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A New Neolignan Glycoside from *Pedicularis armata*

Cheng Shan YUAN, Zhan Xin ZHANG, Xue GAO, Zhong Jian JIA*

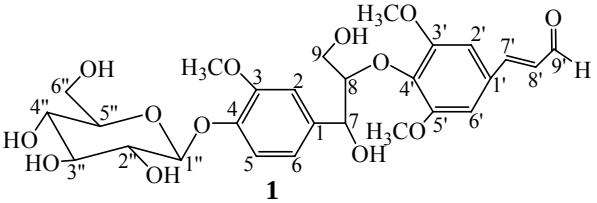
College of Chemistry and Chemical Engineering, State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou 730000

Abstract: A new neolignan glycoside named armaoside **(1)** was isolated from the whole plant of *Pedicularis armata* Maxim. Its structure was elucidated by spectroscopic and chemical methods. Antibacterial assay showed that it has moderately antibacterial activities against *Eschecichia coli*, *Bacillus subtilis* and *Staphylococcus aureus*.

Keywords: *Pedicularis armata*, Scrophulariaceae, neolignan glycoside, armaoside, antibacterial activity.

Pedicularis armata Maxim. has been used for treatment to collapse, exhaustion and senility[1]. Here we report the structure elucidation of a new neolignan glycoside **1** isolated from this plant.

Compound **1**, white amorphous powder, $[\alpha]_D^{20}$ +15 (*c* 0.35, CH_3OH), the IR spectrum (KBr) showed absorptions for hydroxyl (3397 cm^{-1}), a conjugated carbonyl group (1707 cm^{-1}) and aromatic ring (1667, 1582, 1505, 1461 cm^{-1}). The molecular formula was determined as $C_{27}H_{34}O_{13}$ on the basis of its HRESIMS ($C_{27}H_{34}O_{13}Na$, 589.1983, calcd. 589.1982). Its ^{1}H-NMR spectrum showed the presence of two *trans*-double bond protons at δ 7.60 (d, 1H, 15.6Hz, H-7'), and 6.76 (dd, 1H, 15.6, 8.0 Hz, H-8'), an aldehydel proton at δ 9.62 (d, 1H, 8.0 Hz, H-9'), a 1, 3, 4-trisubstituted aromatic ring at δ 7.08 (d, 1H, 1.6Hz, H-2), 7.11 (d, 1H, 8.0, H-5), and 6.91 (dd, 1H, 8.0, 1.6 Hz, H-6), a 1, 3, 4, 5-tetrasubstituted aromatic ring at δ 7.00 (brs, 2H, H-2', 6'), and an anomeric proton of glycose at δ 5.01 (d, 1H, 7.8 Hz, H-1"). The ^{13}C-NMR and DEPT data (**Table 1**) of **1** showed three methoxy groups (δ 55.6), an oxygenated methylene (δ 61.1, C-9), two oxygenated methines (δ 72.8, C-7; 86.1, C-8), and the signals of glucose. On acid hydrolysis with HCl, compound **1** afforded D-glucose (identified by PC). Furt-



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* E-mail: jiazj@lzu.edu.cn

ther analysis of the ^{1}H-^{1}H COSY spectra of compound **1** disclosed that H-8' correlated to H-7' and H-9', while H-8 (δ 4.40, m, 1H) correlated to H-7 (δ 4.94, d, 1H, 4.8Hz) and H-9 (δ 3.90, dd, 1H, 10.8, 4.2 Hz, H-9a; δ 3.63, dd, 1H, 10.8, 5.6 Hz, H-9b). On the basis of such preliminary information, in combination with the observed HMBC correlations from H-7 to the C-1, C-2, and C-6, and from H-7' to C-1', C-2', and C-6', the presence of two C_6-C_3 units in the molecule of compound **1** was evident, and it could be inferred that this compound is an 8-*O*-4 neolignan derivative. The location of the methoxyl and glycose were assigned on the basis of HMBC correlations from δ_H 3.85 (9H, s, MeO-3, MeO-3', and MeO-5') to δ_C 149.3 (C-3) and 153.6 (C-3' and C-5'), and H-1'' to δ_C 146.7 (C-4). The coupling constant of H-1''(*J*=7.8Hz), suggested the D-glucose was in *β*-orientation. The relatively small coupling constant between H-7 and H-8 (4.8 Hz), indicated the *erythro* form of the 1-phenyl-2-aryloxypropane-1,3-diol moiety[2]. Thus compound **1** was elucidated structurally as *erythro*-1-(4-O-*β*-D-glucopyranosyl-3-methoxyphenyl)-2-{2, 6-demethoxyl-4-[(E)-formylvinyl] phenoxyl} propane-1, 3-diol, which was named as armaoside.

The antibacterial screening was carried out employing the cup-plate method. Chloramphenicol was used as a positive control. The results indicated that compound **1** exhibited moderately antibacterial activities against *E. coli*, *B. subtilis* and *S. aureus*.

Table 1 ^{1}H-NMR (400 MHz), ^{13}C-NMR (100 MHz) and DEPT data of **1** (CD_3OD, TMS, δ_{ppm}, J_{Hz})

No.	^{1}H-NMR	^{13}C-NMR	No.	^{1}H-NMR	^{13}C-NMR
1	-	130.2 (C)	4'	-	138.7 (C)
2	7.08 (d, 1.6)	111.3 (CH)	5'	-	153.6 (C)
3	-	149.3 (C)	6'	7.00 (brs)*	106.1 (CH)*
4	-	146.7 (C)	7'	7.60 (d, 15.6)	154.0 (CH)
5	7.11 (d, 8.0)	116.4 (CH)	8'	6.76 (dd, 15.6, 8.0)	127.9 (CH)
6	6.91 (dd, 8.0, 1.6)	119.8 (CH)	9'	9.62 (d, 8.0)	194.9 (CH)
7	4.94 (d, 4.8)	72.8 (CH)	1''	5.01 (d, 7.8)	101.8 (CH)
8	4.40 (m)	86.1 (CH)	2''	3.38-3.82	73.7 (CH)
9a	3.90 (dd, 10.8, 4.2)	61.1 (CH_2)	3''	3.38-3.82	76.6 (CH)
9b	3.63 (dd, 10.8, 5.6)		4''	3.38-3.82	70.2 (CH)
1'	-	136.3 (C)	5''	3.38-3.82	77.0 (CH)
2'	7.00 (brs)*	106.1 (CH)*	6''	3.38-3.82	61.3 (CH_2)
3'	-	153.6 (C)	3×-OMe	3.85 (s)*	55.6 (CH_3)*

The signals of H-7, H-8, and H-9 were assigned by TOCSY 1D. * Overlapped singals.

Acknowledgments

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