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Full Papers

Bisabolane-Type Sesquiterpenes: Liginvolones A–D from *Ligusticum involucratum*

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Four new bisabolane-type sesquiterpenes, liginvolones A–D (**1–4**), a new coumarin, 4'-octanoyloxyosthenol (**5**), and 20 known constituents were isolated from *Ligusticum involucratum*. Their structures were elucidated on the basis of spectroscopic analyses and chemical methods.

Ligusticum involucratum Franch. (Umbelliferae) grows in altitudinal meadows and forests (about 2800–4000 m above sea level) from Yunnan to Sichuan Province, China.¹ We learned that the roots have been used as folk medicine for the treatment of inflammation and fever on our field survey, but no suggestion about the constituents of this plant has been made as yet. In the course of our studies on the phenolic components of umbelliferous plants, we investigated the constituents of this plant and isolated four new bisabolane-type sesquiterpenes, liginvolones A–D (**1–4**) along with the new coumarin 4'-octanoyloxyosthenol (**5**), 16 known coumarins [umbelliferone, scopoletin, psoralen, bergapten, xanthotoxin, isoimpinellin, isopsoralen, lomatin isovalerate,² nuttallin,³ peguangxienin,⁴ suksdorfin,⁵ isosamidin,⁶ pteryxin,⁵ ostruthin, (*E*)-6-(7-hydroxy-3,7-dimethylocta-2,5-dienyl)-7-hydroxycoumarin, 6-(6-hydroxy-3,7-dimethylocta-2,7-dienyl)-7-hydroxycoumarin], ferulic acid, 4-hydroxy-3-methoxycinnamaldehyde, ligustilide, and faltarindiol. This report deals with the isolation and structural elucidation of the five new natural products.

Results and Discussion

Liginvolone A (**1**) was obtained as a pale yellow viscous oil, $[\alpha]_D^{25} +180.6^\circ$ (*c* 0.498, EtOH), showing a green spot on TLC when sprayed with 5% sulfuric acid reagent

followed by heating on a hot plate. The molecular formula was determined as C₂₀H₂₈O₅ on the basis of HREIMS (*m/z* 348.1930, [M]⁺, calcd 348.1937). The IR spectrum showed a strong OH band at 3451 cm⁻¹ and ester and α , β -unsaturated carbonyl bands at 1738 and 1678 cm⁻¹, respectively.

The ¹H NMR spectrum of **1** showed the presence of six methyl groups [δ 0.95 (6H, d, *J* = 6.6 Hz), 1.62 (3H, s), 1.75 (3H, brs), 1.82 (3H, brs), 1.99 (3H, s)], two methylene groups [δ 2.23 (1H, dd, *J* = 15.0, 7.2 Hz), 2.15 (1H, dd, *J* = 15.0, 7.0 Hz), 2.87 (1H, dd, *J* = 18.1, 8.0 Hz), 2.78 (1H, ddq, *J* = 18.1, 8.0, 1.4 Hz)], two methine groups [δ 4.98 (1H, t, *J* = 8.0 Hz), 2.05 (1H, ddq, *J* = 7.2, 7.0, 6.6, 6.6 Hz)], and three olefinic protons [δ 5.43 (1H, d, *J* = 11.2 Hz), 6.07 (1H, dq, *J* = 11.2, 1.4, 1.4 Hz), 6.07 (1H, brs)]. These data were similar to those of bisabolangelone (**6**),^{7–10} one of the sesquiterpenes from *Angelica silvestis* L., except for the presence of an isovaleryl spin system [δ 2.23 (1H, dd, *J* = 15.0, 7.2 Hz), 2.15 (1H, dd, *J* = 15.0, 7.0 Hz), 2.05 (1H, ddq, *J* = 7.2, 7.0, 6.6, 6.6 Hz), 0.95 (6H, d, *J* = 6.6 Hz)] instead of a C-9 methine signal [δ 2.65 (1H, d, *J* = 6.9 Hz)] in **6**.

