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A New Sesquiterpene Lactone from *Scorzonera austriaca*

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Abstract: A new guaianolide was isolated from the roots of *Scorzonera austriaca*. The structure was elucidated on the basis of spectral methods including 2D NMR.

Keywords: *Scorzonera austriaca*, compositae, sesquiterpene, guaianolide.

Scorzonera austriaca occurs in the northwestern mountainous regions in China. Its root is used as Tibetan traditional medicine for the treatment of many diseases, such as curing fever, carbuncle and mastitis[1]. No phytochemical studies have been described for *S. austriaca*. In this paper, we report the structural elucidation of a new guaianolide isolated from the acetone extract of its roots.

Compound **1** afforded as colorless crystal, $[\alpha]_D^{26}$- 41(c 0.18, $CHCl_3$). Its HR-ESIMS provided a quasi-molecular ion $[M+NH_4]^+$ at *m/z* 284.1859 (calcd. 284.1856), suggesting the molecular formula of $C_{15}H_{22}O_4$ and 5 degrees of unsaturation. The IR (KBr) bands were at 3377 (OH), 1758 (γ-lactone), 1640 cm^{-1} (double bond). The ^{13}C NMR and DEPT spectra contained 15 carbon signals. The ^1H NMR spectrum showed exocyclic double bond at δ 5.01, 4.98 (s, 1H, each); α-methyl-γ-lactone group at δ 4.41 (dd, 1H, *J*=11.2, 9.2 Hz, H-6), 1.80 (ddd, 1H, *J*=11.2, 9.2, 3.2 Hz, H-7), 1.44 (s, 3H, H-13) and methyl at δ 1.00 (d, 3H, *J*=7.2 Hz, H-15). All those data indicated a guaianolide-type skeleton with a terminal double bond[2]. Its structure was further confirmed by HMBC correlations: H-2/C-1, C-3, C-4, C-5; H-4/C-1, C-2, C-5, C-15; H-5/C-1, C-4, C-6, C-7, C-15; H-14/C-1, C-9; H-15/C-3, C-4, C-5 and H-13/C-11, C-7. The signal for the bearing oxygen carbon at δ 73.8 (C-3) correlated with H-1, H-2, H-4, H-15 and that at 74.5 (C-11) correlated with H-13 respectively, which indicated two hydroxyl groups located at C-3 and C-11 respectively. Finally, the relative stereochemistry of **1** was established by a selective NOE difference experiments (**Figure 1**). When H-6 was assigned as β-orientation, NOEs supported β-orientation of the hydroxyl group at C-3, the methyl groups at C-4 and C-11, while H-1, H-5, H-7 and the hydroxyl group at C-11 had α-orientation respectively. Thus, compound **1** was assigned as 3β, 11α-dihydroxy-4β- methyl-guaia-10 (14)-en-12, 6α-oli-

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Figure 1 The structure and significant 1D NOE corrections of **1**

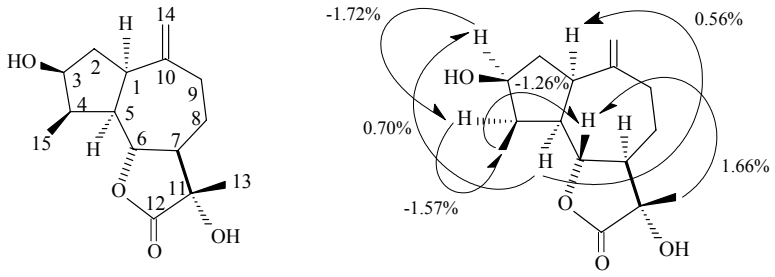

Table 1 ^{1}H NMR (400 MHz), ^{13}C NMR(75 MHz) data of **1** ($CDCl_3$, δ ppm, *J* Hz)

No.	δ_H	δ_C	DEPT	No.	δ_H	δ_C	DEPT
1	2.71 (m)	41.4	CH	9	2.68 (dd,12.4, 8.0, 4.4,1.8)	38.6	CH_2
2’	1.99 (ddd, 13.6, 10.8, 7.6)			10	-	148.1	C
3	4.24 (ddd, 12.4, 10.4, 6.8)	73.8	CH	11		74.5	C
4	2.35 (m)	40.5	CH	12	-	177.4	C
5	2.16 (ddd, 11.6, 11.2, 6.8)	47.3	CH	13	1.44 (s)	22.4	CH_3
6	4.4 1(dd, 11.2, 9.2)	82.7	CH	14	5.01 (brs)	111.9	CH_2
7	1.80 (ddd, 11.2, 9.2, 3.2)	53.2	CH	14’	4.98 (brs)		
8	1.73 (m)	25.7	CH_2	15	1.00 (d, 7.2)	8.3	CH_3
8’	1.66 (m)						

de[3,4]. Analysis of ^{1}H-^{1}HCOSY and HMBC spectra allowed the assignments of the proton and carbon signals of **1** in **Table 1.**

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