, br s, H-3b), 4.88 (1H, br s, H-3a), 4.89 (1H, d, J = 17, H-2*t*), 4.92 (1H, d, J = 10, H-2*c*), 5.30 (1H, br s, H-8), 5.60 (1H, br s, H-13b), 5.80 (1H, dd, J = 10; 17, H-1), 6.27 (1H, br s, H-13a); OTigl: 1.78 (3H, br d, H-4′), 1.80 (3H, br s, H-5′), 6.78 (1H, br q, H-3′) [1]

References

1. F. Bohlmann, J. Jakupovic, A. Schuster, Phytochemistry **22**(7), 1637 (1983)

8α-(3′,4′,5′-Trimethoxybenzoyloxy)-4α,5α-epoxy-1(10)-germacren-6β-ol (Ugaferin)

CAS Registry Number: 63026-58-4



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Ferula ugamica* Korov. [1]; *F. kuhistanica* Korov. [2]; *F. leucographa* Korov. [3]

$C_{25}H_{36}O_7$: 448.2461

Mp: 125–126° [1]

$[\alpha]_D$ −24.5° (*c* 1.0, $CHCl_3$) [1]

UV (EtOH) 270 (4.06) [1]

IR (KBr): 3400–3600, 1735, 1615, 1560, 1520, 1250 [1]

^{1}H NMR (100 MHz, $CDCl_3$, HMDS): 1.0 and 1.18 (each 3H, d, J = 7, H-12, H-13), 1.02 (3H, s, H-15), 1.55 (3H, s, H-14), 2.90 (1H, d, J = 6, H-5), 3.64 (2H, m, H-1, H-6), 5.10 (1H, t, J = 6, H-1), 5.60 (1H, q, J = 10; 5, H-8); acyl group: 3.45 (6H, s, 2 × OCH_3), 3.82 (3H, s, OCH_3), 7.45 (2H, s, H-2′, H-6′) [1]

X-ray: [4]

Pharm./Biol.: Estrogenic activity [5]

References

1. A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **14**, 614 (1978)

2. A.I. Babekov, A.I. Saidkhodzhaev, B.M. Keneshov, Chem. Nat. Comp. **36**, 219 (2000)
3. M.N. Kobilov, A.I. Saidkhodzhaev, N.D. Abdullaev, Chem. Nat. Comp. **31**, 530 (1995)
4. M.K. Makhmudov, B. Tashkhodjaev, A.I. Saidkhodzhaev, V.M. Yagudaev, Chem. Nat. Comp. **26**, 157 (1990)
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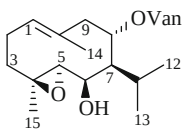
8α-Vanilloyloxy-4β,5α-epoxy-1(10)-germacren-6β-ol (Rubaferinin)

CAS Registry Number: 70476-16-3



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Ferula rubroarenosa* Korov. [1]; *F. tenuisecta* Korov. [2]; *F. calcarea* M. Pimen. [3]; *F. kopetdagensis* Korov. [4]

$C_{23}H_{32}O_6$: 404.2199

Mp: 105–106°C (hexane – ether, 9:1) [1]

$[\alpha]_D$ −36° (*c* 1.0, $CHCl_3$) [1]

UV (EtOH): 265 (4.01), 295 (3.79) [1]

IR (KBr): 3200–3400, 1710–1675, 1620–1515 [1]

^{1}H NMR (100 MHz, $CDCl_3$, HMDS): 0.92 (3H, d, J = 6, H-12 or H-13), 1.15 (3H, d, J = 6, H-13 or H-12), 1.15 (3H, s, H-15), 1.77 (3H, s, H-14), 2.8 (1H, d, J = 7, H-5), 3.84 (1H, d, J = 7, H-6), 5.3 (2H, m, H-1, H-8); OVan: signals of vanillic acid, 3.88 (3H, s, OCH_3) [1]

References

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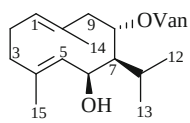
2. A.I. Saidkhodzjaev, L.A. Golovina, V.M. Malikov, S. Melibaev, U. Rakhmankulov, Chem. Nat. Comp. **21**, 388 (1985)
3. S.Sh. Kerimov, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **23**, 641 (1987)
4. A.I. Saidkhodzhaev, Kh.M. Kamilov, M.A. Pimenov, Chem. Nat. Comp. **23**, 640 (1987)

8α-Vanilloyloxy-1(10),4-germacradien-6β-ol (Tschimganidin; Chimganidin; 8α-Vanillyloxy-6β-hydroxy-6,7-H-germacrene C)

CAS Registry Number: 39380-16-0



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Monoesters

Biological sources: *Ferula tschimganica* Korov. [1]; *F. rubroarenosa* Korov. [2]; *F. calcarea* M. Pimen. [3]; *F. tenuisecta* Korov. [4]; *F. karakalensis* Korov. [5]; *F. angreni* Korov. [6]; *F. kopetdagensis* Korov. [7]; *F. lapidosa* Korov. [8]; *F. kyzylkumica*

Korov., *F. karategina* Lipsky ex Korov. [9]; *F. ferganensis* Lipsky ex Korov. [10]

$C_{23}H_{32}O_5$: 388.2250

Mp: 140–141°C (hexane – ether, 7:1) [1]; 140–141°C (ether) [7]

$[\alpha]_D$ −97.9° (*c* 1.2, $CHCl_3$) [1]; −80° (*c* 1.0, $CHCl_3$) [3]; $[\alpha]_D^{20}$ −96.8° (*c* 1.0, $CHCl_3$) [7]

UV (EtOH): 267 (4.10), 298 (3.86) [1]

IR (KBr): 3180–3450, 1690, 1680, 1610, 1590 [1]

TLC: petrol – EtOAc, R_f 0.55 [1]

^{1}H NMR (100 MHz, $CDCl_3$, HMDS): 1.00 and 1.10 (6H, d, J = 6.5, H-12, H-13), 1.42 (3H, s, H-15), 1.66 (3H, w.s, H-14), 4.40 (1H, q, J = 11.4; 5.3, H-6), 5.22 (2H, m, H-1, H-8), 5.05 (1H, d, J = 6, H-5); OVan: 3.84 (3H, s, OCH_3), 6.91 (1H, d, J = 10, H-3′), 7.55 (1H, q, J = 10, H-2′), 7.60 (1H, d, J = 2, H-6′) [1]

X-ray [11]

Pharm./Biol.: Estrogenic activity [12]

References

1. A.Sh. Kadyrov, T.Kh. Khasanov, A.I. Saidkhodzjaev, G.K. Nikonov, Chem. Nat. Comp. **8**, 796 (1972)
2. L.I. Golovina, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **14**, 606 (1978)
3. S.Sh. Kerimov, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **23**, 641 (1987)
4. A.I. Saidkhodzjaev, L.A. Golovina, V.M. Malikov, S. Melibaev, U. Rakhmankulov, Chem. Nat. Comp. **21**, 388 (1985)
5. A.I. Saidkhodzjaev, V.M. Malikov, M.G. Pimenov, Chem. Nat. Comp. **29**, 187 (1993)
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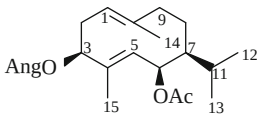
12. S.S. Nazrullaev, Z.A. Khushbaktova, V.N. Syrov, Kh.S. Akhmedkhodzhaeva, A.I. Saidkhodzhaev, The Chemistry and Biological Activity of Synthetic and Natural Compounds, in *Oxygen- and Sulfur-Containing Heterocycles*, ed. by V.G. Kartsev, vol. 1 (IBS PRESS, Moscow, 2003), p. 329

Germacranes

Diesters

6β-Acetoxy-3β-angeloyloxy-6α,7α(H)-germacra-1(10),4-diene (6β-Acetoxy-3β-angeloyloxy-6.7(H)-germacrene C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Senecio ficoides* Harv. [1]; *S. vitalis* [2]; *S. crassissimus* Humbert [3]

$C_{22}H_{34}O_4$: 362.2457

Mp: colorless oil [1]

$[\alpha]^{24}$ (λ, nm): −99.2° (589), −104.8° (578), −126.2° (546), −261.8° (436) (*c* 0.5, $CHCl_3$) [1]

IR (CCl_4): 1740, 1715, 1650 [1]

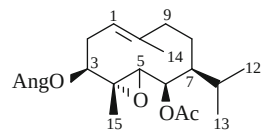
MS: 362.246 $[M]^+$ (2) (calc. for $C_{22}H_{34}O_4$: 362.246), 262 $[M - C_4H_7COOH]^+$ (2), 202 $[262 - AcOH]^+$ (75), 159 $[202 - C_3H_7]^+$ (95), 83 $[C_4H_7CO]^+$ (100) [1]

^{1}H NMR (270 MHz, C_6D_6, TMS): 1.12 (3H, d, J = 7, H-13), 1.19 (3H, d, J = 7, H-12), 1.31 (3H, s, H-15), 1.49 (3H, s, H-14), 1.75 (3H, s, OAc), 5.21 (1H, br d, J = 12, H-1), 5.33 (1H, d, J = 7, H-5), 5.86 (1H, dd, J = 5; 11, H-3), 5.98 (1H, dd, J = 7; 1, H-6); OAng: 1.95 (3H, dq, H-5′), 2.10 (3H, dq, H-4′), 5.78 (1H, qq, H-3′) [1]

References

1. F. Bohlmann, K.-H. Knoll, C. Zdero, P.K. Mahanta, M. Grenz, A. Suwita, D. Ehlers, N.L. Van, W.-R. Abraham, A. A. Natu, Phytochemistry **16**(7), 965 (1977)
2. F. Bohlmann, J. Ziesche, Phytochemistry **19**(8), 1851 (1980)
3. F. Bohlmann, J. Ziesche, Phytochemistry **20**(3), 469 (1981)

6β-Acetoxy-3β-angeloyloxy-4α,5-epoxy-7α(H)-germacr-1(10)-ene (6β-Acetoxy-3β-angeloyloxy-4.5.6.7H-4.5-epoxygermacrene C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Senecio ficoides* Harv. [1]; *S. cylindricus* (A. Berger) Jacobsen [2]; *S. crassissimus* Humbert [3]; *Senecio balbinifolius* DC. [4]; *Kleinia mandraliscae* Tin. ex Lojac. [5]

$C_{22}H_{34}O_5$: 378.2406

Mp: colorless oil [1]

$[\alpha]^{24}$ (λ, nm): −41.2° (589), −43.4° (578), −50.6° (546), +98.0° (436) (*c* 1.0, $CHCl_3$) [1]

IR (CCl_4): 1740, 1712, 1650 [1]

MS: 378.240 $[M]^+$ (0.5) (calc. for $C_{22}H_{34}O_5$: 378.241), 278 $[M - C_4H_7COOH]^+$ (1), 203 $[278 - AcOH - CH_3]^+$ (5), 160 $[203 - C_3H_7]^+$ (12), 83 $[C_4H_7CO]^+$ (100) [1]

^{1}H NMR (270 MHz, C_6D_6, 76°C, TMS): 1.08 (3H, d, J = 7, H-13), 1.15 (3H, d, J = 7, H-12), 1.16 (3H, s, H-14), 1.59 (3H, s, H-15), 1.75 (3H, s, OAc), 2.97 (1H, d, J = 7, H-5), 5.23 (1H, m, H-1), 5.30 (1H, dd, J = 7; 1.5, H-6), 5.75 (1H, ddd, J = 5; 12, H-3α), OAng: 1.89 (3H, dq, H-5′), 2.04 (3H, dq, H-4′), 5.79 (1H, qq, H-3′) [1]

References

1. F. Bohlmann, K.-H. Knoll, C. Zdero, P.K. Mahanta, M. Grenz, A. Suwita, D. Ehlers, N.L. Van, W.-R. Abraham, A. A. Natu, Phytochemistry **16**(7), 965 (1977)
2. F. Bohlmann, J. Ziesche, Phytochemistry **18**(9), 1489 (1979)
3. F. Bohlmann, J. Ziesche, Phytochemistry **20**(3), 469 (1981)

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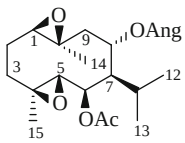
6β-Acetoxy-8α-angeloyloxy-1β,10β;4β,5β-diepoxy-germacrane



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Thapsia villosa* L. var. *villosa* [1]

$C_{22}H_{34}O_6$: 394.2355

Mp: oil [1]

$[\alpha]_D$ −10.5° (*c* 0.6, $CHCl_3$) [1]

IR (film): 2950, 1750, 1720, 1640, 1460, 1390, 1370, 1250, 1160, 1130, 1100, 990, 940, 900, 820, 680 [1]

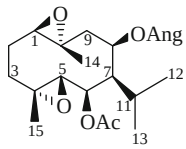
EI-MS: 394 $[M]^+$ (2), 354 (2), 294 (10), 234 (10), 209 (30), 191 (30), 147 (40), 137 (40), 123 (50), 109 (50), 99 (50), 83 (100), 55 (80) [1]

^{1}H NMR (60 MHz, CCl_4, TMS): 1.05* (3H, d, J = 6, H-13), 1.20* (3H, d, J = 6, H-12), 1.28 (3H, s, H-15), 1.45 (3H, s, H-14), 1.90 (3H, s, OAc), 3.10 (1H, m, H-1), 3.15 (1H, d, J = 7, H-5), 4.90 (1H, d, J = 7, H-6), 5.58 (1H, dd, J = 12; 5, H-8); OAng: 1.93 (3H, s, H-5′), 2.00 (3H, d, J = 7, H-4′), 6.00 (1H, q, J = 7, H-3′), * – Assignment may be interchanged [1]

References

1. J. de Pascual Teresa, J.R. Moran, J.M. Hernandez, M. Grande, Phytochemistry **24**(8), 1779 (1985)

6β-Acetoxy-8β-angeloyloxy-1β,10α;4α,5β-diepoxy-germacrane



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Kleinia articulata* Haw. [1]

$C_{22}H_{34}O_6$: 394.2355

Mp: colorless gum [1]

$[\alpha]^{24}$ (λ, nm): −10.5° (365) (*c* 0.59, $CHCl_3$) [1]

IR (CCl_4): 1750, 1725, 1650, 1240 [1]

MS: 394.236 $[M]^+$ (1), 334 (0.5), 295 (1), 235 (2), 83 (100), 55 (71) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.01 (3H, d, J = 6.5, H-13), 1.20 (3H, d, J = 6.5, H-12), 1.32 (3H, s, H-14), 1.33 (1H, ddd, J = 13; 14, H-3b), 1.50 (1H, dddd, J = 15; 3.5; 13, H-2α), 1.50 (3H, s, H-15), 1.67 (1H, br d, J = 1.3; 10, H-7), 1.97 (2H, m, H-9α, H-11), 1.97 (3H, s, OAc), 2.12 (1H, ddd, J = 10; 15, H-2β), 2.22 (1H, ddd, J = 3.5; 14, H-3a), 2.27 (1H, dd, J = 12.5, H-9β), 3.14 (1H, br d, J = 10, H-1), 3.18 (1H, d, J = 6.5, H-5), 4.97 (1H, dd, J = 6.5; 1.3, H-6), 5.68 (1H, br dd, J = 5.5; 12.5, H-8); OAng: 1.90 (3H, dq, H-5′), 2.02 (3H, dq, H-4′), 6.10 (1H, qq, H-3′) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS) (its 6-hydroxy deriv.): 1.00 (3H, d, J = 6.5, H-13), 1.16 (3H, d, J = 6.5, H-12), 1.27 (3H, s, H-14), 1.3 (1H, m, J = 13; 14, H-3b), 1.38 (1H, dddd, J = 15; 3.5; 13, H-2α), 1.51 (3H, s, H-15), 1.60 (1H, br d, J = 2; 10, H-7), 1.86 (2H, m, H-9α, H-11), 2.11 (1H, ddd, J = 10; 15, H-2β), 2.24 (1H, ddd, J = 3.5; 14, H-3a), 2.48 (1H, dd, J = 12.5, H-9β), 3.04 (1H, br d, J = 10, H-1), 3.14 (1H, d, J = 7.5, H-5), 3.31 (1H, d, J = 9, OH), 3.57 (1H, ddd, J = 7.5; 2; 9, H-6), 5.43 (1H, br dd, J = 5.5; 12.5, H-8); OAng: 1.89

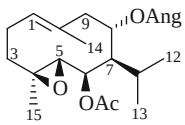
(3H, dq, H-5′), 2.02 (3H, dq, H-4′), 6.19 (1H, qq, H-3′) [1]

References

1. F. Bohlmann, M. Ahmed, J. Jakupovic, C. Jeffrey, Phytochemistry **20**(2), 251 (1981)

6β-Acetoxy-8α-angeloyloxy-4β,5β-epoxy-1(10)-germacrene (6β-*O*-Acetyl-8α-*O*-angeloylshiromodiol; Shiromodiol-6-*O*-acetate-8-*O*-angelate)

CAS Registry Number: 98941-64-1



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Thapsia villosa* L. var. *villosa* [1]; *Laserpitium halleri* subsp. *halleri* Crantz [2]

$C_{22}H_{34}O_5$: 378.2406

Mp: oil [1, 2]

$[\alpha]_D^{25}$ −54° (*c* 1.1, $CHCl_3$) [2]

UV 218 (3.9) [2]

IR (film): 2950, 1750, 1720, 1240, 1160, 1050 [1]; ($CHCl_3$): 1750–1250, 1720 [2]

MS: 378.240594 $[M]^+$ (2) (calc for $C_{22}H_{34}O_5$: 378.24609), 83 (100) [2]

^{1}H NMR (60 MHz, $CDCl_3$, TMS): 0.95* (3H, d, J = 6.5, H-13), 1.16* (3H, d, J = 6.5, H-12), 1.22 (3H, s, H-15), 1.77 (3H, s, H-14), 1.94 (3H, s, OAc), 2.88 (1H, d, J = 7, H-5), 4.90 (1H, d, J = 7, H-6), 5.30 (1H, m, H-1), 5.45 (1H, dd, J = 12; 5, H-8); OAng: 1.96 (3H, s, H-5′), 1.99 (3H, d, J = 7, H-4′), 6.05 (1H, q, J = 7, H-3′), * – Assignment may be interchanged [1]

^{1}H NMR (200 MHz, $CDCl_3$, 25°C, TMS): 0.89 (3H, d, J = 7.0, H-12), 1.10 (3H, d, J = 7.0, H-13), 1.14 (3H, s, H-15), 1.76 (3H, br s, H-14), 2.03 (3H, s, OAc), 2.60 (1H, br s, H-9a), 2.86 (1H, d, J = 7.2, H-5), 4.90 (1H, dd, J = 7.2; 1.8, H-6), 5.32 (1H, t, J = 8.0, H-1), 5.49 (1H, br dd, J = 12; 5.0, H-8); OAng: 1.88 (3H, quint, J = 1.5; 1.5, H-5′), 2.00 (3H, dq, J = 7.0; 1.5, H-4′), 6.10 (1H, qq, J = 7.0; 1.5, H-3′) [2]

^{1}H NMR (200 MHz, C_6D_6, TMS): 0.93 (3H, s, H-15), 1.02 (3H, d, J = 7.0, H-12), 1.08 (3H, d, J = 7.0, H-13), 1.46 (3H, br s, H-14), 1.70 (3H, s, OAc), 2.50 (1H, br s, H-9a), 2.96 (1H, d, J = 7.2, H-5), 5.13 (1H, br t, J = 8.0, H-1), 5.30 (1H, br d, J = 7.2H-6), 5.69 (1H, br dd, J = 12; 5.0, H-8); OAng: 1.86 (3H, q, J = 1.5; 1.5, H-5′), 1.98 (3H, dq, J = 7.0; 1.5, H-4′), 5.78 (1H, qq, J = 7.0; 1.5, H-3′) [2]

^{13}C NMR (50.30 MHz, $CDCl_3$, 25°C, TMS) [2]:

Table 1

C-1	128.48 d	C-9	41.62 t	OAng: 1′	166.52 s
2	24.18 t	10	130.87 s	2′	127.84 s
3	38.22 t	11	26.27 d	3′	137.85 d
4	59.14 s	12	23.19 q[a]	4′	15.56 q
5	66.46 d	13	21.31 q[a]	5′	20.68 q
6	73.74 d	14	20.38 q	OAc: 1″	169.56 s
7	48.16 d	15	16.72 q	2″	20.30 q
8	71.53 d				

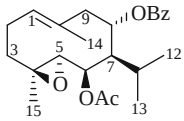
[a]Assignment may be interchanged

X-ray (shiromodiol): [3]

References

1. J. de Pascual Teresa, J.R. Moran, J.M. Hernandez, M. Grande, Phytochemistry **24**(8), 1779 (1985)
2. G. Appendino, M.G. Valle, P. Gariboldi, J. Chem. Soc. Perkin Trans. **1**, 1363 (1986)
3. R.J. McClure, G.A. Sim, P.Coggon, A.T. Phail, J. Chem. Soc. D. 128 (1970)

6β-Acetoxy-8α-benzoyloxy-4β,5α-epoxy-1(10)-germacrene (6-Acetyl-8-benzoylshiromodiol)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Ferulago antiochia* O. Saya et M. Miski [1]

$C_{24}H_{32}O_5$: 400.2250

Mp: gum [1]

IR (NaCl): 1720, 1610, 1590, 1450, 1270, 1240, 730, 710, 690 [1]

EI-MS: 400 $[M]^+$ (0.2), 236 (6.5), 218 (23.0), 200 (23.4), 175 (63.3), 122 (41.3), 105 (100), 77 (65.6), 43 (92.5) [1]

CI-MS: 399 $[M - H]^+$ (14.9), 357 (13.4), 295 (28.3), 277 (13.2), 235 (42.2), 219 (62.9), 201 (100), 123 (9.8), 105 (49.7) [1]

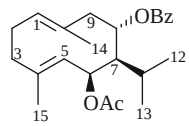
^{1}H NMR (200 MHz, $CDCl_3$, TMS): 1.02 (3H, d, J = 6.5, H-13), 1.24 (3H, s, H-15), 1.28 (3H, d, J = 6.5, H-12), 1.55–2.40 (4H, m, H-2, H-3), 1.80 (3H, s, OAc), 1.83 (3H, br s, H-14), 2.78 (2H, br m, H-9), 2.94 (1H, br d, J = 6.5, H-5), 4.98 (1H, br d, J = 6.5, H-6), 5.43 (1H, br dd, J = 8.5, H-1), 5.68 (1H, br dd, J = 6; 12.5, H-8); OBz: 7.50 (3H, m, H-3′, H-4′, H-5′), 8.05 (2H, dd, J = 2; 8, H-2′, H-6′); * – Overlapping signals [1]

X-ray (shiromodiol): [2]

References

1. M. Miski, H.A. Moubasher, T.J. Mabry, Phytochemistry **29**(3), 881 (1990)
2. R.J. McClure, G.A. Sim, P. Coggon, A.T. Phail, J. Chem. Soc. D. 128 (1970)

6β-Acetoxy-8α-benzoyloxy-1(10),4-germacradiene (6-Acetyl-8-benzoyltovarol; 6β-Acetoxy-8α-benzoyloxy-6,7(H)-germacrene C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Ferulago antiochia* O. Saya et M. Miski [1]

$C_{24}H_{32}O_4$: 384.2301

Mp: gum [1]

IR (NaCl): 1720, 1610, 1590, 1450, 1270, 1235, 710, 690 [1]

EI-MS: 218 [M – HOAc – benzoate acylium – H]$^+$ (12.5), 202 (77.4), 187 (41.7), 159 (90.3), 145 (51.8), 122 (28.9), 105 (100.0), 77 (71.0), 43 (87.9) [1]

CI-MS: 383 $[M - H]^+$ (4.5), 341 (11.0), 279 (34.3), 237 (35.1), 219 (100.0), 201 (86.1), 123 (58.6), 105 (58.0) [1]

^{1}H NMR (200 MHz, $CDCl_3$, TMS): 1.04 (3H, d, J = 6.5, H-13), 1.28 (3H, d, J = 6.5, H-12), 1.46 (1H, br d, J = 10.5, H-7), 1.55 (3H, br s, H-15), 1.70–2.50 (4H, m, H-2, H-3), 1.72 (3H, br s, H-14), 1.80 (3H, s, OAc), 1.98 (1H, dd, J = 13; 13, H-9b), 2.80 (1H, dd, J = 5; 13, H-9a), 5.21* (1H, br d, J = 6.5, H-5), 5.21* (1H, m, H-1), 5.64 (1H, br d, J = 6.5, H-6), 5.70 (1H, dd, J = 5; 13, H-8); OBz: 7.50 (3H, m, H-3′, H-4′, H-5′), 8.05 (2H, dd, J = 2; 8, H-2′, H-6′); * – Overlapping signals [1]

^{13}C NMR (22.6 MHz, $CDCl_3$, TMS) [1]:

Table 1

C-1	129.8 d	C-8	74.3 d	OBz	165.7 s
2	24.8 t	9	41.4 t	OAc	131.0 s

(*continued*)

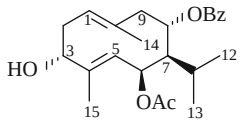
Table 1 (continued)

3	39.0 t	10	135.5 s	129.5 (× 2) d
4	129.5 s	11	26.5 d	128.6 (× 2) d
5	132.1 d	12	21.5 q	132.9 d
6	71.4 d	13	20.9 q	170.6 s
7	52.4 d	14	23.3 q	20.9 q
		15	16.7 q	

References

1. M. Miski, H.A. Moubasher, T.J. Mabry, Phytochemistry **29**(3), 881 (1990)

6α-Acetoxy-8α-benzoyloxy-1(10),4-germacradien-3α-ol (6-Acetyl-8-benzoyl-antakyatriol; 3α-Hydroxy-6α-acetoxy-8α-benzoyloxy-6,7(H)-germacrene C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Ferulago antiochia* O. Saya et M. Miski [1]

$C_{24}H_{32}O_5$: 400.2250

Mp: gum [1]

IR (NaCl): 3480, 1745, 1720, 1610, 1590, 1450, 1275, 1240, 1110, 710, 690 [1]

EI-MS: 340 $[M - HOAc]^+$ (1.4), 252 (0.8), 236 (2.6), 218 (18.2), 200 (6), 189 (8.5), 175 (48.7), 136 (28.5), 122 (12.2), 105 (100.0), 43 (68.7) [1]

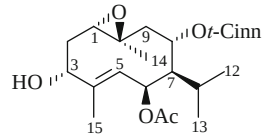
CI-MS: 399 $[M - H]^+$ (3.0), 383 (7.7), 341 (10.1), 323 (2.8), 277 (2.8), 261 (7.8), 235 (9.6), 219 (100), 201 (81.2), 191 (9.3), 175 (16.3), 161 (9.6), 149 (9.8), 123 (5.7), 105 (27.3) [1]

^{1}H NMR (200 MHz, $CDCl_3$, TMS): 1.03 (3H, d, J = 6.5, H-13), 1.28 (3H, d, J = 6.5, H-12), 1.43 (1H, br d, J = 10.5, H-7), 1.59 (3H, br s, H-15), 1.73 (3H, br s, H-14), 1.81 (3H, s, OAc), 2.00 (1H, dd, J = 11.5; 12, H-9b), 2.46 (2H, m, H-2), 2.78 (1H, br dd, J = 6; 12, H-9a), 4.34 (1H, dd, J = 6.5; 8.5, H-3), 5.15 (1H, m, H-1), 5.28 (1H, br d, J = 6.5, H-5), 5.58 (1H, dd, J = 6; 11.5, H-8), 5.66 (1H, br d, J = 6.5, H-6); OBz: 7.51 (3H, m, H-3′, H-4′, H-5′), 8.06 (2H, dd, J = 2; 8, H-2′, H-6′); * - Overlapping signals [1]

References

1. M. Miski, H.A. Moubasher, T.J. Mabry, Phytochemistry **29**(3), 881 (1990)

6β-Acetoxy-8α-*trans*-cinnamoyloxy-1α,10β-epoxy-4-germacren-3α-ol (6-Acetyl-8-*trans*-cinnamyl-1α,10β-epoxyantakyatrol)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Ferulago antiochia* O. Saya et M. Miski [1]

$C_{26}H_{34}O_6$: 442.2355

Mp: gum [1]

IR (NaCl): 3450, 1740, 1710, 1640, 1580, 1450, 1270, 1260, 1240, 1170, 770, 735, 710, 700, 680 [1]

EI-MS: 251 [M – *trans*-cinnamate acylium – $HOAc]^+$ (3.9), 234 (10.5), 216 (20.3), 201 (11.7), 173 (35.7),

161 (17.7), 159 (18.7), 148 (35.2), 131 (100), 119 (43.0), 103 (80.9), 77 (50.6), 43 (85.7) [1]

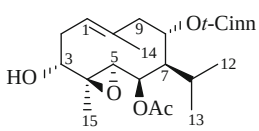
CI-MS: 443 $[M + H]^+$ (5.1), 425 (3.4), 383 (8.0), 313 (7.6), 295 (45.7), 277 (10.5), 235 (100), 217 (39.9), 205 (29.4), 173 (27.2), 149 (34.8), 131 (55.2), 123 (29.1), 107 (66.2), 105 (95.1) [1]

^{1}H NMR (200 MHz, $CDCl_3$, TMS): 1.05 (3H, d, J = 6.5, H-13), 1.23 (3H, d, J = 6.5, H-12), 1.38 (3H, s, H-14), 1.71 (3H, s, H-15), 1.94 (3H, s, OAc), 2.23 (1H, dd, J = 12; 13, H-9b), 2.33 (1H, br dd, J = 6; 13, H-9a), 2.93 (1H, dd, J = 1; 10.5, H-1), 4.50 (1H, dd, J = 5.5; 11, H-3), 5.53 (1H, dd, J = 6; 10.5, H-8), 5.57 (1H, br d, J = 6, H-5), 5.67 (1H, br d, J = 6, H-6); O^{t}Cinn: 6.42 (1H, d, J = 16, H-8′), 7.40 (3H, m, H-3′, H-4′, H-5′), 7.53 (2H, m, H-2′, H-6′), 7.66 (1H, d, J = 16, H-7′) [1]

References

1. M. Miski, H.A. Moubasher, T.J. Mabry, Phytochemistry **29**(3), 881 (1990)

6β-Acetoxy-8α-*trans*-cinnamoyloxy-4β,5α-epoxy-1(10)-germacren-3α-ol (6-Acetyl-8-*trans*-cinnamyl-4β,5α-epoxyantakyatriol)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Ferulago antiochia* O. Saya et M. Miski [1]

$C_{26}H_{34}O_6$: 442.2355

Mp: gum [1]

IR (NaCl): 3450, 1740, 1710, 1640, 1580, 1450, 1370, 1275, 1230, 1170, 770, 735, 710, 685 [1]

EI-MS: 252 [M – *trans*-cinnamate acylium – HOAc + $H]^+$ (1.1), 234 (3.5), 216 (5.6), 201 (3.7), 191 (14.2), 173 (13.1), 161 (15.9), 148 (26.4), 131 (100), 119 (27.9), 103 (67.6), 91 (41.4), 77 (44.9), 43 (70.6) [1]

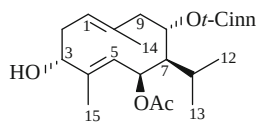
CI-MS: 441 $[M - H]^+$ (9.4), 425 (42.0), 383 (9.1), 295 (29.1), 277 (10.2), 235 (100), 217 (95.6), 205 (35.9), 173 (29.4), 149 (23.7), 131 (69.3), 123 (46.5), 107 (62.2), 105 (22.8) [1]

^{1}H NMR (200 MHz, $CDCl_3$, 55°C, TMS): 0.99 (3H, d, J = 6.5, H-13), 1.22 (3H, d, J = 6.5, H-12), 1.27 (3H, s, H-15), 1.72 (3H, br s, H-14), 1.95 (3H, s, OAc), 2.08 (1H, dd, J = 12; 12.5, H-9b), 2.63 (1H, br dd, J = 4.5; 12.5, H-9a), 2.89 (1H, d, J = 6.5, H-5), 3.38 (1H, dd, J = 6.5; 10.5, H-3), 4.99 (1H, br d, J = 6.5, H-6), 5.33 (1H, br dd, J = 5; 10.5, H-1), 5.47 (1H, dd, J = 4.5; 11, H-8); O^{t}Cinn: 6.43 (1H, d, J = 16, H-8′), 7.41 (3H, m, H-3′, H-4′, H-5′), 7.53 (2H, m, H-2′, H-6′), 7.69 (1H, d, J = 16, H-7′) [1]

References

1. M. Miski, H.A. Moubasher, T.J. Mabry, Phytochemistry **29**(3), 881 (1990)

6β-Acetoxy-8α-*trans*-cinnamoyloxy-1(10),4-germacradien-3α-ol (6-Acetyl-8-*trans*-cinnamylantakyatriol; 3α-Hydroxy-6β-acetoxy-8α-*trans*-cinnamoyloxy-6,7-H-germacrene C)



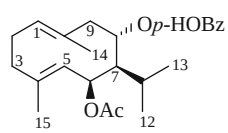
Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Ferulago antiochia* O. Saya et M. Miski [1]
$C_{26}H_{34}O_5$: 426.2406
Mp: gum [1]
IR (NaCl): 3450, 1740, 1710, 1640, 1580, 1450, 1370, 1270, 1260, 1245, 1170, 770, 700, 680 [1]
EI-MS: 366 $[M - HOAc]^+$ (0.8), 251 (1.7), 234 (3.5), 218 (9.4), 200 (4.8), 175 (23.0), 157 (18.0), 148 (30.8), 131 (100), 103 (65.4), 91 (45.2), 77 (52.8), 43 (83.9) [1]
CI-MS: 425 $[M - H]^+$ (3.5), 409 (3.9), 367 (3.3), 277 (4.7), 235 (21.8), 219 (22.5), 201 (12.3), 191 (7.1), 175 (8.6), 149 (31.6), 131 (42.7) [1]
^{1}H NMR (200 MHz, $CDCl_3$, TMS): 1.02 (3H, d, J = 6.5, H-13), 1.22 (3H, d, J = 6.5, H-12), 1.38 (1H, br d, J = 10.5, H-7), 1.58 (3H, br s, H-15), 1.72 (3H, br s, H-14), 1.93* (3H, s, OAc), 1.99* (1H, m, H-9b), 2.42 (2H, m, H-2), 2.71 (1H, br dd, J = 6; 13, H-9a), 4.33 (1H, dd, J = 6.5; 8.5, H-3), 5.12 (1H, br dd, J = 5; 10.5, H-1), 5.27 (1H, br d, J = 6.5, H-5), 5.46 (1H, dd, J = 6; 11.5, H-8), 5.63 (1H, br d, J = 6.5, H-6); O^{t}Cinn: 6.46 (1H, d, J = 16, H-8′), 7.41 (3H, m, H-3′, H-4′, H-5′), 7.55 (2H, m, H-2′, H-6′), 7.69 (1H, d, J = 16, H-7′), * - Overlapping signals [1]

References

1. M. Miski, H.A. Moubasher, T.J. Mabry, Phytochemistry **29**(3), 881 (1990)

6β-Acetoxy-8α-(4′-hydroxy-benzoyloxy)-1(10),4-germacradiene (Federin; 6β-Acetoxy-8α-[4-hydroxy-benzoyloxy]-6,7-H-germacrene C)

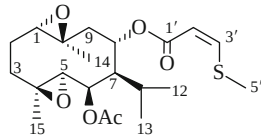


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters
Biological sources: *Ferula fedtschenkoana* K.-Pol. [1]; *F. rubroarenosa* Korov. [2]; *F. karakalensis* Korov. [3]
$C_{24}H_{32}O_5$: 400.2250
Mp: 179–180°C (ether) [1]; 178–179°C (hexane–ether, 5:1) [2]
$[\alpha]_D$ −90.9° (*c* 0.99, EtOH) [1]; −86.0° (*c* 1.0, EtOH) [2]
UV 260 (4.27) [1]
IR: 3250–3350, 1745, 1610, 1590, 1525 [1]
MS: 400 $[M]^+$ [1]
^{1}H NMR: 1.78 (3H, s, OAc), 5.14 (2H, d), 5.59 (2H, m) [1]

References

1. Kh.M. Kamilov, G.K. Nikonov, N.N. Sharakhimov, Chem. Nat. Comp. **10**, 540 (1974)
2. L.I. Golovina, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **14**, 606 (1978)
3. A.I. Saidkhodzjaev, V.M. Malikov, M.G. Pimenov, Chem. Nat. Comp. **29**, 187 (1993)

6β-Acetoxy-8α-(3′-methylthioacryloyloxy)-1α,10β;4β,5α-diepoxy-germacrane



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters
Biological sources: *Thapsia villosa* L. [1]
$C_{21}H_{32}O_6S$: 412.1920
Mp: amorphous white powder [1]
$[\alpha]_D^{25}$ –18.3° (*c* 0.25, $CHCl_3$) [1]

IR (film): 21 2960, 1740, 1698, 1558, 1387, 1235, 1161, 992, 796 [1]

EI-MS: 412 $[M]^+$ (1), 235 $[M - HOAc - C_4H_5O_2S]^+$ (1), 195 $[M - OAc - C_3H_7 - C_4H_5O_2S]^+$ (4), 193 (2), 163 (4), 149 (5), 101 $[C_4H_5O_S]^+$ (100) [1]

HR-EI-MS: 412.1905 $[M]^+$ (calc. for $C_{21}H_{32}O_6S$: 412.1920) [1]