Each partial structure was obtained by the analyses of ¹H–¹H COSY cross-peaks, and they were connected on the basis of the HMBC spectrum to establish the planar structure (Figure 2).

The ¹H and ¹³C NMR signals were assigned by HSQC and DEPT experiments, as shown in Tables 1 and 2.

Liginvolone B (**2**) was obtained as a pale yellow viscous oil, $[\alpha]_D^{25} +83.4^\circ$ (*c* 0.500, EtOH), and showed a green spot

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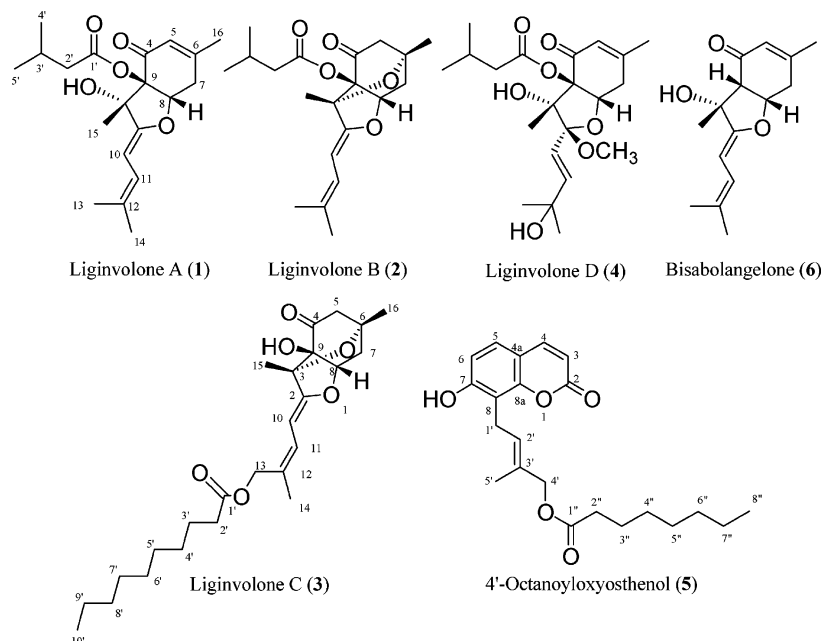


Figure 1. Structures of liginvolones A–D, 4'-octanoyloxyosthenol, and bisabolangelone.

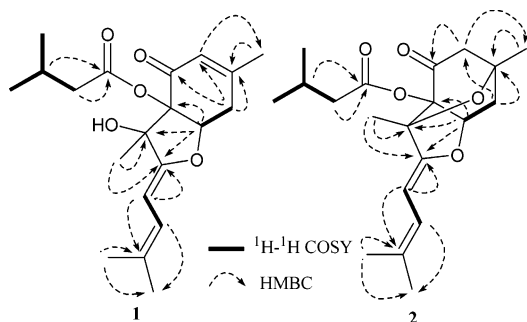


Figure 2. Selected ^1H - ^1H COSY and HMBC correlations in **1** and **2**.

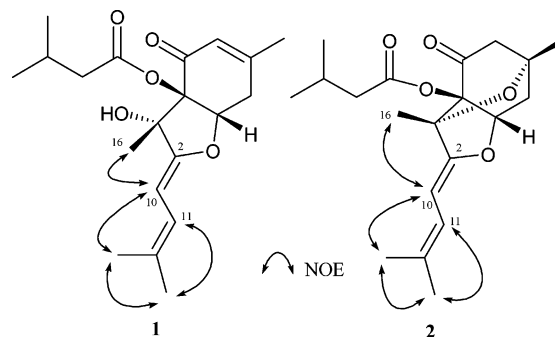


Figure 3. Selected NOESY correlations in **1** and **2**.

on TLC when sprayed with 5% sulfuric acid reagent followed by heating. The molecular formula was established as $\text{C}_{20}\text{H}_{28}\text{O}_5$ on the basis of HREIMS (m/z 348.1924, $[\text{M}]^+$, calcd 348.1937). The IR spectrum showed strong ester and carbonyl bands at 1739 and 1682 cm^{-1} , respectively.

