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Two New Triterpenoids from *Saussurea petrovii*

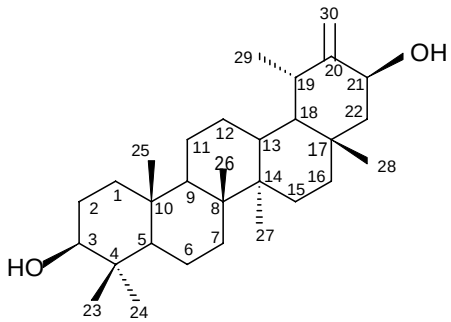
Jing Qiu DAI, Bo ZHOU, Yu Li WANG, Li YANG*, Zhong Li LIU

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

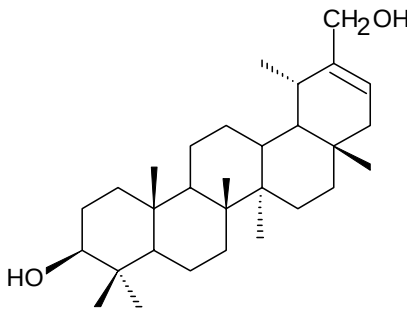
Abstract: Two new taraxastane-type triterpenes, 3β, 21β-dihydroxyl-20(30)-en-taraxastane **1** and 3β, 30-dihydroxy-20(21)-en-taraxastane **2**, were isolated from *Saussurea petrovii*. Their structures were elucidated by spectral methods (EIMS, IR, 1D and 2DNMR).

Keywords: *Saussurea petrovii*, Compositae, taraxastane-type triterpenoid, 3β, 21β-dihydroxyl-20(30)-en-taraxastane, 3β, 30-dihydroxyl-20(21)-en-taraxastane.

Saussurea petrovii Lipsch (Compositae) is a perennial herb mainly distributed in Gansu and Inner Mongolia provinces of China. Its whole herb has been used as a folk remedy for the treatment of rheumatism and bleeding[1]. In order to find active principles, the chemical constituents of *Saussurea petrovii* were studied and two new triterpenoids **1** and **2** were isolated from the acetone extract of the rhizome. In this paper, we report the structural elucidation of the compound **1** and **2**.



1



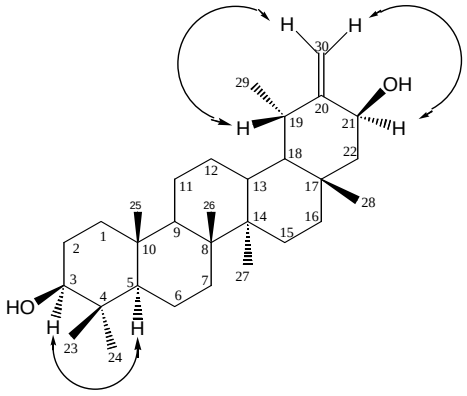
2

Compound **1** was obtained as colorless crystals, mp 256-258^0 C, $[\alpha]_D^{25}$ +225 (c 0.09, $CHCl_3$). The EIMS revealed the molecular ion peak *m/z* 442. the ^{13}C NMR and DEPT spectrum of **1** exhibited 30 carbon signals (7×CH_3, 10×CH_2, 7×CH, 6×C). Then the molecular composition of **1** was deduced to be $C_{30}H_{50}O_2$, which was proved by HREIMS (*m/z* 442.3819, calcd. 442.3811). The ^{1}H NMR (**Table 1**) spectrum indicated the presence of seven methyl groups, of which six were singlets (δ 0.77, 0.77, 0.85, 0.94, 0.97, 1.02) and one was a doublet (δ 1.21, d, J = 7.2). These data suggested that **1** was

an ursane-type or a taraxastane-type triterpenoid, and the signal at δ 48.4 (C-18) confirmed **1** to be a taraxastane-type triterpenoid [2].

Absorption for hydroxyl (3234 cm^{-1}) and double bond (1637 cm^{-1}) were observed in IR. The ^1H NMR spectrum of **1** further revealed two exomethylene proton at δ 4.89, 4.99 (each br. s) and two secondary hydroxyl groups (δ 3.21, 1H, dd, J=11.2, 4.9 Hz; δ 4.40, 1H, dd, J = 10.1, 5.2 Hz), whose chemical shifts and splitting pattern were typical of 3β, 21β equatorial hydroxyl in a conventional taraxastane-type triterpenoid [3,4,5]. The signal at δ 3.21 (H-3α) showed correlation with the signal at δ 1.56 (1H, m, H-2α) and the signal at δ 4.40 (H-21α) showed correlation with H-22α (δ 1.99, dd, J=13.9, 9.0) in the ^1H-^1H COSY sprctrum of **1,** revealing the following partial structure -CH_2(1)-CH_2(2)-CH(3)- and –CH(21)-CH_2(22)-. The C-C interconnectivity of all the fragments was established through HMBC experiment, for example, H-2α and Me-23, 24 correlating to C-3 (δ 78.9); H-22 and Me-28 correlating to C-17 (δ 34.2); H-19 and H-21 correlating to C-20 (δ 156.6). Moreover, in the NOESY spectrum, the correlation between H-3 and H-5α (**Figure 1**) suggested that H-3 must be α-oriented. The above information suggested compound **1** to be 3β, 21β-dihydroxyl-20(30)-en-taraxastane.