^{1}H NMR: 0.95 (3H, d, J = 6.5, H-13), 1.13 (3H, d, J = 6.5, H-12), 1.26 (1H, m, H-3β), 1.26 (3H, s, H-15), 1.45 (1H, m, H-2α), 1.45 (3H, s, H-14), 1.6 (1H, d, J = 8.7, H-8), 1.84 (1H, m, H-11), 1.85 (1H, dd, J = 5.8; 13.7, H-9β), 1.92 (3H, s, OAc), 2.07 (1H, dt, J = 14.6; 3.4, H-2β), 2.17 (1H, dt, J = 13.2; 3.4, H-3α), 2.23 (1H, t, J = 12.2, H-9α), 3.08 (1H, d, J = 10.4, H-1), 3.16 (1H, d, J = 6.8, H-5), 4.89 (1H, dd, J = 6.8; 1.0, H-6); OCOCH = CHSCH$_3$: 2.38 (3H, s, -SCH$_3$), 5.80 (1H, d, J = 10.0, H-2′), 7.05 (1H, d, J = 10.0, H-3′) [1]

^{13}C NMR [1]:

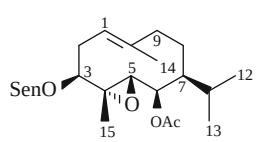
Table 1

C-1	61.5	C-8	69.3	C-15	17.2
2	23.8	9	42.5	1′	165.6
3	36.6	10	58.7	2′	112.9
4	58.8	11	26.5	3′	153.1
5	66.6	12	23.2	-SCH$_3$	19.6
6	73.2	13	21.5	-OCOCH$_3$	170.4
7	48.5	14	22.4	-OCOCH$_3$	21.0

References

1. J.J. Rubal, F.M. Guerra, F. Javier Moreno-Dorado, M. Akssira, F. Mellouki, A.J. Pujadas, Z.D. Jorge, G.M. Massanet, Tetrahedron **60**, 159 (2004)

6β-Acetoxy-3β-senecioyloxy-4α,5-epoxy-7α(H)-germacr-1(10)-ene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Senecio vitalis* N.E.Br. [1]

$C_{22}H_{34}O_5$: 378.2406

Mp: colorless gum [1]

$[\alpha]^{24}$ (λ, nm): −47.8° (589), −50.0° (578), −58.7° (546), −113.0° (436) (*c* 0.2, $CHCl_3$) [1]

IR (CCl_4): 1745, 1710, 1655, 1230 [1]

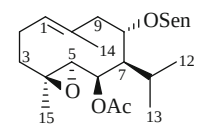
MS: 378 $[M]^+$ (0.2), 83 (100) [1]

^{1}H NMR (270 MHz, $CDCl_3$): 1.09 (3H, d, J = 7, H-13), 1.16 (3H, d, J = 7, H-12), 1.54 (3H, br s, H-14), 1.73 (3H, s, H-15), 2.0 (2H, m, H-9), 2.0 (2H, m, J = 5; 11, H-2), 2.96 (1H, d, J = 7, H-5), 5.24 (1H, m, H-1), 5.29 (1H, br d, J = 7; 1.5, H-6), 5.72 (1H, dd, J = 5; 11, H-3); OSen: 1.73 (3H, br s, H-4′), 2.16 (3H, br s, H-5′), 5.72 (1H, br s, H-2′) [1]

References

1. F. Bohlmann, J. Ziesche, Phytochemistry **19**(8), 1851 (1980)

6β-Acetoxy-8α-senecioyloxy-4β,5α-epoxy-1(10)-germacrene (6-*O*-Acetyl-8-*O*-senecioylshiromodiol; 8α-*O*-(3-Methyl-2-butenoyl)-6β-acetyl-4,5-epoxy-1(10)-germacrene)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Ligularia persica* Boiss. [1]

$C_{22}H_{34}O_5$: 378.2406

Mp: oil [1]
$[\alpha]_D$ −72° (*c* 0.5, $CHCl_3$) [1]
IR (film): 1740, 1700, 1645, 1235, 1145, 1075 [1]
EI-MS: 378 $[M]^+$ (10), 278 (12), 236 (10), 218 (9), 205 (8), 177 (25), 175 (40), 160 (32), 150 (35), 136 (36), 121 (30), 93 (40), 83 (100), 55 (56) [1]
HPLC [1]
^{1}H NMR (400 MHz, $CDCl_3$, TMS, 57°C): 0.98 (3H, d, J = 6.5, H-12 or H-13), 1.12 (3H, d, J = 6.5, H-12 or H-13), 1.22 (3H, s, H-15), 1.55 (1H, br d, J = 1.5, H-7), 1.79 (3H, br s, H-14), 1.90 (1H, m, overlapped by other signals, H-11), 1.95 (3H, s, OAc), 2.00 (1H, m, overlapped by other signals, H-9b), 2.10 (2H, ddd, J = 6; 2; 13, H-3), 2.30 (2H, m, H-2), 2.60 (1H, br dd, J = 5; 13, H-9a), 2.88 (1H, d, J = 8, H-5), 4.92 (1H, dd, J = 8; 1.5, H-6), 5.37 (1H, ddq, J = 8; 1.5; 8, H-1), 5.48 (1H, ddd, J = 1.5; 5; 12, H-8); OSen: 1.92 (3H, d, J = 1.5, H-4′), 2.20 (3H, d, J = 1.5, H-5′), 5.67 (1H, qq, J = 1.5, H-2′) [1]
^{13}C NMR (50.32 MHz, $CDCl_3$) [1]:

Table 1

C-1	128.46	C-8	70.97	C-15	16.78
2	24.18	9	42.30	OSen	165.56
3	38.36	10	131.47	OAc	156.23
4	59.17	11	26.41		116.42
5	66.74	12	23.32[a]		27.16
6	73.81	13	21.21[a]		20.66
7	48.40	14	26.41[b]		169.79
					20.14

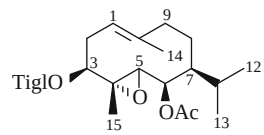
[a]Signals may be interchanged within the same column
[b]The signal of C-14 is coincident with either that of C-11 (as in this Table) or with one of the other methyl signals. The proposed assignment is only tentative

X-ray (shiromodiol): [2]

References

1. J.A. Marco, J.F. Sanz, A. Garcia-Sarrion, A. Rustaiyan, Phytochemistry **30**(7), 2325 (1991)
2. R.J. McClure, G.A. Sim, P. Coggon, A.T. Phail, J. Chem. Soc. D. 128 (1970)

6β-Acetoxy-3β-tigloyloxy-4α,5-epoxy-7α(H)-germacr-1(10)-ene (6β-Acetoxy-3β-tiglinoyloxy-4.5.6.7H-4.5-epoxygermacrene C)

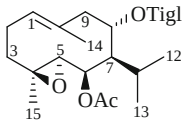


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters
Biological sources: *Senecio ficoides* Harv. [1]; *Kleinia mandraliscae* Tin. ex Lojac. [2]
$C_{22}H_{34}O_5$: 378.2406
Mp: colorless oil [1]
$[\alpha]^{24}$ (λ, nm): +58.1° (589), +60.8° (578), +68.5° (546), +113.0° (436) (*c* 1.0, $CHCl_3$) [1]
IR (CCl_4): 1740, 1712, 1650 [1]
MS: 378.244 $[M]^+$ (0.5) (calc. for $C_{22}H_{34}O_5$: 378.241), 278 $[M - C_4H_7COOH]^+$ (1), 218 $[278 - AcOH]^+$ (5), 175 $[218 - C_3H_7]^+$ (14), 83 $[C_4H_7CO]^+$ (100) [1]
^{1}H NMR (270 MHz, C_6D_6, 76°C, TMS): 1.07 (3H, s, H-14), 1.11 (3H, d, J = 7, H-13), 1.21 (3H, d, J = 7, H-12), 1.60 (3H, s, H-15), 1.75 (3H, s, OAc), 2.99 (1H, d, J = 7, H-5), 5.24 (1H, m, H-1), 5.33 (1H, dd, J = 7; 1.5, H-6), 5.76 (1H, ddd, J = 5; 12, H-3α); OTigl: 1.52 (3H, dq), 1.88 (3H, dq), 6.96 (1H, qq, H-3′) [1]

References

1. F. Bohlmann, K.-H. Knoll, C. Zdero, P.K. Mahanta, M. Grenz, A. Suwita, D. Ehlers, N.L. Van, W.-R. Abraham, A. A. Natu, Phytochemistry **16**(7), 965 (1977)
2. F. Bohlmann, M. Ahmed, J. Jakupovic, C. Jeffrey, Phytochemistry **20**(2), 251 (1981)

6β-Acetoxy-8α-tigloyloxy-4,5-epoxy-5β,7α(H)-germacr-1(10)-ene (6-*O*-Acetyl-8-*O*-tigloyl-shiromodiol; 8α-*O*-tigloyl-6β-acetyl-4,5-epoxy-1(10)-germacrene)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Ligularia persica* Boiss. [1]

$C_{22}H_{34}O_5$: 378.2406

Mp: oil [1]

$[\alpha]_D$ −44° (*c* 0.1, $CHCl_3$) [1]

IR (film): 1735, 1700, 1645, 1260, 1140, 1060 [1]

EI-MS: 378 $[M]^+$ (12), 278 (15), 236 (12), 218 (9), 205 (9), 177 (20), 175 (44), 160 (33), 150 (38), 136 (40), 121 (20), 93 (46), 83 (100), 55 (65) [1]

HPLC [1]

^{1}H NMR (400 MHz, $CDCl_3$, 57°): 0.99 (3H, d, J = 6.5, H-12 or H-13), 1.18 (3H, d, J = 6.5, H-12 or H-13), 1.21 (3H, s, H-15), 1.57 (1H, br d, J = 1.5, H-7), 1.78 (3H, br s, H-14), 1.90 (1H, m, overlapped by other signals, H-11), 1.93 (1H, s, OAc), 2.00 (1H, m, H-9b), 2.10 (2H, ddd, J = 6; 2; 13, H-3), 2.30 (2H, m, H-2), 2.60 (1H, br dd, J = 5; 13, H-9a), 2.80 (1H, d, J = 8, H-5), 4.93 (1H, dd, J = 8; 1.5, H-6), 5.47 (1H, ddd, J = 1.5; 5; 12, H-8), 5.32 (1H, ddq, J = 8; 1.5; 8, H-1); OTigl: 1.81 (3H, dq, J = 1.5; 7.5, H-4′), 1.87 (3H, dq, J = 1.5; 1.5, H-5′), 6.83 (1H, qq, J = 1.5; 7.5, H-3′) [1]

^{13}C NMR (50.32 MHz, $CDCl_3$) [1]:

Table 1

C-1	128.41	C-8	71.92	C-15	16.70
2	24.10	9	42.28	OTigl	166.92
3	38.27	10	131.32		136.51
4	59.09	11	26.34		128.41
5	66.65	12	23.18[a]		14.13
6	73.74	13	21.32[a]		11.85
7	48.72	14	26.34[b]	OAc	169.67
					20.10

[a]Signals my be interchanged within the same column

[b]The signal of C-14 is coincident with either that of C-11 (as in this Table) or with one of the other methyl signals. The proposed assignment is only tentative

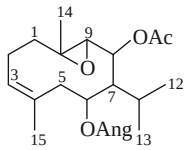
X-ray (shiromodiol): [2]

References

1. J.A. Marco, J.F. Sanz, A. Garcia-Sarrion, A. Rustaiyan, Phytochemistry **30**(7), 2325 (1991)
2. R.J. McClure, G.A. Sim, P. Coggon, A.T. Phail, J. Chem. Soc. D. 128 (1970)

8-Acetoxy-6-angeloyloxy-9(10)-epoxy-3-germacrene (Fecorine; Fekorin)

CAS Registry Number: 56581-77-2



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

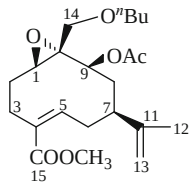
Biological sources: *Ferula korshinskyi* Korov. [1]; *F. leucographa* Korov. [2]

$C_{22}H_{34}O_5$: 378.2406
$[n]_D^{24}$ 1.491 [1]
$[\alpha]_D^{23}$ −29° (*c* 0.94, $CHCl_3$) [1]
UV: 222 (3.94) [1]
IR: 2960–2880, 1745, 1720, 1660, 1270–1230 [1]
MS: 378 $[M]^+$, 318 $[M - CH_3COOH]^+$, 279 $[M - C_5H_7O_2]^+$ [1]
TLC: petrol – EtOAc (3:1) × 2, R_f 0.8 [1]
^{1}H NMR (100 MHz, $CDCl_3$, HMDS): 0.95 (3H, d, J = 6, H-12), 1.10 (3H, d, J = 6, H-13), 1.10 (3H, s, H-14), 1.76 (3H, s, H-15), 1.8 (3H, s, OAc), 2.72 (1H, d, J = 6, H-9), 4.75 (1H, d, J = 6, H-8), 5.30 (2H, d, J = 6, H-3, H-6); OAng: 1.87 (3H, d, J = 3, H-5′), 1.9 (3H, s, H-4′), 5.96 (1H, qd, J = 3, H-3′) [1]

References

1. A.Sh. Kadyrov, A.I. Saidkhodzjaev, G.K. Nikonov, Chem. Nat. Comp. **11**, 167 (1975)
2. M.N. Kobilov, A.I. Saidkhodzhaev, N.D. Abdullaev, Chem. Nat. Comp. **31**, 530 (1995)

9β-Acetoxy-14-butyroyloxy-1β,10α-epoxy-4,11-germacradien-15-oic Acid Methyl Ester (Methyl-9β-acetoxy-14-*O*-*n*-butyryl-oxyphylloate)

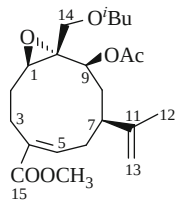


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters
Biological sources: *Oxyphyllum ulicinum* Phil. [1]
$C_{22}H_{32}O_7$: 408.2148
Mp: colorless oil [1]
IR (CCl_4): 1740, 1720 [1]
MS: 408.215 $[M]^+$ (4), 376 (0.6), 348 (0.3), 260 (3), 247 (3.7), 71 (100) [1]
HPLC [1]
^{1}H NMR (400 MHz, $CDCl_3$): 1.61 (1H, dddd, J = 11; 13; 12; 5, H-2β), 1.68 (1H, br d, J = 14; 1, H-8α), 1.73 (3H, br s, H-12), 1.98 (1H, ddd, J = 12; 14; 9, H-8β), 2.05 (3H, s, OAc), 2.16 (1H, dddd, J = 2.5; 13; 2; 2, H-2α), 2.26 (1H, m, J = 12; 12, H-7), 2.26 (1H, m, J = 2; 12; 13.5, H-3α), 2.39 (1H, br d, J = 4, H-6α), 2.75 (1H, br d, J = 2; 5; 13.5, H-3β), 2.92 (1H, dd, J = 2.5; 11, H-1), 3.15 (1H, br q, J = 11; 14; 12, H-6β), 3.80 (3H, s, OCH_3), 3.95 (1H, d, J = 12, H-14b), 4.43 (1H, d, J = 12, H-14a), 4.47 (1H, dd, J = 1; 9, H-9), 4.67 (1H, dq, J = 1; 1, H-13b), 4.73 (1H, br s, H-13a), 5.97 (1H, dd, J = 4; 11, H-5); O^{n}Bu: 0.96 (3H, t, J = 7, H-4′), 1.67 (2H, tq, J = 7, H-3′), 2.33 (2H, t, J = 7, H-2′) [1]

References

1. C. Zdero, F. Bohlmann, H.M. Niemeyer, Phytochemistry **27**(7), 2165 (1988)

9β-Acetoxy-14-isobutyroyloxy-1β,10α-epoxy-4*E*,11-germacradien-15-oic Acid Methyl Ester (Methyl-4*E*-9β-acetoxy-14-*O*-isobutyryl-oxyphylloate)



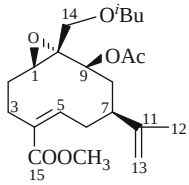
Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters
Biological sources: *Oxyphyllum ulicinum* Phil. [1]

$C_{22}H_{32}O_7$: 408.2148
Mp: colorless oil [1]
$[\alpha]_D^{24}$ −92° (*c* 0.54, $CHCl_3$) [1]
IR (CCl_4): 1745, 1715 [1]
HPLC [1]
MS: 408.215 $[M]^+$ (4.5), 348 (0.4), 260 (3.2), 247 (2.7), 71 (100) [1]
^{1}H NMR (400 MHz, C_6D_6): 1.60 (3H, br s, H-12), 1.63 (1H, dddd, J = 10, H-2′), 1.73 (3H, s, OAc), 1.80 (1H, dd, J = 8; 11, H-6b), 2.09 (1H, m, H-6a), 2.19 (1H, m, H-2), 2.55 (1H, m, H-7), 2.75 (1H, dd, J = 4; 10, H-1), 3.54 (3H, s, OCH_3), 4.55 (1H, br d, J = 11, H-14b), 4.57 (1H, dd, J = 11; 2.5, H-9), 4.67 (1H, br d, J = 11, H-14a), 4.73 (1H, br s, H-13b), 4.77 (1H, br s, H-13a), 6.98 (1H, br dd, J = 10; 8, H-5); O^{i}Bu: 1.14 (6H, d, J = 7, H-3′, H-4′), 2.47 (1H, qq, J = 7, H-2′), [1]

References

1. C. Zdero, F. Bohlmann, H.M. Niemeyer, Phytochemistry **27**(7), 2165 (1988)

9β-Acetoxy-14-isobutyroyloxy-1β,10α-epoxy-4*Z*,11-germacradien-15-oic Acid Methyl Ester (Methyl-9β-acetoxy-14-*O*-isobutyryl-oxyphylloate)

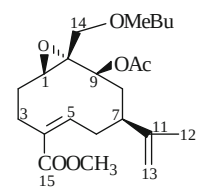


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters
Biological sources: *Oxyphyllum ulicinum* Phil. [1]
$C_{22}H_{32}O_7$: 408.2148
Mp: colorless oil [1]
$[\alpha]_D^{24}$ −92°C (*c* 2.86, $CHCl_3$) [1]
IR (CCl_4): 1740, 1720 [1]
MS: 408.215 $[M]^+$ (4.5), 376 (0.6), 348 (0.3), 307 (0.3), 260 (2.9), 247 (4.3), 71 (100) [1]
HPLC [1]
^{1}H NMR (400 MHz, $CDCl_3$): 1.61 (1H, dddd, J = 11; 13; 12; 5, H-2β), 1.68 (1H, br d, J = 14; 1, H-8α), 1.73 (3H, br s, H-12), 1.98 (1H, ddd, J = 12; 14; 9, H-8β), 2.05 (3H, s, OAc), 2.16 (1H, dddd, J = 2.5; 13; 2; 2, H-2α), 2.26 (1H, m, J = 12; 12, H-7), 2.26 (1H, m, J = 2; 12; 13.5, H-3α), 2.39 (1H, br d, J = 4, H-6α), 2.75 (1H, br d, J = 2; 5; 13.5, H-3β), 2.92 (1H, dd, J = 2.5; 11, H-1), 3.15 (1H, br q, J = 11; 14; 12, H-6β), 3.80 (3H, s, OCH_3), 3.86 (1H, d, J = 12, H-14b), 4.46 (1H, d, J = 12, H-14a), 4.48 (1H, dd, J = 1; 9, H-9), 4.67 (1H, dq, J = 1; 1, H-13b), 4.73 (1H, br s, H-13a), 5.97 (1H, dd, J = 4; 11, H-5); O^{i}Bu: 1.18 (3H, d, J = 7, H-3′), 1.19 (3H, d, J = 7, H-4′), 2.59 (1H, qq, J = 7, H-2′) [1]

References

1. C. Zdero, F. Bohlmann, H.M. Niemeyer, Phytochemistry **27**(7), 2165 (1988)

9β-Acetoxy-14-(2′-methylbutyroyloxy)-1β,10α-epoxy-4,11-germacradien-15-oic Acid Methyl Ester (Methyl-9β-acetoxy-14-*O*-[2-methylbutyryl]-oxyphylloate)



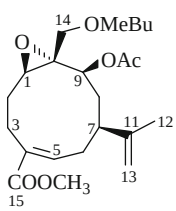
Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Oxyphyllum ulicinum* Phil. [1]
$C_{23}H_{34}O_7$: 422.2305
Mp: colorless oil [1]
$[\alpha]_D^{24}$ −93°C (*c* 0.92, $CHCl_3$) [1]
IR (CCl_4): 1740, 1240, 1720 [1]
MS: 422.230 $[M]^+$ (5), 390 (0.6), 362 (0.3), 307 (0.3), 260 (3), 247 (3.5), 85 (56), 57 (100) [1]
HPLC [1]
^{1}H NMR (400 MHz, $CDCl_3$): 1.61 (1H, dddd, J = 11; 13; 12; 5, H-2β), 1.68 (1H, br d, J = 14; 1, H-8α), 1.73 (3H, br s, H-12), 1.98 (1H, ddd, J = 12; 14; 9, H-8β), 2.05 (3H, s, OAc), 2.16 (1H, dddd, J = 2.5; 13; 2; 2, H-2α), 2.26 (1H, m, J = 12; 12, H-7), 2.26 (1H, m, J = 2; 12; 13.5, H-3α), 2.39 (1H, br d, J = 4, H-6α), 2.75 (1H, br d, J = 2; 5; 13.5, H-3β), 2.92 (1H, dd, J = 2.5; 11, H-1), 3.15 (1H, br q, J = 11; 14; 12, H-6β), 3.80 (3H, s, $COOCH_3$), 3.88 (1H, d, J = 12, H-14b), 4.45 (1H, d, J = 12, H-14a), 4.48 (1H, dd, J = 1; 9, H-9), 4.67 (1H, dq, J = 1; 1, H-13b), 4.73 (1H, br s, H-13a), 5.97 (1H, dd, J = 4; 11, H-5); OMeBu: 0.90 (3H, t, J = 7, H-4′), 1.16 (3H, d, J = 7, H-5′), 2.42 (3H, tq, J = 7, H-2′, H-3′) [1]

References

1. C. Zdero, F. Bohlmann, H.M. Niemeyer, Phytochemistry **27**(7), 2165 (1988)

9β-Acetoxy-14-(2′-methylbutyroyloxy)-1β,10α-epoxy-4*E*,11-germacradien-15-oic Acid Methyl Ester (Methyl-4*E*-9β-acetoxy-14-*O*-[2-methylbutyryl]-oxyphylloate)

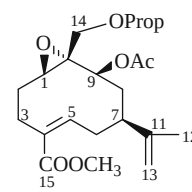


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters
Biological sources: *Oxyphyllum ulicinum* Phil. [1]
$C_{23}H_{34}O_7$: 422.2305
Mp: colorless oil [1]
$[\alpha]_D^{24}$ −82° (*c* 0.36, $CHCl_3$) [1]
IR (CCl_4): 1745, 1715 [1]
MS: 422.230 $[M]^+$ (7), 362 (0.4), 260 (3), 247 (1.8), 228 (2), 85 (51), 57 (100) [1]
HPLC [1]
^{1}H NMR (400 MHz, C_6D_6): 1.60 (3H, br s, H-12), 1.63 (1H, dddd, J = 10, H-2′), 1.76 (3H, s, OAc), 1.80 (1H, dd, J = 8; 11, H-6b), 2.09 (1H, m, J = 10; 4, H-6a), 2.19 (1H, m, J = 10, H-2), 2.55 (1H, br ddd, J = 4; 11; 11, H-7), 2.79 (1H, dd, J = 4; 10, H-1), 3.56 (3H, s, OCH_3), 4.55 (1H, br d, J = 11, H-14b), 4.57 (1H, dd, J = 11; 2.5, H-9), 4.65 (1H, br d, J = 11, H-14a), 4.73 (1H, br s, H-13b), 4.77 (1H, br s, H-13a), 6.98 (1H, br dd, J = 10; 8, H-5); OMeBu: 0.90 (3H, t, J = 7, H-4′), 1.15 (3H, d, J = 7, H-5′), 2.37 (3H, tq, J = 7, H-2′, H-3′) [1]

References

1. C. Zdero, F. Bohlmann, H.M. Niemeyer, Phytochemistry **27**(7), 2165 (1988)

9β-Acetoxy-14-propionyloxy-1β,10α-epoxy-4,11-germacradien-15-oic Acid Methyl Ester (Methyl-9β-acetoxy-14-*O*-propionyl-oxyphylloate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Oxyphyllum ulicinum* Phil. [1]

$C_{21}H_{30}O_7$: 394.1992

Mp: colorless oil [1]

IR (CCl_4): 1740, 1715 [1]

MS: 394.199 $[M]^+$ (3.7), 362 (0.6), 334 (0.3), 260 (2.5), 247 (3.7), 228 (2.5), 57 (100) [1]

HPLC [1]

^{1}H NMR (400 MHz, $CDCl_3$): 1.61 (1H, dddd, J = 11; 13; 12; 5, H-2β), 1.68 (1H, br d, J = 14; 1, H-8α), 1.73 (3H, br s, H-12), 1.98 (1H, ddd, J = 12; 14; 9, H-8β), 2.05 (3H, s, OAc), 2.16 (1H, dddd, J = 2.5; 13; 2; 2, H-2α), 2.26 (1H, m, J = 12; 12, H-7), 2.26 (1H, m, J = 2; 12; 13.5, H-3α), 2.39 (1H, br d, J = 4, H-6α), 2.75 (1H, br d, J = 2; 5; 13.5, H-3β), 2.92 (1H, dd, J = 2.5; 11, H-1), 3.15 (1H, br q, J = 11; 14; 12, H-6β), 3.80 (3H, s, OCH_3), 3.97 (1H, d, J = 12, H-14b), 4.43 (1H, d, J = 12, H-14a), 4.47 (1H, dd, J = 1; 9, H-9), 4.67 (1H, dq, J = 1; 1, H-13b), 4.73 (1H, br s, H-13a), 5.97 (1H, dd, J = 4; 11, H-5); OProp: 1.16 (3H, t, J = 7, H-3′), 2.38 (2H, q, J = 7, H-2′) [1]

References

1. C. Zdero, F. Bohlmann, H.M. Niemeyer, Phytochemistry **27**(7), 2165 (1988)

Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Oxyphyllum ulicinum* Phil. [1]

$C_{23}H_{32}O_7$: 420.2148

Mp: colorless oil [1]

IR (CCl_4): 1740, 1720 [1]

MS: 420.215 $[M]^+$ (2.3), 388 (0.3), 360 (0.2), 260 (1), 247 (1.2), 83 (100) [1]

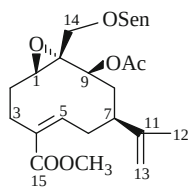
HPLC [1]

^{1}H NMR (400 MHz, $CDCl_3$): 1.61 (1H, dddd, J = 11; 13; 12; 5, H-2β), 1.68 (1H, br d, J = 14; 1, H-8α), 1.73 (3H, br s, H-12), 1.98 (1H, ddd, J = 12; 14; 9, H-8β), 2.05 (3H, s, OAc), 2.16 (1H, dddd, J = 2.5; 13; 2; 2, H-2α), 2.26 (1H, m, J = 12; 12, H-7), 2.26 (1H, m, J = 2; 12; 13.5, H-3α), 2.39 (1H, br d, J = 4, H-6α), 2.75 (1H, br d, J = 2; 5; 13.5, H-3β), 2.92 (1H, dd, J = 2.5; 11, H-1), 3.15 (1H, br q, J = 11; 14; 12, H-6β), 3.80 (3H, s, OCH_3), 4.09 (1H, d, J = 12, H-14b), 4.35 (1H, d, J = 12, H-14a), 4.46 (1H, dd, J = 1; 9, H-9), 4.67 (1H, dq, J = 1; 1, H-13b), 4.73 (1H, br s, H-13a), 5.97 (1H, dd, J = 4; 11, H-5); OSen: 1.92 (3H, d, J = 1, H-4′), 2.20 (3H, d, J = 1, H-5′), 5.73 (1H, br s, H-2′) [1]

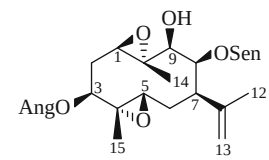
References

1. C. Zdero, F. Bohlmann, H.M. Niemeyer, Phytochemistry **27**(7), 2165 (1988)

9β-Acetoxy-14-senecioyloxy-1β,10α-epoxy-4,11-germacradien-15-oic Acid Methyl Ester (Methyl-9β-acetoxy-14-*O*-senecioyl-oxyphylloate)



3β-Angeloyloxy-8β-senecioyloxy-1β,10α,4α,5β-diepoxy-5α,7α(H)-germacr-11(13)-en-9β-ol



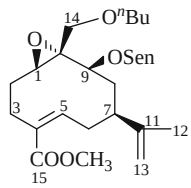
Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Senecio galpinii* Hook. f. [1]
$C_{25}H_{36}O_7$: 448.2461
Mp: colorless gum [1]
$[\alpha]^{24}$ (λ, nm): −16° (589), −16° (578), −19° (546), −35° (436) (*c* 0.54, $CHCl_3$) [1]
IR (CCl_4): 3585, 1720, 1650 [1]
MS: 433 $[M - CH_3]^+$ (5), 349.202 $[M - OAng]^+$ (0.3) ($C_{20}H_{29}O_5$), 348 $[M - AngOH]^+$ (0.3), 248 $[348 - SenOH]^+$ (1), 230 $[248 - H_2O]^+$ (1), 83 $[C_4H_7CO]^+$ (100), 55 $[83 - CO]^+$ (35) [1]
TLC: C_6H_6 – $CHCl_3$ – Et_2O (2:2:1) [1]
HPLC: MeOH – H_2O (3:1), reversed phase [1]
^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.27 (3H, s, H-12), 1.27 (3H, s, H-15), 1.43 (3H, s, H-14), 1.88 (1H, m, H-2b), 2.0 (1H, m, H-2a), 2.0 (1H, m, H-6b), 2.13 (1H, dd, J = 13; 12, H-6a), 2.27 (1H, d, J = 9.5, OH), 2.37 (1H, br dd, J = 7; ∼1, H-7), 2.77 (1H, dd, J = 6; 5, H-1), 3.21 (1H, d, J = 4, H-5), 3.97 (1H, dd, J = 3.5; 9.5, H-9), 5.01 (1H, s, H-13b), 5.21 (1H, s, H-13a), 5.31 (1H, br d, J = ∼1, H-8), 5.38 (1H, dd, J = 8; 6, H-3), OAng: 1.90 (3H, dq, H-5′), 1.99 (3H, dq, H-4′), 6.11 (1H, qq, H-3′); OSen: 1.88 (3H, d, H-4″), 2.13 (3H, d, H-5″), 5.71 (1H, qq, H-2″) [1]

References

1. F. Bohlmann, C. Zdero, Phytochemistry **21**(10), 2537 (1982)

14-Butyroyloxy-9β-senecioyloxy-1β,10α-epoxy-4*E*,11-germacradien-15-oic Acid Methyl Ester (Methyl-9β-senecioyloxy-14-*O*-*n*-butyryl-oxyphylloate)

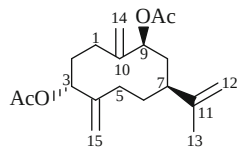


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters
Biological sources: *Oxyphyllum ulicinum* Phil. [1]
$C_{25}H_{36}O_7$: 448.2461
Mp: colorless oil [1]
IR (CCl_4): 1735, 1715 [1]
MS: 448.246 $[M]^+$ (4), 360 (0.1), 348 (0.4), 247 (1.5), 260 (1.3), 83 (100), 71 (24) [1]
HPLC [1]
^{1}H NMR (400 MHz, $CDCl_3$): 1.61 (1H, dddd, J = 11; 13; 12; 5, H-2β), 1.68 (1H, br d, J = 14; 1, H-8α), 1.73 (3H, br s, H-12), 1.98 (1H, ddd, J = 12; 14; 9, H-8β), 2.16 (1H, dddd, J = 2.5; 13; 2; 2, H-2α), 2.26 (1H, m, J = 12; 12, H-7), 2.26 (1H, m, J = 2; 12; 13.5, H-3α), 2.39 (1H, br d, J = 4, H-6α), 2.75 (1H, br d, J = 2; 5; 13.5, H-3β), 2.92 (1H, dd, J = 2.5; 11, H-1), 3.15 (1H, br q, J = 11; 14; 12, H-6β), 3.80 (3H, s, OCH_3), 3.99 (1H, d, J = 12, H-14b), 4.42 (1H, d, J = 12, H-14a), 4.53 (1H, dd, J = 1; 9, H-9), 4.67 (1H, dq, J = 1; 1, H-13b), 4.73 (1H, br s, H-13a), 5.97 (1H, dd, J = 4; 11, H-5); O^{n}Bu: 0.97 (3H, t, J = 7, H-4′), 1.69 (2H, tq, J = 7, H-3′), 2.34 (2H, t, J = 7, H-2′); OSen: 1.88 (3H, d, J = 1, H-4″), 2.15 (3H, d, J = 1, H-5″), 5.66 (1H, br s, H-2″) [1]

References

1. C. Zdero, F. Bohlmann, H.M. Niemeyer, Phytochemistry **27**(7), 2165 (1988)

3α,9β-Diacetoxy-7α(H)-germacra-4(15),10(14),11(12)-triene (Chrysanthediacetate C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Chrysanthemum morifolium* Ramat. [1]
$C_{19}H_{28}O_4$: 320.1988
Mp: oil [1]
$[\alpha]_D^{17}$ –46.64° (*c* 0.729, CH_3OH) [1]
IR (KBr): 2935, 1735, 1650, 1240, 900 [1]
EI-MS: 320, 278, 260, 218, 200, 157, 131 [1]
^{1}H NMR (400 MHz, $CDCl_3$): 1.56 (1H, m, H-6b), 1.60 (1H, m, H-8b), 1.63 (3H, br s, H-13), 1.68 (1H, m, H-6a), 1.78 (1H, ddd, J = 12.7; 8.4; 3.0, H-8a), 1.89 (1H, m, H-5b), 1.90 (1H, m, H-2b), 1.96 (3H, s, OAc), 2.01 (3H, s, OAc), 2.07 (1H, m, H-1b), 2.10 (1H, m, H-7), 2.22 (1H, m, H-5a), 2.26 (1H, m, H-2a), 2.39 (1H, ddd, J = 17.2; 4.4; 3.0, H-1a), 4.63 (1H, br s, H-12b), 4.66 (1H, br s, H-12a), 4.83 (1H, dd, J = 11.2; 5.4, H-9), 5.08 (1H, br s, H-15b), 5.14 (1H, br s, H-14b), 5.20 (1H, br s, H-14a), 5.22 (1H, br s, H-15a), 5.24 (1H, dd, J = 10.9; 4.8, H-3) [1]
^{13}C NMR (100 MHz, $CDCl_3$) [1]:

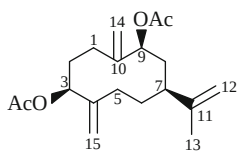
Table 1

C-1	28.9 t	C-7	39.3 d	C-13	18.5 t
2	29.6 t	8	38.1 t	14	112.3 t
3	72.8 d	9	76.8 d	15	115.6 t
4	146.9 s	10	147.8 s	2 × OAc	170.2 s
5	33.1 t	11	147.9 s		169.7 s
6	29.9 t	12	110.6 t		21.3 q

References

1. L. Hu, Z. Chen, Phytochemistry **44**(7), 1287 (1997)

3β,9β-Diacetoxy-7α(H)-germacra-4(15),10(14),11(12)-triene (Chrysanthediacetate B)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Chrysanthemum morifolium* Ramat. [1]
$C_{19}H_{28}O_4$: 320.1988
Mp: oil [1]
$[\alpha]_D^{17}$ +45.53° (*c* 0.797, CH_3OH) [1]
IR (KBr): 2930, 1735, 1645, 1245, 900 [1]
EI-MS: 320, 278, 261, 218, 200, 185, 157, 131 [1]
^{1}H NMR (400 MHz, $CDCl_3$): 1.53 (1H, m, H-6b), 1.65 (1H, m, H-6a), 1.65 (1H, m, H-8b), 1.83 (3H, br s, H-13), 1.87 (1H, ddd, J = 13.7; 11.9; 3.8, H-8a), 1.96 (3H, s, OAc), 1.97 (1H, m, H-5b), 2.01 (3H, s, OAc), 2.05 (1H, m, H-1b), 2.05 (1H, m, H-2a), 2.05 (1H, m, H-2b), 2.18 (1H, m, H-7), 2.25 (1H, m, H-1a), 2.31 (1H, ddd, J = 14.5; 6.6; 5.1, H-5a), 4.68 (1H, br s, H-12b), 4.70 (1H, br s, H-12a), 5.05 (1H, dd, J = 11.7; 4.0, H-9), 5.12 (1H, br s, H-15b), 5.14 (1H, br s, H-14b), 5.17 (1H, br s, H-14a), 5.23 (1H, br s, H-15a), 5.36 (1H, dd, J = 7.7; 5.6, H-3) [1]
^{13}C NMR (100 MHz, $CDCl_3$) [1]:

Table 1

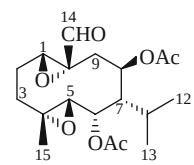
C-1	24.8 t	C-7	40.6 d	C-13	19.4 q
2	29.7 t	8	34.4 t	14	116.9 t
3	76.0 d	9	78.4 d	15	116.6 t
4	145.2 s	10	145.3 s	2 × OAc	170.2 s
5	30.4 t	11	148.1 s		169.6 s
6	31.2 t	12	110.5 t		21.3 q