The ^1H NMR spectrum was similar to that of **1**, except for the presence of a methylene signal [δ 2.44 (1H, d, $J = 19.0$ Hz), 2.53 (1H, ddd, $J = 19.0, 3.3, 0.9$ Hz)] adjacent to a carbonyl group instead of the C-5 olefinic proton [δ 6.07 (1H, brs)] of **1**. Moreover *W*-type long-range coupling was observed between $5\alpha\text{-H}$ and $7\alpha\text{-H}$. The chemical shifts of the C-5 (δ 51.4) and C-6 (δ 70.9) signals were shielded to 75.8 and 87.5 ppm compared to those of **1**, while the C-4 carbonyl signal (δ 200.4) was deshielded by 8.9 ppm, suggesting the formation of a bridge structure between C-3

and C-6 through an oxygen atom. The planar structure of **2** was thus elucidated, as shown in Figure 2. This structure was supported by ^1H - ^1H COSY, HSQC, HMBC, and DEPT spectra.

The geometry of the olefinic C-2–C-10 bonds in **1** and **2** was determined as *Z* by NOE correlation between the C-16 methyl protons and the C-10 olefinic proton (Figure 3). Moreover, the C-10–C-11 bond possessed *s-trans* conformation on the basis of the vicinal coupling constant ($J = 11.2$ Hz).

Only one relative configuration for **2** exists from its complex cross-linkage structure as shown in Figure 1. Moreover the relative configuration of **1** was estimated from the formation of **2** by the biosynthesis as shown in Scheme 1. However the absolute configurations of **1** and **2** are still being investigated.

