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Two New Sesquiterpenes from *Ligularia veitchiana*

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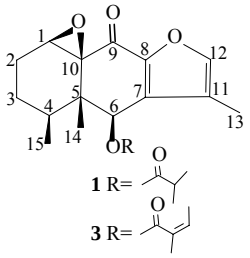
Abstract: A new furanoeremophilane and a new eudesmane were isolated from the roots of *Ligularia veitchiana*. Their structures were elucidated as 1β, 10β-epoxy-6β-isobutyryloxy-9-oxo-furanoeremophilane and 8α-hydroxy-4 (15), 11-eudesmadiene by spectroscopic methods.

Keywords: *Ligularia veitchiana*, Compositae, furanoeremophilane, eudesmane.

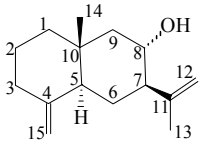
Ligularia veitchiana has long been used as Chinese folk medicine for the treatment of influenza, cough, ulcer, and tuberculosis[1]. Here we report the structure elucidation of a new furanoeremophilane **1** and a new eudesmane **2** from the roots of *L.veitchiana*.

Compound **1**, colorless oil, $[\alpha]_D^{21}$ –17.6 (*c* 0.50, $CHCl_3$). Its EIMS exhibited a molecular ion peak at *m/z* 332. The molecular formula $C_{19}H_{24}O_5$ was deduced by the support of its MS, ^{13}C-NMR and DEPT spectra (5×CH_3, 2×CH_2, 5×CH, and 7×C). The ^{1}H- and ^{13}C-NMR spectra of compound **1** (**Table 1**) were very similar with those of the known compound **3** except for the presence of an isobutyryl group instead of the angeloyl group at C-6 in **3**[2], this was confirmed by the fragment (*m/z* 262 [M-$COCH(CH_3)_2]^+$) in the EIMS spectrum. Its IR bands (1738, 1690 cm^{-1}) and the UV absorption (286 nm) further evidenced that compound **1** possesses the 9-oxo-furanoeremophilane character. The stereochemistry of **1** was identical with that of **3** by comparing their ^{1}H-NMR data and coupling constants (**Table 1**). Thus, the structure of compound **1** was proved to be 1β, 10β-epoxy-6β-isobutyryloxy-9-oxofuranoeremophil-ane.



1 R=

3 R=



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Compound **2**, colorless oil, $[\alpha]_D^{20}$ +14.8 (*c*, 1.19, $CHCl_3$). The molecular formula $C_{15}H_{24}O$ was deduced by its EIMS (*m/z* 220 $[M]^+$) together with the ^{13}C-NMR and DEPT spectra (2×CH_3, 7×CH_2, 3×CH and 3×C). A hydroxyl group was indicated by the IR absorption band (3420 cm^{-1}) and the fragment (*m/z* 202 $[M-H_2O]^+$) in EIMS spectrum. Its ^{1}H-NMR spectrum showed the presence of –C(CH_3)=CH_2 (δ 4.71, 4.72, each 1H, br and 1.75, 3H, br), >C=CH_2 (δ 4.54, 4.82, each 1H, br) and a methyl group (δ 0.73, 3H, s). The above information and the ^{13}C-NMR data (**Table 1**) suggested that compound **2** was an eudesmane, and Me-10 and isoallyl-7 groups were in β configurations[3]. H-5 was deduced to be α configuration by its coupling constants: $J_{5,\ 6\beta}$=11.2 Hz (**Table 1**). Therefore, the only position for the hydroxyl group was 8α, which confirmed by the *J* values of H-8: $J_{8,\ 9\alpha}=J_{8,\ 7\alpha}$=11.2 Hz, $J_{8,\ 9\beta}$=5.0 Hz. Thus, the structure of **2** was elucidated as 8α-hydroxy-4 (15), 11-eudesmadiene.

Table 1 ^{1}H-NMR (400 MHz), ^{13}C-NMR (100 MHz) and DEPT data of **1,2** ($CDCl_3$, δ_{ppm}, J_{Hz})

No.	**1** δ_H (α/β)	**2** δ_H (α/β)	**1** δ_C (DEPT)	**2** δ_C (DEPT)
1	3.31 (d, 4.8)	1.31 (m)/1.60 (m)	62.4(CH)	45.6(CH_2)
2	1.42(m)/2.03 (m)	1.60 (m)/1.45 (m)	24.7(CH_2)	26.3(CH_2)
3	2.00(m)/1.53 (m)	1.72-1.87 (m)	18.8(CH_2)	40.7(CH_2)
4	1.79 (m)	-	31.6(CH)	147.7(C)
5	-	1.82 (brd, 11.2)	45.2(C)	49.1(CH)
6	6.60 (s)	1.57(dt, 12.0, 5.0)/1.23 (dt, 12.0, 11.2)	68.6 (CH)	29.0(CH_2)
7	-	2.67 (dt, 5.0, 11.2)	136.8(C)	46.4(CH)
8	-	3.89 (dt, 5.0, 11.2)	146.4(C)	68.0(CH)
9	-	1.98 (dd, 12.0, 11.2)/1.63 (dd, 12.0, 5.0)	181.0(C)	51.0(CH_2)
10	-	-	65.7(C)	35.3(C)
11	-	-	121.5(C)	150.5(C)
12	7.44 (brs)	4.71 (brs)/4.72 (brs)	146.6(CH)	108.0(CH_2)
13	1.91 (brs)	1.75 (brs)	8.4(CH_3)	21.0(CH_3)
14	1.20 (s)	0.73 (s)	16.1(CH_3)	17.2(CH_3)
15	1.00 (d, 7.3)	4.54 (brs)/4.82 (brs)	15.2(CH_3)	108.3(CH_2)
*16			176.5(C)	

*isobutyryl δ_H 2.69(qq, 7.2, 6.8), 1.25 (d, 7.2), 1.23 (d, 6.8); δ_C 34.1(CH), 19.3(CH_3), 18.5(CH_3).

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