References

1. L. Hu, Z. Chen, Phytochemistry **44**(7), 1287 (1997)

6α,8β-Diacetoxy-1β,10α;4α,5β-diepoxy-5α,6β,7β(H)-germacr-14-al (Pulicanaral B)

CAS Registry Number: 851595-70-5



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Pulicaria canariensis* Bolle. subsp. *canariensis* [1]

$C_{19}H_{28}O_7$: 368.1835

Mp: 205–210°C, colorless needles [1]

$[\alpha]_D^{25}$ –60.0° (*c* 0.005, $CHCl_3$) [1]

UV (EtOH) 208 (2.3) [1]

IR (KBr): 2932, 1737, 1715, 1432, 1373, 1244, 1130, 1090, 1033, 894, 767 [1]

EI-MS: 309 (3), 308 (1), 297 (4), 279 (3), 266 (6) 255 (27), 248 (4), 237 (12), 223 (15), 220 (18), 219 (28), 209 (10), 207 (13), 205 (27), 195 (34), 191 (14), 187 (11), 177 (44), 166 (27), 163 (28), 159 (14), 151 (24), 149 (47), 141 (30), 139 (66), 127 (50), 123 (44), 109 (59), 99 (76), 97 (100), 95 (74), 85 (58), 83 (100), 81 (83), 71 (53), 69 (60), 55 (90) [1]

HR-FAB-MS: 391.1738 $[M + Na]^+$ (calc. for $C_{19}H_{28}O_7Na$: 391.1733) [1]

^{1}H NMR: 0.96 (3H, d, J = 6.7, H-13), 1.10 (3H, s, OAc), 1.29 (1H, m, H-3a), 1.29 (3H, d, J = 6.7, H-12), 1.52 (1H, m, H-7), 1.55 (1H, m, H-9b), 1.70 (1H, m, H-2a), 1.95 (1H, m, H-11), 2.06 (s, H-15), 2.22 (1H, ddd, J = 3.5, 7.1, 13.8, H-3b), 2.38 (1H, m, H-2b), 2.84 (1H, t, J = 12.6, H-9a), 3.04 (1H, d, J = 6.7, H-5), 3.05 (1H, d, J = 11.2, H-1), 4.87 (1H, dd, J = 1.0; 6.7, H-6), 5.44 (1H, dd, J = 4.6; 12.1, H-8), 9.38 (1H, s, H-14) [1]

^{13}C NMR [1]:

Table 1

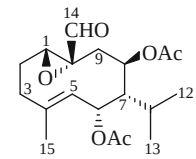
C-1	62.3	C-8	69.2	C-13	21.0
2	23.1	9	33.3	14	199.8
3	35.7	10	61.8	15	16.7
4	58.0	11	26.3	2 × OAc	20.8
5	66.2	12	21.9		20.9
6	72.5				169.7
7	47.9				169.8

References

1. J. Triana, M. Lopez, F.J. Perez, J. Gonzalez-Platas, J. Quintana, F. Estevez, F. Leon, J. Bermejo, J. Nat. Prod. **68**, 523 (2005)

6α,8β-Diacetoxy-1β,10α-epoxy-6β,7β(H)-germacr-4*E*-en-14-al (Pulicanaral A)

CAS Registry Number: 851595-69-2



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Pulicaria canariensis* Bolle. subsp. *canariensis* [1]

$C_{19}H_{28}O_6$: 352.1886

Mp: 183–184° C, colorless needles [1]

$[\alpha]_D^{25}$ 11.1° (*c* 0.108, $CHCl_3$) [1]

UV (EtOH): 209 (3.1), 272 (1.9) [1]

IR (KBr): 2928, 1732, 1716, 1375, 1243, 1025, 935 [1]

EI-MS: 352 $[M]^+$ (0.5), 337 (0.6), 292 (6), 249 (10), 232 (68), 203 (21), 189 (66), 175 (31), 171 (20), 166 (28), 161 (45), 153 (47), 145 (33), 143 (100), 135 (22), 129 (58), 109 (46), 107 (28), 105 (28), 95 (42), 84 (56), 81 (61), 69 (36), 55 (50) [1]

HR-EI-MS: 352.1905 $[M]^+$ (calc. for $C_{19}H_{28}O_6$ 352.1886) (12), 185 (9), 175 (56), 160 (17), 159 (25), 157 (30), 145 (44), 133 (42), 131 (41), 123 (39), 107 (58), 105 (69), 95 (55), 93 (64), 91 (72), 81 (79), 69 (79), 57 (84), 55 (100) [1]

^{1}H NMR ($CDCl_3$): 0.97 (3H, d, J = 6.6, H-13), 1.32 (3H, d, J = 6.6, H-12), 1.43 (1H, d, J = 4.20, H-9b), 1.45 (3H, s, H-15), 1.58 (1H, br d, J = 9.3, H-7), 1.75 (1H, m, H-2a), 1.96 (1H, m, H-11), 2.00 (3H, s, OAc), 2.08 (3H, s, OAc), 2.33 (1H, m, H-3a), 2.38 (1H, m, H-2b), 2.44 (1H, m, H-3b), 2.79 (1H, t, J = 12.8, H-9a), 3.34 (1H, d, J = 11.6, H-1), 5.40 (1H, dd, J = 4.2; 12.6, H-8), 5.43 (1H, d, J = 7.2, H-5), 5.54 (1H, d, J = 6.1, H-6), 9.28 (1H, s, H-14) [1]

^{13}C NMR ($CDCl_3$) [1]:

Table 1

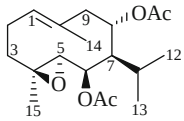
C-1	63.9	C-8	68.8	C-13	21.1
2	23.7	9	34.6	14	199.7
3	35.9	10	61.1	15	16.4
4	133.6	11	26.3	2 × OAc	20.9
5	129.7	12	22.0		21.1
6	71.2				169.8
7	51.4				170.4

References

1. J. Triana, M. Lopez, F.J. Perez, J. Gonzalez-Platas, J. Quintana, F. Estevez, F. Leon, J. Bermejo, J. Nat. Prod. **68**, 523 (2005)

6β,8α-Diacetoxy-4,5-epoxy-1(10)-germacrene (Shiromodiol Diacetate)

CAS Registry Number: 20071-58-3



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Parabenzoin trilobum* Nakai (=*Lindera triloba* (Siebold & Zucc.) Blume) [1, 2]

$C_{19}H_{30}O_5$: 338.2093

Mp: 112°C [1, 3]

$[\alpha]_D^{25}$ −61.9° (*c* 1.06, $CHCl_3$) [1, 3]

UV: end absorption [1]

IR (KBr): 1735, 1240 [1]

EI-MS: 338 $[M]^+$ (7), 278 (37), 236 (47), 218 (45), 201 (62), 175 (100), 160 (73), 139 (66), 109 (48), 93 (44) [3]

^{1}H NMR (100 MHz, $CDCl_3$, TMS): 0.9 (3H, d, J = 6, H-12), 1.1 (3H, d, J = 6, H-13), 1.2 (3H, s, H-15), 1.8 (3H, s, H-14), 2.0 (3H, s, OAc), 2.1 (3H, s, OAc), 2.8 (1H, d, J = 7, H-5), 4.9 (1H, dd, J = 7; 1.5, H-8), 5.4 (2H, m, H-1, H-6) [1]

^{1}H NMR (400 MHz, $CDCl_3$) [3]

^{1}H NMR (200 MHz, $CDCl_3$) [4]

^{13}C NMR (100 MHz, $CDCl_3$) [3]

Chemistry of shiromodiol diacetate [5]

Microbiol biotransformation of shiromodiol diacetate from *Neolitsea serisea koids* [3]

X-ray: [6]

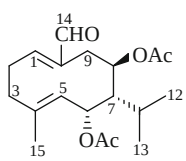
Pharm./Biol.: Showed 100% antifeeding activity against *Prodenia litura* at 0.5% concentration; on entomological test against an *Oligophagous* insect, *Trimeresia Miranda* Butler, the former showed 100% antifeeding activity at 0.13% concentration, while the latter showed only weak activity even at 0.25% [1]; inhibitors against a polyphagous insect, *Spodoptera littoralis* Boisd, and an oligophagous insect, *Trimeresia miranda* Butler. [2]

References

1. K. Wada, Y. Enomoto, K. Matsui, K. Munakata, Tetrahedron Lett. **9**, 4673 (1968)
2. K. Wada, K. Matsui, Y. Enomoto, O. Ogiso, K. Munakata, Agr. Biol. Chem. **34**, 941 (1970)
3. K. Hayashi, K. Asano, M. Tanaka, D. Takaoka, H. Nosaki, Phytochemistry **48**(3), 461 (1998)
4. J. de Pascual Teresa, J.R. Moran, J.M. Hernandez, M. Grande, Phytochemistry **24**(8), 1779 (1985)
5. K. Wada, Y. Enomoto, K. Munakata, Agr. Biol. Chem. **34**, 946 (1970)
6. K. Wada, K. Munakata, Tetrahedron Lett. **9**, 4677 (1968)

6α,8β-Diacetoxy-7β(H)-germacra-1(10)*E*,4*E*-dien-14-al (Pulicanadiene B)

CAS Registry Number: 851595-65-8



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Pulicaria canariensis* Bolle. subsp. *canariensis* [1]

$C_{19}H_{28}O_5$: 336.1937

Mp: colorless oil [1]

$[\alpha]_D^{25}$ 35.7° (*c* 0.042, $CHCl_3$) [1]

UV (EtOH): 209 (3.2), 222 (2.7), 251 (2.1) [1]

IR (KBr): 2932, 1732, 1687, 1433, 1372, 1243, 1141, 1023, 960 [1]

EI-MS: 277 (35), 235 (10), 217 (74), 216 (72), 199 (79), 187 (82), 173 (93), 150 (62), 145 (94), 131 (41), 123 (83), 109 (38), 107 (100), 95 (39), 93 (33), 91 (33), 84 (45), 55 (49) [1]

HR-FAB-MS: 359.1874 $[M + Na]^+$ (calc. for $C_{19}H_{28}O_5Na$: 359.1834) [1]

^{1}H NMR: 1.09 (3H, d, J = 6.3, H-13), 1.28 (3H, d, J = 6.3, H-12), 1.70 (1H, m, H-2a), 1.70 (2H, m, H-3), 1.72 (3H, s, OAc), 1.77 (3H, s, OAc), 1.80 (1H, m, H-11), 1.80 (1H, m, H-2b), 1.80 (1H, m, H-7), 1.98 (3H, s, H-15), 2.34 (1H, br s, H-9a), 2.61 (1H, dd, J = 5.3; 14.0, H-9b), 5.11 (1H, d, J = 8.6, H-5), 5.86 (1H, t, J = 8.4, H-1), 6.02 (1H, dd, J = 1.8; 8.8, H-6), 6.09 (1H, br s, H-8), 9.26 (1H, s, H-14) [1]

^{13}C NMR [1]:

Table 1

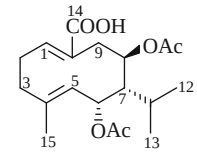
C-1	150.4	C-8	70.1	C-14	193.6
2	27.1	9	30.2	15	20.6
3	36.8	10	143.6	2 × OAc	169.0
4	136.6	11	26.7		169.0
5	124.3	12	22.6		20.5
6	70.0	13	21.6		17.9
7	52.6				

References

1. J. Triana, M. Lopez, F.J. Perez, J. Gonzalez-Platas, J. Quintana, F. Estevez, F. Leon, J. Bermejo, J. Nat. Prod. **68**, 523 (2005)

6α,8β-Diacetoxy-7β(H)-germacra-1(10)*E*,4*E*-dien-14-oic Acid (Pulicanadiene A)

CAS Registry Number: 851595-64-7



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Pulicaria canariensis* Bolle. subsp. *canariensis* [1]

$C_{19}H_{28}O_6$: 352.1886

Mp: amorphous solid [1]

$[\alpha]_D^{25}$ 21.4° (*c* 0.014, $CHCl_3$) [1]

UV (EtOH): 206 (3.2), 250 (2.3), 273 (1.8) [1]

IR (KBr): 3067, 2937, 1731, 1693, 1554, 1430, 1372, 1245, 1023, 960 [1]

EI-MS: 352 $[M]^+$ (1), 316 (1), 292 (1), 281 (0.5), 274 (1), 250 (12), 233 (15), 232 (66), 217 (24), 203 (12), 189 (100), 187 (41), 176 (16), 171 (17), 161 (19), 145 (89), 143 (44), 131 (40), 123 (56), 105 (34), 91 (49), 81 (42), 69 (30), 55 (30) [1]

HR-EI-MS: 352.1877 $[M]^+$ (calc. for $C_{19}H_{28}O_6$: 352.1886) [1]

^{1}H NMR: 0.97 (3H, d, J = 4.5, H-13), 1.06 (3H, d, J = 5.6, H-12), 1.80 (1H, m, H-7), 1.80 and 2.10 (2H, m, H-3), 1.84 (3H, s, H-15), 2.00 (3H, s, OAc), 2.05 (3H, s, OAc), 2.10 (1H, m, H-11), 2.10 and 2.35 (2H, m, H-2), 2.35 (1H, m, H-9a), 2.66 (1H, d, J = 11.2, H-9b), 5.18 (1H, d, J = 8.9, H-5), 5.63 (1H, br s, H-8), 5.77 (1H, d, J = 9.1, H-6), 6.78 (1H, t, J = 8.0, H-1) [1]

^{13}C NMR [1]:

Table 1

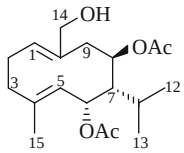
C-1	141.6	C-8	70.1	C-14	173.0
2	26.7	9	31.6	15	20.6
3	36.5	10	137.3	2 × OAc	18.0
4	132.2	11	26.7		20.6
5	123.7	12	22.4		169.1
6	70.0	13	21.3		169.1
7	52.2				

References

1. J. Triana, M. Lopez, F.J. Perez, J. Gonzalez-Platas, J. Quintana, F. Estevez, F. Leon, J. Bermejo, J. Nat. Prod. **68**, 523 (2005)

6α,8β-Diacetoxy-7β(H)-germacra-1(10)*E*,4*E*-dien-14-ol (Pulicanadiene C)

CAS Registry Number: 851595-66-9



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Pulicaria canariensis* Bolle. subsp. *canariensis* [1]

$C_{19}H_{30}O_5$: 338.2093

Mp: colorless oil [1]

$[\alpha]_D^{25}$ −75.0° (*c* 0.008, $CHCl_3$) [1]

UV (EtOH): 205 (3.2), 271 (1.9) [1]

IR (KBr): 3414, 3020, 2928, 2854, 1728, 1502, 1411, 1381, 1332, 1219, 1159, 1107, 1028, 766 [1]

EI-MS: 338 $[M]^+$ (1), 290 (10), 279 (10), 241 (13), 218 (48), 203 (25), 200 (78), 193 (11), 187 (100), 178 (59), 175 (99), 161 (44), 157 (71), 149 (45), 143 (46), 135 (38), 131 (35), 122 (28), 109 (23), 105 (30), 97 (33), 95 (26), 91 (25), 83 (36), 81 (30), 69 (33), 57 (45), 55 (95) [1]

HR-EI-MS: 338.2019 $[M]^+$ (calc. for $C_{19}H_{30}O_5$: 338.2093) [1]

^{1}H NMR: 0.97 (3H, d, J = 6.9, H-13), 1.13 (3H, d, J = 6.8, H-12), 1.40 (2H, m, H-3), 1.52 (3H, s, H-15), 1.70 and 2.01 (2H, m, H-2), 1.78 (3H, s, OAc), 1.85 (3H, s, OAc), 1.92 (1H, br dd, J = 3.3; 13.4, H-7), 2.12 (1H, t, J = 6.3, H-11), 2.50 (1H, m, H-9a), 2.68 (1H, m, H-9b), 4.12 (2H, br d, J = 17.8, H-14), 5.11 (1H, m, H-5), 5.34 (1H, t, J = 8.5, H-1), 5.76 (1H, t, J = 9.2, H-8), 6.13 (1H, br d, J = 5.9, H-6) [1]

^{13}C NMR [1]:

Table 1

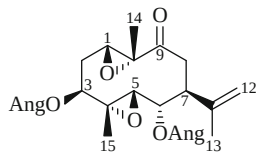
C-1	126.7	C-8	71.1	C-14	69.7
2	26.0	9	30.0	15	20.0
3	31.0	10	135.0	2 × OAc	21.5
4	136.1	11	27.0		21.5
5	127.0	12	19.9		170.2
6	71.0	13	21.4		170.2
7	50.0				

References

1. J. Triana, M. Lopez, F.J. Perez, J. Gonzalez-Platas, J. Quintana, F. Estevez, F. Leon, J. Bermejo, J. Nat. Prod. **68**, 523 (2005)

3β,6α-Diangeloyloxy-1β,10α;4α,5β-diepoxy-6β,7α(H)-germacr-11-en-9-one (Ligularinone A)

CAS Registry Number: 64185-20-2



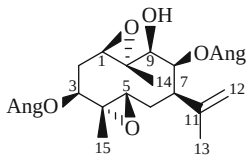
Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Ligularia hodgsoni* Hook. f., *L. brachyphylla* Hand.-Mazz. [1]
$C_{25}H_{34}O_7$: 446.2305
Mp: colorless oil [1]
IR (CCl_4): 1740, 1725, 1655, 850 [1]
MS: 446.232 $[M]^+$ (0.7), 347 (1), 346 (0.8), 246 (2), 83 (100) [1]
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.26 (3H, s, H-14), 1.26 (3H, s, H-15), 1.48 (3H, s, H-13), 1.85 (2H, m, H-2), 2.23 (1H, dd, J = 4; 1.5, H-6), 2.71 (1H, ddd, J = 10; 15; 5, H-6), 2.76 (1H, m, H-1), 2.76 (1H, m, J = 6, H-7), 3.47 (1H, d, J = 4, H-5), 5.11 (1H, br.s, H-12′), 5.26 (1H, dd, J = 4; 8.5, H-3), 5.27 (1H, br s, H-12), 5.88 (1H, d, J = 12, H-8); 2 × OAng: 1.85 (3H, dq, J = 1; 1, H-5′), 1.92 (3H, dq, J = 1; 1, H-5″), 1.96 (3H, dq, J = 7; 1, H-4′), 2.01 (3H, dq, J = 7; 1, H-4″), 6.05(1H, qq, J = 7; 1, H-3′), 6.13 (1H, qq, J = 7; 1, H-3″) [1]
^{1}H NMR (270 MHz, C_6D_6, TMS): 2.60 (1H, ddd, J = 10; 7.5; 12, H-7), 2.75 (1H, t, J = 6, H-1) [1]

References

1. F. Bohlmann, D. Ehlers, C. Zdero, M. Crenz, Chem. Ber. **110**, 2640 (1977)

3β,8β-Diangeloyloxy-1β,10α;4α,5β-diepoxy-11(12)-germacren-9β-ol

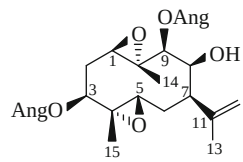


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters
Biological sources: *Senecio galpinii* Hook. f. [1]
$C_{25}H_{36}O_7$: 448.2461
TLC: C_6H_6 – $CHCl_3$ – Et_2O (2:2:1) [1]
HPLC: MeOH – H_2O (3:1), reversed phase [1]
Its data is analogical with the rhomboidol in [2]

References

1. F. Bohlmann, C. Zdero, Phytochemistry **21**(10), 2537 (1982)
2. F. Bohlmann, C. Zdero, Phytochemistry **17**(8), 1337 (1978)

3β,9β-Diangeloyloxy-1β,10α;4α,5β-diepoxy-11(12)-germacren-8α-ol (Rhomboidol)

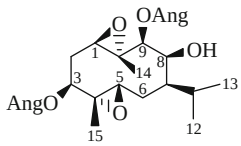


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters
Biological sources: *Senecio rhomboideus* Harv. [1]
$C_{25}H_{36}O_7$: 448.2461
Mp: colorless oil [1]
IR (CCl_4): 3580, 1720, 1650 [1]
MS: 448.246 $[M]^+$ (0.2), 430 (0.3), 348 (3), 330 (1), 83 (100) [1]
^{1}H NMR (270 MHz, C_6D_6, TMS): 1.16 (3H, s, H-13), 1.22 (3H, s, H-15), 1.26 (3H, s, H-14), 1.74 (1H, m, J = 5.5; 14; 5, H-6α), 2.00 (1H, m, J = 14; 14, H-6β), 2.00 (2H, m, H-2), 2.33 (1H, dd, J = 5; 14, H-7α), 2.43 (1H, d, OH), 2.77 (1H, d, J = 5.5, H-5α), 2.81 (1H, dd, J = 5.5; 5.5, H-1α), 3.68 (1H, dd, J = 4.5, H-8α), 4.94 (1H, s, H-12b), 5.20 (1H, s, H-12a), 5.58 (1H, d, J = 4.5, H-9α), 5.59 (1H, dd, J = 5.5; 8, H-3α); OAng: 1.90 (3H, dq, J = 1; 1, H-5′), 2.00 (3H, dq, J = 7; 1, H-4′), 5.77 (1H, qq, J = 7; 1, H-3′); OAng: 1.89 (3H, dq, J = 1; 1, H-5″), 1.99 (1H, dq, J = 7; 1, H-4″), 5.74 (1H, qq, J = 7; 1, H-3″) [1]

References

1. F. Bohlmann, C. Zdero, Phytochemistry **17**(8), 1337 (1978)

3β,9β-Diangeloyloxy-1β,10α;4α,5β-diepoxy-7α(H)-germacr-8β-ol



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Senecio petraeus* (R.E.Fr.) Jacobsen [1]

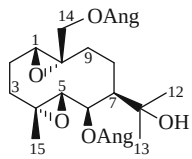
$C_{25}H_{38}O_7$: 450.5420

References

1. F. Bohlmann, J. Ziesche, Phytochemistry **18**(9), 1489 (1979)

6β,14-Diangeloyloxy-1β,10α;4α,5β-diepoxy-7α(H)-germacr-11-ol ((1*R*,4*R*,5*R*,6*R*,10*R*)-1,10;4,5-Diepoxy-11-hydroxygermacrane-6,14-diyl di-[(*Z*)-2-methylbut-2-enoate])

CAS Registry Number: 114176-09-9



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Nanothamnus sericeous* Thomson [1]

$C_{25}H_{38}O_7$: 450.2618

Mp: gum [1]

IR (nujol): 3440, 1720, 1650 [1]

MS: 450 $[M]^+$, 432, 292, 233, 83 (100), 55 [1]

^{1}H NMR (90 MHz, $CDCl_3$, TMS): 1.22 (3H, s, H-12), 1.28 (3H, s, H-13), 1.56 (3H, s, H-15), 3.0 (1H, br d, J = 10, H-1), 3.20 (1H, d, J = 6.5, H-5), 3.83 (1H, br d, J = 12, H-14a), 4.79 (1H, d, J = 12, H-14b), 5.33 (1H, dd, J = 6.5; 1, H-6); OAng: 2.14 (6H, dq, J = 7; 1.5, H-4′, H-4″), 6.16 (2H, qq, J = 7; 1.5, H-3′, H-3″) [1]

^{13}C NMR (23.63 MHz, $CDCl_3$, TMS) [1]:

Table 1

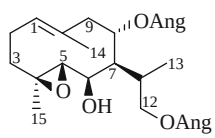
C-1	61.68 d	C-10	61.81 s[a]	2′, 2″	127.64 s
2	37.07 t[a]	11	73.44 s		127.64 s
3	23.40 t[a]	12	27.82 q	3′, 3″	139.53 d
4	59.92 s[a]	13	28.99 q		139.99 d
5	66.87 d	14	62.33 t	4′, 4″	20.60 q
6	72.14 d	15	23.07 q		20.60 q
7	48.35 d	2 × OAng			16.05 q
8	23.20 t[a]	1′, 1″	167.15 s	5′, 5″	16.05 q
9	31.26 t[a]		167.87 s		

[a]Assignments may be interchanged [1]

References

1. U.G. Bhat, V.G. Puranik, N.N. Dhaneshwar, S.S. Tavale, T.N. Guru Row, B.A. Nagasampagi, J. Chem. Soc., Perkin Trans. **1**, 657 (1988)

8α,12-Diangeloyloxy-4,5-epoxy-1(10)-germacren-6β-ol (12-Angeloxy-8-*O*-angeloylshiromodiol)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic

Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Thapsia villosa* var. *minor* (Hoff. et Link) Cout. [1]

$C_{25}H_{38}O_6$: 434.2668

Mp: oil [1]

$[\alpha]_D$ −38.00° (*c* 0.9, $CHCl_3$) [1]

IR (film): 3500, 1720, 1660, 1460, 1400, 1360, 1250, 1170, 1100, 1050, 1000, 840 [1]

EI-MS: 234 (1), 203 (7), 170 (60), 150 (40), 141 (70), 77 (100), 58 (80), 51 (30), 43 (70), 41 (50), 39 (30), 29 (10) [1]

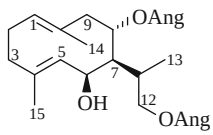
^{1}H NMR (60 MHz, $CDCl_3$): 1.20 (3H, d, J = 6.5, H-13), 1.25 (3H, s, H-15), 1.80 (3H, s, H-14), 2.82 (4H, br d, J = 7, H-5), 3.42 (1H, br d, J = 7, H-6), 4.15 (2H, m, H-12), 5.28 (m, H-1, H-8); 2 × OAng: 1.90 (6H, br s, H-5′, H-5″), 1.95 (6H, m, H-4′, H-4″), 5.95 (1H, br q, J = 6, H-3″), 6.05 (1H, br q, J = 6, H-3′) [1]

X-ray (shiromodiol): [2]

References

1. J. de Pascual Teresa, J.R. Moran, J.M. Hernandez, M. Grande, Phytochemistry **25**(5), 1167 (1986)
2. R.J. McClure, G.A. Sim, P. Coggon, A.T. Phail, J. Chem. Soc. D. 128 (1970)

8α,12-Diangeloyloxy-1(10),4-germacradien-6β-ol (12-Angeloyloxy-8-*O*-angeloyltovarol; 6β-Hydroxy-8α,12-diangeloyloxy-6,7-H-germacrene C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Thapsia villosa* var. *minor* (Hoff. et Link) Cout. [1]

$C_{25}H_{38}O_5$: 418.2719

Mp: oil [1]

$[\alpha]_D$ −132.0° (*c* 7.3, $CHCl_3$) [1]

IR (film): 3400, 1700, 1640, 1380, 1220, 1150, 1070, 1030, 1000, 850 [1]

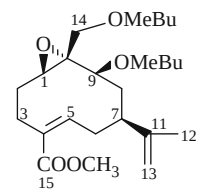
EI-MS: 218 (10), 203 (3), 200 (10), 203 (3), 200 (4), 169 (15), 134 (25), 121 (10), 119 (10), 107 (40), 105 (20), 93 (60), 83 (100), 57 (50), 55 (50), 43 (20), 41 (20) [1]

^{1}H NMR (60 MHz, CCl_4): 1.15 (3H, d, J = 6.5, H-13), 1.38 (3H, s, H-15), 1.62 (3H, s, H-14), 2.12 (4H, br s, H-2 and H-3), 4.20 (3H, m, H-8, H-12), 5.10 (m, H-1, H-5, H-6); 2 × OAng: 1.90 (6H, br s, H-5′, H-5″), 1.96 (6H, br d, J = 6, H-4′, H-4″), 6.05 (1H, br q, J = 6, H-3′), 5.95 (1H, br q, J = 6, H-3″) [1]

References

1. J. de Pascual Teresa, J.R. Moran, J.M. Hernandez, M. Grande, Phytochemistry **25**(5), 1167 (1986)

9β,14-di(2′-Methylbutyroyloxy)-1β,10α-epoxy-4,11-germacradien-15-oic Acid Methyl Ester (Methyl-9β-[2-methylbutyryloxy]-14-*O*-[2-methylbutyryl]-oxyphylloate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Oxyphyllum ulicinum* Phil. [1]

$C_{26}H_{40}O_7$: 464.2774

Mp: colorless oil [1]

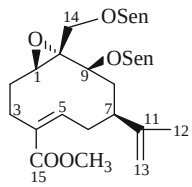
$[\alpha]_D^{24}$ −71° (*c* 0.41, $CHCl_3$) [1]

IR (CCl_4): 1730, 1720 [1]
MS: 464.277 $[M]^+$ (5), 432 (0.5), 362 (0.5), 330 (0.5), 260 (2.8), 247 (2.7), 85 (48), 57 (100) [1]
HPLC [1]
^{1}H NMR (400 MHz, $CDCl_3$): 1.61 (1H, dddd, J = 11; 13; 12; 5, H-2β), 1.68 (1H, br d, J = 14; 1, H-8α), 1.73 (3H, br s, H-12), 1.98 (1H, ddd, J = 12; 14; 9, H-8β), 2.16 (1H, dddd, J = 2.5; 13; 2; 2, H-2α), 2.26 (1H, m, J = 12; 12, H-7), 2.26 (1H, m, J = 2; 12; 13.5, H-3α), 2.39 (1H, br d, J = 4, H-6α), 2.75 (1H, br d, J = 2; 5; 13.5, H-3β), 2.92 (1H, dd, J = 2.5; 11, H-1), 3.15 (1H, br q, J = 11; 14; 12, H-6β), 3.80 (3H, s, OCH_3), 3.85 (1H, d, J = 12, H-14b), 4.44 (1H, d, J = 12, H-14a), 4.55 (1H, dd, J = 1; 9, H-9), 4.67 (1H, dq, J = 1; 1, H-13b), 4.73 (1H, br s, H-13a), 5.97 (1H, dd, J = 4; 11, H-5); 2 × OMeBu: 0.89 (6H, t, J = 7, H-4′, H-4″), 1.13 (3H, d, J = 7, H-5′), 1.14 (3H, d, J = 7, H-5″), 2.37 (4H, tq, J = 7, H-3′, H-3″), 2.43 (2H, tq, J = 7, H-2′, H-2″) [1]

References

1. C. Zdero, F. Bohlmann, H.M. Niemeyer, Phytochemistry **27**(7), 2165 (1988)

9β,14-Disenecioyloxy-1β,10α-epoxy-4,11-germacradien-15-oic Acid Methyl Ester (Methyl-9β-senecioyloxy-14-*O*-senecioyloxy-oxyphylloate)

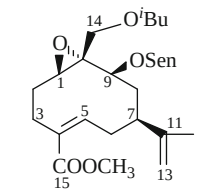


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters
Biological sources: *Oxyphyllum ulicinum* Phil. [1]
$C_{26}H_{36}O_7$: 460.2461
Mp: colorless oil [1]
IR (CCl_4): 1730 [1]
MS: 460.246 $[M]^+$ (5.5), 360 (0.5), 260 (2.3), 247 (2), 83 (100) [1]
HPLC [1]
^{1}H NMR (400 MHz, $CDCl_3$): 1.61 (1H, dddd, J = 11; 13; 12; 5, H-2β), 1.68 (1H, br d, J = 14; 1, H-8α), 1.73 (3H, br s, H-12), 1.98 (1H, ddd, J = 12; 14; 9, H-8β), 2.16 (1H, dddd, J = 2.5; 13; 2; 2, H-2α), 2.26 (1H, m, J = 12; 12, H-7), 2.26 (1H, m, J = 2; 12; 13.5, H-3α), 2.39 (1, br d, J = 4, H-6α), 2.75 (1H, br d, J = 2; 5; 13.5, H-3β), 2.92 (1H, dd, J = 2.5; 11, H-1), 3.15 (1H, br q, J = 11; 14; 12, H-6β), 3.80 (3H, s, OCH_3), 4.11 (1H, d, J = 12, H-14b), 4.51 (1H, d, J = 12, H-14a), 4.51 (1H, dd, J = 1; 9, H-9), 4.67 (1H, dq, J = 1; 1, H-13b), 4.73 (1H, br s, H-13a), 5.97 (1H, dd, J = 4; 11, H-5); 2 × OSen: 1.86 (3H, d, J = 1, H-4′), 1.92 (3H, d, J = 1, H-4″), 2.14 (3H, d, J = 1, H-5′), 2.19 (3H, d, J = 1, H-5″), 5.63 (1H, br s, H-2′), 5.73 (1H, br s, H-2″) [1]

References

1. C. Zdero, F. Bohlmann, H.M. Niemeyer, Phytochemistry **27**(7), 2165 (1988)

14-Isobutyroyloxy-9β-senecioyloxy-1β,10α-epoxy-4,11-germacradien-15-oic Acid Methyl Ester (Methyl-9β-senecioyloxy-14-*O*-isobutyryl-oxyphylloate)



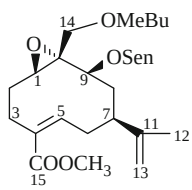
Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters
Biological sources: *Oxyphyllum ulicinum* Phil. [1]

$C_{25}H_{36}O_7$: 448.2461
Mp: colorless oil [1]
IR (CCl_4): 1735, 1715 [1]
MS: 448.246 $[M]^+$ (3), 360 (0.1), 348 (0.2), 247 (1.2), 260 (1.3), 83 (100), 71 (20) [1]
HPLC [1]
^{1}H NMR (400 MHz, $CDCl_3$): 1.61 (1H, dddd, J = 11; 13; 12; 5, H-2β), 1.68 (1H, br d, J = 14; 1, H-8α), 1.73 (3H, br s, H-12), 1.98 (1H, ddd, J = 12; 14; 9, H-8β), 2.16 (1H, dddd, J = 2.5; 13; 2; 2, H-2α), 2.26 (1H, m, J = 12; 12, H-7), 2.26 (1H, m, J = 2; 12; 13.5, H-3α), 2.39 (1H, br d, J = 4, H-6α), 2.75 (1H, br d, J = 2; 5; 13.5, H-3β), 2.92 (1H, dd, J = 2.5; 11, H-1), 3.15 (1H, br q, J = 11; 14; 12, H-6β), 3.80 (3H, s, OCH_3), 3.92 (1H, d, J = 12, H-14b), 4.44 (1H, d, J = 12, H-14a), 4.53 (1H, dd, J = 1; 9, H-9), 4.67 (1H, dq, J = 1; 1, H-13b), 4.73 (1H, br s, H-13a), 5.97 (1H, dd, J = 4; 11, H-5); O^{i}Bu: 1.19 (3H, d, J = 7, H-3′), 1.20 (3H, d, J = 7, H-4′), 2.61 (1H, qq, J = 7, H-2′); OSen: 1.88 (3H, d, J = 1, H-4), 2.15 (3H, d, J =1, H-5″), 5.66 (1H, br s, H-2″) [1]

References

1. C. Zdero, F. Bohlmann, H.M. Niemeyer, Phytochemistry **27**(7), 2165 (1988)

14-(2′-Methylbutyroyloxy)-9β-senecioyloxy-1β,10α-epoxy-4*Z*,11-germacradien-15-oic Acid Methyl Ester (Methyl-9β-senecioyloxy-14-*O*-[2-methylbutyryl]-oxyphylloate)



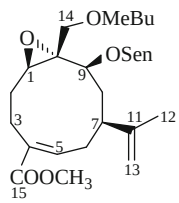
Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Oxyphyllum ulicinum* Phil. [1]
$C_{26}H_{38}O_7$: 462.2618
Mp: colorless oil [1]
$[\alpha]_D^{24}$ −79°C (*c* 2.07, $CHCl_3$) [1]
IR (CCl_4): 1730, 1720 [1]
MS: 462.262 $[M]^+$ (7.4), 430, (0.3), 362 (0.3), 247 (2.1), 260 (2.3), 85 (18), 83 (100) [1]
HPLC [1]
^{1}H NMR (400 MHz, $CDCl_3$): 1.61 (1H, dddd, J = 11; 13; 12; 5, H-2β), 1.68 (1H, br d, J = 14; 1, H-8α), 1.73 (3H, br s, H-12), 1.98 (1H, ddd, J = 12; 14; 9, H-8β), 2.16 (1H, dddd, J = 2.5; 13; 2; 2, H-2α), 2.26 (1H, m, J = 12; 12, H-7), 2.26 (1H, m, J = 2; 12; 13.5, H-3α), 2.39 (1H, br d, J = 4, H-6α), 2.75 (1H, br d, J = 2; 5; 13.5, H-3β), 2.92 (1H, dd, J = 2.5; 11, H-1), 3.15 (1H, br q, J = 11; 14; 12, H-6β), 3.80 (3H, s, OCH_3), 3.88 (1H, d, J = 12, H-14b), 4.46 (1H, d, J = 12, H-14a), 4.52 (1H, dd, J = 1; 9, H-9), 4.67 (1H, dq, J = 1; 1, H-13b), 4.73 (1H, br s, H-13a), 5.97 (1H, dd, J = 4; 11, H-5); OMeBu: 0.91 (3H, t, J = 7, H-4′), 1.16 (3H, d, J = 7, H-5′), 2.43 (3H, tq, J = 7, H-2′, H-3′); OSen: 1.86 (3H, d, J = 1, H-4″), 2.14 (3H, d, J = 1, H-5″), 5.65 (1H, br s, H-2″) [1]

References

1. C. Zdero, F. Bohlmann, H.M. Niemeyer, Phytochemistry **27**(7), 2165 (1988)

14-(2′-Methylbutyroyloxy)-9β-senecioyloxy-1β,10α-epoxy-4*E*,11-germacradien-15-oic Acid Methyl Ester (Methyl-4*E*-9β-senecioyloxy-14-*O*-[2-methylbutyryl]-oxyphylloate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Diesters

Biological sources: *Oxyphyllum ulicinum* Phil. [1]