Scheme 1. Presumed Biosynthetic Formation of **2** from **1**

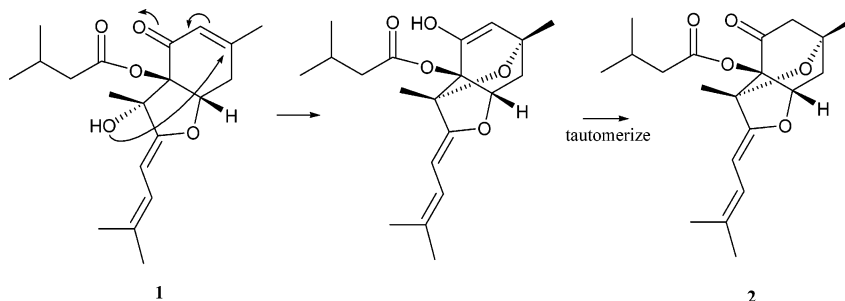


Table 1. ^1H NMR Data for **1–4** and **6** (δ ppm, in CDCl_3 , TMS)^a

	1	2	4	6^b	3
2					2
3					3
4					4
5	6.07 brs	α : 2.53 dd (19.0, 3.3) β : 2.44 d (19.0)	6.08 brt (1.1)	6.00 m	5 α : 2.57 dd (19.4, 3.1) β : 2.44 d (19.4)
6					6
7	α : 2.78 ddq (18.1, 8.0, 1.4) β : 2.87 dd (18.1, 8.0)	α : 2.28 dd (14.9, 3.3) β : 2.35 dd (14.9, 6.9)	α : 2.54 d (18.8) β : 3.07 dd (18.8, 6.6)	α : 2.78 dd (18.3, 5.1) β : 2.70 dd (18.3, 5.7)	7 α : 2.27 dd (15.0, 3.0) β : 2.17 dd (15.0, 7.0)
8	4.98 t (8.0)	5.27 d (6.9)	4.19 dd (6.6, 1.1)	4.87 ddd (6.9, 5.7, 5.1)	8 4.50 d (7.0)
9				2.65 d (6.9)	9
10	5.43 d (11.2)	5.40 d (11.2)	5.51 d (16.0)	5.37 d (11.3)	10 5.46 d (11.4)
11	6.07 dq (11.2, 1.4, 1.4)	6.04 dq (11.2, 1.4, 1.4)	6.11 d (16.0)	6.00 m (11.3)	11 6.33 dd (11.4, 1.4)
12					12
13	1.82 brs	1.81 brs	1.35 s	1.79 s	13 4.67 s
14	1.75 brs	1.74 brs	1.36 s	1.72 s	14 1.84 d (1.4)
15	1.62 s	1.33 s	1.41 s	1.62 s	15 1.28 s
16	1.99 s	1.33 s	2.02 brs	2.02 s	16 1.34 s
OH			1.69 brs		OH 3.92 s
OCH ₃			1.78 brs 3.14 s		
1'					1'
2'	2.15 dd (15.0, 7.0) 2.23 dd (15.0, 7.2)	2.27 dd (15.0, 6.9) 2.31 dd (15.0, 6.9)	2.28 dd (14.6, 7.1) 2.33 dd (14.6, 7.1)		2' 2.32 t (7.4) 3' 1.62 tt (7.4, 7.4)
3'	2.05 ddq (7.2, 7.0, 6.6, 6.6)	2.09 ddq (6.9, 6.9, 6.9, 6.9)	2.11 ddq (7.1, 7.1, 6.7, 6.7)		4' } 5' } 6' } 7' } 8' } 9' } 10' 0.88 t (7.0)
4'	0.95 d (6.6)	0.99 d (6.9)	0.98 d (6.7)		
5'	0.95 d (6.6)	0.99 d (6.9)	0.99 d (6.7)		

^a Values in parentheses are coupling constants in Hz. ^b These are literature data by Liu, J.-H., et al.⁸

Table 2. ^{13}C NMR Data for **1–4** and **6** (δ ppm, in CDCl_3 , TMS)

	1	2	4	6^a	3
2	156.6 s	153.5 s	107.8 s	158.2 s	2 156.2 s
3	80.5 s	82.8 s	83.9 s	78.6 s	3 83.1 s
4	191.5 s	200.4 s	191.9 s	196.8 s	4 208.0 s
5	127.2 d	51.4 t	126.5 d	127.2 d	5 49.9 t
6	158.5 s	71.0 s	157.7 s	160.0 s	6 70.8 s
7	37.8 t	43.7 t	34.7 t	34.9 t	7 43.6 t
8	81.5 d	76.0 d	79.4 d	76.1 d	8 79.6 d
9	84.3 s	88.6 s	85.6 s	53.6 d	9 84.3 s
10	96.2 d	96.5 d	119.8 d	94.4 d	10 95.1 d
11	117.7 d	117.8 d	144.7 d	117.7 d	11 122.8 d
12	133.7 s	133.7 s	70.8 s	132.6 s	12 129.9 s
13	26.1 q	26.1 q	29.7 q	26.0 q	13 63.0 t
14	18.2 q	18.3 q	29.9 q	18.2 q	14 21.7 q
15	20.7 q	17.0 q	16.8 q	27.4 q	15 16.6 q
16	24.5 q	25.6 q	24.7 q	24.6 q	16 25.6 q
OCH ₃			49.0 q		
1'	172.0 s	171.3 s	172.7 s		1' 173.9 s
2'	42.9 t	43.3 t	43.0 t		2' 34.3 t
3'	25.7 d	25.7 d	25.9 d		3' 25.0 t
4'	25.2 q	22.2 q	22.3 q		4' } 5' } 6' } 7' } 8' } 9' } 10' 14.1 q
5'	22.3 q	22.3 q	22.3 q		

