Chinese Chemical Letters Vol. 13, No. 8, pp 752 – 753, 2002
http://www.imm.ac.cn/journal/ccl/html

A New Sesquiterpene from *Saussurea parviflora*

Zhong Duo YANG, Shuo LI, Cheng Shan YUAN, Zhong Jian JIA*

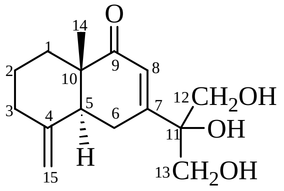
Department of Chemistry, National Laboratory of Applied Organic chemistry, Lanzhou University
Lanzhou 730000

Abstract: A new sesquiterpene: 11,12,13-trihydroxy-4(15),7(8)-eudesmdien-9-one was isolated from *Saussurea parviflora*. The structure was elucidated on the basis of spectral evidence.

Keywords: Composite, *Saussurea parviflora*, eudesmane, sesquiterpene.

A new eudesmane sesquiterpene was obtained from the whole plant of *Saussurea parviflora* and its structure was elucidated to be 11,12,13-trihydroxy-4(15),7(8)-eudesmdien-9-one (**1**).

Compound **1,** colorless gum, $[\ ]^{20}_{D}$ +64.9 (c 0.15, $CHCl_3$), UV λ max($CHCl_3$) 324. The IR spectrum revealed absorptions of α, β-unsaturated carbonyl (1655cm^{-1}) and hydroxy groups (3450,3434,3321cm^{-1}). The molecular formula $C_{15}H_{22}O_4$ was deduced from FABMS spectrum at *m/z* 267 $[M+1]^+$ in coupled with its ^{1}H, ^{13}CNMR and DEPT data (**Table 1**). Five unsaturations, two of which were attributed to the α, β unsaturated carbonyl groups, δ_H 6.13 (s), δ_C 206.06, 162.52, 123.59, and one of which caused by the terminal double bond δ_H 4.93, 4.69 (br s) δc 147.78, 108.48, implied presence of bicyclic carbon skeleton. In the ^{13}CNMR spectrum of **1** a tertiary hydroxyl δ_C78.01 (C_{11}) and two hydroxymethyl groups δ_C 65.78 (C_{12}) and 65.61 (C_{13}), indicated that **1** contained a glyceryl moiety which was also confirmed by the fragment peaks at *m/z* 235$[M\text{-}CH_2OH]^+$ and *m/z* 175$[M\text{-}(CH_2OH)_2COH]^+$ in the EIMS spectrum. An angular methyl δ_H 0.88 (s) δ_C 15.28 and a quaternary carbon atom δc 45.97 showed that **1** belonged to a structure of eudesmane and the angular methyl should be β orientated[1, 2]. The positions of the terminal double bond and carbonyl group were determined to be C-15 and C-9 respectively, by HMBC which showed the cross peaks: C-15 to H-5, H-3;



1

---

[*] E-mail: zhengrl@lzu.edu.cn

C-4 to H-5, H-3 and C-9 to Me-14. In ^{1}HNMR, H-8 gave a singlet at δ_H 6.13, which showed that the carbonyl group and glyceryl moiety should be at C-9 and C-7 respectively. A quartet at δ_H 2.47 (J=10.0, 5.0 Hz, H-5) suggested H-5 should be α orientated. Thus, the structure of compound **1** was confirmed.

Table 1 ^{1}HNMR (400MHz), ^{13}CNMR (100MHz) and DEPT date of **1** ($CDCl_3$)

H	δ_H	C	δ_C	DEPT
1α	1.41(br dt, 13.2, 3.2)	1	32.5	CH_2
1β	1.52(br d, 13.2)	2	22.70	CH_2
2	1.71(m)	3	35.95	CH_2
3α	1.93(br dt, 13.2, 3.2)	4	147.78	C
3β	1.98(br d, 13.2)	5	46.32	CH
5	2.47(dd, 10.0, 5.0)	6	25.87	CH_2
6α	2.34(dd, 13.2, 5.0)	7	162.52	C
6β	2.36(dd, 13.2, 10.0)	8	123.59	CH
8	6.13(s)	9	206.06	C
12	3.79(d, 8.4)	10	45.97	C
12'	3.77(d, 8.4)	11	78.01	C
13	3.76(d, 9.0)	12	65.78	CH_2
13'	3.73(d, 9.0)	13	65.61	CH_2
14	0.88(s)	14	15.28	CH_3
15	4.93(br s)	15	108.48	CH_3
15'	4.69(br s)			

Acknowledgments

This work was financed by The NNSFC (No. 29972017) and the FMEC (No. 98073003).

References

1. C. Zdero, F. Bohlmann, R. M. King, *Phytochemistry*, **1990**, *29* (10), 3201.
2. X. Hong, B. G. Wang, J. Zhou, X. J. Hao*, *Chin. Chem. Lett.*,**1998**,*9* (10), 939.

Received 13 November, 2001