$C_{26}H_{38}O_7$: 462.2618

Mp: colorless oil [1]

$[\alpha]_D^{24}$ −82° (*c* 0.69, $CHCl_3$) [1]

IR (CCl_4): 1730, 1720 [1]

MS: 462.262 $[M]^+$ (3), 362 (0.3), 260 (1.4), 247 (1), 85 (35), 83 (100), 57 (64), 55 (16) [1]

HPLC [1]

^{1}H NMR (400 MHz, C_6D_6): 1.58 (3H, br s, H-12), 2.11 (1H, dd, J = 4; 10, H-1), 3.77 (3H, s, $COOCH_3$), 4.44 (1H, dd, J = 11; 2.5, H-9), 4.77 (2H, m, H-14), 4.81 (2H, br s, H-13), 6.88 (1H, dd, J = 10; 8, H-5), H-2a, H-2b, H-6a, H-6b, H-7 – obscured signals; OMeBu: 0.94 (3H, t, J = 7, H-4′), 1.20 (3H, d, J = 7, H-5′), 2.45 (3H, tq, J = 7, H-2′, H-3′); OSen: 1.89 (3H, br s, H-4″), 2.15 (3H, br s, H-5″), 5.68 (1H, br s, H-2″) [1]

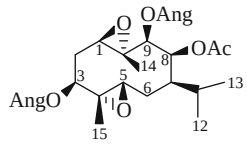
References

1. C. Zdero, F. Bohlmann, H.M. Niemeyer, Phytochemistry **27**(7), 2165 (1988)

Germacranes

Triesters

8β-Acetoxy-3β,9β-diangeloyloxy-1β,10α;4α,5β-diepoxy-7α(H)-germacrane



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Triesters

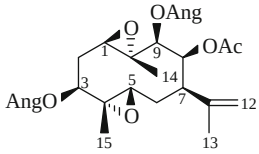
Biological sources: *Senecio petraeus* (R.E.Fr.) Jacobsen [1]

$C_{27}H_{40}O_8$: 492.2723

References

1. F. Bohlmann, J. Ziesche, Phytochemistry **18**(9), 1489 (1979)

8β-Acetoxy-3β,9β-diangeloyloxy-1β,10α;4α,5β-diepoxy-11-germacrene (Rhomboidol Acetate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Triesters

Biological sources: *Senecio rhomboideus* Harv. [1]; *S. galpinii* Hook. [2]

$C_{27}H_{38}O_8$: 490.2567

Mp: colorless oil [1]

$[\alpha]^{24}$ (λ, nm): −26.2° (589), −27.2° (578), −30.6° (546), −52.9° (436) (*c* 1.11, $CHCl_3$) [1]

IR (CCl_4): 1750, 1720, 1650, 1235 [1]

MS: 490.257 $[M]^+$ (0.1) (calc. for $C_{27}H_{30}O_8$), 430 (0.3), 390 (2), 83 (100) [1]

TLC: C_6H_6 – $CHCl_3$ – Et_2O (2:2:1) [2]

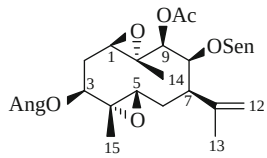
HPLC: MeOH – H_2O (3:1), reversed phase [2]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.30 (6H, s, H-14, H-15), 1.33 (3H, s, H-13), 1.81 (1H, m, H-2a), 2.00 (1H, m, H-2b), 2.00 (2H, m, H-6), 2.06 (3H, s, OAc), 2.49 (1H, dd, J = 8; 11.5, H-7α), 2.76 (1H, dd, J = 5.5; 5.5, H-1α), 3.21 (1H, br d, J = 4.5, H-5α), 5.05 (1H, s, H-12b), 5.25 (1H, s, H-12a), 5.28 (1H, d, J = 4.5, H-9α), 5.37 (1H, dd, J = 5.5; 8, H-3α), 5.40 (1H, br d, J = 4.5, H-8α); 2 × OAng: 1.93 and 1.94 (each 3H, dq, J = 1; 1, H-5′, H-5″), 2.00 (6H, dq, J = 7; 1, H-4′, H-4″), 6.05 and 6.12 (each 1H, qq, J = 7; 1, H-3′, H-3″) [1]

References

1. F. Bohlmann, C. Zdero, Phytochemistry **17**(8), 1337 (1978)
2. F. Bohlmann, C. Zdero, Phytochemistry **21**(10), 2537 (1982)

9β-Acetoxy-3β-angeloyloxy-8β-senecioyloxy-1β,10α,4α,5β-diepoxy-germacr-11-ene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Triesters

Biological sources: *Senecio galpinii* Hook. f. [1]

$C_{27}H_{38}O_8$: 490.2567

Mp: colorless gum [1]

IR (CCl_4): 1745, 1720, 1650, 1240 [1]

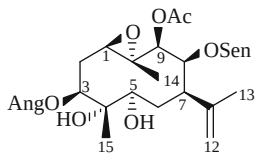
MS: 490.257 $[M]^+$ (0.5) ($C_{27}H_{38}O_8$), 391 [M − OAng or OSen]$^+$ (5), 390 [M − AngOH or SenOH]$^+$ (5), 331 [391 − AcOH]$^+$ (2), 231 [331 − SenOH or AngOH]$^+$ (12), 83 $[C_4H_7CO]^+$ (100) [1]

CI-MS: 491 $[M + 1]^+$ (17), 391 [491 − AngOH or SenOH]$^+$ (100), 331 [391 − HOAc]$^+$ (38), 231 [331 − SenOH or AngOH]$^+$ (31) [1]
TLC: C_6H_6 – $CHCl_3$ – Et_2O (2:2:1) [1]
HPLC: MeOH – H_2O (3:1), reversed phase [1]
^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.27 (6H, s, H-14, H-15), 1.29 (3H, s, H-13), 1.85 (1H, m, H-2b), 2.0 (1H, m, H-2a), 2.02 (1H, m, H-6b), 2.05 (3H, s, OAc), 2.13 (1H, dd, J = 4; 13, H-6a), 2.44 (1H, br dd, J = 12; 6; ∼1, H-7), 2.74 (1H, dd, J = 6; 5, H-1), 3.20 (1H, d, J = 4, H-5), 5.04 (1H, s, H-12b), 5.21 (1H, s, H-12a), 5.24 (1H, d, J = 4.5, H-9), 5.31 (1H, br d, J = 4.5, H-8), 5.37 (1H, dd, J = 8; 6, H-3); OAng: 1.86 (3H, dq, H-5′), 1.99 (3H, dq, H-4′), 6.11 (1H, qq, H-3′); OSen: 1.93 (3H, d, H-4″), 2.12 (3H, d, H-5″), 5.71 (1H, qq, H-2″) [1]

References

1. F. Bohlmann, C. Zdero, Phytochemistry **21**(10), 2537 (1982)

9β-Acetoxy-3β-angeloyloxy-8β-senecioyloxy-1β,10α-epoxy-germacr-11-ene-4α,5α-diol

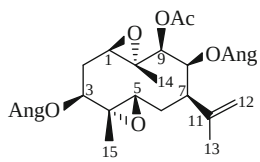


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Triesters
Biological sources: *Senecio galpinii* Hook. f. [1]
$C_{27}H_{40}O_9$: 508.2672
Mp: colorless gum, which could not be separated [1]
IR (CCl_4): 3570, 1750, 1720, 1650, 1235 [1]
MS: 508.267 $[M]^+$ (0.3) ($C_{27}H_{40}O_9$), 409 [M − OAng or OSen]$^+$ (1), 408 [M − AngOH or SenOH]$^+$ (1), 390 [408 − H_2O]$^+$ (0.6), 308 [408 − SenOH or AngOH]$^+$ (1.2), 249 [308 − OAc]$^+$ (1.8), 231 [249 − H_2O]$^+$ (1.4), 83 $[C_4H_7CO]^+$ (100), 55 [83 − CO]$^+$ (42) [1]
TLC: C_6H_6 – $CHCl_3$ – Et_2O (2:2:1) [1]
HPLC: MeOH – H_2O (3:1), reversed phase [1]
^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.23 (3H, s, H-15), 1.26 (3H, s, H-13), 1.26 (3H, s, H-14), 2.02 (3H, s, OAc), 2.74 (1H, t, J = 6, H-1), 3.00 (1H, br d, J = 2.5, H-7), 3.15 (1H, s, OH), 3.90 (1H, br s, H-5), 5.06 (1H, s, H-12′), 5.07 (1H, d, J = 2.5, H-9), 5.26 (1H, s, H-12), 5.52 (1H, m, H-3), 5.50 (1H, m, H-8); OAng: 1.85 (3H, dq, H-5′), 1.97 (3H, dq, H-4′), 6.13 (1H, qq, H-3′); OSen: 1.88 (3H, d, H-4′), 2.11 (3H, d, H-5′), 5.63 (1H, qq, H-2′); H-2, H-6 − overlapping multiplets [1]
^{1}H NMR (400 MHz, C_6D_6, TMS): 1.10 (3H, s, H-15), 1.11 (3H, s, H-14), 1.39 (3H, s, H-13), 1.60 (3H, s, OAc), 1.70 (1H, m, H-6b), 1.89 (1H, m, H-2b), 2.07 (1H, m, H-2a), 2.45 (1H, ddd, J = 2.5; 14; 14, H-6a), 2.62 (1H, t, J = 6, H-1), 3.27 (1H, br d, J = 2.5, H-7), 3.78 (1H, br dd, J = 2.5; 2.5, H-5), 4.97 (1H, s, H-12′), 5.21 (1H, s, H-12), 5.49 (1H, d, J = 2.5, H-9), 5.74 (1H, t, J = 7, H-3), 5.93 (1H, br dd, J = 2.5, H-8); OAng: 2.02 (3H, br s, H-5′), 2.10 (3H, dq, H-4′), 5.82 (1H, qq, H-3′); OSen: 1.38 (3H, d, H-4″), 2.02 (3H, d, H-5″), 5.56 (1H, br s, H-2″) [1]

References

1. F. Bohlmann, C. Zdero, Phytochemistry **21**(10), 2537 (1982)

9β-Acetoxy-3β,8β-diangeloyloxy-1β,10α;4α,5β-diepoxy-11-germacrene (Isorhombiodol Acetate)



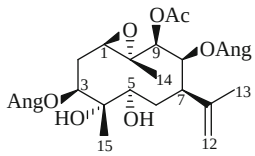
Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Triesters

Biological sources: *Kleinia fulgens* Hook. [1]; *Senecio galpinii* Hook. f. [2]
$C_{27}H_{38}O_8$: 490.2567
Mp: colorless gum [1]
IR (CCl_4): 1750, 1720, 1650, 1250 [1]
MS: 490.257 $[M]^+$ (0.2) ($C_{27}H_{38}O_8$), 391 (1), 331 (0.5), 231 (1), 83 (100) [1]
TLC: C_6H_6 – $CHCl_3$ – Et_2O (2:2:1) [2]
HPLC: MeOH – H_2O (3:1), reversed phase [2]
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.26 (3H, s, H-15), 1.29 (3H, s, H-14), 1.32 (3H, s, H-13), 1.83 (1H, m, H-2β), 2.02 (3H, s, OAc), 2.13 (2H, m, H-6), 2.15 (1H, m, H-2α), 2.49 (1H, br dd, J = 12; 6.5, H-7α), 2.75 (1H, dd, J = 6; 5, H-1), 3.20 (1H, br d, J = 4.5, H-5α), 5.08 (1H, s, H-12b), 5.27 (1H, s, H-12a), 5.35 (2H, m, H-8α, H-9α), 5.39 (1H, dd, J = 8; 6, H-3α); 2 × OAng: 1.88 (3H, dq, H-5″), 1.93 (3H, dq, H-5′), 1.99 (6H, dq, H-4′, H-4″), 6.11 (2H, qq, H-3′, H-3″) [1]

References

1. F. Bohlmann, M. Ahmed, J. Jakupovic, C. Jeffrey, Phytochemistry **20**(2), 251 (1981)
2. F. Bohlmann, C. Zdero, Phytochemistry **21**(10), 2537 (1982)

9β-Acetoxy-3β,8β-diangeloyloxy-1β,10α-epoxy-germacr-11-ene-4α,5α-diol

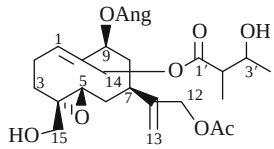


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Triesters
Biological sources: *Senecio galpinii* Hook. f. [1]
$C_{27}H_{40}O_9$: 508.2672
Mp: colorless gum, which could not be separated [1]
IR (CCl_4): 3570, 1750, 1720, 1650, 1235 [1]
MS: 508.267 $[M]^+$ (0.3) ($C_{27}H_{40}O_9$), 409 $[M - OAng]^+$ (1), 408 $[M - AngOH]^+$ (1), 390 $[408 - H_2O]^+$ (0.6), 308 $[408 - AngOH]^+$ (1.2), 249 $[308 - OAc]^+$ (1.8), 231 $[249 - H_2O]^+$ (1.4), 83 $[C_4H_7CO]^+$ (100), 55 $[83 - CO]^+$ (42) [1]
TLC: C_6H_6 – $CHCl_3$ – Et_2O (2:2:1) [1]
HPLC: MeOH – H_2O (3:1), reversed phase [1]
^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.23 (3H, s, H-15), 1.27 (3H, s, H-13), 1.27 (3H, s, H-14), 2.04 (3H, s, OAc), 2.77 (1H, t, J = 6, H-1), 3.04 (1H, br d, J = 2.5, H-7), 3.30 (1H, s, OH), 3.90 (1H, br s, H-5), 5.08 (1H, s, H-12b), 5.20 (1H, d, J = 2.5, H-9), 5.30 (1H, s, H-12a), 5.50 (1H, m, H-3), 5.50 (1H, m, H-8); 2 × OAng: 1.92 (6H, dq, H-5′, H-5″), 2.00 (6H, dq, H-4′, H-4″), 6.11 (1H, qq, H-3′), 6.13 (1H, qq, H-3″); H-2, H-6 – overlapping multiplets [1]
^{1}H NMR (400MHz, C_6D_6, TMS): 1.10 (3H, s, H-15), 1.12 (3H, s, H-14), 1.40 (3H, s, H-13), 1.70 (1H, m, H-6b), 1.79 (3H, s, OAc), 1.89 (1H, m, H-2b), 2.07 (1H, m, H-2a), 2.56 (1H, ddd, J = 14; 14; 2.5, H-6a), 2.64 (1H, t, J = 6, H-1), 3.31 (1H, br d, J = 2.5, H-7), 3.81 (1H, br dd, J = 2.5; 2.5, H-5), 5.14 (1H, s, H-12′), 5.26 (1H, s, H-12), 5.56 (1H, d, J = 2.5, H-9), 5.74 (1H, t, J = 7, H-3), 5.99 (1H, br dd, J = 2.5; 2.5, H-8); 2 × OAng: 1.91 (3H, dq, H-5′), 2.02 (3H, dq, H-5″), 2.10 (3H, dq, H-4′), 2.12 (3H, dq, H-4″), 6.13 (2H, qq, H-3′, H-3″) [1]

References

1. F. Bohlmann, C. Zdero, Phytochemistry **21**(10), 2537 (1982)

12-Acetoxy-9β-angeloyloxy-14-(3″-hydroxy-2″-methylbutyroyloxy)-4,5-epoxy-1(10),11(13)-germacradien-15-ol (Vautheriol Angelate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Triesters

Biological sources: *Trixis vautheri* DC. [1]

$C_{27}H_{40}O_9$: 508.2672

Mp: colorless gum [1]

$[\alpha]^{24}$ (λ, nm): −34.5° (589), −36° (578), −40.5° (546), −61° (436) (*c* 0.8, $CHCl_3$) [1]

IR (CCl_4): 3500, 1740, 1720, 1650 [1]

CI-MS: 509 $[M + 1]^+$ (3), 409 (11), 391 (10), 291 (100), 231 (85), 213 (47), 101 (42), 83 (10) [1]

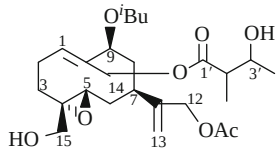
HPLC [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.5 (1H, m, H-3β), 1.7 (1H, m, H-6α), 2.0 (1H, m, H-8β), 2.08 (3H, s, OAc), 2.15 (1H, m, H-2α), 2.20 (1H, m, H-8α), 2.28 (1H, m, H-6β), 2.5 (1H, m, H-3α), 2.50 (1H, m, H-7), 2.82 (1H, m, H-2β), 3.35 (1H, br d, J = 11; 2, H-5), 3.58 (1H, br d, J = 12, H-15b), 3.79 (1H, br d, J = 12, H-15a), 4.48 (1H, d, J = 12.5, H-14b), 4.54 (2H, br s, H-12), 4.83 (1H, d, J = 12.5, H-14a), 4.95 (1H, br s, H-13b), 5.05 (1H, br s, H-13a), 5.81 (1H, br dd, J = 7; 10, H-1), 5.93 (1H, br d, J = ~5, H-9); OAng: 1.88 (1H, dq, J = 1.5; 1.5, H-5′), 1.99 (1H, dq, J = 7; 1.5, H-4′), 6.12 (1H, qq, J = 7; 1.5, H-3′); OMeBu (OH): 1.19 (3H, d, J = 7, H-5″), 1.24 (3H, d, J = 7, H-4″), 2.50 (1H, dq, J = 7; 7, H-2″), 3.92 (1H, dq, J = 7; 7, H-3″) [1]

References

1. F. Bohlmann, A. Suwita, J. Jakupovic, R.M. King, H. Robinson, Phytochemistry **20**(7), 1649 (1981)

12-Acetoxy-14-(3′-hydroxy-2′-methylbutyroyloxy)-9β-isobutyroyloxy-4,5-epoxy-1(10),11(13)-germacradien-15-ol (Vautheriol Isobutyrate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Triesters

Biological sources: *Trixis vautheri* DC. [1]

$C_{26}H_{40}O_9$: 496.2672

Mp: colorless gum [1]

$[\alpha]^{24}$ (λ, nm): −30° (589), −32° (578), −36° (546), −58° (436) (*c* 0.58, $CHCl_3$) [1]

IR (CCl_4): 3480, 1735 [1]

CI-MS: 497 $[M + 1]^+$ (5), 409 (21), 291 (100), 231 (72), 119 (11), 101 (11) [1]

HPLC [1]

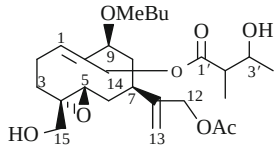
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.5 (1H, m, H-3β), 1.65 (1H, m, H-6α), 2.0 (1H, m, H-8β), 2.10 (3H, s, OAc), 2.2 (1H, m, H-2α), 2.2 (1H, m, H-8α), 2.26 (1H, m, H-6β), 2.5 (1H, m, H-3α), 2.5 (1H, m, H-7), 2.8 (1H, m, H-2β), 3.32 (1H, br d, J = 11; 2, H-5), 3.58 (1H, br d, J = 12, H-15b), 3.78 (1H, br d, J = 12, H-15a), 4.46 (1H, d, J = 12.5, H-14b), 4.53 (2H, br s, H-12), 4.80 (1H, d, J = 12.5, H-14a), 4.95

(1H, br s, H-13b), 5.06 (1H, br s, H-13a), 5.80 (1H, br dd, J = 7; 10, H-1), 5.84 (1H, br d, J = ~5, H-9); OMeBu(OH): 1.16 (3H, d, J = 7, H-5′), 1.24 (3H, d, J = 7, H-4′), 2.48 (1H, dq, J = 7; 7, H-2′), 3.93 (1H, dq, J = 7; 7, H-3′); O^{i}Bu: 1.18 (6H, d, J = 7, H-3″, H-4″), 2.53 (1H, qq, J = 7; 7, H-2″) [1]

References

1. F. Bohlmann, A. Suwita, J. Jakupovic, R.M. King, H. Robinson, Phytochemistry **20**(7), 1649 (1981)

12-Acetoxy-14-(3′-hydroxy-2′-methylbutyroyloxy)-9β-(2″-methylbutyroyloxy)-4,5-epoxy-1(10),11(13)-germacradien-15-ol (Vautheriol-2′-methylbutyrate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Triesters

Biological sources: *Trixis vautheri* DC. [1]

$C_{27}H_{42}O_9$: 510.2829

Mp: colorless gum [1]

$[\alpha]^{24}$ (λ, nm): −33.5° (589), −35° (578), −39.5° (546), −64° (436) (*c* 4.7, $CHCl_3$) [1]

IR (CCl_4): 3480, 1740, 1660 [1]

MS: 290 (14), 85 (58), 57 (100) [1]

CI-MS: 511 $[M + 1]^+$ (4), 409, 291 (100) [1]

HPLC [1]

^{1}H NMR (270 MHz, C_6D_6, TMS): 1.35 (1H, m, H-3β), 1.58 (1H, ddd, J = 11; 10; 12, H-6α), 1.81 (3H, s, OAc), 1.85 (1H, m, H-2α), 1.93 (1H, m, H-8β), 2.21 (1H, br d, J = 2, H-6β), 2.21 (1H, m, H-8α), 2.26 (1H, br dd, J = 10; ~5, H-7), 2.48 (1H, m, H-3α), 2.78 (1H, m, H-2β), 3.03 (1H, dd, J = 11; 2, H-5), 3.62 (1H, br d, J = 12, H-15b), 3.89 (1H, br d, J = 12, H-15a), 4.51 (1H, d, J = 12.5, H-14b), 4.57 (2H, Abq, H-12), 4.86 (1H, d, J = 12.5, H-14a), 4.90 (1H, br s, H-13b), 5.00 (1H, br s, H-13a), 5.73 (1H, br dd, J = 7; 10, H-1), 6.01 (1H, br d, J = ~5, H-9); OMeBu(OH): 1.07 (3H, d, J = 7, H-5′), 1.14 (3H, d, J = 7, H-4′), 2.48 (1H, dq, J = 7; 7, H-2′), 3.97 (1H, dq, J = 7; 7, H-3′); OMeBu: 0.89 (3H, t, J = 7, H-4″), 1.07 (3H, d, J = 7, H-5″), 1.37 (1H, ddd, J = 7; 7; 14, H-3″b), 1.67 (1H, ddd, J = 7; 7; 14, H-3″a), 2.27 (1H, tq, J = 7; 7, H-2″) [1]

^{13}C NMR (C_6D_6) [1]:

Table 1

11.7 q	40.4 t	72.3 d
14.1 q	41.3 d	111.5 t
16.6 q	48.3 d	130.3 d
20.5 q	60.9 d	135.5 s
21.0 q	63.7 t	148.8 s
25.4 t	64.2 t	170.1 s

(*continued*)

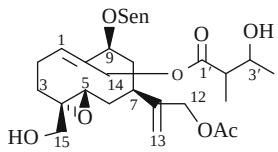
Table 1 (continued)

27.0 t	64.7 s	175.6 s
31.7 t	65.6 t	175.7 d
35.1 t	69.8 d	

References

1. F. Bohlmann, A. Suwita, J. Jakupovic, R.M. King, H. Robinson, Phytochemistry **20**(7), 1649 (1981)

12-Acetoxy-14-(3′-hydroxy-2′-methylbutyroyloxy)-9β-senecioyloxy-4,5-epoxy-1(10),11(13)-germacradien-15-ol (Vautheriol Senecioate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Triesters

Biological sources: *Trixis vautheri* DC. [1]

$C_{27}H_{40}O_9$: 508.2672

Mp: not separated colorless gum (mix. with vautheriol tiglate) [1]

IR (CCl_4) (mix.): 3500, 1740, 1720, 1655 [1]

CI-MS (mix.): 509 $[M + 1]^+$ (4), 409 (18), 391 (12), 291 (100), 231 (92), 213 (51), 101 (52), 83 (8) [1]

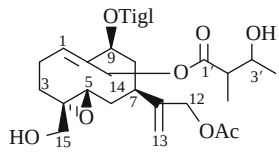
HPLC [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS) (mix.): 1.5 (1H, m, H-3β), 1.68 (1H, m, H-6α), 2.0 (1H, m, H-8β), 2.08 (3H, s, OAc), 2.15 (1H, m, H-2α), 2.2 (1H, m, H-8α), 2.28 (1H, m, H-6β), 2.5 (1H, m, H-3α), 2.50 (1H, m, H-7), 2.80 (1H, m, H-2β), 3.34 (1H, br d, J = 11; 2, H-5), 3.58 (1H, br d, J = 12, H-15b), 3.78 (1H, br d, J = 12, H-15a), 4.47 (1H, d, J = 12.5, H-14b), 4.53 (2H, br s, H-12), 4.80 (1H, d, J = 12.5, H-14a), 4.95 (1H, br s, H-13b), 5.06 (1H, br s, H-13a), 5.80 (1H, br dd, J = 7; 10, H-1), 5.89 (1H, br d, J = ∼5, H-9); OMeBu(OH): 1.17 (3H, d, J = 7, H-5′), 1.23 (3H, d, J = 7, H-4′), 2.48 (1H, dq, J = 7; 7, H-2′), 3.91 (1H, dq, J = 7; 7, H-3′); OSen: 1.90 (1H, d, J = 1, H-4″), 2.17 (1H, d, J = 1, H-5″), 5.66 (1H, qq, J = 1, H-2″) [1]

References

1. F. Bohlmann, A. Suwita, J. Jakupovic, R.M. King, H. Robinson, Phytochemistry **20**(7), 1649 (1981)

12-Acetoxy-14-(3′-hydroxy-2′-methylbutyroyloxy)-9β-tigloyloxy-4,5-epoxy-1(10),11(13)-germacradien-15-ol (Vautheriol Tiglate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Triesters

Biological sources: *Trixis vautheri* DC. [1]

$C_{27}H_{40}O_9$: 508.2672

Mp: not separated colorless gum (mix. with vautheriol senecioate) [1]

IR (CCl_4) (mix.): 3500, 1740, 1720, 1655 [1]

CI-MS (mix.): 509 $[M + 1]^+$ (4), 409 (18), 391 (12), 291 (100), 231 (92), 213 (51), 101 (52), 83 (8) [1]

HPLC [1]

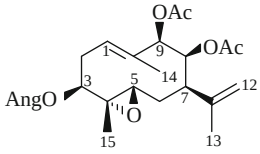
^{1}H NMR (270 MHz, $CDCl_3$, TMS) (mix.): 1.5 (1H, m, H-3β), 1.68 (1H, m, H-6α), 2.0 (1H, m, H-8β), 2.07 (3H, s, OAc), 2.15 (1H, m, H-2α), 2.2 (1H, m, H-8α), 2.28 (1H, m, H-6β), 2.5 (1H, m, H-3α), 2.50 (1H, m, H-7), 2.80 (1H, m, H-2β), 3.34 (1H, br d, J = 11; 2, H-5), 3.58 (1H, br d, J = 12, H-15b), 3.78 (1H, br d, J = 12, H-15a), 4.47 (1H, d, J = 12.5, H-14b), 4.53 (2H, br s, H-12), 4.82 (1H, d, J = 12.5,

H-14a), 4.95 (1H, br s, H-13b), 5.06 (1H, br s, H-13a), 5.80 (1H, br dd, J = 7; 10, H-1), 5.89 (1H, br d, J = ~5, H-9); OMeBu(OH): 1.17 (3H, d, J = 7, H-5′), 1.23 (3H, d, J = 7, H-4′), 2.48 (1H, dq, J = 7; 7, H-2′), 3.91 (1H, dq, J = 7; 7, H-3′); OTigl: 1.80 (1H, br d, J = 7, H-4″), 1.82 (1H, br s, H-5″), 6.86 (1H, qq, J = 7, H-3″), [1]

References

1. F. Bohlmann, A. Suwita, J. Jakupovic, R.M. King, H. Robinson, Phytochemistry **20**(7), 1649 (1981)

8β,9β-Diacetoxy-3β-angeloyloxy-4α,5β-epoxy-4α,5α,6α,7α(H)-germacra-1(10),11-diene (8β,9β-Diacetoxy-3β-angeloyloxy-4.5.6.7H-4.5-epoxygermacrene C)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Triesters

Biological sources: *Senecio platyphylloides* Somm. et Levier [1]

$C_{24}H_{34}O_7$: 434.2305

Mp: colorless oil [1]

$[\alpha]^{24}$ (λ, nm): −12° (589), −12° (578), −14° (546), −15° (436) (*c* 2.9, $CHCl_3$) [1]

IR (CCl_4): 1750, 1720, 1650, 1255 [1]

MS: 434.230 $[M]^+$ (0.1) (calc. for $C_{24}H_{34}O_7$: 434.230), 334 $[M - C_4H_7COOH]^+$ (3), 274 $[334 - AcOH]^+$ (1), 214 $[274 - AcOH]^+$ (3), 83 $[C_4H_7CO]^+$ (100) [1]

^{1}H NMR (270 MHz, C_6D_6, TMS): 1.12 (3H, s, H-14), 1.61 (3H, br s, H-13), 1.66 (3H, br s, H-15), 1.79 (3H, s, OAc), 1.82 (3H, s, OAc), 2.35 (1H, ddd, J = 6.5; 13; 6.5, H-2b), 2.50 (1H, ddd, J = 6.5; 13; 6.5, H-2a), 2.67 (1H, d, J = 6, H-5α), 5.00 (1H, br s, H-12b), 5.17 (1H, dd, J = 6.5, H-3α), 5.19 (1H, br s, H-12a), 5.31 (1H, d, J = 4, H-8), 5.37 (1H, t, J = 6.5, H-1), 5.55 (1H, br d, J = 4, H-9); OAng: 2.01 (6H, m, H-4′, H-5′), 5.76 (1H, qq, H-3′) [1]

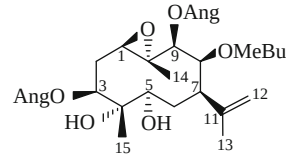
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.34 (3H, s, H-14), 1.65 (3H, br s, H-13), 1.70 (3H, br s, H-15), 2.07 (3H, s, OAc), 2.09 (3H, s, OAc), 2.4 (2H, m, H-2), 3.21 (1H, d, J = 6, H-5α), 5.04 (1H, br s, H-12b), 5.16 (1H, t, J = 6.5, H-1), 5.2 (1H, m, H-3α), 5.2 (2H, m, H-8, H-9), 5.21 (1H, br s, H-12a); OAng: 1.91 (3H, dq, H-5′), 1.99 (3H, dq, H-4′), 6.08 (1H, qq, H-3′) [1]

References

1. F. Bohlmann, K.-H. Knoll, C. Zdero, P.K. Mahanta, M. Grenz, A. Suwita, D. Ehlers, N.L. Van, W.-R. Abraham, A.A. Natu, Phytochemistry **16**(7), 965 (1977)

3β,9β-Diangeloyloxy-8β-(2‴-methylbutyroyloxy)-1β,10α-epoxy-11-germacrene-4α,5α-diol (4α,5α-Dihydroxy-kleinifulgin)

CAS Registry Number: 79383-72-5



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Triesters

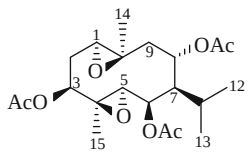
Biological sources: *Kleinia fulgens* Hook. [1]

$C_{30}H_{46}O_9$: 550.3142
Mp: colorless gum [1]
$[\alpha]^{24}$ (λ, nm): −31.9° (589), −31.9° (578), −36.2° (546), −62.2° (436) (*c* 0.91, $CHCl_3$) [1]
IR (CCl_4): 3560, 1740, 1720, 1650 [1]
MS: 550.314 $[M]^+$ (1), 532 (0.5), 451 (2), 450 (1), 432 (1), 348, 85 (16), 83 (100), 57 (55), 55 (53) [1]
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.27 (3H, s, H-15), 1.29 (3H, s, H-13), 1.29 (3H, s, H-14), 1.70 (1H, m, H-2β), 2.00 (1H, m, H-6β), 2.10 (1H, ddd, J = 6.5; 7; 15, H-2α), 2.42 (1H, ddd, J = 2.5; 14; 14, H-6α), 2.75 (1H, dd, J = 6.5; 5, H-1), 3.09 (1H, br d, J = 14; 3; 3, H-7α), 3.27 (1H, s, OH), 3.90 (1H, br dd, J = 2.5; 2.5, H-5β), 5.08 (1H, s, H-12b), 5.23 (1H, d, J = 3, H-9α), 5.31 (1H, s, H-12a), 5.53 (1H, dd, J = 7; 7, H-3α), 5.58 (1H, br dd, J = 3; 3, H-8α); 2 × OAng: 1.87 (3H, dq, H-5′), 1.95 (3H, dq, H-5″), 1.99 (3H, dq, H-4′), 2.01 (3H, dq, H-4″), 6.06 (1H, qq, H-3′), 6.10 (1H, qq, H-3″); OMeBu: 0.88 (3H, t, H-5‴), 1.14 (3H, d, H-4‴), 1.42 (1H, ddq, H-3‴b), 1.67 (1H, ddq, H-3‴a), 2.34 (1H, tq, H-2‴) [1]

References

1. F. Bohlmann, M. Ahmed, J. Jakupovic, C. Jeffrey, Phytochemistry **20**(2), 251 (1981)

3β,6β,8α-Triacetoxy-4β,5α;1α,10β-diepoxy-germacrane



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Triesters
Biological sources: *Salvia roborowskii* Maxim. [1]
$C_{21}H_{32}O_8$: 412.2097
Mp: colorless gum [1]
$[\alpha]_D^{26}$ +5.0° (*c* 2.0, $CHCl_3$) [1]
IR (KBr): 2962, 1743, 1371, 1240, 1041 [1]
FAB-MS: 413 $[M + 1]^+$ [1]
EI-MS: 395 (2), 353 (5), 337 (2), 253 (3), 249 (35), 43 (100) [1]
^{1}H NMR (400.13 MHz, $CDCl_3$, TMS): 0.82 (3H, d, J = 6.4, H-13), 1.00 (3H, d, J = 6.4, H-12), 1.20 (3H, s, H-15), 1.32 (3H, s, H-14), 1.47 (1H, br d, J = 8.7, H-7), 1.70 (1H, m, H-11), 1.70 (1H, m, H-2β), 1.70 (1H, m, H-9α), 2.08 (1H, m, H-2α), 2.08 (1H, m, H-9β), 3.13 (1H, d, J = 10.6, H-1), 3.19 (1H, d, J = 6.8, H-5), 4.83 (1H, d, J = 6.8, H-6), 5.08 (1H, t, J = 2.5, H-3α), 5.35 (1H, dd, J = 12.0; 5.6, H-8); 3 × OAc: 1.86 (3H, s), 1.91 (3H, s), 1.93 (3H, s) [1]
^{13}C NMR (100.62 MHz, $CDCl_3$) [1]:

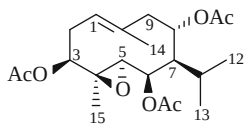
Table 1

C-1	56.3 d	C-8	68.8 d	C-15	15.5 q
2	26.4 t	9	41.3 t	3 × OAc	169.1 s
3	67.9 d	10	57.4 s		20.6 q
4	57.5 s	11	25.6 d		169.0 s
5	59.6 d	12	21.4 q		20.4 q
6	72.0 d	13	20.4 q		168.7 s
7	74.4 d	14	22.2 q		20.2 q

References

1. Y. Li, W. Yan-Qi, D. Xin, Y.-P. Shi, Planta Med. **69**, 782 (2003)

3β,6β,8α-Triacetoxy-4β,5α-epoxy-germacr-1(10)*E*-ene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Triesters

Biological sources: *Salvia roborowskii* Maxim. [1, 2]
$C_{21}H_{32}O_7$: 396.2148
Mp: colorless gum [1]
$[\alpha]_D^{26}$ −12.7° (*c* 16.5, $CHCl_3$) [1, 2]
IR: 1740, 1239 [1]; (KBr): 2964, 1740, 1367, 1239, 1022 [2]
HR-SI-MS: found 397.2221 (calc. 397.2180) [1]
EI-MS: 396 $[M]^+$ (5), 354 (4), 336 (4), 294 (7), 252 (5), 234 (29), 226 (31), 43, (100) [2]
^{1}H NMR (400 MHz, $CDCl_3$, TMS): 0.80 (3H, d, J = 6.4, H-13), 0.99 (3H, d, J = 6.4, H-12), 1.10 (3H, s, H-15), 1.32 (1H, br d, J = 7.0, H-7), 1.65 (3H, s, H-14), 1.80 (1H, m, H-11), 2.25 (1H, br d, J = 12.0, H-2β), 2.52 (1H, m, H-2α), 2.52 (1H, m, H-9β), 3.00 (1H, d, J = 6.8, H-5), 4.83 (1H, br d, J = 6.8, H-6), 5.05 (1H, t, J = 3.0, H-3), 5.35 (1H, m, H-1), 5.35 (1H, m, H-8); 3 × OAc: 1.92 (3H, s), 1.95 (3H, s), 2.00 (3H, s) [1]
^{1}H NMR (400.13 MHz, $CDCl_3$, TMS): 0.80 (3H, d, J = 6.4, H-13), 0.99 (3H, d, J = 6.4, H-12), 1.10 (3H, s, H-15), 1.32 (1H, br d, J = 7.0, H-7), 1.65 (3H, br s, H-14), 1.80 (1H, m, H-11), 1.99 (1H, m, H-9α), 2.25 (1H, dd, J = 12.0; 3.0, H-2β), 2.52 (1H, m, H-2α), 2.52 (1H, m, H-9β), 3.00 (1H, d, J = 6.8, H-5), 4.83 (1H, d, J = 6.8, H-6), 5.05 (1H, t, J = 3.0, H-3α), 5.35 (1H, m, H-1), 5.35 (1H, m, H-8); 3 × OAc: 1.92 (3H, s), 1.95 (3H, s), 2.00 (3H, s) [2]
^{13}C NMR (100 MHz, $CDCl_3$) [1]:

