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A Minor New Flavone from *Scutellaria baicalensis* Georgi

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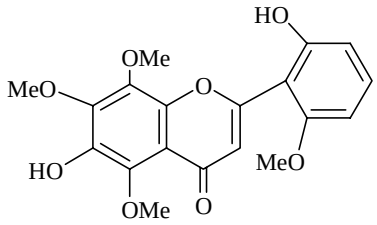
Abstract: A new flavone, 6, 2′-dihydroxy-5, 7, 8, 6′-tetramethoxyflavone, was isolated from the roots of *Scutellaria baicalensis*. Its structure was established on the basis of spectral evidences.

Keywords: Flavone, 6,2′-dihydroxy-5,7,8,6′-tetramethoxyflavone, *Scutellaria baicalensis* Georgi.

In our previous paper[1], we have reported $GABA_A$ receptor BZ-site binding assay of several flavones from the roots of *Scutellaria baicalensis* Georgi. In this study, we report the isolation of a minor new flavone from this plant.



Compound **1**

Compound **1**, a white amorphous powder, exhibited $[M-H]^-$ peak at *m/z* 373 ($C_{19}H_{18}O_8$) in negative ESI-MS and showed the presence of hydroxyl (3374 cm^{-1}) and carbonyl (1629 cm^{-1}) groups in its IR spectrum. In EI-MS, two fragment ions appearing at *m/z* 225 and 149 derived from *retro*-Diels-Alder fragmentation suggested the presence of a hydroxyl and three methoxyl groups in ring A and a hydroxyl and a methoxyl group in ring B.

The ^1H NMR spectrum (**Table 1**) of **1** showed four methoxyl, a non-coupled olefinic, ABC-type aromatic and two hydroxyl proton signals. Due to the lack of a chelated OH signal near δ 13.0 in the ^1H NMR and no shifts on addition of $AlCl_3$ in UV spectrum, one of the four methoxyl groups should be located at C-5. This signal pattern resembled that **1** has a 5(OMe), 6, 7, 8, 2′, 6′-substituted flavone structure.

The ^{13}C NMR spectrum of **1** (**Table 2**) exhibited 17 carbons whose A-ring carbon chemical shifts were in good agreement with those of 6-hydroxy-5, 7, 8, 4′-tetramethoxyflavone (**1a**)[2] and

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B-ring carbon chemical shifts were in good agreement with those of 2′-hydroxy-5, 6, 7, 8, 6′-pentamethoxyflavone (**1b**)[3]. This structural assignment was further confirmed by HMBC experiments which showed long range correlations between C-6-OH (δ 9.27) and C-5 (δ 141.5), C-7 (δ 146.4) and C-6 (δ 140.8) and between C-2′-OH (δ 10.03) and C-1′(δ 109.4), C-3′(δ 108.8) and C-2′(δ 156.6). Based on the above these data, compound **1** was concluded to be 6, 2′-dihydroxy-5, 7, 8, 6′-tetramethoxyflavone.

Table 1 ^{1}H NMR spectral data of **1** (in DMSO-d_6, 300 MHz)

No.	δppm	No.	δppm
3	6.06, *s*	2′-OH	10.03, *s*
5-OMe	3.74, *s*	3′	6.62, *d* (8)
6-OH	9.27, *s*	4′	7.32, *t* (8)
7-OMe	3.94, *s*	5′	6.62, *d* (8)
8-OMe	3.82, *s*	6′-OMe	3.74, *s*

Table 2 ^{13}C NMR spectral data of **1, 1a** and **1b** (in DMSO-d_6 ,300 MHz δppm)

No.	**1**	**1a**	**1b**	No.	**1**	**1a**	**1b**
2	158.4	160.1	162.0	1′	109.4	123.2	108.6
3	114.3	105.7	114.4	2′	156.6	127.6	156.4
4	175.9	175.9	175.5	3′	108.8	114.5	106.1
5	141.2	141.2	143.2	4′	132.0	161.8	131.8
6	140.8	140.7	137.4	5′	102.3	114.5	102.1
7	146.4	146.3	150.7	6′	158.4	127.6	158.2
8	137.8	137.8	137.4	5-OMe	61.66	61.7	61.4
9	144.8	143.6	147.3	7-OMe	60.98	61.4	61.4
10	114.3	114.1	114.4	8-OMe	61.53	60.8	61.4
				6′-OMe	55.88	55.3	55.7

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