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A New Iridoid Glycoside and a New Iridoid from *Pedicularis kansuensis* f. *albiflora*

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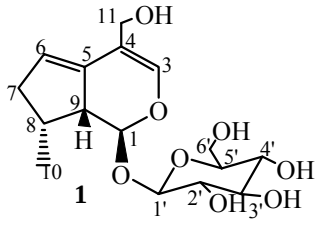
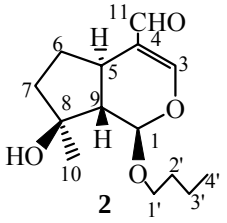
Abstract: A new iridoid glycoside **1** and a new iridoid **2** were isolated from the whole plant of *Pedicularis kansuensis* f. *albiflora*. Their structures were elucidated by spectroscopic methods.

Keywords: *Pedicularis kansuensis* f. *albiflora*, Scrophulariaceae, iridoid glycoside, iridoid.

Pedicularis kansuensis f. *albiflora* has been used for treatment of collapse, exhaustion and senility[1]. Here we report the structure elucidation of a new iridoid glycoside **1** and a new iridoid **2** isolated from this plant.



1



2

Compound **1**, white amorphous powder, $[\alpha]_D^{24}$ –10 (*c* 1.44, CH_3OH), UV λ_{max}^{MeOH} 249 (0.65) nm, the IR spectrum (KBr) showed absorptions for hydroxyl (3464, 3200 cm^{-1}), double bond (1637 cm^{-1}) and C-O-C (1077, 1007 cm^{-1}), FABMS showed quasimolecular ion peaks at *m/z* 351 $[M+Li]^+$ and *m/z* 367 $[M+Na]^+$, suggesting the molecular formula to be $C_{16}H_{24}O_8$, which was supported by ^{13}C NMR and DEPT spectra. The NMR spectra supported **1** was an iridoid glycoside. ^1H NMR spectra of compound **1** (**Table 1**) showed the presence of two methines at δ 5.07 (d, 10Hz, H-1), 6.52 (s, H-3) and a methylene connected with oxygen at 4.02 (brs, H-11), ^1H and ^{13}C NMR showed that except double bond between C-3 and C-4, there was another double bond between C-5 and C-6, the carbons of the double bond were a methine and quaternary carbon. The anomeric proton of glucose at 4.57(d, 7.8Hz, H-1') suggested the glucose was in β-orientation. The D-glucose was confirmed by PC after acid hydrolysis of **1**. C-10 (δ14.8) in **1** was in α-orientation[2]. The relative stereochemistry of **1** was further determined by the NOESY

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experiment. The correlations of δ 2.42 (H-8) with δ 2.58 (H-9), δ 0.84 (H-10) with δ 5.07 (H-1), and no correlation between δ 5.07 (H-1) and δ 2.58 (H-9), δ 0.84 (H-10) and δ 2.58 (H-9), suggested that the H-8 and H-9 were in β-orientation, and the H-1 was in α-orientation. Hence, the structure of the iridiod glycoside was assigned to be **1**.

Compound **2**, $[\alpha]_D^{23}$ – 62 (*c*, 0.23, CH_3OH) colorless needle. Its EIMS exhibited a molecular ion peak at *m/z* 254. The molecular formula was deduced as $C_{14}H_{22}O_4$ by its MS, ^{13}C-NMR and DEPT spectra. The ^{13}C-NMR spectra of compound **2** (**Table 1**) was similar with those of the known compound ixoroside[3] except for the presence of an *n*-butyl group instead of the β-D-glucopyranosyl at C-1 in ixoroside. The ^{13}C NMR data δ 51.3 (C-9) suggested the -OH at C-8 was in β-orientation[4], the NOESY experiment showed that δ 4.95 (H-1) correlated with 3.55 (H-5) and 1.34 (H-10), and 3.20 (H-9) did not correlate with them. This result suggested that the H-1, H-5, and the -CH_3 at C-8 were α and the H-9 was β-orientated. Thus, the structure of compound **2** was confirmed.

Table 1 ^{1}H-NMR (400 MHz), ^{13}C-NMR (100 MHz) and DEPT data of **1** and **2**(δ_{ppm}, J_{Hz})

No.	^{1}H(α/β)		^{13}C (DEPT)	
	1	**2**	**1**	**2**
1	5.07 (brd, 10.0)	4.95 (d, 4.4)	97.8 (CH)	100.2 (CH)
3	6.50 (s)	7.15 (s)	141.8 (CH)	160.7 (CH)
4	-	-	114.4 (C)	124.1 (C)
5	-	3.55 (m)	133.4 (C)	29.7 (CH)
6	5.53 (brs)	2.34 (m)/1.72 (m)	118.6 (CH)	28.8 (CH_2)
7	1.92 (m)/2.48 (m)	2.21 (m)/1.58 (m)	40.6 (CH_2)	40.5 (CH_2)
8	2.42 (m)	-	32.8 (CH)	79.9 (C)
9	2.58 (dd, 10.0, 6.5)	3.20 (m)	48.6 (CH)	51.3 (CH)
10	0.84 (d, 6.8)	1.34 (s)	14.8 (CH_3)	24.8 (CH_3)
11	4.02 (brs)	9.25 (s)	58.3 (CH_2)	190.4 (CH)
1'	4.57 (d, 7.8)	3.87 (m)	98.8 (CH)	69.3 (CH_2)
2'	2.90-3.37	1.45 (m)	73.2 (CH)	31.5 (CH_2)
3'	2.90-3.37	1.38 (m)	76.7 (CH)	19.2 (CH_2)
4'	2.90-3.37	0.93 (t, 7.2)	70.1 (CH)	13.8 (CH_3)
5'	2.90-3.37	-	77.2 (CH)	-
6'	3.65 (d, 11.2)	-	61.3 (CH_2)	-

DMSO-d6 as solvent for **1** and $CDCl_3$ as solvent for **2**.

Acknowledgments

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