Table 1

C-1	123.8 d	C-8	71.9 d	C-15	15.4 q
2	29.8 t	9	40.1 t	3 × OAc	169.4 s
3	71.0 d	10	132.6 s		20.7 q
4	58.1 s	11	25.7 d		169.3 s
5	60.1 d	12	20.8 q		20.7 q
6	73.6 d	13	20.8 q		169.1 s
7	47.3 d	14	22.9 q		20.4 q

^{13}C NMR (100.62 MHz, $CDCl_3$) [2]:

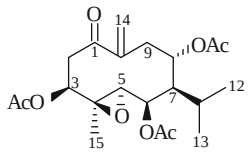
Table 2

C-1	123.8 d	C-8	71.9 d	C-15	15.4 q
2	29.8 t	9	40.1 t	3 × OAc	169.4 s
3	71.0 d	10	132.6 s		20.7 q
4	58.1 s	11	25.7 d		169.3 s
5	60.1 d	12	20.8 q		20.7 q
6	73.6 d	13	20.8 q		169.1 s
7	47.3 d	14	22.9 q		20.4 q

References

1. Y. Li, N. Lou, W. Yan Qi, X. Feng Lin, Y. Li, Chin. Chem. Lett. **14**, 1156 (2003)
2. Y. Li, W. Yan-Qi, D. Xin, Y.-P. Shi, Planta Med. **69**, 782 (2003)

3β,6β,8α-Triacetoxy-4β,5α-epoxy-5β,7α(H)-germacr-10(14)-en-1-one



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Triesters
Biological sources: *Salvia roborowskii* Maxim. [1, 2]
$C_{21}H_{30}O_8$: 410.1941
Mp: colorless gum [1, 2]
$[\alpha]_D^{26}$ +29.0° (*c* 2.0, $CHCl_3$) [1, 2]
IR: 1743, 1240, 1677 [1]; (KBr): 2962, 1743 (ester), 1677 (α,β-unsaturated ketone), 1623, 1371, 1240, 1029 [2]
FAB-MS: 411 $[M + 1]^+$ [1, 2]
EI-MS: 368 (1), 350 (1), 308 (6), 266 (6), 205 (20), 43 (100) [2]
^{1}H NMR (400 MHz, $CDCl_3$, TMS): 0.85 (3H, d, J = 6.4, H-13), 1.13 (3H, d, J = 6.4, H-12), 1.37 (3H, s, H-15), 1.47 (1H, br d, J = 8.6, H-7), 1.81 (1H, m, H-11), 2.54 (1H, t, J = 11.4, H-9α), 2.80 (1H, br d, J = 13.6, H-2β), 2.90 (1H, br d, J = 11.4, H-9β), 3.07 (1H, d, J = 7.2, H-5), 3.32 (1H, dd, J = 13.6, 3.8, H-2α), 4.82 (1H, br d, J = 7.2, H-6), 5.17 (1H, t, J = 3.8, H-3), 5.35 (1H, m, H-1), 5.41 (1H, m, H-8), 5.99 (1H, s, H-14a), 6.05 (1H, s, H-14b); 3 × OAc: 1.97 (3H, s), 2.06 (3H, s), 2.06 (3H, s) [1]
^{1}H NMR (400.13 MHz, $CDCl_3$, TMS): 0.85 (3H, d, J = 6.4, H-13), 1.13 (3H, d, J = 6.4, H-12), 1.37

(3H, s, H-15), 1.47 (1H, br d, J = 8.6, H-7), 1.81 (1H, m, H-11), 2.54 (1H, t, J = 12.0, H-9α), 2.80 (1H, dd, J = 13.6; 3.8, H-2β), 2.90 (1H, dd, J = 11.4; 2.8, H-9β), 3.07 (1H, d, J = 7.2, H-5), 3.32 (1H, dd, J = 13.6; 3.8, H-2α), 4.82 (1H, d, J = 7.2, H-6), 5.17 (1H, t, J = 3.8, H-3α), 5.41 (1H, dd, J = 11.2; 2.8, H-8), 5.99 (1H, s, H-14b), 6.05 (1H, s, H-14a); 3 × OAc: 1.97 (3H, s), 2.06 (6H, s) [2]

^{13}C NMR (100 MHz, $CDCl_3$) [1]:

Table 1

C-1	199.4 s	C-9	38.4 t	3 × OAc	169.8 s
2	38.4 t	10	147.5 s		20.9 q
3	69.2 d	11	26.0 d		169.8 s
4	57.3 s	12	22.8 q		20.6 q
5	59.6 d	13	20.9 q		169.4 s
6	72.2 d	14	129.3 t		20.5 q
7	47.5 d	15	16.3q		
8	68.4 d				

^{13}C NMR (100.62 MHz, $CDCl_3$) [2]:

Table 2

C-1	199.4 s	C-8	68.4 d	C-15	16.3 q
2	38.4 t	9	38.4 t	3 × OAc	169.8 s
3	69.2 d	10	147.5 s		20.9 q
4	57.3 s	11	26.0 d		169.8 s
5	59.6 d	12	22.8 q		20.6 q
6	72.2 d	13	20.9 q		169.4 s
7	47.5 d	14	129.3 t		20.5 q

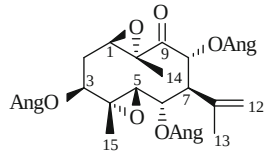
^{1}H-^{1}H COSY [2]

^{1}H-^{1}H NOESY [2]

References

1. Y. Li, N. Lou, W. Yan-Qi, X. Feng Lin, Y. Li, Chin. Chem. Lett. **14**, 1156 (2003)
2. Y. Li, W. Yan-Qi, D. Xin, Y.-P. Shi, Planta Med. **69**, 782 (2003)

3β,6α,8α-Triangeloyloxy-1β,10α;4α,5β-diepoxy-11-germacren-9-one (8α-Angeloyloxy-ligularinone A)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Triesters

Biological sources: *Ligularia hodgsoni* Hook.f., *L. brachyphylla* Hand.-Mazz., *L. dentata* (A. Gray) Hara., *L. clivorum* Maxim. [1]

$C_{30}H_{40}O_9$: 544.2672

Mp: colorless oil [1]

$[\alpha]^{24}$ (λ, nm): +17.3° (589), +18.6° (578), +22.1° (546) (*c* 9.0, $CHCl_3$) [1]

IR (CCl_4): 1725, 1655, 850 [1]

MS: 544.267 $[M]^+$ (1), 455 (2), 444 (1.5), 344 (1), 244 (1), 83 (100) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.22 (3H, s, H-15), 1.26 (3H, s, H-14), 1.51 (3H, s, H-13), 1.9 (2H, m, H-2), 2.78 (1H, m, J = 6, H-1), 2.96 (1H, dd, J = 7; 11.5, H-7), 3.40 (1H, d, J = 1, H-5), 5.32 (1H, br s, H-12b), 5.40 (1H, br s, H-12a), 5.47 (1H, dd, J = 3.5; 8, H-3), 5.54 (1H, dd, J = 1; 7, H-6), 5.89 (1H, d, J = 11.5, H-8); 3 × OAng: 1.85 (3H, dq, J = 1; 1, H-5′), 1.88 (3H, dq, J = 1; 1, H-5″), 1.90 (3H, dq, J = 1; 1, H-5‴), 1.93 (3H, dq, J = 7; 1, H-4′), 1.96 (3H, dq, J = 7; 1, H-4″), 1.99 (3H, dq, J = 7; 1, H-4‴), 6.13 (1H, qq, J = 7; 1, H-3′), 6.15 (1H, qq, J = 7; 1, H-3″), 6.19 (1H, qq, J = 7; 1, H-3‴) [1]

^{13}C NMR [1]:

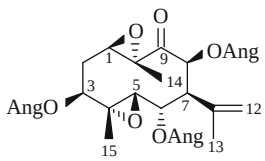
Table 1

C-1	60.9 d	C-10	145.7 s	2″	126.9 s
2	33.7 t	11	114.5 t	2‴	124.0 s
3	72.2 d	12	24.6 q	3′	140.6 s
4	58.9 s	13	14.1 q	3″	139.3 s
5	65.6 d	14	14.4 q	3‴	139.2 s
6	50.1 d	15	166.6 s	4′, 4″, 4‴	16.0 q
7	71.5 c	3 × OAng	166.3 s	5′, 5″, 5‴	15.8 q
8	199.8 s	1′,1″,1‴	127.4 s		20.5 q
9	61.5 s	2′			18.9 q

References

1. F. Bohlmann, D. Ehlers, C. Zdero, M. Crenz, Chem. Ber. **110**, 2640 (1977)

3β,6α,8β-Triangeloyloxy-1β,10α;4α,5β-diepoxy-11-germacren-9-one (8β-Angeloyloxy-ligularinone A)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Triesters

Biological sources: *Ligularia hodgsoni* Hook. f., *L. brachyphylla* Hand.-Mazz. [1]

$C_{30}H_{40}O_9$: 544.2672

Mp: colorless oil [1]

$[\alpha]^{24}$ (λ, nm): +1° (589), +12° (578), +13° (546) (*c* 2.7, $CHCl_3$) [1]

IR (CCl_4): 1730, 1650, 850 [1]

MS: 544.267 $[M]^+$ (0.3), 444 (6.5), 344 (6.3), 244 (0.7), 83 (100) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.26 (3H, s, H-14), 1.26 (3H, s, H-15), 1.51 (3H, s, H-13), 1.9 (2H, m, H-2), 2.76 (1H, t, J = 6, H-1), 3.07 (1H, dd, J = 7; 4, H-7), 3.41 (1H, d, J = 1, H-5), 5.21 (1H, br.s, H-12′), 5.22 (1H, d, J = 4, H-8), 5.44 (1H, br.s, H-12), 5.55 (1H, dd, J = 6; 7.5, H-3), 5.91 (1H, dd, J = 1; 7, H-6); 3 × OAng: 1.91 (9H, dq, J = 1; 1, H-5′, H-5″, H-5‴), 1.99 (6H, dq, J = 7; 1, H-4′, H-4″), 2.02 (3H, dq, J = 7; 1, H-4‴), 6.13 (1H, qq, J = 7; 1, H-3′), 6.18 (1H, qq, J = 7; 1, H-3″), 6.21 (1H, qq, J = 7; 1, H-3‴) [1]

References

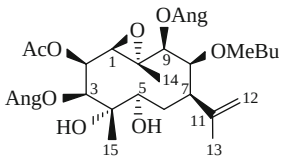
1. F. Bohlmann, D. Ehlers, C. Zdero, M. Crenz, Chem. Ber. **110**, 2640 (1977)

Germacranes

Tetraesters

2β-Acetoxy-3β,9β-diangeloyloxy-8β-(2‴-methylbutyroyloxy)-4α,5α-dihydroxy-1β,10α-epoxy-germacr-11-ene (2β-Acetoxy-4α,5α-dihydroxy-kleinifulgin)

CAS Registry Number: 79383-75-8



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Tetraesters

Biological sources: *Kleinia fulgens* Hook. [1]

$C_{32}H_{48}O_{11}$: 608.3197

Mp: colorless gum [1]

$[\alpha]^{24}$ (λ, nm): −68.5° (589), −72.0° (578), −82.2° (546), −143.4° (436) (*c* 1.15, $CHCl_3$) [1]

IR (CCl_4): 3580, 1750, 1730, 1650, 1235 [1]

MS: 608.320 $[M]^+$ (0.5) ($C_{32}H_{48}O_{11}$), 590 (0.5), 548 (0.5), 509 (1), 448 (0.5), 85 (18), 83 (100), 57 (68), 55 (45) [1]

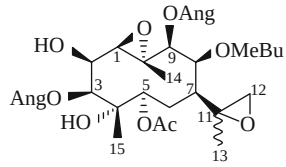
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.26 (3H, s, H-15), 1.27 (3H, s, H-14), 1.42 (3H, s, H-13), 2.00 (1H, m, H-6β), 2.10 (3H, s, OAc), 2.42 (1H, br dd, J = 3; 13; 14, H-6α), 2.90 (1H, d, J = 8, H-1), 3.18 (1H, s, OH), 3.20 (1H, br d, J = 13; 3, H-7α), 3.91 (1H, br dd, J = 3; 3, H-5β), 5.08 (1H, dd, J = 8; 7, H-2α), 5.14 (1H, s, H-12b), 5.24 (1H, d, J = 3, H-9α), 5.29 (1H, s, H-12a), 5.58 (1H, br dd, J = 3; 3, H-8α), 5.62 (1H, d, J = 7, H-3α); 2 × OAng: 1.86 (3H, dq, H-5′), 1.98 (3H, dq, H-5″), 1.97 (3H, dq, H-4′), 2.03 (3H, dq, H-4″), 6.05 (1H, qq, H-3′), 6.18 (1H, qq, H-3″); OMeBu: 0.87 (3H, t, H-4‴), 1.13 (3H, d, H-5‴), 1.40 (1H, m, H-3‴b), 1.65 (1H, m, H-3‴a), 2.34 (1H, tq, H-2‴) [1]

References

1. F. Bohlmann, M. Ahmed, J. Jakupovic, C. Jeffrey, Phytochemistry **20**(2), 251 (1981)

5α-Acetoxy-3β,9β-diangeloyloxy-8β-(2‴-methylbutyroyloxy)-2β,4α-dihydroxy-1β,10α;11,12-diepoxy-germacrane (5α-Acetoxy-2β,4α-dihydroxy-11,12-epoxy-11,12-dihydroxy-kleinifulgin)

CAS Registry Number: 79383-77-0



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Tetraesters

Biological sources: *Kleinia fulgens* Hook. [1]

$C_{32}H_{48}O_{12}$: 624.3146

Mp: colorless gum [1]

IR (CCl_4): 3580, 1750, 1730, 1650, 1235 [1]

MS: 624.316 $[M]^+$ (0.5) ($C_{32}H_{48}O_{12}$), 606 (0.1), 523 (0.2), 363 (0.2), 322 (0.5), 305 (0.3), 85 (10), 83 (100), 57 (26), 55 (28) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.15 (3H, s, H-13), 1.26 (3H, s, H-14), 1.30 (3H, s, H-15), 2.05 (2H, m, H-6), 2.07 (3H, s, OAc), 2.77 (1H, d, H-12b), 2.83 (1H, d, J = 7, H-1), 2.90 (1H, br dd, J = 12; 5; 3, H-7α), 2.94 (1H, d, H-12a), 3.17 (1H, s, OH), 3.54 (1H, dd, J = 7; 8, H-2), 5.06 (1H, d, J = 3, H-9α), 5.06 (1H, dd, J = 2.5; 2.5, H-5β), 5.32 (1H, d, J = 8, H-3α), 5.83 (1H, br dd, J = 3; 3, H-8α); 2 × OAng: 1.88 (3H, dq, H-5′), 1.95 (3H, dq, H-5″), 2.01 (3H, dq, H-4′), 2.04 (3H, dq, H-4″), 6.13 (1H, qq, H-3′), 6.20 (1H, qq, H-3″); OMeBu: 0.92 (3H, t, H-4‴), 1.17 (3H, d, H-5‴), 1.44 (1H, ddq, H-3‴b), 1.71 (1H, ddq, H-3‴a), 2.37 (1H, tq, H-2‴) [1]

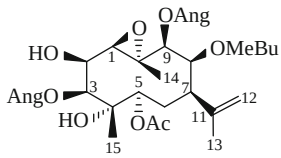
^{1}H NMR (270 MHz, C_6D_6, TMS): 1.11 (3H, s, H-13), 1.21 (3H, s, H-14), 1.32 (3H, s, H-15), 1.70 (3H, s, OAc), 2.05 (1H, m, H-6β), 2.19 (1H, ddd, J = 2.5; 12, H-6α), 2.32 (1H, s, OH), 2.67 (1H, d, H-12b), 2.82 (1H, d, J = 7, H-1), 2.85 (1H, d, H-12a), 3.24 (1H, br dd, J = 12; 5; 3, H-7α), 3.63 (1H, dd, J = 7; 8, H-2), 5.36 (1H, d, J = 3, H-9α), 5.41 (1H, dd, J = 2.5; 2.5, H-5β), 5.52 (1H, d, J = 8, H-3α), 6.26 (1H, br dd, J = 3; 3, H-8α); 2 × OAng: 1.90 (3H, dq, H-5′), 1.95 (3H, dq, H-5″), 2.03 (6H, dq, H-4′, H-4″), 5.75 (1H, qq, H-3′), 5.81 (1H, qq, H-3″); OMeBu: 0.82 (3H, t, H-4‴), 1.02 (3H, d, H-5‴), 1.31 (1H, ddq, H-3‴b), 1.67 (1H, ddq, H-3‴a), 2.0 (1H, m, H-2‴) [1]

References

1. F. Bohlmann, M. Ahmed, J. Jakupovic, C. Jeffrey, Phytochemistry **20**(2), 251 (1981)

5α-Acetoxy-3β,9β-diangeloyloxy-8β-(2‴-methylbutyroyloxy)-1β,10α-epoxy-germacr-11-ene-2β,4α-diol (5α-Acetoxy-2β,4α-dihydroxy-kleinifulgin)

CAS Registry Number: 79383-74-7



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Tetraesters

Biological sources: *Kleinia fulgens* Hook. [1]

$C_{32}H_{48}O_{11}$: 608.3197

Mp: colorless gum [1]

$[\alpha]^{24}$ (λ, nm): −45.3° (589), −47.3° (578), −54.1° (546), −94.1° (436) (*c* 1.1, $CHCl_3$) [1]

IR (CCl_4): 3585, 1750, 1730, 1650, 1230 [1]

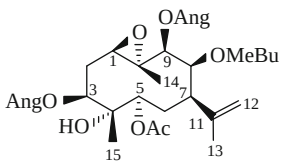
MS: 608.320 $[M]^+$ (0.3) ($C_{32}H_{48}O_{11}$), 508 (0.3), 408 (1), 348 (0.2), 306 (0.5), 246 (1), 85 (8), 83 (100), 57 (25), 55 (41) [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.17 (3H, s, H-15), 1.29 (3H, s, H-14), 1.36 (3H, s, H-13), 2.0 (1H, m, H-6β), 2.10 (3H, s, OAc), 2.41 (1H, br dd, J = 3; 12, H-6α), 2.79 (1H, d, J = 7, H-1), 3.08 (1H, br d, J = 12; 2.5; 3, H-7α), 3.35 (1H, s, OH), 3.79 (1H, dd, J = 7; 7, H-2), 5.05 (1H, dd, J = 3; 3, H-5β), 5.10 (1H, s, H-12b), 5.16 (1H, d, J = 3, H-9α), 5.31 (1H, s, H-12a), 5.36 (1H, d, J = 7, H-3α), 5.63 (1H, br dd, J = 3; 3, H-8α); 2 × OAng: 1.86 (3H, dq, H-5′), 1.95 (3H, dq, H-5″), 1.99 (3H, dq, H-4′), 2.01 (3H, dq, H-4″), 6.10 (1H, qq, H-3′), 6.15 (1H, qq, H-3″); OMeBu: 0.87 (3H, t, H-4‴), 1.15 (3H, d, H-5‴), 1.42 (1H, ddq, H-3‴b), 1.67 (1H, ddq, H-3‴a), 2.35 (1H, tq, H-2‴) [1]

References

1. F. Bohlmann, M. Ahmed, J. Jakupovic, C. Jeffrey, Phytochemistry **20**(2), 251 (1981)

5α-Acetoxy-3β,9β-diangeloyloxy-8β-(2‴-methylbutyroyloxy)-1β,10α-epoxy-germacr-11-en-4α-ol (5α-Acetoxy-4α-hydroxy-kleinifulgin)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Tetraesters

Biological sources: *Kleinia fulgens* Hook. [1]

$C_{32}H_{48}O_{10}$: 592.3247

Mp: colorless gum [1]

IR (CCl_4): 3600, 1750, 1730, 1650, 1230 [1]

MS: 592.325 $[M]^+$ (1) ($C_{32}H_{48}O_{10}$), 575 (0.5), 493 (2), 492 (2), 390 (1), 330 (1), 231 (3), 213 (3), 85 (18), 83 (100), 57 (52), 55 (68) [1]

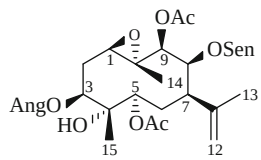
^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.16 (3H, s, H-15), 1.27 (3H, s, H-13), 1.27 (3H, s, H-14), 2.0 (2H, m, H-2), 2.10 (3H, s, OAc), 2.31 (1H, dd, J = 2.5; 3; 14, H-6β), 2.38 (1H, ddd, J = 2.5; 12; 14, H-6α), 2.73 (1H, dd, J = 7; 4, H-1), 2.90 (1H, br d, J = 12; 3, H-7α), 3.36 (1H, s, OH), 5.07 (1H, dd, J = 2.5; 2.5, H-5β), 5.07 (1H, s, H-12b), 5.16 (1H, d, J = 3, H-9α), 5.32 (1H, s, H-12a), 5.52 (1H, dd, J = 7; 7, H-3α), 5.61 (1H, br dd, J = 3; 3, H-8α); 2 × OAng: 1.87 (3H, dq, H-5′), 1.93 (3H, dq, H-5″), 2.00 (6H, dq, H-4′, H-4″), 6.11 (2H, qq, H-3′, H-3″) [1]

^{1}H NMR (270 MHz, C_6D_6, TMS): 1.07 (3H, s, H-14), 1.07 (3H, s, H-15), 1.32 (3H, s, H-13), 1.67 (3H, s, OAc), 2.0 (2H, m, H-2), 2.37 (2H, ddd, J = 2.5; 12; 3; 14, H-6), 2.54 (1H, dd, J = 7; 4, H-1), 3.13 (1H, br d, J = 12; 3; 3, H-7α), 3.33 (1H, s, OH), 4.89 (1H, s, H-12b), 5.31 (1H, s, H-12a), 5.38 (1H, dd, J = 2.5; 2.5, H-5β), 5.45 (1H, d, J = 3, H-9α), 5.71 (1H, dd, J = 7; 7, H-3α), 5.99 (1H, br dd, J = 3; 3, H-8α); 2 × OAng: 1.85 (3H, dq, H-5′), 1.97 (3H, dq, H-5″), 2.03 (3H, dq, H-4′), 2.04 (3H, dq, H-4″), 5.70 (1H, qq, H-3′), 5.78 (1H, qq, H-3″); OMeBu: 0.75 (3H, t, H-4‴), 0.99 (3H, d, H-5‴), 1.20 (1H, ddq, H-3‴b), 1.60 (1H, ddq, H-3‴a), 2.0 (1H, m, H-2‴) [1]

References

1. F. Bohlmann, M. Ahmed, J. Jakupovic, C. Jeffrey, Phytochemistry **20**(2), 251 (1981)

5α,9β-Diacetoxy-3β-angeloyloxy-8β-senecioyloxy-4α-hydroxy-1β,10α-epoxy-germacr-11-ene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Tetraesters

Biological sources: *Senecio galpinii* Hook. f. [1]

$C_{29}H_{42}O_{10}$: 550.2778

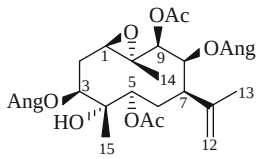
Mp: colorless gum [1]

$[\alpha]^{24}$ (λ, nm): −56 (589), −57 (578), −66 (546), −116 (436) (*c* 0.62, $CHCl_3$) [1]
IR (CCl_4): 3580, 1760, 1725, 1655, 1240 [1]
MS: 550.278 $[M]^+$ (0.2) ($C_{29}H_{42}O_{10}$), 450 [M − AngOH or SenOH]$^+$ (1), 390 [450 − HOAc]$^+$ (0.4), 350 [450 − SenOH or AngOH]$^+$ (1.4), 290 [350 − HOAc]$^+$ (0.5), 230 [290 − HOAc]$^+$ (2), 83 $[C_4H_7CO]^+$ (100), 55 [83 − CO]$^+$ (58) [1]
TLC: C_6H_6 – $CHCl_3$ – Et_2O (2:2:1) [1]
HPLC: MeOH – H_2O (3:1), reversed phase [1]
^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.12 (3H, s, H-15), 1.23 (3H, s, H-14), 1.25 (3H, s, H-13), 1.77 (1H, ddd, J = 14; 2.5; 2.5, H-6b), 1.9 (1H, m, H-2b), 2.0 (1H, m, H-2a), 2.06 (3H, s, OAc), 2.09 (3H, s, OAc), 2.34 (1H, ddd, J = 14; 14, H-6a), 2.72 (1H, t, J = 6, H-1), 2.81 (1H, br d, J = 14; 2.5, H-7), 3.44 (1H, s, OH), 4.99 (1H, d, J = 2.5, H-9), 5.02 (1H, dd, J = 2.5; 2.5, H-8), 5.05 (1H, s, H-12′), 5.26 (1H, s, H-12), 5.45 (1H, dd, J = 8; 6, H-3), 5.51 (1H, br dd, J = 2.5, H-5); OAng: 1.90 (3H, dq, H-5′), 1.99 (3H, dq, H-4′), 6.11 (1H, qq, H-3′); OSen: 1.89 (3H, d, H-4″), 2.12 (3H, d, H-5″), 5.63 (1H, qq, H-2″) [1]

References

1. F. Bohlmann, C. Zdero, Phytochemistry **21**(10), 2537 (1982)

5α,9β-Diacetoxy-3β,8β-diangeloyloxy-4α-hydroxy-1β,10α-epoxygermacr-11-ene



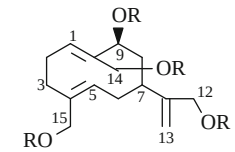
Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Tetraesters
Biological sources: *Senecio galpinii* Hook. f. [1]
$C_{29}H_{42}O_{10}$: 550.2778

Mp: colorless gum [1]
IR (CCl_4): 3580, 1755, 1720, 1650, 1235 [1]
MS: 550.278 $[M]^+$ (0.1) ($C_{29}H_{42}O_{10}$), 490 [M − HOAc]$^+$ (0.1), 390 [490 − AngOH]$^+$ (0.2), 291 [390 − OAng]$^+$ (0.5), 231 [291 − HOAc]$^+$ (1), 83 $[C_4H_7CO]^+$ (100), 55 [83 − CO]$^+$ (48) [1]
TLC: C_6H_6 – $CHCl_3$ – Et_2O (2:2:1) [1]
HPLC: MeOH – H_2O (3:1), reversed phase [1]
^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.24 (3H, s, H-15), 1.25 (3H, s, H-14), 1.27 (3H, s, H-13), 1.77 (1H, ddd, J = 2.5; 14; 2.5, H-6b), 1.9 (1H, m, H-2b), 2.0 (1H, m, H-2a), 2.04 (3H, s, OAc), 2.09 (3H, s, OAc), 2.35 (1H, ddd, J = 14; 14, H-6a), 2.76 (1H, t, J = 6, H-1), 2.85 (1H, br d, J = 14; 2.5, H-7), 3.26 (1H, s, OH), 5.04 (1H, dd, J = 2.5; 2.5, H-8), 5.06 (1H, s, H-12b), 5.13 (1H, d, J = 2.5, H-9), 5.31 (1H, s, H-12a), 5.49 (1H, dd, J = 8; 6, H-3), 5.53 (1H, br dd, J = 2.5, H-5); 2 × OAng: 1.86 (3H, dq, H-5′), 1.90 (3H, dq, H-5″), 2.00 (each 3H, dq, H-4′, H-4″), 6.11 (each 1H, qq, H-3′, H-3″) [1]

References

1. F. Bohlmann, C. Zdero, Phytochemistry **21**(10), 2537 (1982)

(7*S**,9*S**)-9,12,14,15-Diacetoxy-(2′-hydroxy-isovaleroyloxy)-isobutyroyloxy-germacra-1(10),4,11(13)-triene



R = Ac, Ac, ^{i}Bu, ^{i}Val(2′-OH)

Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Tetraesters

Biological sources: *Trixis grisebachii* Kuntze (= *T. frutescens* var. *cacalioides* Griseb.) [1]

$C_{28}H_{42}O_{10}$: 538.2778

Mp: gum, not free (2*R**,3*S**,4*R**,6*R**,7*R**,8*R**,10*R**,11*R**,14*S**)-14-isovaleroyloxy-14,15-epoxytrix-5(15)-en-12-onic acid [1]

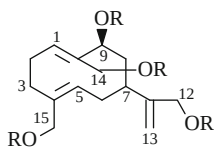
HPLC [1]

^{1}H NMR (270 MHz, $CDCl_3$, TMS): 1.89 (1H, dd, J = 15; 5, H-8a), 2.03 and 2.00 (each 3H, s, OAc), 4.20 (1H, d, J = 12, H-14a or H-14b), 4.53 (1H, d, J = 13.5, H-15a or H-15b), 4.61 (1H, d, J = 13.5, H-15a or H-15b), 4.64 (1H, d, J = 14, H-13b), 4.71 (1H, d, J = 14, H-13a), 4.73 (1H, d, J = 12, H-14a or H-14b), 5.00 (1H, br s, H-12b), 5.10 (1H, br s, H-12a), 5.51 (1H, dd, J = 5; 1.5, H-9), ~5.60 (1H, m, H-5), 5.66 (1H, dd, J = 10; 7, H-1), H-2, H-3, H-6, H-7, H-8b obsc.; O^{i}Val(2′-OH): 0.89 (3H, d, J = 7, H-5′), 1.03 (3H, d, J = 7, H-4′), 2.13 (1H, dq, J = 7; 4, H-3′), 4.07 (1H, d, J = 4, H-2′); O^{i}Bu: 1.19 (6H, d, J = 7, H-3″, H-4″), 2.59 (1H, hept, J = 7, H-2″) [1]

References

1. C.E. De Riscala, C.A.N. Catalan, P.R. Legname, A.B. Gutierrez, W. Herz, Phytochemistry **28**(8), 2155 (1989)

(7*S**,9*S**)-9,12,14,15-Diacetoxy-(2′-hydroxy-isovaleroyloxy)-(2″-methylbutyroyloxy)-germacra-1(10),4,11(13)-triene



R = Ac, Ac, MeBu, ^{i}Val(2′-OH)

Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Tetraesters

Biological sources: *Trixis grisebachii* Kuntze (= *T. frutescens* var. *cacalioides* Griseb.) [1]

$C_{29}H_{44}O_9$: 536.2985

Mp: gum [1]

IR (KBr): 3480, 1735 [1]

EI-MS: 536 $[M]^+$ (0.2), 477 (28.9), 435 (2.3), 419 (9.4), 418 (26.3), 404 (9.9), 403 (25.3), 316 (11.7), 315 (47.6), 314 (35.2), 257 (12.0), 216 (11.6), 215 (48.4), 214 (50.89), 213 (12.9), 199 (28.6), 198 (52.1), 197 (100), 196 (81.2), 195 (16.8), 183 (33.0), 157 (37.1), 143 (31.9), 85 (32.7), 73 (13.0), 57 (28.2) [1]

PCI-MS: 537 $[M + 1]^+$ (0.6), 478 (28), 477 (100), 435 (3), 419 (30.0), 417 (8.5), 405 (5.9), 375 (21.3), 315 (69.2), 299 (3.0), 277 (9.9), 257 (11.9), 215 (25.8), 197 (27.4), 119 (6.2), 103 (9.1) [1]

HPLC [1]

^{1}H NMR (270MHz, $CDCl_3$, TMS): 1.88 (1H, dd, J = 15; 5, H-8a), 2.04 and 2.00 (each 3H, s, OAc), 2.58 (1H, m, H-2a), 4.22 (1H, d, J = 12, H-14a or H-14b), 4.50 (1H, d, J =, H-15a or H-15b), 4.62 (1H, d, J = 14, H-15a or H-15b), 4.63 (1H, d, J = 14, H-13b), 4.69 (1H, d, J = 14, H-13a), 4.72 (1H, d, J = 12, H-14a or H-14b), 5.00 (1H, br s, H-12b), 5.10 (1H, br s, H-12a), 5.52 (1H, br d, J = 5, H-9), ~5.60 (1H, m, H-5), 5.66 (1H, dd, J = 10; 7, H-1), H-2b, H-3, H-6, H-7, H-8b obsc.; O^{i}Val(2′-OH): 0.89 (3H, d, J = 7, H-5′), 1.04 (3H, d, J = 7, H-4′), 2.10 (1H, dq, J = 7; 4, H-3′), 3.96 (1H, d, J = 4, H-2′); OMeBu: 0.92 (3H, t, J = 7, H-4″), 1.17 (3H, d, J = 7, H-5″), 1.52 (1H, ddq, J = 14; 7; 7, H-3b″), 1.71 (1H, ddq, J = 14; 7; 7, H-3a″), 2.36 (1H ddq, J = 7; 7; 7, H-2″) [1]

^{1}H NMR (270 MHz, C_6D_6, TMS)** (from mix. (7*S**,9*S**)-9,12,14,15-diacetoxy)-[2-hydroxy-3-methylbutanoyloxy], isobutanoyloxygermacra-1(10),4,11(13)-triene and (2*R**,3*S**,4*R**,6*R**,7*R**,8*R**,10*R**,11*R**,14*S**)-14-isovaleryloxy-14,15-epoxytrix-5(15)-en-12-oic acid): ~1.70 (1H, m, H-8b), 1.71 and 1.66 (each 3H, s, OAc), 1.83 (1H, m, H-3b), 1.94 (1H, dd, J = 15; 5, H-8a), ~1.95 (1H, m, H-2b), ~2.20–2.25 (2H, m, H-6), 2.21 (1H, m, H-3a), 2.45 (1H, m, H-7), 2.56 (1H, m, H-2a), 4.29 (1H, d, J = 12, H-

13b or 13a), 4.51 (1H, d, J = 12.5, H-15a or H-15b), 4.61 (1H, d, J = 12, H-14a or H-14b), 4.61 (1H, d, J = 13.5, H-15a or H-15b), 4.76 (1H, d, J = 12.5, H-14a or H-14b), 4.83 (1H, d, J = 12, H-13a or H-13b), 4.85 (1H, br s, H-12b), 4.91 (1H, br s, H-12a), 5.34 (1H, br t, J = 8, H-5), 5.50 (1H, br dd, J = 10; 7, H-1), 5.67 (1H, dd, J = 5; 1.5, H-9); O^{i}Val(2′-OH): 0.96 (3H, d, J = 7, H-5′), 1.04 (3H, d, J = 7, H-4′), 2.13 (1H, dq, J = 7; 4, H-3′), 4.11 (1H, d, J = 4, H-2′); OMeBu: 0.88 (3H, t, J = 7, H-4″), 1.14 (3H, d, J = 7, H-5″), 1.43 (1H, ddq, J = 14; 7; 7, H-3″b), 1.75 (1H, ddq, J = 14; 7; 7, H-3″a), 2.26 (1H ddq, J = 7; 7; 7, H-2″) [1]

** No change on addition of TA1 except for O-(HO)^{i}Val: 0.92 (3H, d, J = 7, H-5′), 0.97 (3H, d, J = 7, H-4′), 5.00 (1H, s, OH-2′), and the AB system from 4.61-4.51 to 4.72 (d, J = 12), -4.41 (d, J = 12) [1]

^{13}C NMR (67.89 MHz, $CDCl_3$): [1]

Table 1

C-1	129.95 d[a]	C-11	147.74 s	O^{i}Val(2′-OH)	170.90 s
2	28.44 t	12	112.94 t		41.22 d[a]
3	34.32 t	13	63.64 t[a]		26.72 t
4	134.78 s[a]	14	63.90 t[a]		11.54 q
5	130.19 d[a]	15	66.92 t[a]		16.10 q
6	30.91 t	OMeBu	174.54 s	2 × OAc	170.59 s
7	41.22 d[a]		73.14 d[a]		170.59 s
8	40.10 t		32.20 d		21.12 q
9	75.29 d[a]		18.85 q		20.89 q
10	135.21 s[a]		16.57 q		

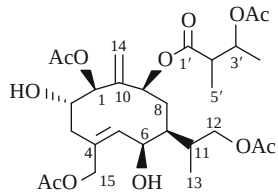
[a]Assignments may be interchanged

References

1. E.C. de Riscala, C.A.N. Catalan, P.R. Legname, A.B. Gutierrez, W. Herz, Phytochemistry **28**(8), 2155 (1989)

1β,12,15-Triacetoxy-9β-(3′-acetoxy-2′-methylbutyroyloxy)-7α(H)-germacra-4,10(14)-diene-2α,6β-diol (Salviadienol A)

CAS Registry Number: 1064085-05-7



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Tetraesters

Biological sources: *Salvia chinensis* Benth. [1]

$C_{28}H_{42}O_{12}$: 570.2676

Mp: colorless oil [1]

$[\alpha]_D^{25}$ +0.8° (*c* 0.36, Py) [1]

IR (KBr): 3470, 2952, 1744, 1694, 1383, 1242, 1184, 1135, 1054, 1030 [1]

HR-ESI-MS: 593.2574 $[M + Na]^+$ (calc. for $C_{28}H_{42}O_{12}Na$ 593.2574; found: 593.2546) [1]

ESI-MS: 593 $[M + Na]^+$ [1]

