

A New Lignan Glucoside from *Lancea tibetica*

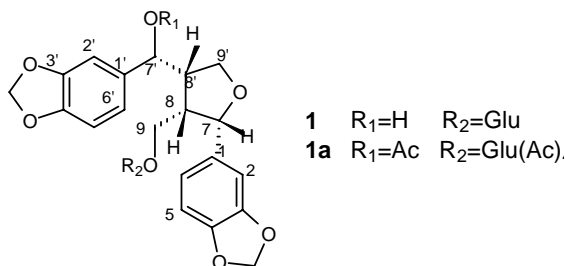
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Abstract: A new 7-9'-monoepoxy tetrahydrofuran type lignan glucoside with the cis-relationship of H-7 and H-8, named tibeticoside A **1**, was isolated from the medicinal whole plants of *Lancea tibetica*. Its structure was elucidated by spectroscopic methods and chemical transformation.

Keywords: *Lancea tibetica*; scrophulariaceae; tibeticoside A.

L. tibetica Hook. f. et Thoms. is an important Tibetan medicine used for treatment of many diseases¹. The lignan glycosides and triterpenes from this plant have been reported^{2,3} by Huidi Zhang et al. This paper describes the structure elucidation of a new lignan glucoside, named tibeticoside A **1**.



Compound **1** was obtained as a white amorphous powder, $[\alpha]_{\text{D}}^{20} -120$ (c 0.50, MeOH), UV $\lambda_{\text{max}}^{\text{MeOH}}$ (log ϵ): 207 (4.52), 235 (3.34), 286 (3.32) nm. The IR spectrum (KBr) showed absorptions for hydroxyl (3422-3461 cm^{-1}) and aromatic ring (1635, 1502 cm^{-1}). The molecular formula of **1** was determined to be C₂₆H₃₀O₁₂ on the basis of NMR spectral data and elemental analysis. ¹HNMR spectrum of **1** showed the presence of aromatic rings at δ 6.73-6.87, two methylenedioxy groups at δ 6.96 (2H, brs) and 6.97 (2H, brs), two methines connected with oxygen at δ 5.05 (1H, s, H-7) and 4.37 (1H, d, J=9.7Hz, H-7'), the anomeric proton of glucose at δ 4.24 (1H, d, J=7.6Hz). ¹³CNMR and DEPT data (**Table 1**) of **1** showed the presence of four methines and two methylenes except two aromatic rings, two methylenedioxy groups and the signals of a glucose. On acid hydrolysis with HCl, compound **1** afforded glucose (identified by PC). From the above results, **1** seemed to be a 7-9'-monoepoxy tetrahydrofuran type lignan glucoside.

^1H and ^{13}C NMR data of **1** were assigned on the basis of the ^1H - ^1H COSY and HMQC. Furthermore, the correlations of ^1H - ^1H COSY confirmed the structure skeleton given. In the HMBC spectrum of **1**, the correlations of H-7 (δ 5.05) with C-8, C-9, C-9', C-2, C-6 and C-1; H-7' (δ 4.37) with C-8', C-2', C-6' and C-1'; H-1 of Glu. (δ 4.24) with C-9, all of these correlations were in agreement with the structure.

Compound **1** has been acetylated to **1a** by using acetic anhydride and pyridine (1:1). ^1H and ^{13}C NMR spectra of **1a** showed five acetyls. Furthermore, the chemical shift values of H-7' and H-8' of **1a** appeared significantly downfield when comparison with **1**, suggesting C-7' of **1** to be connected with a hydroxyl. The correlations of δ 4.96 (H-7) with 2.36 (H-8) and δ 2.36 (H-8) with 2.92 (H-8') in the NOESY spectrum of **1a** indicated that H-7, H-8 and H-8' were cis-relationship. Thus, the structure of **1** has been determined.

Table 1. ^{13}C NMR data of **1** (DMSO- d_6) and **1a** (CDCl_3) (100MHz, δ , ppm, TMS)

C	1	1a	C	1	1a	C	1	1a
1	138.3	133.6	1'	139.3	136.9	Glu. 1	102.6	101.1
2	105.8	105.9	2'	106.2	106.8	2	73.5	71.9
3	147.1	147.8	3'	147.1	147.8	3	76.9	74.0
4	145.8	146.7	4'	146.2	147.5	4	69.9	68.3
5	107.7	108.0	5'	107.8	108.2	5	76.6	72.7
6	118.0	118.6	6'	119.0	120.6	6	61.0	61.7
7	82.5	83.4	7'	70.2	71.2	OCH ₂ O	100.6	100.8, 100.9
							100.6	
8	47.4	48.9	8'	48.3	45.6	OCOMe		169.1, 169.3, 169.5, 170.3, 170.5
9	66.3	67.3	9'	69.1	70.2			20.6, 20.6, 20.7, 20.7, 21.1

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