^a These are literature data by Liu, J.-H., et al.⁸

Liginvolone C (**3**) was obtained as a pale yellow viscous oil, $[\alpha]_{\text{D}}^{25} +1.8^\circ$ (*c* 0.500, EtOH), showing a reddish purple spot on TLC when sprayed with 5% sulfuric acid reagent followed by heating. The molecular formula was determined as $\text{C}_{25}\text{H}_{38}\text{O}_6$ on the basis of HREIMS (m/z 434.2650, $[\text{M}]^+$, calcd 434.2668). The IR spectrum showed strong OH, ester, and carbonyl bands at 3462, 1732, and 1674 cm^{-1} , respectively.

Table 3. ^1H and ^{13}C NMR Data of **5**

	δ_{H}	δ_{C}
2		161.4 s
3	6.24 d (9.5)	112.6 d
4	7.62 d (9.5)	144.0 d
4a		112.7 s
5	7.22 d (8.4)	126.6 d
6	6.79 d (8.4)	112.9 d
7		157.8 s
8		114.5 s
8a		153.3 s
1'	3.64 d (7.2)	21.7 t
2'	5.59 tq (7.2, 1.3)	125.1 d
3'		132.7 s
4'	4.47 s	69.6 t
5'	1.89 d (1.3)	14.2 q
1''		174.0 s
2''	2.31 t (7.3)	34.4 t
3''	1.61 tt (7.3, 7.3)	25.0 t
4''		28.9 t
5''	1.28 m	30.0 t
6''		31.6 t
7''		22.6 t
8''	0.87 t (6.9)	14.0 q

The ^1H NMR spectrum was similar to that of **2**, except that **3** had an oxymethylene signal [δ 4.67 (2H, s)], a decanoyloxy spin pattern [δ 2.32 (2H, t, $J = 7.4$ Hz), 1.62 (2H, tt, $J = 7.4, 7.4$ Hz), 1.36–1.20 (12H, brm), 0.88 (3H, t, $J = 7.0$ Hz)], and a hydroxyl proton [δ 3.92 (1H, s)] instead of an isovaleryl spin pattern. A *W*-type long-range coupling was also observed between $5\alpha\text{-H}$ and $7\alpha\text{-H}$, as seen in **2**. The chemical shift of C-13 (δ 63.0) was deshielded by 36.92 ppm from that of **2**. The HMBC was observed between H-13 and C-1'. Consequently, liginvolone C was elucidated to have the structure shown in Figure 1. The signals were assigned using ^1H – ^1H COSY, HSQC, HMBC, and DEPT as shown in Tables 1 and 2. The structure was

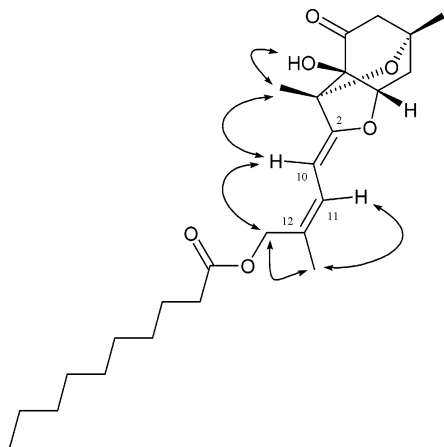


Figure 4. Selected NOESY correlations in **3**.

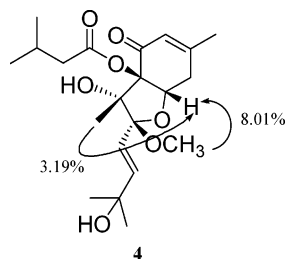


Figure 5. NOE difference experiment for **4**.

supported by the ^{13}C NMR spectrum of an acetate (**3a**): C-9 (δ 88.7) was deshielded by 4.45 ppm from that of **3**, but C-4 (δ 200.1) was shielded by 7.90 ppm.