^{1}H NMR (600 MHz, Py-d_5): 1.33 (3H, d, J = 6.0, H-13), 1.93 (1H, m, H-7), 1.98 (3H, s, OAc-15), 2.06 (1H, m, H-8b), 2.08 (1H, m, H-3b), 2.17 (3H, s, OAc-12), 2.23 (3H, s, OAc-1), 2.43 (1H, m, H-11), 2.47 (1H, m, H-3a), 2.52 (1H, m, H-8a), 4.36 (1H, d, J = 12.6, H-15b), 4.46 (1H, dd, J = 10.8; 1.8, H-12b), 4.46 (1H, m, H-2), 4.60 (1H, dd, J = 10.8; 4.2, H-12a), 4.78 (1H, d, J = 12.6, H-15a), 5.08 (1H, overlapped, H-6), 5.44 (1H, s, H-14b), 5.67 (1H, s, H-14a), 5.76 (1H, d, J = 10.8, H-9), 6.15 (1H, d, J = 6.0, H-5), 6.33 (1H, dd, J = 10.8; 1.8, H-1);

OMeBu(OAc): 1.30 (3H, d, J = 6.0, H-5′), 1.33 (3H, d, J = 6.0, H-4′), 1.99 (3H, s, 3′-OAc), 2.95 (1H, dq, J = 12.0; 6.0, H-2′), 5.46 (1H, dq, J = 12.0; 6.0, H-3′) [1]

^{13}C NMR (150 MHz, Py-d_5) [1]:

Table 1

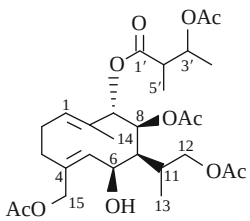
C-1	68.6 d	C-11	31.3 d	C-5′	12.4 q
2	68.7 d	12	67.9 t	1-OAc	21.2 q
3	33.4 t	13	18.4 q		170.4 s
4	132.3 s	14	119.6 t	12-OAc	20.8 q
5	137.7 d	15	61.3 t		171.2 s
6	66.3 d	1′	173.4 s	15′-OAc	20.6 q
7	47.7 d	2′	45.6 d		170.6 s
8	33.5 t	3′	71.4 d	3′-OAc	21.0 q
9	81.9 d	4′	18.3 q		170.2 s
10	146.8 s				

References

1. Y. Wang, Z. Li, H. Zhang, Y. Sha, Y. Pei, H. Hua, Chem. Pharm. Bull. **56**, 843 (2008)

8β,12,15-Triacetoxy-9α-(3′-acetoxy-2′-methylbutyroyloxy)-7α(H)-germacra-1(10),4-dien-6β-ol (Salviadienol B)

CAS Registry Number: 1064085-09-1



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Tetraesters

Biological sources: *Salvia chinensis* Benth. [1]

$C_{28}H_{42}O_{11}$: 554.2727

Mp: colorless oil [1]

$[\alpha]_D^{25}$ −5.3° (*c* 0.33, $CHCl_3$) [1]

IR (KBr): 3466, 2940, 1736, 1382, 1237, 1027 [1]

HR-ESI-MS: 553.2649 $[M - H]^+$ (calc. for $C_{28}H_{41}O_{11}$; found: 553.2626) [1]

FAB-MS: 577 $[M + Na]^+$ [1]

^{1}H NMR (600 MHz, $CDCl_3$): 1.14 (3H, d, J =6.0, H-13), 1.55 (1H, m, H-7), 1.80 (3H, s, H-14), 1.84 (1H, m, H-11), 2.08 (3H, s, OAc-15), 2.10 (1H, overlapped, H-3b), 2.11 (3H, s, OAc-12), 2.13 (3H, s, OAc-8), 2.18 (1H, m, H-2b), 2.34 (1H, ddd, J = 12.6; 10.8; 4.8, H-2a), 2.55 (1H, dd, J = 10.8; 3.0, H-3a), 4.21 (1H, dd, J = 11.0; 3.6, H-12b), 4.27 (1H, dd, J = 11.0; 1.8, H-12a), 4.28 (1H, d, J = 12.6, H-15b), 4.46 (1H, d, J = 12.6, H-15a), 4.57 (1H, *t*-like, J = 7.8, H-6), 4.87 (1H, d, J =10.2, H-9), 5.29 (1H, dd, J = 10.2; 1.2, H-8), 5.38 (1H, dd, J = 10.8; 1.4, H-1), 5.52 (1H, d, J = 7.8, H-5); OMeBu(OAc): 1.14 (3H, d, J = 6.0, H-5′), 1.22 (3H, d, J = 6.0, H-4′), 2.04 (3H, s, OAc-3′), 2.58 (1H, m, H-2′), 5.03 (1H, dt, J = 12.6; 6.0, H-3′) [1]

^{13}C NMR (150 MHz, Py-d_5) [1]:

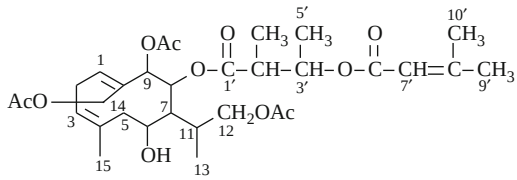
Table 1

C-1	132.5 d	C-11	30.8 d	C-5′	12.4 q
2	24.4 t	12	67.0 t	1-OAc	21.0 q
3	33.4 t	13	17.7 q		172.4 s
4	131.8 s	14	19.0 q	12-OAc	20.9 q
5	138.0 d	15	59.8 t		171.0 s
6	66.2 d	1′	172.5 s	15-OAc	20.6 q
7	49.4 d	2′	44.7 d		170.6 s
8	73.8 d	3′	70.9 d	3′-OAc	20.7 q
9	77.8 d	4′	18.0 q		170.1 s
10	132.9 s				

References

1. Y. Wang, Z. Li, H. Zhang, Y. Sha, Y. Pei, H. Hua, Chem. Pharm. Bull. **56**, 843 (2008)

9β,12,14-Triacetoxy-8α-(3′-senecioyloxy-2′-methylbutyroyloxy)-7α(H)-germacra-1(10),3-dien-6α-ol



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Germacranes – Tetraesters

Biological sources: *Salvia miltiorrhiza* Bunge [1]

$C_{31}H_{46}O_{11}$: 594.3040

Mp: amorphous [1]

$[\alpha]_D$ –23° (*c* 1.06, MeOH) [1]

IR: 3500 (br), 1730, 1380, 1220, 1050 [1]

HR-MS: 594.3062 $[M]^+$ (calc. for $C_{31}H_{46}O_{11}$: 594.3040) [1]

CI-MS: 594 $[M]^+$ (7.5), 535 (14.4), 395 (8.6), 334 (12.5), 316 (14.8), 274 (44.7), 256 (45.3), 215 (68.6), 214 (65.3), 183 (97.8), 164 (37.8), 155 (17.7), 83 (100), 55 (34.4) [1]

^{1}H NMR (CD_3OD): 1.12 (3H, d, J = 6.7, H-13), 1.51 (1H, br d, J = 10, H-7), 1.66 (3H, s, H-15), 1.84 (1H, t, J 12, H-5a), 2.03 (3H, s, 12-OAc), 2.04 (3H, s, 14-OAc), 2.07 (3H, s, 9-OAc), 2.15 (1H, m, H-11), 2.33 (1H, br d, J = 14.3, H-2b), 2.64 (1H, m, H-2a), 2.66 (1H, m, H-5b), 3.92 (1H, dd, J = 11.4; 3.7, H-12b), 4.10 (1H, dd, J = 11.4; 2.4, H-12a), 4.28 (1H, dd, J = 12; 5.8, H-6), 4.33 (1H, d, J = 13, H-14b), 4.63 (1H, d, J = 13, H-14a), 5.22 (1H, br d, J = 11.2, H-3), 5.50 (1H, m, H-1), 5.51 (1H, m, H-9), 5.69 (1H, br d, J = 7.3, H-8); acyl group: 1.18 (3H, d, J = 7.1, H-4′), 1.27 (3H, d, J = 6.4, H-5′), 1.79 (3H, s, H-10′), 1.80 (3H, s, H-9′), 2.81 (1H, q, H-2′), 5.10 (1H, q, H-3′), 6.84 (1H, m, H-7′) [1]

^{13}C NMR (CD_3OD) [1]:

Table 1

C-1	134.6 d	C-12	69.2 t	C-7′	139.3 d
2	31.7 t	13	18.8 q	8′	129.8 s
3	126.4 d	14	61.1 t	9′	12.1 q
4	135.6 s	15	21.6 q	3 × OAc	14.5 q
5	46.3 t	1′	174.9 s		173.0 s
6	72.4 d	2′	46.2 d		20.7 q
7	51.0 d	3′	73.2 d		171.1 s
8	72.0 d	4′	13.4 q		20.8 q
9	73.8 d	5′	17.5 q		172.3 s
10	133.4 s	6′	168.7 s		21.0 q
11	31.7 d				

^{1}H-^{1}H COSY [1]

^{1}H-^{13}C COSY [1]

COLOC [1]

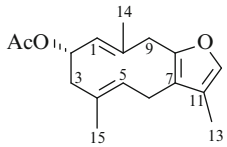
References

1. J. Liu, J. Zapp, H. Becker, Planta Med. **61**, 453 (1995)

Furanogermacranes

Monoesters

2α-Acetoxy-1(10),4-furanogermacradiene (2α-Acetylfurodiene)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Furanogermacranes – Monoesters

Biological sources: *Commiphora myrrha* (Nees) Engl. [1, 2]; *C. erythraea* Engl. [1]; *Smyrnium cordifolium* Boiss. [3]; *C. molmol* (Engl.) Engl. [4]; *C. kua* (J. F. Royle) Vollesen [5]

$C_{17}H_{22}O_3$: 274.1569

Mp: 82–83°C [1]; amorphous [3]

$[\alpha]_D$ +75° (*c* 0.93, $CHCl_3$) [1]

UV (MeOH) 218 (4.45) [3]

IR (KBr): 3000, 2920, 2850, 1730, 1660, 1555, 1450, 1370, 1240, 1140, 1020, 880 [3]

MS: 274 $[M]^+$ (0.3) (calc. for $C_{17}H_{22}O_3$: 274), 214 (0.76), 159 (1), 108 (4), 91 (4.7), 43 (100) [1]

MS: 274 $[M]^+$ (63), 232 (30), 214 (100), 108 (45) [3]

FT-NMR (90 MHz, C_6D_6): 1.17 (3H, s, H-15), 1.35 (3H, br s, H-14), 1.60 (3H, d, J = 1.1, H-13), 1.66 (3H, s, OAc), 1.85 (1H, dd, J = 10.4; 11.28, H-3α), 2.43 (1H, dd, J = 11.28; 4.5, H-3β), 2.98 (2H, m, H-6), 3.23 (1H, d, J = 15.2, H-9α), 3.84 (1H, d, J = 15.2, H-9β), 4.86 (1H, br dd, H-5), 4.9 (1H, br d, J = 10.4, H-1), 5.62 (1H, td, J = 10.4; 4.5, H-2), 6.95 (1H, br s, H-12) [1]

^{1}H NMR (60 MHz, $CDCl_3$, TMS): 1.44 (3H, br d, J = ~1.1, H-14), 1.72 (3H, br d, J = ~1.2, H-15), 1.96 (3H, d, J = 1.5, H-13), 2.13 (3H, s, OAc), 3.08 (2H, br d, J = 8, H-6), 3.56 (2H, br s, H-9), 5.0 (1H, br d, J = 10.4, H-1), 5.20 (1H, br dd, H-5), 5.63 (1H, ddd, J = 10.4; 4.5, H-2), 7.22 (1H, br s, H-12) [1]

^{1}H NMR (NT-FT, 200 MHz, $CDCl_3$): 1.40 (3H, s, H-15), 1.67 (3H, s, H-14), 1.92 (3H, d, J = 1, H-13), 2.08 (3H, s, OAc), 2.35 (1H, t, H-3b), 2.52 (1H, dd, H-3a), 3.00 (1H, br d, H-6b), 3.08 (1H, br dd, H-6a), 3.42 (1H, d, J = 16, H-9b), 3.55 (1H, d, J = 16, H-9a), 4.95 (1H, ddd, J = 4; 11; 12, H-2), 5.07 (1H, br d, H-1), 5.22 (1H, br d, H-5), 7.06 (1H, br s, H-12) [3]

^{1}H NMR [6]

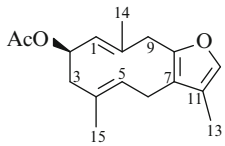
HPLC: isopropanol-acetonitrile (7:3), R_t = 18 min [2]

Pharm./Biol.: (LD_{50} 10%) toxic to larvae of *Rhipicephalus appendiculatus* ticks responsible for transmitting organisms causing East Coast Fever in cattle [1]; antihyperglycemic compound, using *in vitro* bioassayguided fractionation (C57BL/K_s-*db*/*db* mice were used as a model for type 2 diabetes) [7]

References

1. A. Maradufu, Phytochemistry **21**(3), 677 (1982)
2. R.P. Ubillias, C.D. Mendez, S.D. Jolad, J. Luo, S.R. King, T. J. Carlson, D.M. Fort, Planta Med. **65**, 778 (1999)
3. A. Ulubelen, S. Oksuz, N. Tanker, Phytochemistry **23**(8), 1793 (1984)
4. C.H. Brieskorn, P. Noble, Phytochemistry **22**(5), 1207 (1983)
5. L.O.A. Manguro, K.M. Mukonyi, J.K. Githiomi, Planta Med. **62**, 84 (1996)
6. C.H. Brieskorn, P. Noble, Phytochemistry **22**(1), 187 (1983)
7. A.Y. Oubre, T.J. Carlson, S.R. King, G.M. Reaven, Diabetologia **40**, 614 (1997)

2β-Acetoxy-1(10),4-furanogermacradiene (2β-Acetoxyfuranodiene)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Furanogermacranes – Monoesters

Biological sources: *Commiphora molmol* (Engl.) Engl. [1]

$C_{17}H_{22}O_3$: 274.1569

Mp: colorless wax, RR_t (capillary column) 2.0 [1]
IR (film): 2930, 2870, 2835, 1735, 1600, 1550, 1450, 1435, 1375, 1365, 1240, 1140, 1023, 985, 965, 765 [1]
MS: 274 $[M]^+$ (10) ($C_{17}H_{22}O_3$), 214 (50), 119 (44), 149 (23), 147 (29), 146 (28), 135 (39), 119 (24), 109 (41), 108 (67), 106 (39), 105 (24), 91 (37), 79 (27), 77 (22), 43 (100), 41 (28) [1]
TLC: *n*-hexane – Et_2O (1:1), R_f 0.67 [1]
^{1}H NMR (90 MHz, $CDCl_3$, TMS): 1.41 (3H, br s, H-14), 1.67 (3H, br s, H-15), 1.92 (3H, d, J = 1.2, H-13), 2.06 (3H, s, OAc), 2.52 (2H, dd, J = 10.5; 4.5, H-3), 3.08 (2H, d, J = 7.5, H-6), 3.50 (2H, br s, H-9), 5.04 (1H, d, J = 10.5, H-1), 5.09 (1H, t, J = 7.5, H-5), 5.53 (1H, dt, J = 10.5; 4.5, H-2), 7.07 (1H, br s, H-12) [1]
^{13}C NMR (62.89 MHz, $CDCl_3$, TMS) [1]:

Table 1

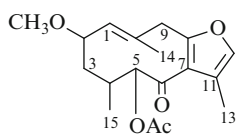
C-1	130.6 d[a]	C-7	121.9 d[a]	C-13	8.8 q
2	72.5 d	8	148.6 s	14	17.3 q[a]
3	45.0 t[a]	9	24.4 t[a]	15	17.2 q[a]
4	136.0 s[a]	10	127.8 d[a]	$OCOCH_3$	170.7 s
5	129.2 s[a]	11	119.4 s[a]	$OCOCH_3$	21.2 q
6	40.8 t[a]	12	136.2 d		

[a]Assignment may be interchanged [1]

References

1. C.H. Brieskorn, P. Noble, Phytochemistry **22**(5), 1207 (1983)

5-Acetoxy-2-methoxy-6-oxo-1(10)-Furanogermacrene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Furanogermacranes – Monoesters

Biological sources: *Commiphora molmol* (Engl.) Engl. [1]
$C_{18}H_{24}O_5$: 320.1624
Mp: 116°C [1]
UV (EtOH) 279 [1]
IR (KBr): 1745, 1735, 1680, 1230 [1]
^{1}H NMR (90 MHz, $CDCl_3$, TMS): 1.07 (3H, d, J = 7.5, H-14), 1.92 (6H, br s, H-13, H-15), 3.25 (3H, s, OCH_3), 3.30 (1H, AB system, J = 16.5, H-9b), 3.66 (1H, AB system, J = 16.5, H-9a), 4.12 (1H, m, H-2), 5.29 (1H, br d, J = 9, H-1), 5.57 (1H, br d, J = 8.5, H-5), 7.03 (1H, br s, H-12) [1]
^{13}C NMR (22.64 MHz, $CDCl_3$, TMS) [1]:

Table 1

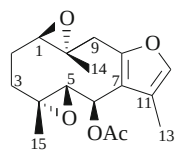
C-1	132.8 d	C-8	154.2 s	C-15	20.6 q[a]
2	73.8 d	9	37.9 t[a]	OAc	170.1 s
3	38.1 t[a]	10	135.1 s	1′	18.8 q[a]
4	30.6 d	11	123.2 s	2′	55.7 q
5	78.9 d	12	138.0 d	OCH_3	
6	195.4 s	13	8.7 q		
7	121.2 s	14	17.3 q[a]		

[a]Assignment may be interchanged [1]

References

1. C.H. Brieskorn, P. Noble, Tetrahedron Lett. **21**, 1511 (1980)

6β-Acetoxy-1β,10α;4α,5β-diepoxy-furanogermacrane (6β-Acetoxy-glechomafurane)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Germacranes – Furanogermacranes – Monoesters

Biological sources: *Salvia roborowskii* Maxim. [1]
$C_{17}H_{22}O_5$: 306.1467
Mp: colorless gum [1]
EI-MS: 306 $[M]^+$ (14), 264 (2), 246 (6), 203 (38), 188 (24), 43 (100) [1]
^{1}H NMR (400.13 MHz, $CDCl_3$, TMS): 1.32 (1H, m, H-3α), 1.38 (3H, s, H-15), 1.49 (2H, m, H-2β), 1.50 (3H, s, H-14), 1.92 (3H, s, H-13), 2.06 (3H, s, OAc), 2.14 (1H, m, H-2β), 2.20 (1H, dt, J = 12.7; 3.6, H-3β), 2.70 (1H, d, J = 16.3, H-9α), 2.83 (1H, dd, J = 10.8; 1.5, H-1), 3.06 (1H, d, J = 1.5, H-5), 3.39 (1H, d, J = 16.1, H-9β), 6.50 (1H, br s, H-6), 7.02 (1H, s, H-12) [1]
^{13}C NMR (100.62 MHz, $CDCl_3$) [1]:

Table 1

C-1	66.0 d	C-8	148.4 s	C-15	18.2 q
2	23.1 t	9	37.6 t	OAc	169.2 s
3	37.5 t	10	59.6 s		20.8 q
4	61.8 s	11	117.8 s		
5	63.7 d	12	137.6 d		
6	65.0 d	13	8.9 q		
7	121.5 s	14	17.7 q		

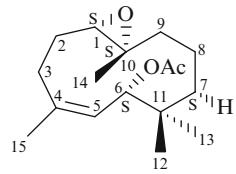
References

1. Y. Li, W. Yan-Qi, D. Xin, Y.-P. Shi, Planta Med. **69**, 782 (2003)

Humulanes

Monoesters

(1*S*,6*S*,10*S*)-6-Acetoxy-1,10-epoxy-humul-4(*Z*)-ene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Torilis scabra* DC. [1]

$C_{17}H_{28}O_3$: 280.2038

Mp: 125–130°C; colorless needles [1]

$[\alpha]_D$ +21.4° (*c* 0.36) [1]

IR: 3000, 2970, 2930, 2870, 1730, 1655, 1465, 1450, 1385, 1370, 1245, 1130, 1065, 1010, 965 [1]

MS: 280 $[M]^+$ (0.4), 265 (0.3), 283 (3), 220 (3), 177 (5), 126 (25), 109 (25), 95 (25), 84 (80), 43 (100) [1]

^{1}H NMR: 0.86 (3H, s, H-13), 0.94 (3H, s, H-12), 1.36 (3H, s, H-14), 1.82 (3H, s, H-15), 2.03 (3H, s, OAc), 2.84 (1H, dd, J = 4; 11, H-1), 5.29 (1H, d, J = 10, H-6), 5.52 (1H, d, J = 10, H-5) [1]

^{13}C NMR [1]:

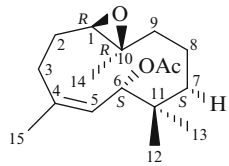
Table 1

16.66 q	25.02 t	60.60 d
19.72 t	29.12 t	73.40 d
21.16 q	37.02 s	122.58 d
22.72 q	37.59 t	140.86 s
23.01 q	38.69 t	170.44 s
24.04 q	60.60 s	

References

1. H. Itokawa, H. Matsumoto, S. Mihashi, Y. Itaka, A. Kasuya, A. Itai, Chem. Pharm., Bull. **33**, 2204 (1985)

(1*R*,6*S*,10*R*)-6-Acetoxy-1,10-epoxy-humul-4(*Z*)-ene



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Torilis scabra* DC. [1]

$C_{17}H_{28}O_3$: 280.2038

Mp: colorless oil [1]

$[\alpha]_D$ −175.5° (*c* 0.33) [1]

IR: 2970, 2950, 2860, 1730, 1665, 1460, 1365, 1245, 1120, 1070, 1015, 655, 905, 860 [1]

MS: 280 $[M]^+$ (0.3), 238 (4), 220 (5), 205 (8), 126 (32), 109 (48), 94 (34), 84 (100), 81 (58), 79 (58), 55 (49) [1]

^{1}H NMR: 0.87 (3H, s, H-13), 0.98 (3H, s, H-12), 1.28 (3H, s, H-14), 1.76 (3H, s, H-15), 2.02 (3H, s, OAc), 2.70 (1H, m, H-1), 5.30 (1H, d, J = 10, H-6), 5.51 (1H, d, J = 10, H-5) [1]

^{13}C NMR [1]:

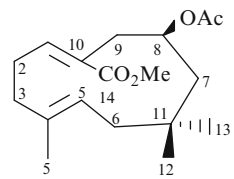
Table 1

21.20 q	24.85 t	62.62 s
21.59 q	28.41 t	74.46 d
21.98 t	36.69 s	122.56 d
22.66 q	37.04 t	141.22 s
23.78 q	37.04 t	170.31 s
23.98 q	62.13 d	

References

1. H. Itokawa, H. Matsumoto, S. Mihashi, Y. Itaka, A. Kasuya, A. Itai, Chem. Pharm., Bull. **33**, 2204 (1985)

8β-Acetoxyhumula-1(10)*Z*,4*E*-dien-14-oic Acid Methyl Ester (Methyl-8β-acetoxyhumula-1(10)*Z*,4*E*-dien-14-oate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Heterotheca villosa* (Pursh) Shinners [1]

$C_{18}H_{28}O_4$: 308.1988

Mp: colorless oil [1]

IR (CCl_4): 1740, 1720, 1250 [1]

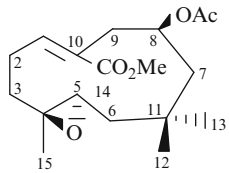
MS: 308.199 $[M]^+$ (3.5) (calc. for $C_{18}H_{28}O_4$: 308.199), 276 (3.5), 248 (25), 233 (12), 216 (18), 189 (42), 121 (44), 61 (100) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 0.86 (3H, s, H-13), 0.93 (3H, s, H-12), 1.35 (1H, br dd, J = 16; 9, H-7β), 1.40 (3H, br s, H-15), 1.63 (1H, br d, J = 16, H-7α), 1.81 (1H, dd, J = 5.5; 16, H-6α), 1.91 (1H, br dd, J = 8.5; 16, H-6β), 2.01 (3H, s, OAc), 2.31 (1H, dd, J = 9; 13.5, H-9β), 2.36 (1H, br dd, J = 4; 13.5, H-9α), 3.73 (3H, s, OCH_3), 4.86 (1H, ddd, J = 9; 9; 4, H-8), 5.04 (1H, br dd, J = 5.5; 8.5, H-5), 6.00 (1H, br dd, J = 10.5; 7, H-1) [1]

References

1. J. Jakupovic, R. Boeker, F. Bohlmann, R.M. King, H. Robinson, Phytochemistry **26**(2), 445 (1987)

8β-Acetoxy-4β,5α-epoxyhumul-1(10)*Z*-en-14-oic Acid Methyl Ester (Methyl-8β-acetoxy-4β,5α-epoxyhumul-1(10)*Z*-en-14-oate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Heterotheca villosa* (Pursh) Shinners [1]

$C_{18}H_{28}O_5$: 324.1937

Mp: colorless oil [1]

IR ($CHCl_3$): 1730, 1720, 1250 [1]

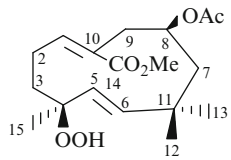
MS: 264.173 $[M - HOAc]^+$ (22) (calc. for $C_{16}H_{24}O_3$: 264.173), 249 (17), 232 (28), 189 (41), 121 (42), 55 (100) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 0.93 (3H, s, H-13), 0.99 (3H, s, H-12), 1.15 (3H, br s, H-15), 1.30 (1H, dd, J = 15; 10, H-6α), 1.50 (1H, br dd, J = 16; 9, H-7α), 1.53 (1H, br d, J = 15; ~ 0.5, H-6β), 1.72 (1H, br d, J = 16, H-7β), 2.03 (3H, s, OAc), 2.41 (1H, br dd, J = 5; 14, H-9α), 2.48 (1H, dd, J = 10; 14, H-9β), 2.84 (1H, d, J = 10; ~ 0.5, H-5), 3.77 (3H, s, OMe), 4.90 (1H, br ddd, J = 9; 5; 10, H-8), 6.17 (1H, br dd, J = 12; 4, H-1) [1]

References

1. J. Jakupovic, R. Boeker, F. Bohlmann, R.M. King, H. Robinson, Phytochemistry **26**(2), 445 (1987)

8β-Acetoxy-4β-hydroperoxyhumula-1(10)*Z*-5*E*-dien-14-oic Acid Methyl Ester (Methyl-8β-acetoxy-4β-hydroperoxy-humula-1(10)*Z*-5*E*-dien-14-oate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Heterotheca villosa* (Pursh) Shinners [1]

$C_{18}H_{28}O_6$: 340.1886

Mp: colorless oil [1]

MS (its 4β-hydroxy deriv.): 264.172 $[M - HOAc]^+$ (10) (calc. for $C_{16}H_{24}O_3$: 264.173), 246 (10), 232 (14), 189 (20), 57 (100) [1]

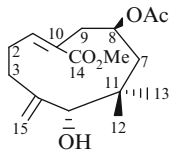
^{1}H NMR (400 MHz, $CDCl_3$, TMS): 0.94 (3H, s, H-13), 0.96 (3H, s, H-12), 1.36 (3H, br s, H-15), 1.67 (2H, m, H-7), 2.03 (3H, s, OAc), 2.32 (1H, dd, J = 12; 13, H-9β), 2.51 (1H, br d, J = 3.5, H-9α), 3.76 (3H, s, OCH_3), 4.64 (1H, dddd, J = 3.5; 3.5; 3.5; 12, H-8), 5.10 (1H, d, J = 16, H-6), 5.26 (1H, d, J = 16, H-5), 6.03 (1H, br dd, J = 9; 8, H-1), 7.39 (1H, s, OOH) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS) (its 4β-hydroxy deriv.): 0.94 (3H, s, H-13), 0.98 (3H, s, H-12), 1.24 (3H, br s, H-15), 1.69 (2H, m, H-7), 2.02 (3H, s, OAc), 2.26 (1H, dd, J = 12; 13, H-9β), 2.61 (1H, br d, J = 3.5, H-9α), 3.80 (3H, s, OCH_3), 4.55 (1H, dddd, J = 3.5; 3.5; 3.5; 12, H-8), 5.24 (1H, d, J = 16, H-6), 5.30 (1H, d, J = 16, H-5), 5.82 (1H, br dd, J = 9; 8, H-1) [1]

References

1. J. Jakupovic, R. Boeker, F. Bohlmann, R.M. King, H. Robinson, Phytochemistry **26**(2), 445 (1987)

8β-Acetoxy-5α-hydroxyhumula-1(10)*Z*,4(15)-dien-14-oic Acid Methyl Ester (Methyl-8β-acetoxy-5α-hydroxyhumula-1(10)*Z*,4(15)-dien-14-oate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Heterotheca villosa* (Pursh) Shinners [1]

$C_{18}H_{28}O_5$: 324.1937

Mp: colorless oil [1]

IR (CCl_4): 3620, 1740, 1720, 1240 [1]

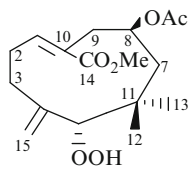
MS: 264.172 $[M - HOAc]^+$ (24) (calc. for $C_{16}H_{24}O_3$: 264.173), 249 (24), 232 (27), 121 (54), 83 (100) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 0.79 (3H, s, H-13), 1.01 (3H, s, H-12), 1.16 (1H, ddd, J = 8; 16; 2, H-6β), 1.41 (1H, ddd, J = 16; 2; 6.5, H-7α), 1.79 (1H, dd, J = 2.5; 16, H-6α), 1.80 (1H, br d, J = 16, H-7β), 2.01 (3H, s, OAc), 2.34 (1H, dd, J = 12; 14, H-9β), 2.51 (1H, br dd, J = 4; 14, H-9α), 3.75 (3H, s, OCH_3), 4.04 (1H, dd, J = 2.5; 8, H-5), 4.84 (1H, ddd, J = 6.5; 4; 12, H-8), 4.91 (1H, br s, H-15b), 5.10 (1H, br s, H-15a), 6.08 (1H, ddd, J = 6; 10; 1.5, H-1) [1]

References

1. J. Jakupovic, R. Boeker, F. Bohlmann, R.M. King, H. Robinson, Phytochemistry **26**(2), 445 (1987)

8β-Acetoxy-5α-hydroperoxyhumula-1(10)*Z*-4(15)-dien-14-oic Acid Methyl Ester (Methyl-8β-acetoxy-5α-hydroperoxy-humula-1(10)*Z*-4(15)-dien-14-oate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Heterotheca villosa* (Pursh) Shinners [1]

$C_{18}H_{28}O_6$: 340.1886

Mp: colorless oil [1]

IR (CCl_4) (its 5α-hydroxy deriv.): 3620, 1740, 1720, 1240 [1]

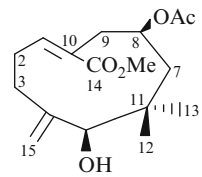
MS (its 5α-hydroxy deriv.): 264.172 $[M - HOAc]^+$ (24) (calc. for $C_{16}H_{24}O_3$: 264.173), 249 (24), 232 (27), 121 (54), 83 (100) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS) (its 5α-hydroxy deriv.): 0.79 (3H, s, H-13), 1.01 (3H, s, H-12), 1.16 (1H, ddd, J = 8; 16; 2, H-6β), 1.41 (1H, ddd, J = 16; 2; 6.5, H-7α), 1.79 (1H, dd, J = 2.5; 16, H-6α), 1.80 (1H, br d, J = 16, H-7β), 2.01 (3H, s, OAc), 2.34 (1H, dd, J = 12; 14, H-9β), 2.51 (1H, br dd, J = 4; 14, H-9α), 3.75 (3H, s, OCH_3), 4.04 (1H, dd, J = 2.5; 8, H-5), 4.84 (1H, ddd, J = 6.5; 4; 12, H-8), 4.91 (1H, br s, H-15b), 5.10 (1H, br s, H-15a), 6.08 (1H, ddd, J = 6; 10; 1.5, H-1) [1]

References

1. J. Jakupovic, R. Boeker, F. Bohlmann, R.M. King, H. Robinson, Phytochemistry **26**(2), 445 (1987)

8β-Acetoxy-5β-hydroxyhumula-1(10)*Z*-4(15)-dien-14-oic Acid Methyl Ester (Methyl-8β-acetoxy-5β-hydroxyhumula-1(10)*Z*-4(15)-dien-14-oate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Heterotheca villosa* (Pursh) Shinners [1]

$C_{18}H_{28}O_5$: 324.1937

Mp: colorless oil [1]

IR ($CHCl_3$): 3510, 1730, 1710, 1240 [1]

MS: 264.173 $[M - HOAc]^+$ (26) (calc. for $C_{16}H_{24}O_3$: 264.173), 249 (23), 232 (24), 121 (56), 83 (100) [1]

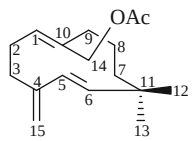
^{1}H NMR (400 MHz, $CDCl_3$, TMS): 0.91 (3H, s, H-13), 0.95 (3H, s, H-12), 1.42 (1H, dd, J = 3.5; 15, H-6β), 1.47 (1H, br dd, J = 17; 5, H-7α), 1.58 (1H, br dd, J = 9; 15, H-6α), 1.97 (1H, br d, J = 17, H-7β), 2.03

(3H, s, OAc), 2.42 (1H, dd, J = 11; 13, H-9β), 2.55 (1H, br dd, J = 4; 13, H-9α), 3.74 (3H, s, OCH_3), 4.14 (1H, dd, J = 3.5; 9, H-5), 4.90 (1H, br s, H-15b), 5.05 (1H, br s, H-15a), 5.10 (1H, br ddd, J = 5; 4; 11, H-8), 6.36 (1H, br dd, J = 5; 10, H-1) [1]

References

1. J. Jakupovic, R. Boeker, F. Bohlmann, R.M. King, H. Robinson, Phytochemistry **26**(2), 445 (1987)

14-Acetoxy-humula-1(10),4(15),5-triene (14-Acetoxy-γ-humulene)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Acritopappus prunifolius* R.M. King & H.Rob. [1]

$C_{17}H_{26}O_2$: 262.1933

Mp: colorless oil, $bp_{0.1}$ 130° (bath temp.) [1]

IR (CCl_4): 3080, 1740, 1645, 1605, 1240, 980 [1]

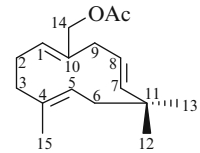
MS: 262.193 $[M]^+$ (0.5) ($C_{17}H_{26}O_2$), 202 $[M - HOAc]^+$ (27), 187 $[202 - \cdot CH_3]^+$ (39), 159 $[202 - C_3H_7]^+$ (86), 91 $[C_7H_7]^+$ (100) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 0.95 (6H, s, H-12, H-13), 1.44 (4H, m, H-7, H-8), 2.04 (2H, m, H-9), 2.04 (3H, s, OAc), 2.30 (2H, m, H-3), 2.38 (2H, m, H-2), 4.43 (2H, br s, H-14), 4.88 (1H, br s, H-15b), 4.91 (1H, br s, H-15a), 5.38 (1H, d, J = 16, H-5), 5.43 (1H, d, J = 16, H-6), 5.52 (1H, br dd, J = 8, H-1) [1]

References

1. F. Bohlmann, C. Zdero, R.M. King, H. Robinson, Phytochemistry **21**(1), 147 (1982)

14-Acetoxy-humula-1(10),4,7-triene (14-Acetoxy-α-humulene)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Lychnophora columnaris* Mattf. [1]

$C_{17}H_{26}O_2$: 262.1933

Mp: colorless oil [1]

IR (CCl_4): 1745, 1240, 980 [1]

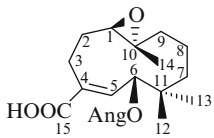
MS: 218.167 $[M - ketene]^+$ (34) ($C_{15}H_{22}O$), 203 (10), 187 (11), 119 (100) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.03 (6H, s, H-12, H-13), 1.43 (3H, d, J = 1, H-15), 1.91 (2H, br t, J = 7.5, H-6), 2.11 (2H, br t, J = 7, H-3), 2.17 (2H, br dt, J = 7.5; 7, H-2), 2.61 (2H, br d, J = 7.5, H-9), 4.76 (2H, s, H-14), 5.12 (1H, br t, J = 7.5; 1, H-5), 5.37 (1H, d, H-7), 5.44 (1H, br t, J = 7.5, H-1), 5.78 (1H, dt, J = 7.5, H-8) [1]

References

1. F. Bohlmann, C. Zdero, H. Robinson, R.M. King, Phytochemistry **21**(3), 685 (1982)

6β-Angeloyloxy-1β,10α-epoxy-4*E*-humulen-15-oic Acid (1β,10α-Epoxykurubaschic Acid Angelate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Ferula haussknechtii* Wolff. ex Rech. [1]

$C_{20}H_{30}O_5$: 350.2093

Mp: gum [1]

IR (NaCl): 3200, 2975, 2930, 2870, 2660, 2520, 1715, 1695, 1645, 1510, 1453, 1385, 1270, 1260, 1230, 1150, 1040, 962, 862, 780, 710 [1]

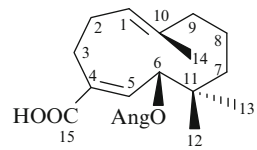
EI-MS: 350 $[M]^+$ (0.1), 250 (4.4), 235 (2.7), 232 (4.2), 205 (5.2), 191 (6), 189 (6.6), 165 (12.9), 151 (17.7), 149 (17.6), 121 (19.3), 105 (28.9), 100 (18.4), 83 (100) [1]