Figure 1. The key correlations of **1** in NOESY



Compound **2** was also obtained as colorless crystals, mp 198~200^{0}C, $[\alpha]_D^{25}$ +116 (c 0.35, $CHCl_3$). The EIMS revealed the molecular ion peak *m/z* 442, as well as the ^1H, ^{13}C NMR and DEPT data (**Table 1**) indicated that molecular formula should be $C_{30}H_{50}O_2$, which was confirmed by HREIMS (*m/z* 442.3811, calcd. 442.3811). The ^1H and ^{13}C NMR spectrum of **2** showed that **2** was another taraxastane-type triterpenoid by comparing with those of **1**. The ^1H and ^{13}C NMR data of **2** were quite similar to those of Pseudotaraxasterol[5], a known taraxastane-type triterpenoid, except that there were differences in the chemical shifts of C-19, C-20, C-30 and an additional hydroxyl group was present. These characteristics indicated that C-30 is hydroxylated. This was also supported by HMQC and HMBC experiments. Thus, compound **2** was deduced as 3β, 30-dihydroxyl-20(21)en-taraxastane.

Table 1 ^{1}H and ^{13}C NMR spectrum data of compounds **1** and **2** in $CDCl_3$

compounds			**1**		**2**	
position	δ_C	δ_H	couplings in HMBC	couplings in ^{1}H-^{1}H COSY	δ_C	δ_H
1α		1.73		H-1β, H-2α, H-2β		1.73
1β	38.7	0.92	H-2, H-3, H-25	H-1α, H-2β	38.8	0.91
2α		1.56		H-1α		1.55
2β	27.4	1.54	H-1, H-3, H-23	H-3, H-1α	27.6	1.54
3	78.9	3.21	H-2, H-23, H-24	H-2α	79.0	3.21
4	38.9		H-3, H-5, H-23, H-24		38.9	
5	55.3	0.70	H-23, H-24, H-25,H-6	H-6	55.3	0.76
6	18.3	1.50	H-5, H-7	H-5, H-7	18.3	1.54
7	34.0	1.36	H-26, H-6	H-6	34.2	1.36
8	40.9		H-7, H-9, H-26, H-27		41.1	
9	50.4	1.40	H-11, H-25, H-26	H-11α, H-11β	50.4	1.36
10	37.1		H-1, H-5, H-9, H-25		37.1	
11α		1.59		H-9, H-11β, H-12α		1.59
11β	21.4	1.26	H-9, H-12, H-13	H-9, H-11α, H-12α, H-12β	21.6	1.27
12α		1.63		H-11α , H-11β, H-12β, H-13		1.62
12β	26.2	0.94	H-11, H-13, H-9, H-18	H-11β, H-13, H-12α	27.0	0.92
13	38.9	1.53	H-12, H-18, H-27	H-12α, H-12β, H-18	39.2	1.55
14	42.2		H-13,H-15, H-26,H-27		42.4	
15α		1.65		H-15β, H-16		1.68
15β	26.4	1.11	H-27, H-16, H-28	H-15α, H-16	27.4	1.11
16	37.7	1.51	H-15, H-28	H-15α, H-15β	36.7	1.54
17	34.2		H-18, H-22, H-28		34.5	
18	48.4	1.24	H-13, H-29, H-19,H-28	H-13, H-19	48.5	1.25
19	38.1	2.17	H-18, H-21, H-29	H-18, H-29	32.0	2.04
20	156.6		H-19, H-30, H-21		143.7	
21	71.3	4.40	H-30, H-22α	H-22α, H-22β	120.7	5.59
22α		1.99		H-21		1.88
22β	48.8	1.31	H-21, H-28	H-21	41.7	1.88
23	15.4	0.77	H-3, H-5		15.4	0.75
24	27.9	0.97	H-3, H-5		27.9	0.96
25	16.2	0.85	H-1, H-9, H-5		16.3	0.85
26	15.9	1.02	H-9, H-7, H-27		16.0	1.04
27	14.8	0.94	H-13, H-15, H-26		14.8	0.95
28	18.2	0.77	H-16, H-22, H-18		17.7	0.76
29	28.4	1.21	H-19, H-18, H-30	H-19	22.5	1.00
30α		4.99				4.13
30β	113.6	4.89	H-19, H-21, H-29		65.5	4.02

Acknowledgments

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References

1. Editorial Board of Flora Inner Mongoliaensis, *Flora Inner Mongolia*, **1982**, *6*, 244.
2. S. B.Mahato, A. P. Kundu, *Phytochemistry*,**1994**, *37*,1517.
3. D. H. S. Horn, L. A. lamberton, *Aust. J.Chem.*, **1964**, *17*,447.
4. F. A. L. Anet, *J. Am. Chem. Soc*.,**1960**, *84*, 1053.
5. W. F. Reynolds, S. McLean, *Tetrahedron*, **1986**, *42*, 3419.

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