The *Z* configuration of the C-2–C-10 and C-11–C-12 bonds in **3** was determined by NOE correlations (Figure 4). Moreover, the vicinal coupling constant ($J = 11.4$ Hz) of H-10 and H-11 established that the C-10–C-11 bond has an *s-trans* conformation.

Liginvolone D (**4**) was obtained as a pale yellow viscous oil, $[\alpha]_{\text{D}}^{25} +127.8^\circ$ (*c* 0.504, EtOH), showing a reddish purple spot on TLC when sprayed with 5% sulfuric acid reagent followed by heating. The molecular formula was determined as $\text{C}_{21}\text{H}_{32}\text{O}_7$ on the basis of high-resolution secondary-ion mass spectroscopy (HR-SIMS) (m/z 419.2046, $[\text{M} + \text{Na}]^+$, calcd 419.2046). The IR spectrum showed strong OH, ester, and α,β -unsaturated carbonyl bands at 3479, 1733, and 1682 cm^{-1} , respectively.

The ^1H NMR spectrum was similar to that of **2**, except that **4** had an *O*-methyl signal [δ 3.14 (3H, s)] and two hydroxyl protons [δ 1.69 (1H, brs), 1.78 (1H, brs)]. The H-10 [δ 5.51 (1H, d, $J = 16.0$ Hz)] and H-11 [6.11 (1H, d, $J = 16.0$ Hz)] coupling constants were larger by 4.8 Hz than those of **2**. Consequently, the structure of liginvolone D was elucidated using the ^1H – ^1H COSY, HSQC, HMBC, and DEPT spectra, as shown in Figure 1. The relative configuration was defined by NOE as shown in Figure 5, although the absolute configuration is still being investigated.

Compound **5** was obtained as a pale yellow viscous oil. The molecular formula was determined as $\text{C}_{22}\text{H}_{28}\text{O}_5$ on the basis of HREIMS (m/z 372.1940, $[\text{M}]^+$, calcd 372.1937). The IR spectrum showed strong OH, carbonyl, and aromatic ring bands at 3479, 1733, 1698, 1607, and 1576 cm^{-1} . In the UV spectrum, two absorption maxima were observed at 332.0 ($\log \epsilon$ 4.01) and 268 nm ($\log \epsilon$ 3.59).

The ^1H NMR spectrum was similar to that of osthenol,^{11,12} except that **5** had an oxymethylene signal [δ 4.47 (2H, s)] and an octanoyloxy spin pattern [δ 2.31 (2H, t,

$J = 7.3$ Hz), 1.61 (2H, tt, $J = 7.3, 7.3$ Hz), 1.28 (8H, m), 0.87 (3H, t, $J = 6.9$ Hz)]. A three-bond HMBC was observed between H-4' and C-1''. Consequently, compound **5** was defined as 4'-octanoyloxyosthenol on the basis of the analyses of ^1H – ^1H COSY, NOESY, HSQC, HMBC, and DEPT spectra, as shown in Figure 1.

Liginvolones B (**2**) and C (**3**) possess a new type of skeleton, in which a bridge was formed between C-3 and C-6 through an oxygen atom of the bisabolane skeleton. These compounds were unstable, similar to bisabolangelone (**6**). Liginvolones A (**1**) and C (**3**) were the main constituents of this plant together with suksdorfin, which is an angular-type pyranocoumarin, as shown in the Experimental Section.

Experimental Section

General Experimental Procedures. The instruments used in this study were a JASCO digital polarimeter (for specific rotation, measured at 23 $^\circ\text{C}$), a JASCO J-820 spectrometer (for CD and ORD measured at 23 $^\circ\text{C}$), a Perkin-Elmer 1720X-FTIR spectrometer (for IR spectra), a Hitachi M-80 spectrometer (for MS spectra), a Varian Mercury 300, unity Inova –500 (for NMR spectra measured in CDCl_3 , on the δ scale using tetramethylsilane as an internal standard), and a Shimadzu UV 2100 spectrophotometer. Chromatography was performed using silica gel PQS 100B (Fuji Silycia), Sephadex LH-20 (Pharmacia), and DIAION HP20 (Mitsubishi Chemical), Merck silica gel F254 plates, and Whatman TLC PLK5F silica gel plates.