^{1}H NMR (200 MHz, $CDCl_3$, TMS): 0.95 (3H, s, H-13), 1.10 (3H, s, H-12), 1.18 (3H, s, H-14), 1.25 (1H, m, H-9b), 1.38 (4H, m, H-7, H-8), 1.58 (1H, br q, J = 14.4, H-2b), 1.82 (1H, br dd, J = 11.6; 14.3, H-9a), 2.25 (1H, ddd, J = 1.5; 6.5; 14.4, H-2a), 2.70 (1H, br dd, J = 6.3; 14.2, H-3b), 2.96 (1H, dt, J = 1.4; 14.2, H-3a), 2.98 (1H, dd, J = 3.4; 11.3, H-1), 5.53 (1H, d, J = 10.6, H-6), 6.88 (1H, d, J = 10.6, H-5); OAng: 1.88 (3H, t, J = 1.4, H-5′), 1.98 (3H, dq, J = 1.4; 7.2, H-4′), 6.10 (1H, qq, J = 1.4; 7.2, H-3′) [1]

References

1. M. Miski, T.J. Mabry, O. Saya, Phytochemistry **26**(6), 1733 (1987)

6β-Angeloyloxy-1(10)*Z*,4*E*-humuladien-15-oic-acid (Kurubaschic Acid Angelate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Ferula haussknechtii* Wolff. ex Rech. [1]

$C_{20}H_{30}O_4$: 334.2144

Mp: gum [1]

IR (NaCl): 3100, 2970, 2940, 2880, 2670, 2520, 1715, 1695, 1640, 1510, 1458, 1385, 1368, 1355, 1270, 1230, 1150, 1040, 960, 938, 845, 795 [1]

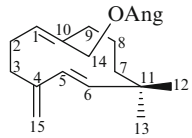
EI-MS: 334 $[M]^+$ (1.1), 234 (13), 219 (15.9), 206 (10.1), 191 (13.2), 149 (67.8), 105 (97), 100 (68.6), 83 (100) [1]

^{1}H NMR (200 MHz, $CDCl_3$, TMS): 0.89 (3H, s, H-13), 1.07 (3H, s, H-12), 1.25 (2H, m, H-7), 1.48 (1H, dt, J = 2.1; 12.6, H-9b), 1.48 (2H, m, H-8), 1.61 (3H, br s, H-14), 2.29 (1H, br d, J = 12.6, H-9a), 2.30 (2H, m, H-2), 2.63 (2H, m, H-3), 5.25 (1H, br t, J = 7.6, H-1), 5.45 (1H, d, J = 10.6, H-6), 6.93 (1H, d, J = 10.6, H-5); OAng: 1.86 (3H, t, J = 1.4, H-5′), 1.96 (3H, dq, J = 1.4; 7.2, H-4′), 6.06 (1H, qq, J = 1.4; 7.2, H-3′) [1]

References

1. M. Miski, T.J. Mabry, O. Saya, Phytochemistry **26**(6), 1733 (1987)

14-Angeloyloxy-humula-1(10),4(15),5-triene (14-Angelyloxy-γ-humulene)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Acritopappus prunifolius* R.M. King et H. Rob. [1]

$C_{20}H_{30}O_2$: 302.2245

Mp: colorless gum [1]

IR (CCl_4): 3080, 1715, 1645, 1605, 975, 895 [1]

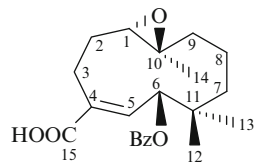
MS: 302.225 $[M]^+$ (0.5) ($C_{20}H_{30}O_2$), 202 $[M - AngOH]^+$ (16), 187 $[202 - \cdot CH_3]^+$ (18), 159 $[202 - C_3H_7]^+$ (28), 93 $[C_4H_7CO]^+$ (100), 55 $[83 - CO]^+$ (88) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 0.95 (6H, s, H-12, H-13), 1.43 (4H, m, H-7, H-8), 2.04 (2H, m, H-9), 2.30 (2H, m, H-3), 2.38 (2H, m, H-2), 4.53 (2H, br s, H-14), 4.88 (1H, br s, H-15b), 4.92 (1H, br s, H-15a), 5.45 (1H, d, J = 16, H-6), 5.52 (1H, br dd, J = 8, H-1), 5.85 (1H, d, J = 16, H-5); OAng: 1.87 (3H, dq, J = 1.5; 1.5, H-5′), 1.97 (3H, dq, J = 7; 1.5, H-4′), 6.03 (1H, qq, J = 7; 1.5, H-3′) [1]

References

1. F. Bohlmann, C. Zdero, R.M. King, H. Robinson, Phytochemistry **21**(1), 147 (1982)

6β-Benzoyloxy-1α,10β-epoxy-4*E*-humulen-15-oic Acid (1α,10β-Epoxykurubaschic Acid Benzoate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Ferula haussknechtii* Wolff. ex Rech. [1]

$C_{22}H_{28}O_5$: 372.1937

Mp: gum [1]

IR (NaCl): 3200, 3070, 2970, 2940, 2870, 2660, 2530, 1720, 1695, 1645, 1602, 1588, 1490, 1465, 1450, 1388, 1370, 1270, 1178, 1110, 1070, 1050, 1028, 960, 865, 775, 710, 688, 678 [1]

EI-MS: 372 $[M]^+$ (0.3), 250 (1.8), 235 (1.4), 191 (3.1), 189 (3.9), 165 (6.4), 151 (3.7), 122 (56), 105 (100) [1]

^{1}H NMR (500 MHz, $CDCl_3$, TMS): 0.83 (1H, br dd, J = 11.6; 12.7, H-9b), 0.98 (3H, s, H-13), 1.16 (3H, s, H-12), 1.22 (1H, m, H-7b), 1.28 (1H, m, H-8b), 1.39 (3H, s, H-14), 1.47 (1H, m, H-2b), 1.47 (1H, m, H-7a), 1.68 (1H, m, H-8a), 2.07 (1H, dd, J = 8.1; 12.7, H-9a), 2.45 (1H, tt, J = 3.7; 13.7, H-2a), 2.69 (1H, td, J = 3.7; 14.1, H-3b), 2.77 (1H, dt, J = 3.3; 14.1, H-3a), 2.89 (1H, dd, J = 4; 10.9, H-1), 5.73

(1H, d, J = 10.5, H-6), 6.88 (1H, d, J = 10.5, H-5); OBz: 7.43 (2H, dt, J = 1.3; 8.2, H-3′, H-5′), 7.54 (1H, dt, J = 1.3; 8.2, H-4′), 7.99 (2H, dd, J = 1.4; 8.1, H-2′, H-6′) [1]

^{13}C NMR (125.8 MHz, $CDCl_3$, TMS) [1]:

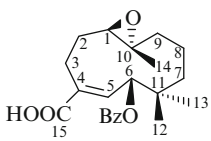
Table 1

C-1	60.8 d	C-9	38.3 t	C-1′	130.0 s
2	26.2 t	10	60.6 s	2′	129.6 d
3	25.1 t	11	37.7 s	3′	128.5 d
4	136.0 s	12	24.5 q	4′	133.2 d
5	138.2 d	13	22.9 q	5′	128.5 d
6	76.7 d	14	16.6 q	6′	129.6 d
7	37.3 t	15	171.7 s	C = O	165.8 s
8	19.8 t				

References

1. M. Miski, T.J. Mabry, O. Saya, Phytochemistry **26**(6), 1733 (1987)

6β-Benzoyloxy-1β,10α-epoxy-4*E*-humulen-15-oic Acid (1β,10α-Epoxykurubaschic Acid Benzoate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Ferula haussknechtii* Wolff. ex Rech. [1]

$C_{22}H_{28}O_5$: 372.1937

Mp: gum [1]

IR (NaCl): 3200, 3060, 2970, 2940, 2875, 2660, 2520, 1720, 1693, 1642, 1602, 1585, 1490, 1450, 1385, 1370, 1320, 1270, 1110, 1070, 1025, 955, 770, 710, 685, 677 [1]

EI-MS: 372 $[M]^+$ (0.12), 250 (2.5), 235 (2.1), 232 (3.9), 205 (2), 191 (3.7), 189 (4.3), 165 (6.6), 151 (5.1), 122 (82.2), 105 (100) [1]

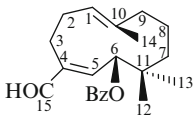
CI-MS: 373 $[M + 1]^+$ (1.1), 371 (1.3), 251 (20.6), 233 (100), 223 (6.7), 215 (16.2), 205 (39.3), 193 (8.7), 187 (19.8), 177 (11.4), 123 (18.2), 105 (25.2) [1]

^{1}H NMR (500 MHz, $CDCl_3$, TMS): 0.98 (3H, s, H-13), 1.17 (3H, s, H-14), 1.19 (3H, s, H-12), 1.22 (1H, dd, J = 8.1; 12.4, H-9b), 1.34 (1H, m, H-8b), 1.41 (3H, m, H-7, H-8a), 1.57 (1H, ddt, J = 1.5; 13; 14.4, H-2b), 1.81 (1H, br dd, J = 11.7; 12.4, H-9a), 2.24 (1H, ddd, J = 3.1; 6.4; 14.1, H-2a), 2.71 (1H, br dd, J = 6.4; 14.2, H-3b), 2.97 (1H, dt, J = 1.4; 14.2, H-3a), 2.98 (1H, dd, J = 3.4; 11.4, H-1), 5.66 (1H, d, J = 10.9, H-6), 6.94 (1H, d, J = 10.9, H-5); OBz: 7.42 (2H, dt, J = 1.3; 8.1, H-3′, H-5′), 7.54 (1H, dt, J = 1.3; 8.1, H-4′), 7.99 (2H, dd, J = 1.4; 8.1, H-2′, H-6′) [1]

References

1. M. Miski, T.J. Mabry, O. Saya, Phytochemistry **26**(6), 1733 (1987)

6β-Benzoyloxy-1(10)*Z*,4*E*-humuladien-15-al (Kurubasch Aldehyde Benzoate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Ferula haussknechtii* Wolff. ex Rech. [1]

$C_{22}H_{28}O_3$: 340.2038

Mp: gum [1]

IR (NaCl): 3060, 2970, 2930, 2865, 2710, 1720, 1695, 1602, 1586, 1490, 1450, 1318, 1270, 1110, 1098, 1028, 950, 935, 800, 710, 688, 672 [1]

EI-MS: 340 $[M]^+$ (6.9), 218 (14.8), 203 (13.6), 189 (8.6), 175 (10), 122 (16.6), 105 (100) [1]

^{1}H NMR (500 MHz, $CDCl_3$, TMS): 0.96 (3H, s, H-13), 1.20 (1H, m, H-7b), 1.20 (3H, s, H-12), 1.33 (1H, m, H-7a), 1.36 (1H, m, H-8b), 1.46 (1H, dt, J = 2.1; 13, H-9b), 1.55 (3H, br s, H-14), 1.64 (1H, m, H-8a), 2.19 (1H, m, H-2b), 2.20 (1H, m, H-9a), 2.28 (1H, m, H-2a), 2.54 (1H, dt, J = 3.8; 12.6, H-3b), 2.61 (1H, td, J = 4.1; 12.6, H-3a), 5.32 (1H, br dd, J = 6.3; 5.8, H-1), 5.72 (1H, d, J = 10.3, H-6), 6.49 (1H, d, J = 10.3, H-5), 9.42 (1H, d, J = 1, H-15); OBz: 7.41 (2H, dt, J = 1.3; 8.6, H-3′, H-5′), 7.53 (1H, dt, J = 1.3; 8.6, H-4′), 7.98 (2H, dd, J = 1.4; 8.7, H-2′, H-6′) [1]

^{13}C NMR (22.6 MHz, $CDCl_3$, TMS) [1]:

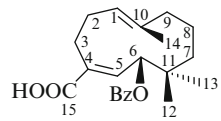
Table 1

C-1	124.4 d	C-9	35.8 t	C-1′	130.2 s
2	25.3 t	10	136.8 s	2′	129.7 d
3	23.6 t	11	37.8 s	3′	128.5 d
4	143.0 s	12	24.3 q	4′	133.2 d
5	143.0 d	13	22.9 q	5′	128.5 d
6	72.8 d	14	19.4 q	6′	129.7 d
7	35.8 d	15	218.1 d	C = O	165.5 s
8	23.8 t				

References

1. M. Miski, T.J. Mabry, O. Saya, Phytochemistry **26**(6), 1733 (1987)

6β-Benzoyloxy-1(10)*Z*,4*E*-humuladien-15-oic Acid (Kurubaschic Acid Benzoate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Ferula haussknechtii* Wolff. ex Rech. [1]

$C_{22}H_{28}O_4$: 356.1988

Mp: gum [1]

IR (NaCl): 3100, 3065, 2970, 2940, 2875, 2660, 2520, 1720, 1692, 1640, 1602, 1585, 1512, 1450, 1388, 1370, 1320, 1270, 1210, 1108, 1070, 1026, 1002, 952, 938, 880, 796, 710, 688, 675 [1]

EI-MS: 356 $[M]^+$ (0.14), 234 (32), 219 (33.9), 206 (5.7), 191 (24.7), 149 (38.5), 122 (82.4), 105 (100) [1]

CI-MS: 355 $[M - 1]^+$ (5.9), 339 (6.4), 251 (9.8), 235 (100), 233 (62.5), 217 (43.2), 205 (20.3), 189 (48), 123 (59.8), 105 (51.5) [1]

^{1}H NMR (500 MHz, $CDCl_3$, TMS): 0.93 (3H, s, H-13), 1.17 (3H, s, H-12), 1.18 (1H, m, H-7b), 1.31 (1H, m, H-7a), 1.32 (1H, m, H-8b), 1.47 (1H, dt, J = 2.1; 12.6, H-9b), 1.61 (3H, s, H-14), 1.63 (1H, m, H-8a), 2.19 (1H, br d, J = 12.6, H-9a), 2.28 (1H, m, H-2), 2.61 (1H, td, J = 4.1; 12.6, H-3b), 2.68 (1H, ddd, J = 5.3; 10; 12.6, H-3a), 5.27 (1H, br t, J = 7.4, H-1), 5.58 (1H, d, J = 10.6, H-6), 6.98 (1H, d, J = 10.6, H-5); OBz: 7.41 (2H, dt, J = 1.3; 8.6, H-3′, H-5′), 7.53 (1H, dt, J = 1.3; 8.6, H-4′), 7.98 (2H, dd, J = 1.4; 8.7, H-2′, H-6′) [1]

^{13}C NMR (125.8 MHz, $CDCl_3$, TMS):

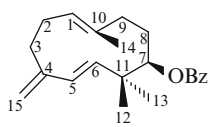
Table 1

C-1	123.9 d	C-9	35.9 t	C-1′	130.2 s
2	26.0 t	10	136.9 s	2′	129.6 d
3	27.7 t	11	37.8 s	3′	128.3 d
4	136.1 s	12	24.3 q	4′	132.9 d
5	138.3 d	13	22.8 q	5′	128.3 d
6	73.2 d	14	19.2 q	6′	129.6 d
7	35.6 t	15	173.4 s	C = O	165.5 s
8	23.7 t				

References

1. M. Miski, T.J. Mabry, O. Saya, Phytochemistry **26**(6), 1733 (1987)

7β-Benzoyloxy-humula-1(10)*z*,5*E*,4(15)-triene (Fervanol Benzoate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Ferula haussknechtii* Wolff. ex Rech. [1]

$C_{22}H_{28}O_2$: 324.2089

Mp: gum [1]

IR (NaCl): 3070, 2970, 2940, 2875, 1720, 1602, 1585, 1450, 1270, 1215, 1040, 880, 830, 710, 688, 675 [1]

EI-MS: 324 $[M]^+$ (1.2), 202 (12.1), 187 (5.6), 159 (9.4), 122 (60), 105 (100) [1]

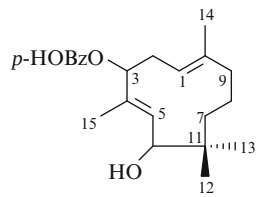
^{1}H NMR (200 MHz, $CDCl_3$, TMS): 1.07 (3H, s, H-13), 1.16 (3H, s, H-12), 1.48 (3H, d, J = 1, H-14), 1.58 (1H, m, H-9b), 1.91 (1H, m, H-8b), 2.17 (1H, m, H-9a), 2.20 (1H, m, H-8a), 2.22 (1H, m, H-2a), 2.33 (1H, m, H-2b), 2.38 (2H, m, H-3), 4.68 (1H, br d, J = 6.9, H-7), 4.90 (1H, d, J = 2.1, H-15b), 4.96 (1H, d, J = 2.1, H-15a), 5.32 (1H, br t, J = 8.5, H-1), 5.59 (1H, d, J = 16.1, H-6), 6.04 (1H, d, J = 16.1, H-5); OBz: 7.46 (1H, dt, J = 2; 8.8, H-3′), 7.46 (1H, dt, J = 2; 8.8, H-5′), 7.60 (1H, dt, J = 2; 8.8, H-4′), 8.03 (1H, dd, J = 2; 8.9, H-2′), 8.03 (1H, dd, J = 2; 8.9, H-6′) [1]

References

1. M. Miski, T.J. Mabry, O. Saya, Phytochemistry **26**(6), 1733 (1987)

3-(4′-Hydroxy-benzoyloxy)-6-hydroxy-humula-1(10)*Z*,4*E*-diene (Juniperdin; Juniferdin)

CAS Registry Number: 74724-29-1



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Ferula juniperina* Korov. [1]

$C_{22}H_{30}O_4$: 358.2144

Mp: 75–77°C [1]

$[\alpha]_D$ −2.8° (*c* 0.53, MeOH) [1]; $[\alpha]_D$ (its diAc) +18.6° (*c* 3.0, MeOH) [1]

UV (EtOH): 211 (4.0), 260 (4.2) [1]

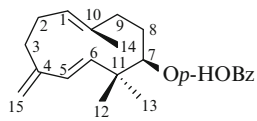
IR (KBr): 3400–3500, 1690, 1610, 1590, 1520 [1]

^{1}H NMR (100 MHz, $CDCl_3$, HMDS): 0.89 and 0.93 (each 3H, s, H-12, H-13), 1.67 (6H, s, H-14, H-15), 4.2 (1H, d, J = 10, H-6), 5.1 (1H, t, J = 7.5, H-1), 5.59 (2H, m, H-3, H-5); O*p*-HOBz: 6.77 (2H, d, J = 9.5, H-3′, H-5′), 7.80 (2H, d, J = 9.5, H-2′, H-6′) [1]

References

1. G.V. Sagitdinova, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **15**, 771 (1979)

7β-(4′-Hydroxy-benzoyloxy)-humula-1(10)*Z*,5*E*,4(15)-triene (Fervanol *p*-Hydroxybenzoate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Ferula haussknechtii* Wolff. ex Rech. [1]

$C_{22}H_{28}O_3$: 340.2038

Mp: gum [1]

IR (NaCl): 3360, 2970, 2940, 2870, 1680, 1610, 1595, 1512, 1450, 1365, 1280, 1220, 1160, 1100, 880, 850, 830, 770, 700 [1]

EI-MS: 340 $[M]^+$ (0.8), 202 (9.4), 187 (4.9), 159 (8.8), 138 (40), 121 (100) [1]

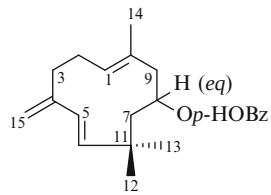
^{1}H NMR (200 MHz, $CDCl_3$, TMS): 1.06 (3H, s, H-13), 1.16 (3H, s, H-12), 1.47 (3H, d, J = 0.9, H-14), 1.58 (1H, m, H-9b), 1.90 (1H, m, H-8b), 2.17 (1H, m, H-9a), 2.19 (1H, m, H-8a), 2.21 (1H, m, H-2a), 2.32 (1H, m, H-2b), 2.36 (2H, m, H-3), 4.68 (1H, br d, J = 6.8, H-7), 4.90 (1H, d, J = 2.1, H-15b), 4.96 (1H, d, J = 2.1, H-15a), 5.31 (1H, br t, J = 8.4, H-1), 5.58 (1H, d, J = 16.1, H-6), 6.04 (1H, d, J = 16.1, H-5); O*p*-HOBz: 6.91 (2H, d, J = 8.8, H-3′, H-5′), 7.99 (2H, d, J = 8.8, H-2′, H-6′) [1]

References

1. M. Miski, T.J. Mabry, O. Saya, Phytochemistry **26**(6), 1733 (1987)

8α-(4′-Hydroxy-benzoyloxy)-humula-1(10),5,4(15)-triene (Juferin)

CAS Registry Number: 70629-76-4



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Ferula juniperina* Korov. [1]

$C_{22}H_{28}O_3$: 340.2038

Mp: 90–91°C (hexane – EtOAc) [1]

$[\alpha]_D^{20}$ +120.4° (*c* 0.77, EtOH) [1]

UV (EtOH): 213.5 (4.3), 255.5 (4.5) [1]

IR (KBr): 3400, 3050, 1680, 1610, 1600, 1520 [1]

TLC: hexane – EtOAc (3:1), R_f 0.5 [1]

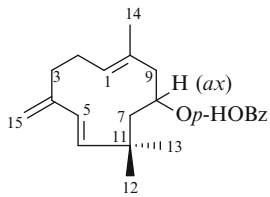
^{1}H NMR (100 MHz, $CDCl_3$, HMDS): 0.98 and 1.07 (each 3H, s, H-12, H-13), 1.37 (3H, s, H-14), 4.52 (1H, m, $W_{1/2}$ = 10, H-8), 5.21 (1H, t, J = 7.5; 7.5, H-1), 5.38 and 5.86 (each 1H, d, J = 16, H-15a, H-15b); O*p*-HOBz: 6.81 (2H, d, J = 10, H-3′, H-5′), 7.82 (2H, d, J = 9, H-2′, H-6′), 8.0 (1H, br s, OH) [2]

References

1. G.V. Sagitdinova, A.I. Saidkhodzjaev, G.K. Nikonov, Chem. Nat. Comp. **12**, 491 (1976)
2. G.V. Sagitdinova, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **14**, 693 (1978)

8β-(4′-Hydroxy-benzoyloxy)-humula-1(10),4(15),5-triene (Ferocin)

CAS Registry Number: 65638-03-1



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Ferula ceratophylla* Regel et Schmalh. [1]; *F. tenusecta* Korov. [2]; *F. lapidosa* Korov. [2]; *F. helenae* U. Rakhmankulov et S. Melibaev [2]; *F. tatarica* Fisch. ex Spreng. [3]

$C_{22}H_{28}O_3$: 340.2038

Mp: 127–128°C (hexane – ether 5:1) [1]

$[\alpha]_D^{20}$ −200° (*c* 1.0, C_6H_6) [1]

UV (EtOH) 253 (4.33) [1]

IR (KBr): 3470–3540, 1710, 1705, 1680, 1610, 1525, 1280, 1240 [1]

MS: 340 $[M]^+$ [1]

TLC: $CHCl_3$, R_f 0.35 [4]

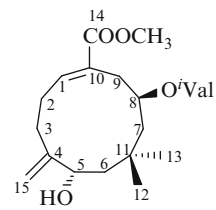
^{1}H NMR (100 MHz, $CDCl_3$, CCl_4, HMDS): 1.07 and 1.00 (each 3H, s, H-12, H-13), 1.55 (3H, s, H-14), 4.80 (1H, s, H-8), 4.80 and 4.86 (each 1H, d, J = 2, H-15), 5.34 (1H, t, J = 7.5, H-1), 5.34 and 5.81 (each 1H, d, J = 16, H-5, H-6); O*p*-HOBz: 6.75 (2H, d, J = 9.5, H-3′, H-5′), 7.86 (2H, d, J = 9.5, H-2′, H-6′) [1]

Pharm./Biol.: Estrogenic activity [5]

References

1. L.I. Golovina, G.K. Nikonov, Chem. Nat. Comp. **13**, 591 (1977)
2. A.I. Saidkhodzjaev, L.I. Golovina, V.M. Malikov, S. Melibaev, U. Rakhmankulov, Chem. Nat. Comp. **21**, 388 (1985)
3. H.H. Najimitdinova, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **31**, 263 (1995)
4. L.I. Golovina, A.I. Saidkhodzjaev, Chem. Nat. Comp. **13**, 796 (1977)
5. S.S. Nazrullaev, Z.A. Khushbaktova, V.N. Syrov, Kh.S. Akhmedkhodzhaeva, A.I. Saidkhodzhaev, The chemistry and biological activity of synthetic and natural compounds, in *oxygen- and sulfur-containing Heterocycles*, ed. by V.G. Kartsev, vol. 1 (IBS PRESS, Moscow, 2003), p. 329

8β-Isovaleroyloxy-5α-hydroxyhumula-1(10)*E*,4(15)-dien-14-oic Acid Methyl Ester (Methyl-8β-isovaleryloxy-5α-hydroxy-humula-1(10)*E*,4(15)-dien-14-oate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

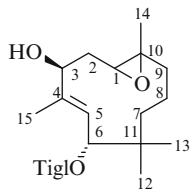
Biological sources: *Heterotheca villosa* (Pursh) Shinners [1]
$C_{21}H_{34}O_5$: 366.2406
Mp: colorless oil [1]
IR (CCl_4): 3600, 1720 [1]
CI-MS: 367 $[M + 1]^+$ (26), 265 (52), 247 (100) [1]
^{1}H NMR (400 MHz, $CDCl_3$, TMS): 0.84 (3H, s, H-13), 1.01 (3H, s, H-12), 1.36 (1H, br dd, J = 6; 15; 1, H-6β), 1.56 (1H, ddd, J = 15; 1; 8.5, H-7α), 1.71 (1H, br d, J = 15, H-7β), 2.00 (1H, br dd, J = 4; 15, H-6α), 2.52 (1H, dd, J = 15; 7, H-9β), 2.73 (1H, br dd, J = 15; 6, H-9α), 3.73 (3H, s, $COOCH_3$), 4.13 (1H, dd, J = 4; 6, H-5), 4.98 (1H, br s, H-15b), 5.04 (1H, br ddd, J = 8.5; 6; 7, H-8), 5.14 (1H, br s, H-15a), 6.95 (1H, dd, J = 8; 8, H-1); O^{i}Val: 0.95 (3H, d, H-5′), 0.96 (3H, d, H-4′), 2.08 (1H, m, H-3′), 2.14 (2H, m, H-2′) [1]

References

1. J. Jakupovic, R. Boeker, F. Bohlmann, R.M. King, H. Robinson, Phytochemistry **26**(2), 445 (1987)

6α-Tigloyloxy-3β-hydroxy-1,10-epoxy-4*E*-humulene (Chatferin)

CAS Registry Number: 89803-99-6



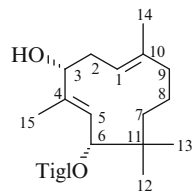
Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters
Biological sources: *Ferula tschatkalensis* M. Pimen. [1]
$C_{20}H_{32}O_4$: 336.2301
$[n]_D^{20}$ 1.5136 [1]
$[\alpha]_D^{20}$ +6.2° (*c* 1.53, EtOH) [1]
IR (KBr): 3600–3400, 1720, 1380, 1360, 1255, 910 [1]
^{1}H NMR (100 MHz, $CDCl_3$, HMDS): 0.88 and 0.95 (each 3H, s, H-12, H-13), 1.35 (3H, s, H-14), 1.75 (3H, s, H-15), 2.50 (1H, q, J = 12; 5, H-1), 4.83 (1H, q, J = 10; 5, H-3), 5.15 (1H, d, J = 10, H-6), 5.30 (1H, d, J = 10, H-5); OTigl: 1.74 (3H, s, H-4′), 1.96 (3H, d, J = 6.5, H-5′), 6.72 (1H, m, H-3′) [1]

References

1. G.V. Sagitdinova, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **19**, 685 (1983)

6α-Tigloyloxy-3α-hydroxy-humula-1(10)*Z*,4*Z*-diene (Fekserin; Fexerin)

CAS Registry Number: 67779-60-6



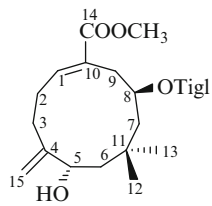
Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters
Biological sources: *Ferula xeromorpha* Korov. [1]; *F. tschatcalensis* M. Pimen. [2]
$C_{20}H_{32}O_3$: 320.2351
$[n]_D$ 1.5095 [1]
$[\alpha]_D^{20}$ −24° (*c* 1.0, $CHCl_3$) [1]
IR: 3600–3300, 1710, 1660, 1240 [1]
MS: 320 $[M]^+$, 237 $[M - 83]^+$, 220 $[M - 100]^+$, 205 $[M - 100 - 15]^+$, 202 $[M - 100 - 18]^+$ [1]
TLC: hexane – ether (3:2), R_f 0.26 [1]
^{1}H NMR (100 MHz, $CDCl_3$, HMDS): 0.77 and 0.92 (each 3H, s, H-12, H-13), 1.62 and 1.68 (each 3H, s, H-14, H-15), 4.65 (1H, q, J = 10; 5, H-3), 4.99 (1H,

t, J = 7.5, H-1), 5.0 (1H, d, J = 10, H-6), 5.15 (1H, d, J = 10, H-5); OTigl: 1.66 (3H, s, H-4′), 1.70 (3H, s, H-5′), 6.66 (1H, m, H-3′) [1]

References

1. K. Bizhanova, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **14**, 495 (1978)
2. G.V. Sagitdinova, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **19**, 685 (1983)

8β-Tigloyloxy-5α-hydroxyhumula-1(10)*E*,4(15)-dien-14-oic Acid Methyl Ester (Methyl-8β-Tigloyloxy-5α-hydroxyhumula-1(10)*E*,4(15)-dien-14-oate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Heterotheca villosa* (Pursh) Shinners [1]

$C_{21}H_{32}O_5$: 364.2250

Mp: colorless oil [1]

IR (CCl_4): 3600, 1720 [1]

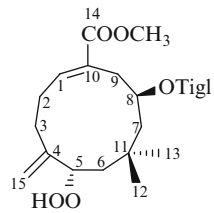
MS: 364 $[M]^+$ (0.2), 264.173 [M – TiglOH]$^+$ (7) (calc. for $C_{16}H_{24}O_3$: 264.173), 249 (3), 246 (7), 232 (5), 121 (7), 83 (100), 55 (49) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 0.82 (3H, s, H-13), 1.01 (3H, s, H-12), 1.37 (1H, br dd, J = 6; 15; 1, H-6β), 1.60 (1H, ddd, J = 15; 1; 8.5, H-7α), 1.73 (1H, br d, J = 15, H-7β), 2.02 (1H, br dd, J = 4; 15, H-6α), 2.61 (1H, dd, J = 15; 7, H-9β), 2.75 (1H, br dd, J = 15; 6, H-9α), 3.71 (3H, s, OCH_3), 4.13 (1H, dd, J = 4; 6, H-5), 4.99 (1H, br s, H-15b), 5.08 (1H, br ddd, J = 8.5; 6; 7, H-8), 5.14 (1H, br s, H-15a), 6.95 (1H, dd, J = 8; 8, H-1); OTigl: 1.78 (3H, d, H-4′), 1.82 (3H, br s, H-5′), 6.83 (1H, qq, H-3′) [1]

References

1. J. Jakupovic, R. Boeker, F. Bohlmann, R.M. King, H. Robinson, Phytochemistry **26**(2), 445 (1987)

8β-Tigloyloxy-5α-hydroperoxyhumula-1(10)*E*,4(15)-dien-14-oic Acid Methyl Ester (Methyl-8β-tigloyloxy-5α-hydroperoxyhumula-1(10)*E*,4(15)-dien-14-oate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Heterotheca villosa* (Pursh) Shinners [1]

$C_{21}H_{32}O_6$: 380.2199

Mp: colorless oil [1]

MS: 246 [M – H_2O_2, TiglOH]$^+$ (4), 231 (3), 83 (100), 55 (38) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 0.84 (3H, s, H-13), 0.97 (3H, s, H-12), 1.49 (1H, br dd, J = 6; 15; 1, H-6β), 1.60 (2H, m, H-7), 1.84 (1H, br dd, J = 4; 15, H-6α), 2.70 (2H, m, H-9), 3.74 (3H, s, $COOCH_3$), 4.33 (1H, dd, J = 4; 6, H-5), 5.08 (1H,

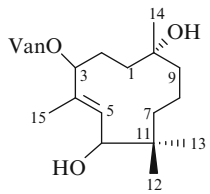
m, H-8), 5.20 (1H, br s, H-15b), 5.22 (1H, br s, H-15a), 6.93 (1H, br dd, J = 8; 8, H-1); OTigl: 1.79 (3H, d, H-4′), 1.82 (3H, br s, H-5′), 6.84 (1H, qq, H-3′) [1]

References

1. J. Jakupovic, R. Boeker, F. Bohlmann, R.M. King, H. Robinson, Phytochemistry **26**(2), 445 (1987)

3-Vanilloyloxy-6,10-dihydroxy-humul-4-ene (Fekseridin; Fexeridin)

CAS Registry Number: 69199-12-8



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Ferula xeromorpha* Korov. [1]

$C_{23}H_{32}O_6$: 404.2199

Mp: 141–143°C [1]

$[\alpha]_D$ +40° (*c* 1.09, MeOH) [1]

UV (EtOH): 267 (4.04), 297 (3.80) [1]

IR (KBr): 3600–3200, 1705, 1620, 1600, 1520 [1]

MS (fexerol): 236 $[M - H_2O]^+$, 221 $[M - H_2O - CH_3]^+$, 218 $[M - 2H_2O]^+$, 200 $[M - 3H_2O]^+$ [1]

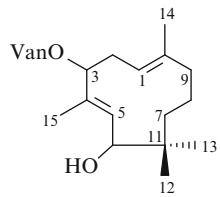
^{1}H NMR (100 MHz, $CDCl_3$, HMDS): 0.88 and 0.98 (each 3H, s, H-12, H-13), 1.20 (3H, s, H-14), 1.78 (3H, s, H-15), 4.50 (1H, d, J = 10, H-6), 5.53 (1H, d, J = 10, H-5), 5.78 (1H, q, J = 12.0; 5, H-3); OVan: 3.87 (3H, s, OCH_3), 6.82 (1H, d, J = 9.5, H-5′), 7.44 (1H, d, J = 2.5, H-2′), 7.52 (1H, q, J = 9.5; 2.5, H-6′) [1]

References

1. K. Bizhanova, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **14**, 495 (1978)

3-Vanilloyloxy-6-hydroxy-humula-1(10)*Z*,4*E*-diene (Juniferin; Juniperin)

CAS Registry Number: 61116-35-6



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Ferula juniperina* Korov. [1]; *F. xeromorpha* Korov. [2]

$C_{23}H_{32}O_5$: 388.2250

Mp: 85–86°C (hexane–EtOAc, 3:1) [1]

$[\alpha]_D^{20}$ −1.6° (*c* 5.8, EtOH) [1]

UV (EtOH): 211 (4.0), 260 (4.2), 286 (4.3) [1]

IR (KBr): 3200–3600, 1690, 1620, 1600, 1520 [1]

TLC: hexane – EtOAc (3:1), R_f 0.35 [1]

^{1}H NMR (100 MHz, CCl_4, HMDS): 0.88 and 0.95 (each 3H, s, H-12, H-13), 1.67 (6H, s, H-14, H-15), 4.18 (1H, d, J = 10, H-6), 5.05 (1H, q, J = 7.5,

H-1), 5.50 (1H, q, J = 10; 5, H-3), 5.52 (1H, d, J = 10, H-5) [3]

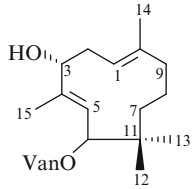
Pharm./Biol.: Estrogenic activity [4]

References

1. G.V. Sagitdinova, A.I. Saidkhodzjaev, G.K. Nikonov, Chem. Nat. Comp. **12**, 491 (1976)
2. K. Bizhanova, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **14**(5), 495 (1978)
3. G.V. Sagitdinova, A.I. Saidkhodzjaev, Chem. Nat. Comp. **13**, 665 (1977)
4. S.S. Nazrullaev, Z.A. Khushbaktova, V.N. Syrov, A.I. Saidkhodzhaev, The chemistry and biological activity of synthetic and natural compounds, in *Oxygen- and Sulfur-Containing Heterocycles*, ed. by V.G. Kartsev, vol. 1 (IBS PRESS, Moscow, 2003), p. 329

6-Vanilloyloxy-3α-hydroxy-humula-1(10)*Z*,4*E*-diene (Fexerinin)

CAS Registry Number: 69199-11-7



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Ferula xeromorpha* Korov. [1]

$C_{23}H_{32}O_5$: 388.2250

$[\alpha]_D$ −64° (*c* 1.33, MeOH) [1]

UV (EtOH): 265 (3.99), 297 (3.71) [1]

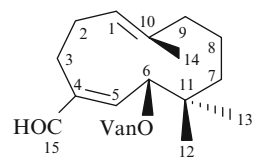
IR (KBr): 3200–3600, 1690, 1620, 1600, 1590, 1520 [1]

^{1}H NMR (100 MHz, $CDCl_3$, HMDS): 0.86 and 1.04 (each 3H, s, H-12, H-13), 1.68 and 1.75 (each 3H, s, H-14, H-15), 4.89 (1H, q, J = 10; 5, H-3), 5.04 (1H, t, J = 7.5, H-1), 5.17 (1H, d, J = 10, H-5), 5.32 (1H, d, J = 10, H-6); OVan: 3.89 (3H, s, OCH_3), 6.86 (1H, d, J = 9.5, H-5′), 7.44 (1H, d, J = 2.5, H-2′), 7.50 (1H, q, J = 9.5; 2.5, H-6′) [1]

