

A New Guaianolide from *Saussurea macrota*

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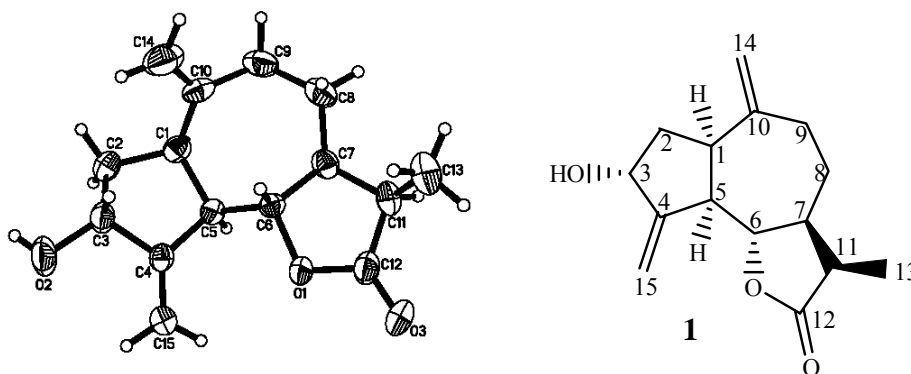
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Abstract: A new guaianolide was isolated from *Saussurea macrota*. Its structure was elucidated by NMR spectroscopic and X-ray diffraction methods.

Keywords: *Saussurea macrota*, Compositae, sesquiterpene, guaianolide.

From the methanol extracts of *Saussurea macrota* Franch, a sesquiterpene **1** was afforded as colorless column crystals mp 122-124°C, $[\alpha]_D^{20} +31.0$ (c 2.5, CHCl₃). The molecular formula was determined as C₁₅H₂₀O₃ by the molecular ion peak $[M]^+ = 248$ in the EIMS spectrum and the ¹³C NMR and DEPT data (**Table 1**). Its IR (KBr) spectrum showed bands at 3457 (OH), 1751 (γ-lactone ring) and 1637 (double bonds) cm⁻¹. In the ¹H NMR, one methyl group appeared at δ 1.15 (d, 3H, J=8.0Hz), two characteristic methylene signals appeared at δ 4.74 (s, 1H), δ 4.90 (s, 1H), δ 5.34 (s, 1H), δ 5.44 (s, 1H), and ¹³C NMR showed two oxygenated groups δ 85.1 (CH), δ 74.6 (CH), corresponding to the signals δ 3.98 (t, 1H, J=9.5Hz) and δ 4.67 (t, 1H, J=6.2Hz) in the ¹H NMR, indicating **1** possessed the guaianolide skeleton, just like those of known 3-hydroxyguaia-4(15), 10(14)-diene-12, 6α-olides^{1,2}.

Figure 1 Structure of compound **1**



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Fortunately, the single crystal was obtained. Compound **1** was detected as 3 α -hydroxy-11 α H-guaia-4(15), 10(14)-dien-12, 6 α -olide by X-ray diffraction analysis.

Table 1 ^1H NMR (400MHz), ^{13}C NMR (75MHz) and DEPT data of **1** (CDCl_3 , TMS, δ , ppm)

H	δ_{H} (α / β), J (Hz)	C	δ_{C}	DEPT
1	3.05m	1	43.6	CH
2	1.87m / 2.15ddd (J=13.5, 6.2, 4.2)	2	39.5	CH ₂
3	4.67dd (J=6.2, 6.2)	3	74.4	CH
		4	154.5	C
5	3.05m	5	49.6	CH
6	3.98dd (J=9.5, 9.5)	6	84.8	CH
7	1.90dddd(10.0, 9.5, 8.0, 4.2)	7	39.3	CH
8	2.42dddd / 1.35dddd (J=12.7, 4.0, 4.0, 4.2 / 12.7, 4.0, 10.0, 10.0)	8	28.8	CH ₂
9	1.95ddd / 2.54ddd (J=12.8, 10.0, 4.0 / 12.8, 4.0, 4.0)	9	37.7	CH ₂
		10	149.3	C
11	2.69dq (J=8.0, 8.0)	11	45.3	CH
		12	179.8	C
13	1.15d (J=8.0)	13	11.4	CH ₃
14	4.74s / 4.90s	14	112.8	CH ₂
15	5.34s / 5.44s	15	112.3	CH ₂

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