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Sesquiterpene Esters from *Salvia roborowskii*

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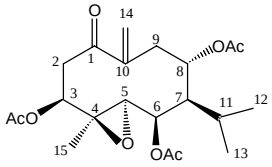
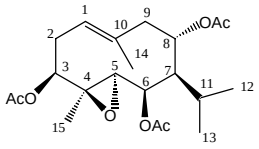
Abstract: Two new sesquiterpene esters, 3β, 6β, 8α-triacetyl-4β, 5α-epoxy -1- oxogermacr-10(14)-ene (**1**) and 3β, 6β, 8α-triacetyl-4β, 5α-epoxygermacr-1(10)-ene (**2**) were isolated from the whole plant of *Salvia roborowskii* Maxim. Their structures were elucidated by means of spectral data (2DNMR and HRMS).

Keywords: *Salvia roborowskii*, Labiatae**,** sesquiterpene, germacrane.

Salvia roborowskii Maxim, with a Chinese name "ye zhi ma", an annual or biennial herb distributed widely in Gansu province of China, has been used as a traditional folk medicine for the treatment of hepatitis and toothache[1]. The chemical constituents isolated from EtOAc and *n*-BuOH extracts of this species have been reported [2], we now report two new sesquiterpenes **1** and **2** isolated from the petroleum ether extract of same plant.



1



2

Compound **1** as colorless gum, $[\alpha]_D^{26}$ +29.0 (c 2.0, $CHCl_3$), has the molecular formula $C_{21}H_{30}O_8$ according to the FABMS ($[M+1]^+$ at *m/z* 411), along with ^{13}CNMR and DEPT spectral data (**Table 1**). The IR spectrum showed the absorptions for esters (1743 and 1240 cm^{-1}) and ketone (1677 cm^{-1}). Its ^{1}H and ^{13}CNMR spectra of **1** displayed some characteristic signals for three acetyl groups and a methylene group (**Table 1 and 2**), and the ^{13}CNMR spectrum also gave a typical signal at δ c 199.4 due to an α,β-unsaturated ketone. By detail observation of ^{1}H and ^{13}CNMR spectra and comparison of its spectral data with those of the known sesquiterpenes [3,4], **1** appears to be a sesquiterpene with germacrane skeleton. The locations of these groups were accomplished using ^{1}H-^{1}H COSY, the H-3 showed correlation with H-2, H-6 showed correlation with H-5 and H-7, H-8 showed correlation with H-7 and H-9. The relative stereochemistry of **1** was

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determined on the basis of the correlations between H-3α and H-15, H-6α and H-15, H-5β and H-8β, H-5β and H-9β, H-7α and H-9α in the NOESY spectrum. Assignment of ^{1}H and $^{13}CNMR$ data was made by the aid of HMQC spectrum. Therefore, **1** was elucidated as 3β, 6β, 8α-triacetyl-4β, 5α-epoxy-1-oxogermacr-10(14)-ene.

Compound **2,** $C_{21}H_{32}O_7$ (HRSIMS: found 397.2221, calcd. 397.2180), was isolated as colorless gum, $[\alpha]_D^{26}$ -12.7 (c 16.5, $CHCl_3$). Its IR spectrum showed the absorption bands for esters (1740 and 1239 cm^{-1}). Comparing the ^{1}H and $^{13}CNMR$ spectra data of **2** with those of **1**, indicated that the most data of **2** were very similar as those of **1** except for the extra signals of a methyl (δ_H 1.65) and a double bond (δ_H 5.35, δ_C 123.8 d, δ_C 132.6 s) in **2**, which replaced the ketone (δ c199.4 s) and methylene (δ c147.5 s, δ c129.3 t) groups in **1**. Thus, **2** was identified as 3β, 6β, 8α-triacetyl-4β, 5α-epoxygermacr-1(10)-ene.

Table 1 $^{1}HNMR$ data for compound **1** and **2** ($CDCl_3$, TMS, δ ppm, 400MHz)

proton	**1**	**2**
1	5.35 (m)	5.35 (m)
2α	3.32 (dd, J=13.6, 3.8Hz)	2.52 (m)
2β	2.80 (brd, J=13.6Hz)	2.25 (brd, J=12.0Hz)
3	5.17 (t, J=3.8Hz)	5.05 (t, J=3.0Hz)
5	3.07 (d, J=7.2Hz)	3.00 (d, J=6.8Hz)
6	4.82 (brd, J=7.2Hz)	4.83 (brd, J=6.8Hz)
7	1.47 (brd, J=8.6Hz)	1.32 (brd, J=7.0Hz)
8	5.41 (m)	5.35 (m)
9α	2.54 (t, J=11.4Hz)	
9β	2.90 (brd, J=11.4Hz)	2.52 (m)
11	1.81 (m)	1.80 (m)
12	1.13 (d, J=6.4Hz)	0.99 (d, J=6.4Hz)
13	0.85 (d, J=6.4Hz)	0.80 (d, J=6.4Hz)
14	6.05(s)	1.65 (s)
14'	5.99(s)	
15	1.37 (s)	1.10 (s)
OAc	2.06 (s), 2.06 (s), 1.97 (s)	2.00 (s), 1.95(s), 1.92 (s)

Table 2 $^{13}CNMR$ data for compound **1** and **2** ($CDCl_3$,TMS, δ ppm,100MHz)

carbon	**1**	**2**	carbon	**1**	**2**
1	199.4s	123.8d	10	147.5s	132.6s
2	38.4t	29.8t	11	26.0d	25.7d
3	69.2d	71.0d	12	22.8q	20.8q
4	57.3s	58.1s	13	20.9q	20.8q
5	59.6d	60.1d	14	129.3t	22.9q
6	72.2d	73.6d	15	16.3q	15.4q
7	47.5d	47.3d	OAc	169.8s, 20.9q	169.4s, 20.7q
8	68.4d	71.9d		169.8s, 20.6q	169.3s, 20.7q
9	38.4t	40.1t		169.4s, 20.5q	169.1s, 20.4q

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