References

1. K. Bizhanova, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **14**, 495 (1978)

6β-Vanilloyloxy-1(10)*Z*,4*E*-humuladien-15-al (Kurubasch Aldehyde Vanillate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Ferula haussknechtii* Wolff. ex Rech. [1]

$C_{23}H_{30}O_5$: 386.2093

Mp: gum [1]

IR (NaCl): 3400, 3080, 2970, 2940, 2870, 2715, 1710, 1692, 1610, 1600, 1512, 1460, 1430, 1388, 1370, 1280, 1215, 1110, 1032, 958, 878, 785, 762, 725 [1]

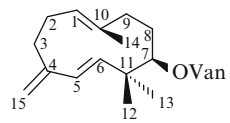
EI-MS: 386 $[M]^+$ (3.3), 218 (5.9), 203 (2.3), 189 (3.1), 175 (4), 168 (15.9), 151 (100) [1]

^{1}H NMR (200 MHz, $CDCl_3$, TMS): 0.97 (3H, s, H-13), 1.21 (3H, s, H-12), 1.38 (1H, m, H-8b), 1.38 (2H, m, H-7), 1.48 (1H, dt, J = 2.1; 13, H-9b), 1.57 (3H, br s, H-14), 1.60 (1H, m, H-8a), 2.21 (1H, m, H-9a), 2.26 (2H, m, H-2), 2.60 (2H, m, H-3), 5.24 (1H, br t, J = 7.6, H-1), 5.70 (1H, d, J = 10.3, H-6), 6.50 (1H, d, J = 10.3, H-5), 9.44 (1H, d, J = 0.9, H-15); OVan: 3.93 (3H, s, OCH_3), 6.93 (1H, d, J = 8.4, H-5′), 7.50 (1H, d, J = 1.9, H-2′), 7.60 (1H, dd, J = 1.9; 8.4, H-6′) [1]

References

1. M. Miski, T.J. Mabry, O. Saya, Phytochemistry **26**(6), 1733 (1987)

7β-Vanilloyloxy-humula-1(10)*Z*,5*E*,4(15)-triene (Fervanol Vanillate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Ferula haussknechtii* Wolff. ex Rech. [1]

$C_{23}H_{30}O_4$: 370.2144

Mp: gum [1]

IR (NaCl): 3400, 3080, 2975, 2938, 2870, 1710, 1610, 1600, 1515, 1460, 1450, 1428, 1283, 1220, 1105, 1030, 880, 830, 785, 762, 725 [1]

EI-MS: 370 $[M]^+$ (4), 202 (13.9), 187 (11.6), 168 (18), 159 (15.8), 151 (100) [1]

^{1}H NMR (500 MHz, $CDCl_3$, TMS): 1.07 (3H, s, H-13), 1.16 (3H, s, H-12), 1.48 (3H, d, J = 1.1, H-14), 1.58 (1H, m, H-9b), 1.92 (1H, m, H-8b), 2.17 (1H, m, H-9a), 2.22 (1H, m, H-2a), 2.24 (1H, m, H-8a), 2.33 (1H, m, H-2b), 2.38 (2H, m, H-3), 4.68 (1H, br d, J = 6.9, H-7), 4.90 (1H, d, J = 2.1, H-15b), 4.96 (1H, d, J = 2.1, H-15a), 5.32 (1H, br t, J = 8.5, H-1), 5.59 (1H, d, J = 16.1, H-6), 6.04 (1H, d, J = 16.1, H-5); OVan: 3.95 (3H, s, OCH_3), 6.96 (1H, d, J = 8.3, H-5′), 7.62 (1H, d, J = 1.8, H-2′), 7.66 (1H, dd, J = 1.8; 8.3, H-6′) [1]

^{13}C NMR (125.8 MHz, $CDCl_3$, TMS) [1]:

Table 1

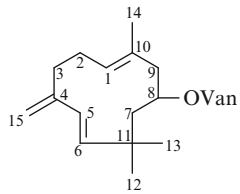
C-1	126.9 d	C-9	40.9 t	C-1′	122.9 s
2	30.2 t	10	135.5 s	2′	114.1 d
3	31.5 t	11	37.7 s	3′	150.0 s
4	148.3 s	12	26.0 q	4′	148.3 s
5	138.5 d	13	26.0 q	5′	111.8 d
6	128.5 d	14	17.0 q	6′	124.0 d
7	83.6 d	15	114.7 t	C = O	166.0 s
8	30.2 t	OCH_3	56.1 q		

References

1. M. Miski, T.J. Mabry, O. Saya, Phytochemistry **26**(6), 1733 (1987)

8-Vanilloyloxy-humula-1(10)*Z*,5*E*,4(15)-triene (Ferocinin)

CAS Registry Number: 65638-04-2



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Monoesters

Biological sources: *Ferula ceratophylla* Regel et Schmalh. [1]; *F. tschatcalensis* M. Pimen. [2]; *F. xeromorpha* Korov. [3]; *F. tenuisecta* Korov. [3];

F. helenae U. Rakhmankulov et S. Melibaev [3]; *F. lapidosa* Korov. [4]; *F. tatarica* Fisch. ex Spreng. [5]

$C_{23}H_{30}O_4$: 370.2144

Mp: 107–108° (hexane) [1]

$[\alpha]_D^{20}$ −197° (*c* 1.0, C_6H_6) [1], $[\alpha]_D^{20}$ −195° (*c* 1.0, EtOH) [2]

UV (EtOH): 252 (4.31), 295 (3.94) [1]

IR (KBr): 3300–3330, 1705, 1680, 1615, 1600, 1525, 1280, 1240 [1]

MS: 370 $[M]^+$ [1]

TLC: $CHCl_3$, R_f 0.5 [6]

^{1}H NMR (100 MHz, $CDCl_3$, CCl_4, HMDS): 0.90 and 1.04 (each 3H, s, H-12, H-13), 1.53 (3H, s, H-14), 4.82 (2H, br s, H-15), 5.1 (1H, m, H-8) 5.28 (1H, t, J = 7.5; 7.5, H-1), 5.40 and 5.94 (each 1H, d, J = 16, H-5, H-6); OVan: 3.83 (3H, s, OCH_3), 6.87 (1H, d, J = 9.5, H-5′), 7.50 (1H, d, J = 9.5, H-2′), 7.55 (1H, q, J = 9.5; 2.5, H-6′) [6]

References

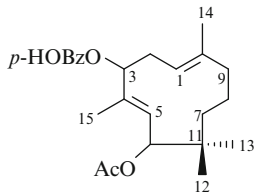
1. L.I. Golovina, G.K. Nikonov, Chem. Nat. Comp. **13**, 591 (1977)
2. G.V. Sagitdinova, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **19**, 685 (1983)
3. K. Bizhanova, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **14**, 495 (1978)
4. A.I. Saidkhodzjaev, L.I. Golovina, V.M. Malikov, S. Melibaev, U. Rakhmankulov, Chem. Nat. Comp. **21**, 388 (1985)
5. H.H. Najimitdinova, A.I. Saidkhodzhaev, V.M. Malikov, Chem. Nat. Comp. **31**, 263 (1995)
6. L.I. Golovina, A.I. Saidkhodzjaev, Chem. Nat. Comp. **13**, 671 (1977)

Humulanes

Diesters

6-Acetoxy-3-(4′-hydroxy-benzoyloxy)-humula-1(10),4-diene (Juniferidin; Juniperidin; Isomer of Juniferinin; Juniperinin)

CAS Registry Number: 70494-82-5



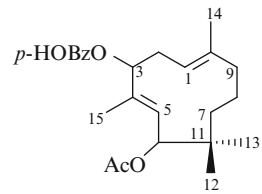
Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Diesters
Biological sources: *Ferula juniperina* Korov. [1]
$C_{24}H_{32}O_5$: 400.2250
Mp: 162–163°C (hexane–ether 9:1) [2]
$[\alpha]_D^{24}$ −2.1° (*c* 0.65, MeOH) [2]
UV (EtOH): 211 (4.0), 260 (4.3) [3]
IR (KBr) (Juniferinin): 3400–3200, 1710, 1695, 1690, 1615, 1520 [3]
TLC: hexane – EtOAc (3:1), R_f 0.27 [3]
^{1}H MMR (100 MHz, $CDCl_3$, HMDS): 0.78 and 0.93 (each 3H, s, H-12, H-13), 1.73 and 1.75 (each 3H, s, H-14, H-15), 2.1 (3H, s, OAc), 5.20 (1H, t, J = 7.5, H-1), 5.42 (2H, s, H-5, H-6), 5.65 (1H, q, J = 10; 5, H-3) [3]
Pharm./Biol.: estrogenic activity [4]

References

1. G.V. Sagitdinova, A.I. Saidkhodzjaev, G.K. Nikonov, Chem. Nat. Comp. **12**, 491 (1976)
2. G.V. Sagitdinova, A.I. Saidkhodzjaev, V.M. Malikov, Chem. Nat. Comp. **14**, 693 (1978)
3. G.V. Sagitdinova, A.I. Saidkhodzjaev, Chem. Nat. Comp. **13**, 665 (1977)
4. S.S. Nazrullaev, Z.A. Khushbaktova, V.N. Syrov, A.I. Saidkhodzhaev, The Chemistry and Biological Activity of Synthetic and Natural Compounds, in *Oxygen- and Sulfur-Containing Heterocycles*, ed. by V.G. Kartsev, vol. 1 (IBS PRESS, Moscow, 2003), p. 329

6-Acetoxy-3-(4′-hydroxy-benzoyloxy)-humula-1(10),4-diene (Juniferinin; Juniperinin; Isomer of Juniferidin; Juniperidin)

CAS Registry Number: 70494-82-5

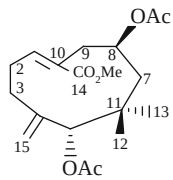


Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Diesters
Biological sources: *Ferula juniperina* Korov. [1]
$C_{24}H_{32}O_5$: 400.2250
Mp: 164–165°C (hexane) [1]
$[\alpha]_D^{20}$ +33.4° (*c* 1.8, EtOH) [1]
UV (EtOH): 211 (4.0), 260 (4.3) [1]
IR (KBr): 3400–3200, 1710, 1695, 1690, 1615, 1520 [1]
TLC: hexane – EtOAc (3:1), R_f 0.21 [2]
^{1}H MMR (100 MHz, $CDCl_3$, HMDS): 0.78 and 0.93 (each 3H, s, H-12, H-13), 1.73 and 1.75 (each 3H, s, H-14, H-15), 2.1 (3H, s, OAc), 5.20 (1H, t, J = 7.5, H-1), 5.42 (2H, s, H-5, H-6), 5.65 (1H, q, J = 10; 5, H-3) [2]
Pharm./Biol.: estrogenic activity [3]

References

1. G.V. Sagitdinova, A.I. Saidkhodzjaev, G.K. Nikonov, Chem. Nat. Comp. **12**, 491 (1976)
2. G.V. Sagitdinova, A.I. Saidkhodzjaev, Chem. Nat. Comp. **13**, 665 (1977)
3. S.S. Nazrullaev, Z.A. Khushbaktova, V.N. Syrov, A.I. Saidkhodzhaev, The chemistry and biological activity of synthetic and natural compounds, in *Oxygen– and Sulfur-Containing Heterocycles*, ed. by V.G. Kartsev, vol. 1 (IBS PRESS, Moscow, 2003), p. 329

5α,8β-Diacetoxyhumula-1(10)*Z*,4(15)-dien-14-oic Acid Methyl Ester (Methyl-5α,8β-diacetoxyhumula-1(10)*Z*,4(15)-dien-14-oate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Diesters

Biological sources: *Heterotheca villosa* (Pursh) Shinners [1]

$C_{20}H_{30}O_6$: 366.2042

IR (CCl_4): 3600, 1750, 1720 [1]

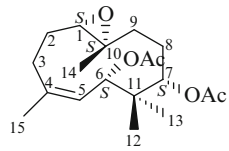
CI-MS: 367 $[M + 1]^+$ (26), 307 (56), 247 (100) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 0.81 (3H, s, H-13), 0.86 (3H, s, H-12), 1.44 (2H, m, H-6β, H-7α), 1.74 (1H, br dd, J = 2.5; 16, H-6α), 1.83 (1H, br d, J = 16, H-7β), 1.98 (3H, s, OAc), 2.02 (3H, s, OAc), 2.39 (1H, dd, J = 12; 14, H-9β), 2.53 (1H, br d, J = 4; 14, H-9α), 3.80 (3H, s, OCH_3), 4.82 (1H, br ddd, J = 6.5; 4; 12, H-8), 4.91 (1H, br s, H-15b), 5.00 (1H, br s, H-15a), 5.08 (1H, br dd, J = 2.5; 8, H-5), 6.13 (1H, br dd, J = 6; 10, H-1) [1]

References

1. J. Jakupovic, R. Boeker, F. Bohlmann, R.M. King, H. Robinson, Phytochemistry **26**(2), 445 (1987)

(1*S*,6*S*,7*S*,10*S*)-6,7-Diacetoxy-6,10-epoxy-humul-4(*Z*)-ene (Caucalol Diacetate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Diesters

Biological sources: *Caucalis scabra* Makino [1]; *Torilis scabra* DC. [2]

$C_{19}H_{30}O_5$: 338.2093

Mp: 124.5–125° C; colorless plates [2]

$[\alpha]_D$ +27.7° (*c* 1.54) [2]

MS: 338.205, 278.185, 236.176, 218.165, 175.148, 175.110 [1]

MS: 278 (5), 237 (11), 235 (8), 218 (14), 203 (12), 175 (24), 151 (18), 135 (22), 125 (22), 121 (22), 109 (100), 81 (60) [2]

IR: 2990, 2890, 1740, 1730, 1665, 1450, 1370, 1240, 1135, 1015, 960, 905, 875 [2]

^{1}H NMR: 0.86 (3H, s, H-12), 0.89 (3H, s, H-13), 1.36 (3H, s, H-14), 1.84 (3H, s, H-15), 2.01 (6H, s, 2 × OAc), 2.99 (1H, dd, J = 4; 11, H-1), 4.90 (1H, m, H-7), 5.29 (1H, d, J = 11, H-6), 5.46 (1H, d, J = 11, H-5) [2]

^{13}C NMR [2]:

Table 1

16.43 q	25.20 t	72.53 d
18. 51 q	27.68 t	76.05 d
18. 51 q	29.29 t	121.66 d

(*continued*)

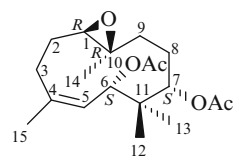
Table 1 (continued)

20.81 q	34.48 t	141.78 s
21.05 q	41.80 s	170.14 s
23.12 q	60.02 s	170.78s
	60.02 d	

References

1. S. Sasaki, Y. Itagaki, H. Moriyama, K. Nakanishi, Tetrahedron Lett. **7**, 623 (1966)
2. H. Itokawa, H. Matsumoto, S. Mihashi, Y. Itaka, A. Kasuya, A. Itai, Chem. Pharm., Bull. **33**, 2204 (1985)

(1*R*,6*S*,7*S*,10*R*)-6,7-Diacetoxy-1,10-epoxy-humul-4(*Z*)-ene (Neocaucalol Diacetate)



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Humulanes – Diesters

Biological sources: *Torilis scabra* DC. [1]

$C_{19}H_{30}O_5$: 338.2093

Mp: 169–171°C; colorless needles [1]

$[\alpha]_D$ –108.3° (*c* 0.29) [1]

MS: 338 $[M]^+$ (3), 323 (1), 278 (4), 236 (9), 218 (15), 203 (20), 175 (38), 135 (30), 109 (100) [1]

IR: 2980, 2930, 2890, 1745, 1660, 1460, 1390, 1370, 1235, 1015, 960, 900 [1]

^{1}H NMR: 0.87 (3H, s, H-12), 0.98 (3H, s, H-13), 1.37 (3H, s, H-14), 1.79 (3H, s, H-15), 2.03 (3H, s, OAc), 2.08 (3H, s, OAc), 2.84 (3H, m, H-1), 4.99 (1H, J = 8, H-7), 5.39 (1H, d, J = 11, H-6), 5.51 (1H, d, J = 11, H-5) [1]

^{13}C NMR [1]:

Table 1

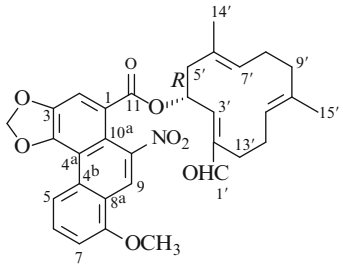
17.99 q	28.37 t	73.17 d
18.10 q	30.21 t	74.96 d
20.93 q	34.02 t	121.37 d
21.10 q	41.96 t	142.82 s
24.10 q	62.33 d	170.09 s
25.02 t	62.62 s	170.90 s

References

1. H. Itokawa, H. Matsumoto, S. Mihashi, Y. Itaka, A. Kasuya, A. Itai, Chem. Pharm., Bull. **33**, 2204 (1985)

Aristoloterpenates

Aristoloterpenate-I



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Other Monocyclic Sesquiterpene Esters – Aristoloterpenates

Biological sources: *Aristolochia heterophylla* Hemsl. [1]

$C_{32}H_{31}NO_8$: 557.2050

Mp: 247–249°C (Me_2CO), yellow needles [1]

$[\alpha]_D$ –39.5° (*c* 0.015, $CHCl_3$) [1]

UV (MeOH): 226 (4.50), 239 (4.40), 250 (4.36), 268 (4.21), 287 (3.98), 322 (3.99), 393 (3.76) [1]

IR (KBr): 2924, 2855.1706,1690, 1645, 1596, 1517, 1463, 1342, 1271, 1242, 1142, 1043, 952, 812, 752 [1]

EI-MS: 557 $[M]^+$ (10), 341 (52), 324 (11), 295 (68), 280 (9), 278 (9), 265 (7), 216 (8) [1]

HR-EI-MS: 557.2045 (calc. for $C_{32}H_{31}NO_8$: 557.2050) [1]

CD: $[\theta]_{237}$ +5017, $[\theta]_{241}$ (0), $[\theta]_{250}$ −12590, $[\theta]_{265}$ −3698, $[\theta]_{285}$ (0) (*c* 3.95×10^{-5}, $CHCl_3$) [1]

^{1}H NMR ($CDCl_3$): 1.34 (3H, s, H-15′), 1.61 (3H, s, H-14′), 1.80 (1H, td, J = 13.0; 4.0, H-13′b), 1.98 (1H, br t, J = 11.2, H-8′b), 2.02 (1H, m, H-9′b), 2.07 (1H, m, H-12′b), 2.20 (2H, m, H-9′a), 2.30 (1H, br t, J = 11.2, H-8′a), 2.39 (1H, br d, J = 12.2, H-5′b), 2.42 (1H, m, H-12′a), 2.72 (1H, br d, J = 12.2, H-5′a), 2.84 (1H, dt, J = 13.0, J = 4.0, H-13′a), 4.81 (1H, br d, J = 8.4, H-11′), 5.04 (1H, br d, J = 11.2, H-7′), 6.08 (1H, d, J = 11.2, H-3′), 6.37 (1H, dd, J = 11.2; 4.6, H-4′), 10.25 (1H, s, H-1′); acyl group: 4.03 (3H, s, OCH_3), 6.34 (2H, s, OCH_2O), 7.04 (1H, d, J = 8.8, H-7), 7.64 (1H, t, J = 8.8, H-6), 7.87 (1H, s, H-2), 8.58 (1H, d, J = 8.8, H-5), 8.79 (1H, s, H-9) [1]

^{13}C NMR [1]:

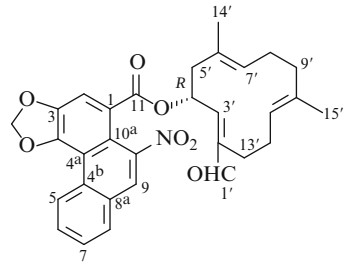
Table 1

C-1	123.2 s	C-10	145.5 s	C-9′	39.6 t
2	112.7 d	10a	118.1 s	10′	134.9 s
3	145.8 s	11	166.0 s	11′	125.2 d
4	146.6 s	1′	191.2 d	12′	25.9 t
4a	118.3 s	2′	141.7 s	13′	31.7 t
4b	130.8 s	3′	144.4 d	14′	15.9 q
5	118.9 d	4′	67.6 d	15′	14.9 q
6	130.9 d	5′	44.9 t	OCH_2O	102.4 t
7	107.8 d	6′	128.5 s	OCH_3	55.9 q
8	156.7 s	7′	130.6 d		
8a	119.9 s	8′	25.0 t		
9	121.2 d				

References

1. Tian-Shung W., Y.-Y. Chan, Y.-L. Leu, Z.-T. Chen, J. Nat. Prod. **62**, 415 (1999)

Aristoloterpenate-II



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Other Monocyclic Sesquiterpene Esters – Aristoloterpenates

Biological sources: *Aristolochia heterophylla* Hemsl. [1]

$C_{31}H_{29}NO_7$: 527.1944

Mp: 241–243°C (Me_2CO), yellow needles [1]

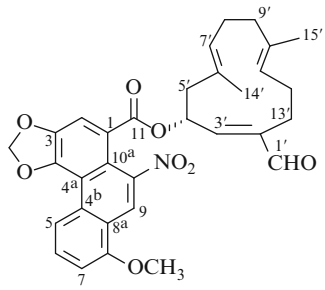
$[\alpha]_D$ −35.4° (*c* 0.016, $CHCl_3$) [1]

UV (MeOH): 1226 (4.57), 241 (4.46), 250 (4.41), 267 (4.27), 283 (4.08), 321 (4.05), 392 (3.82) [1]
IR (KBr): 2928, 2856, 1707, 1680, 1597, 1534, 1518, 1342, 1042, 953 [1]
FAB-MS: 528 $[M + 1]^+$ (3), 527 $[M]^+$ (2), 311 (14), 294 (80), 265 (28), 250 (12), 248 (9), 235 (3) [1]
HR-FAB-MS: 528.2033 $[M + 1]^+$ (calc. for $C_{31}H_{30}NO_7$: 528.2022), 311.0436 $[M - C_{15}H_{20}O]^+$ (calc. for $C_{16}H_9NO_6$: 311.0429) [1]
CD: $[\theta]_{229}$ +2770, $[\theta]_{237}$ (0), $[\theta]_{243}$ −5740, $[\theta]_{253}$ −9583, $[\theta]_{282}$ (0) (*c* 1.84×10^{-4}, $CHCl_3$) [1]
^{1}H NMR ($CDCl_3$): 1.34 (3H, s, H-15′), 1.61 (3H, s, H-14′), 1.80 (1H, br t, J = 12.4, H-13′b), 2.00 (1H, br t, J = 11.2, H-8′b), 2.03 (1H, m, H-9′b), 2.06 (1H, m, H-12′b), 2.18 (1H, m, H-9′a), 2.32 (1H, br t, J = 11.2, H-8′a), 2.40 (1H, br d, J = 11.4, H-5′b), 2.42 (1H, m, H-12′a), 2.73 (1H, br d, 11.4, H-5′a), 2.85 (1H, br d, J = 12.4, H-13′a), 4.82 (1H, br d, J = 8.4, H-11′), 5.05 (1H, br d, J = 11.2, H-7′), 6.08 (1H, td, J = 10.8, H-3′), 6.37 (1H, m, H-4′), 10.25 (1H, s, H-1′); acyl group: 6.40 (2H, s, OCH_2O), 7.70 (1H, t, J = 8.4, H-7), 7.73 (1H, s, H-2), 7.79 (1H, t, J = 8.4, H-6), 8.00 (1H, d, J = 8.4, H-8), 8.35 (1H, s, H-9), 9.13 (1H, d, J = 8.4, H-5) [1]

References

1. T.-S. Wu, Y.-Yi Chan, Y.-L. Leu, Z.-T. Chen, J. Nat. Prod. **62**, 415 (1999)

Aristoloterpenate–III



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Other Monocyclic Sesquiterpene Esters – Aristoloterpenates

Biological sources: *Aristolochia heterophylla* Hemsl. [1]
$C_{32}H_{31}NO_8$: 557.2050
Mp: 245–247° C (Me_2CO), yellow needles [1]
$[\alpha]_D$ −86.0° (*c* 0.038, $CHCl_3$) [1]
UV (MeOH): 225 (4.51), 251 (4.31), 267 (4.18), 284 (3.98), 321 (3.96), 391 (3.74) [1]
IR (KBr): 2922, 2856, 1705, 1695, 1598, 1529, 1452, 1382, 1338, 1263, 1230, 1137, 1043, 948, 806, 756 [1]
EI-MS: 557 $[M]^+$ (3), 341 (24), 324 (26), 309 (13), 295 (62), 293 (100), 278 (83), 265 (13), 250 (30), 216 (21), 187 (10), 164 (23), 137 (18), 105 (27), 91 (47), 79 (38), 67 (42)
HR-FAB-MS: 558.2127 $[M + 1]^+$ (calc. for $C_{32}H_{32}NO_8$: 558.2128), 341.0540 $[M - C_{15}H_{20}O]^+$ (calc. for $C_{17}H_{11}NO_7$: 341.0536) [1]
CD: $[\theta]_{205}$ +19320, $[\theta]_{212}$ (0), $[\theta]_{218}$ −8549, $[\theta]_{221}$ −10260, $[\theta]_{238}$ −32110, $[\theta]_{254}$ −27400 (*c* 4.77×10^{-5}, $CHCl_3$) [1]
^{1}H NMR ($CDCl_3$): 1.40 (3H, s, H-15′), 1.68 (3H, s, H-14′), 2.05 (1H, m, H-9′a), 2.14 (1H, t, 7.0, H-8′a), 2.21 (1H, m, H-12′b), 2.33 (1H, m, H-12′a), 2.40 (1H, t, J = 9.8, H-13′b), 2.43 (1H, t, J = 10.6, H-5′b), 2.63 (1H, dd, J = 9.8; 5.1, H-13′a), 2.80 (1H, dd, J = 10.6; 3.6, H-5′a), 4.85 (1H, t, J = 7.8, H-11′), 5.10 (1H, t, J = 7.0, H-7′), 5.70 (1H, td, J = 10.6; 3.6, H-4′), 6.36 (1H, d, J = 10.6, H-3′), 9.51 (1H, s, H-1′); acyl group: 4.06 (3H, s, OCH_3), 6.36 (2H, s, OCH_2O), 7.10 (1H, dd, J = 8.5; 3.6, H-7), 7.70 (1H, s, H-2), 7.71 (1H, t, J = 8.5, H-6), 8.68 (1H, dd, J = 8.5; 3.6, H-5), 8.84 (1H, s, H-9) [1]
^{13}C NMR [1]:

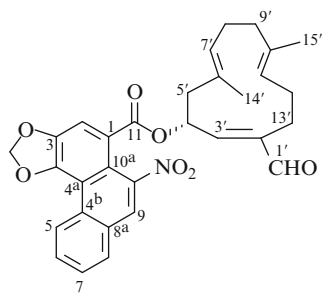
Table 1

C-1	123.3 s	C-10	145.6 s	C-9′	38.4 t
2	112.8 d	10a	118.2 s	10′	133.6 s
3	145.9 s	11	165.8 s	11′	125.5 d
4	146.6 s	1′	195.9 d	12′	25.1 t
4a	118.4 s	2′	145.8 s	13′	25.6 t
4b	130.8 s	3′	148.9 d	14′	18.6 q
5	119.1 d	4′	71.6 d	15′	15.4 q
6	131.0 d	5′	43.6 t	OCH_2O	102.4 t
7	107.9 d	6′	129.0 s	OCH_3	55.9 q
8	156.9 s	7′	129.5 d		
8a	120.1 s	8′	24.9 t		
9	121.3 d				

References

1. T.-S. Wu, Y.-Y. Chan, Y.-L. Leu, Z.-T. Chen, J. Nat. Prod. **62**, 415 (1999)

Aristoloterpenate-IV



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Other Monocyclic Sesquiterpene Esters – Aristoloterpenates

Biological sources: *Aristolochia heterophylla* Hemsl. [1]

$C_{31}H_{29}NO_7$: 527.1944

Mp: 234–236°C (Me_2CO), yellow needles [1]

$[\alpha]_D$ −88.3° (*c* 0.011, $CHCl_3$) [1]

UV (MeOH): 210 (4.60), 219 (4.62), 243 (4.57), 251 (4.60), 266 (4.44), 298 (4.17), 375 (3.74) [1]

IR (KBr): 2924, 2855, 1710, 1694, 1596, 1531, 1519, 1454, 1388, 1351, 1267, 1232, 1118, 1041, 943, 794, 758 [1]

FAB-MS: 528 $[M + 1]^+$ (1), 527 $[M]^+$ (1), 311 (4), 294 (17), 265 (7),250 (3), 248 (3), 235 (2) [1]

HR-FAB-MS: 528.2028 $[M + 1]^+$ (calc. for $C_{31}H_{30}NO_7$: 528.2022), 311.0423 $[M - C_{15}H_{20}O]^+$ (calc. for $C_{16}H_9NO_6$: 311.0429) [1]

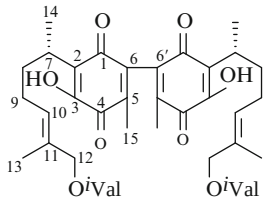
CD: $[\theta]_{209}$ +21760, $[\theta]_{215}$ (0), $[\theta]_{223}$ −20670, $[\theta]_{229}$ −18210, $[\theta]_{248}$ −46970 (*c* 4.22×10^{-5}, $CHCl_3$) [1]

^{1}H NMR ($CDCl_3$): 1.41 (3H, s, H-15′), 1.96 (3H, s, H-14′), 2.06 (2H, m, H-9), 2.15 (1H, t, J = 7.6, H-8′a), 2.22 (1H, m, H-12′b), 2.32 (1H, m, H-12′a), 2.40 (1H, t, J = 9.7, H-13′b), 2.43 (1H, dd, J = 12.8; 9.6, H-5′b), 2.64 (1H, dd, J = 9.8; 4.9, H-13′a), 2.81 (1H, dd, J = 12.8; 3.4, H-5′a), 4.85 (1H, t, J = 7.6, H-11′), 5.11 (1H, t, J = 7.6, H-7′), 5.72 (1H, td, J = 9.6; 3.4, H-4′), 6.36 (1H, d, J = 9.6, H-3′), 9.52 (1H, s, H-1′); acyl group: 6.40 (2H, s, OCH_2O), 7.70 (1H, s, H-2), 7.71 (1H, td, J = 8.4; 2.4, H-7), 7.81 (1H, td, J = 8.4; 2.4, H-6), 7.99 (1H, dd, J = 8.4; 2.4, H-8), 8.34 (1H, s, H-9), 9.13 (1H, d, J = 8.4, H-5) [1]

References

1. T.-S. Wu, Y.-Y. Chan, Y.-L. Leu, Z.-T. Chen, J. Nat. Prod. **62**, 415 (1999)

6′,6-bis-[2-(1,5-Dimethyl-4-hexenyl-6-isovaleroxy)-3-hydroxy-5-methyl-*p*-benzoquinone]



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Other Monocyclic Sesquiterpene Esters – bis-Benzoquinones

Biological sources: *Coreocarpus arizonicus* Gray [1]

$C_{40}H_{54}O_{10}$: 694.3717

Mp: mix. with the 6′,6-bis-[2-(1,5-dimethyl-4-hexenyl-6-(2-methylbutyroxy))-3-hydroxy-5-methyl-*p*-benzoquinone] [1]

^{1}H NMR (200 MHz, $CDCl_3$) (mix.): 1.23 (3H, d, J = 7.0, H-14), 1.59 (3H, br s, H-13), 1.88 (3H, s, H-15), 3.05 (1H, ∼sextet, J = 6.8, H-7), 4.43 (2H, ∼s, H-12), 5.43 (1H, br t, J = 7.0, H-10), 7.09 (1H, s, OH); O^{i}Val: 0.95 (3H, d, J = 6.5, H-4′), ∼1.67 (1H, dq, J = 14.0: 7.0, H-3′), 2.21 (2H, d, J = 6.3, H-2′) [1]

^{13}C NMR (22.63 MHz, $CDCl_3$) (mix.): [1]

Table 1

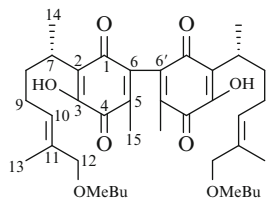
C-1	151.0	C-8	33.5, 33.6	C-15	13.8
2	184.8, 184.9[a]	9	26.7	O-^{i}Val	173.1
3	138.3	10	129.3	1′	43.4
4	140.2	11	130.2	2′	25.7
5	183.2[a]	12	69.8	3′	22.4
6	124.5	13	12.9, 13.0	4′	
7	29.5	14	18.1		

[a]Assignment may be interchanged

References

1. S.D. Jolad, B.N. Timmermann, J.J. Hoffmann, R.B. Bates, F.A. Camou, J.R. Cole, Phytochemistry **27**(11), 3545 (1988)

6′,6-bis-[2-(1,5-Dimethyl-4-hexenyl-6-(2-methylbutyroyloxy))-3-hydroxy-5-methyl-*p*-benzoquinone]



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Other Monocyclic Sesquiterpene Esters – bis-Benzoquinones

Biological sources: *Coreocarpus arizonicus* Gray [1]

$C_{40}H_{54}O_{10}$: 694.3717

Mp: mix. with the 6′,6-bis-[2-(1,5-dimethyl-4-hexenyl-6-isovaleroxy)-3-hydroxy-5-methyl-*p*-benzoquinone] [1]

^{1}H NMR (200 MHz, $CDCl_3$) (mix.): 1.21 (3H, d, J = 6.9, H-14), 1.59 (3H, br s, H-13), 1.88 (3H, s, H-15), 3.05 (1H, ∼sextet, J = 6.8, H-7), 4.43 (2H, ∼s, H-12), 5.43 (1H, br t, J = 7.0, H-10), 7.09 (1H, s, OH); OMeBu: 0.90 (3H, t, J = 7.4, H-4′), 1.14 (3H, d, J = 9, H-5′), ∼1.47 (2H, dq, J = 14.0; 7.0, H-3′), 2.38 (1H, sextet, J = 6.0, H-2′) [1]

^{13}C NMR (22.63 MHz, $CDCl_3$) (mix.): [1]

Table 1

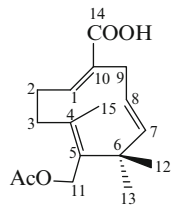
C-1	151.0	C-8	33.5, 33.6	C-15	13.8
2	184.8, 184.9[a]	9	26.7	OMeBu	176.6
3	138.3	10	129.3	1′	41.1
4	140.2	11	130.2	2′	26.3
5	183.2[a]	12	69.8	3′	11.6
6	124.5	13	12.9, 13.0	4′	16.6
7	29.5	14	18.1	5′	

[a]Assignment may be interchanged

References

1. S.D. Jolad, B.N. Timmermann, J.J. Hoffmann, R.B. Bates, F.A. Camou, J.R. Cole, Phytochemistry **27**(11), 3545 (1988)

11-Acetoxylychnen-14-oic Acid



Taxonomy: Physicochemical and Pharmacological Properties of Sesquiterpene Esters – The Monocyclic Sesquiterpene Esters – Other Monocyclic Sesquiterpene Esters – Lychnene

Biological sources: *Lychnophora columnaris* Mattf. [1]

$C_{17}H_{24}O_4$: 292.1675

Mp: colorless gum [1]

IR (CCl_4): 3500–2500, 1730, 1680, 1625, 1240 [1]

MS: 292.167 $[M]^+$ (4) ($C_{17}H_{24}O_4$), 232 (90), 217 (24), 203 (46), 189 (65), 176 (48), 166 (58), 163 (77), 162 (71), 151 (87), 145 (81), 133 (70), 121 (100), 107 (76), 105 (80), 91 (89), 84 (90), 79 (80), 69 (95) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS): 1.02 (3H, s, H-13), 1.10 (3H, s, H-12), 1.67 (3H, br s, H-15), 2.03 (3H, s, OAc), 2.24 (1H, ddd, J = 12; 12.5, H-3β), 2.32 (1H, br dd, J = 5; 12.5, H-3α), 2.49 (1H, br d, J = 5; 13, H-2α), 2.85 (1H, br dd, J = 7; 15, H-9α), 2.92 (1H, m, J = 10; 13, H-2β), 2.97 (1H, br dd, J = 7; 15, H-9β), 5.02 (1H, br d, J = 11, H-11a), 5.16 (1H, d, J = 11, H-11b), 5.17 (1H, d, J = 16, H-7), 5.77 (1H, dt, J = 16; 7, H-8), 6.04 (1H, br dd, J = 5; 10, H-1) [1]

^{1}H NMR (400 MHz, $CDCl_3$, TMS) (its Me-ester): 1.02 (3H, s, H-13), 1.10 (3H, s, H-12), 1.63 (3H, br s, H-15), 2.03 (3H, s, OAc), 2.20 (1H, ddd, J = 12; 12.5, H-3β), 2.31 (1H, br dd, J = 5; 12.5, H-3α), 2.42 (1H, br d, J = 5; 13, H-2α), 2.81 (1H, br dd, J = 7; 15, H-9α), 2.82 (1H, m, J = 10; 13, H-2β), 2.96 (1H, br dd, J = 7; 15, H-9β), 3.76 (3H, s, OCH_3), 5.02 (1H, br d, J = 11, H-11a), 5.16 (1H, d, J = 11, H-11b), 5.18 (1H, d, J = 16, H-7), 5.77 (1H, dt, J = 16; 7, H-8), 5.87 (1H, br dd, J = 5; 10, H-1) [1]

References

1. F. Bohlmann, C. Zdero, H. Robinson, R.M. King, Phytochemistry **21**(3), 685 (1982)