Plant Material. Air-dried roots of *L. involucreatum* (2.7 kg) were collected from plants grown in Lijiang, Yunnan Province, China, in September 2000. A voucher specimen has been deposited in the Institute of Botany, Jiangsu Province, and Academia Sinica, Nanjing, China. The plant was identified by one of the authors (N.W.).

Extraction and Isolation. The roots were chopped into small pieces and extracted with EtOAc (10 L \times 5) under reflux. The combined EtOAc extracts were concentrated to dryness in vacuo. The residue (335 g) was subjected to column chromatography on silica gel (5.5 kg) eluted successively with a hexane–EtOAc solvent system with increasing polarity (5:1 \rightarrow 3:1) to afford 16 fractions [1 (73.3 g), 2 (45.1 g), 3 (2.1 g), 4 (0.7 g), 5 (12.0 g), 6 (16.3 g), 7 (18.5 g), 8 (31.2 g), 9 (13.7 g), 10 (30.1 g), 11 (11.7 g), 12 (3.7 g), 13 (2.9 g), 14 (5.8 g), 15 (10.0 g), 16 (35.9 g)]. Fractions 6, 7, and 8 were rechromatographed on silica gel followed by Sephadex LH-20 to give **1** (4.29 g), **2** (51.4 mg), **3** (3.39 g), **4** (11.4 mg), and **5** (6.9 mg) along with 16 known coumarins [umbelliferone (4.6 mg), scopoletin (1.3 mg), psoralen (29.5 mg), bergapten (40.1 mg), xanthotoxin (8.8 mg), isoimpinellin (8.8 mg), isopsoralen (49.7 mg), lomatin isovalerate² (3.38 g), nuttallin³ (50 mg), peguangienin⁴ (2.1 mg), suksdorfin⁵ (12.61 g), isosamidin⁶ (1.84 g), pteryxin⁵ (63.0 mg), ostruthin (118.2 mg), (*E*)-6-(7-hydroxy-3,7-dimethylocta-2,5-dienyl)-7-hydroxycoumarin (3.1 mg), 6-(6-hydroxy-3,7-dimethylocta-2,7-dienyl)-7-hydroxycoumarin (6.8 mg)], ferulic acid (784.0 mg), 4-hydroxy-3-methoxycinnamaldehyde (4.2 mg), ligustilide (6.4 mg), and falcariindiol (267.8 mg).

Liginvolone A (1): pale yellow viscous oil; $[\alpha]_{\text{D}}^{25} +180.6^\circ$ (*c* 0.498, EtOH); HREIMS m/z 348.1930 $[\text{M}]^+$ (calcd for $\text{C}_{20}\text{H}_{28}\text{O}_5$ 348.1937); UV λ_{max} (MeOH) nm ($\log \epsilon$) 269.0sh (4.22), 260.0 (4.38), 253.4 (4.39); IR ν (cm^{-1}) 3451, 1738, 1678; ^1H and ^{13}C NMR data, see Tables 1 and 2.

Liginvolone B (2): pale yellow viscous oil; $[\alpha]_{\text{D}} +83.4^\circ$ (*c* 0.500, EtOH); HREIMS m/z 348.1924 $[\text{M}]^+$ (calcd for $\text{C}_{20}\text{H}_{28}\text{O}_5$ 348.1937); UV λ_{max} (MeOH) nm ($\log \epsilon$) 260.6sh (4.18), 253.0 (4.19), 210.4 (4.07), 208.0 (4.07); IR ν (cm^{-1}) 1739, 1682; ^1H and ^{13}C NMR data, see Tables 1 and 2.

