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A New Flavone Glycoside from *Isodon enanderianus*

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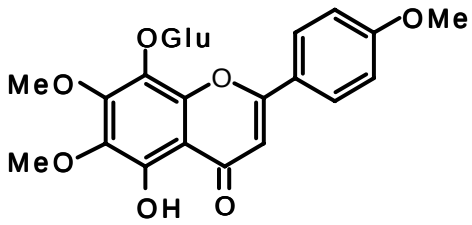
Abstract: A new flavone glycoside, 5,8-dihydroxy-4',6,7-trimethoxyflavone 8-O-β-D-glucopyranoside **1**, together with three known flavonoids, pedalitin **2**, cirsimartin **3** and genkwanin **4**, were isolated from the aerial parts of *Isodon enanderianus*. Their structures were determined on the basis of spectral data.

Keywords: *Isodon enanderianus*, flavonoid, flavone glycoside, 5,8-dihydroxy-4',6,7-trimethoxyflavone 8-O-β-D-glucopyranoside.

Isodon enanderianus (Hand.-Mazz.) H. W. Li, a perennial shrub plant of Labiatae family, is widely distributed in the southern part of Yunnan province. It has long been used as folk medicine to diminish inflammation and detoxify[1]. The *Isodon* genus is known to be rich in *ent*-kaurane diterpenoids, a series of new *ent*-kaurane diterpenoids have been isolated from the dried leaves of *I. enanderianus*[2-4]. During the course on a re-investigation of the chemical constituents of *I. enanderianus*, four flavonoids including a new flavone glycoside were isolated from the 70% acetone extract of the aerial parts of the title plant.

Figure 1 The structure of compound **1**



5,8-dihydroxy-4',6,7-trimethoxyflavone 8-O-β-D-glucopyranoside **1** was obtained as yellow amorphous powder. It was established to have a molecular formula of $C_{24}H_{26}O_{12}$, which was deduced by negative FAB-MS (ion at *m/z* 505 $[M-H]^-$) and ^{13}C NMR data including DEPT technique. $[\alpha]_D^{25}$ -39.0 (*c*= 0.250, C_5H_5N). The analysis of ^1H and ^{13}C NMR spectra (**Table 1**) suggested **1** was a flavone glycoside with a tetrasubstituted ring A and 4'-substituted ring B. FAB-MS exhibited an ion peak at *m/z* 343[aglycone-H]$^-$,

which showed that the aglylone($C_{18}H_{16}O_7$) was a flavone containing two hydroxyl groups and three methoxyl groups. A characteristic proton signal at δ 12.83 on ^{1}H NMR spectrum showed the presence of a free hydroxyl group at C-5 position. The coupling constant of the doublet for H-1" in the ^{1}H NMR spectrum (J = 7.6Hz) indicated β-D-glucose. By comparison of ^{13}C NMR spectrum of aglycone[5], a downfield shift of C-5 (3.5 ppm), C-7 (4.3ppm) and C-9 (3.3 ppm), and an upfield shift of C-8 (2.2 ppm) also indicated that the sugar moiety was linked at C-8[6], which was confirmed by HMBC experiments. Therefore, compound **1** was elucidated as 5,8-dihydroxy-4',6,7-trimethoxyflavone 8-O-β-D-glucopyranoside. The structures of other three known compounds were identified by comparison of the spectral data (MS, ^{1}H and ^{13}C NMR) with literature.

Table 1 ^{1}H (400 MHz) and ^{13}C (100.6 MHz) NMR data of **1** (in DMSO-d_6)

No	C	H (J in Hz)	No	C	H (J in Hz)
2	163.3(s)		5'	113.7(d)	7.06(d, 8.8)
3	103.1(d)	6.92(s)	6'	128.2(d)	8.23(d, 8.4)
4	181.8(s)		4'-OCH_3	54.8	3.81(s)
5	148.2(s)	12.82(s, OH-5)	6-OCH_3	60.4	3.84(s)
6	135.3(s)		7-OCH_3	60.8	4.01(s)
7	152.3(s)		1"	102.2(d)	4.83(d, 7.6)
8	128.3(s)		2"	73.3(d)	
9	144.6(s)		3"	75.7(d)	
10	105.4(s)		4"	69.4(d)	
1'	122.0(s)		5"	76.5(d)	3.10-3.63
2'	128.2(d)	8.23(d, 8.4)	6"	60.4(t)	(6H, m, overlapped)
3'	113.7(d)	7.06(d, 8.8)			
4'	161.8(s)				

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