Liginvolone C (3): pale yellow viscous oil; $[\alpha]_{\text{D}} +1.8^\circ$ (*c* 0.500, EtOH); HREIMS m/z 434.2650 $[\text{M}]^+$ (calcd for $\text{C}_{25}\text{H}_{38}\text{O}_6$ 434.2668); UV λ_{max} (MeOH) nm ($\log \epsilon$) 269.5 (4.33); IR ν (cm^{-1}) 3462, 1732, 1674; ^1H and ^{13}C NMR data, see Tables 1 and 2.

Acetylation of 3. Compound **3** (20 mg) was treated with Ac₂O (0.5 mL) in pyridine at room temperature for 12 h. After workup, the products were subjected to preparative TLC (CH₂-Cl₂-MeOH, 50:1). Acetate (**3a**) was obtained as a pale yellow viscous oil (4.1 mg). **3a**: ¹H NMR (CDCl₃) δ 2.54 (1H, dd, *J* = 19.1, 2.8 Hz, H-5α), 2.45 (1H, d, *J* = 19.1 Hz, H-5β), 2.27 (1H, dd, *J* = 15.1, 2.8 Hz, H-7α), 2.36 (1H, dd, *J* = 15.1, 7.1 Hz, H-7β), 5.30 (1H, d, *J* = 7.1 Hz, H-8), 5.47 (1H, d, *J* = 11.4 Hz, H-10), 6.28 (1H dd, *J* = 11.4, 1.2 Hz, H-11), 4.72 (1H, d, *J* = 12.4 Hz, H-13), 4.66 (1H, d, *J* = 12.4 Hz, H-13), 1.86 (1H, d, *J* = 1.2 Hz, H-14), 1.32 (1H, s, H-15), 1.33 (1H, s, H-16), 2.16 (3H, s, COCH₃), 2.32 (2H, t, *J* = 7.4 Hz, H-2'), 1.62 (2H, tt, *J* = 7.4, 7.4 Hz, H-3'), 1.23–1.34 (12H, brs, H-4'-9'), 0.88 (3H, t, *J* = 7.0 Hz, H-10'); ¹³C NMR (CDCl₃) δ 155.9 s (C-2), 82.8 s (C-3), 200.1 s (C-4), 51.3 t (C-5), 71.2 s (C-6), 43.5 t (C-7), 76.5 d (C-8), 88.7 s (C-9), 94.9 d (C-10), 122.6 d (C-11), 130.3 s (C-12), 63.0 t (C-13), 21.8 q (C-14), 16.9 q (C-15), 25.6 q (C-16), 169.4 s (COCH₃), 21.1 q (COCH₃), 173.9 s (C-1'), 34.3 t (C-2'), 25.0 t (C-3'), 22.6–31.8 t (C-4'-9'), 14.1 q (C-10').

Liginvolone D (4): pale yellow viscous oil; [α]_D +127.8° (*c* 0.504, EtOH); HR-SIMS *m/z* 419.2046 [M + Na]⁺ (calcd for C₂₁H₃₂O₇Na 419.2046); UV λ_{max} (MeOH) nm (log ε) 236.0 (3.93); IR ν (cm⁻¹) 3479, 1733, 1682; ¹H and ¹³C NMR data, see Tables 1 and 2.

4'-Octanoyloxyosthenol (5): pale yellow viscous oil; HRE-IMS *m/z* 372.1940 [M]⁺ (calcd for C₂₂H₂₈O₅ 372.1937); UV λ_{max} (MeOH) nm (log ε) 332.0 (4.01), 268.0 (3.59), 227.6sh (4.04), 211.2 (4.53); IR ν (cm⁻¹) 3290, 1733, 1698, 1607, 1576; ¹H and ¹³C NMR data, see Tables 1 and 2.

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