Mahuangchiside, a New Flavone Glycoside from Chirita fimbrisepala

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Abstract: A new flavone glycoside, named mahuangchiside, was isolated from the root of *Chirita fimbrisepala* Hand.-Mazz. The structure was elucidated as 5,4'-dihydroxy-6-methoxy-flavone-7-O- β -D-xylopyranosyl(1 \rightarrow 2)- β -D-xylopyranoside on the basis of spectral analysis (¹H-¹H COSY, ¹³C-¹H HETCOR and HMBC) and chemical evidence.

Keywords: Chirita fimbrisepala, Gesneriaceae, mahuangchiside, flavone, flavonoid.

Chirita fimbrisepala Hand.-Mazz. (Gesneriaceae), commonly called "Mahuangchi" in China, is distributed mainly in Southern China. As an anti-inflammatory Chinese folk medicine, the root is used for the treatment of inflammations, such as hepatitis and gastroenteritis. The characteristic constituents of the family are flavonoids.

Mahuangchiside **1** was obtained as yellow granular crystals (MeOH) from the extract of 90%EtOH, mp. 212-213°C. It is positive to Mg-HCl and Molish tests. The UV absorption bands at 273 (3.24) and 326 (3.36) nm (log ε). The IR absorption bands (v, cm⁻¹) at 3400, 2920, 1655, 1605, 1585, 1505, 1485, 1455, 1350, 1280, 1250, 1180, 1075, 990 and 835. The EIMS gave the molecular ion peak of the aglycone of **1** at *m*/*z* 300 (100) and fragments 285 (62), 282 (51), 257 (63), 254 (14), 167 (18), 139 (24), 132 (20), 119 (25), 73 (63), and 69 (81). The main peak of the negative MALDI-TOF at *m*/*z* 563 indicated that **1** had a molecular weight of 564. The ¹³C NMR, ¹HNMR (according to¹³C-¹H HETCOR), HMBC and ¹H-¹H COSY data of **1** are shown in **Table I**.



Acid hydrolysis of **1** afforded D-xylose and the aglycone (identified by authentic samples on TLC). According to the spectral references^{1, 2, 3}, **1** was elucidated as a new flavone glycoside, 4H-1-benzopyran-4-one-5-hydroxy-2-(4-hydroxyphenyl)-6-methoxy-7-[(2-O- β -D-x ylo-pyranosyl- β -D-xylopyranosyl)oxy], and named as mahuangchiside.

C/H	δC	δ H (J in Hz)	HMBC(observed)	¹ H- ¹ H COSY
2	164.3	-	3-Н, 2'6'-Н	-
3	102.6	6.86 s	-	-
4	182.3	-	-	-
5	152.6	OH, 12.95 s	5-OH	-
6	132.5	-	6-OCH ₃ , 8-H, 5-OH	-
7	155.7	-	1"-H, 8-H	-
8	93.8	7.00 s	-	-
9	152.1	-	8-H	-
10	105.7	-	3-H, 8-H, 5-OH	-
1'	121.1	-	3-Н, З'5'-Н	-
2'	128.6	7.98 d (8.8)	6'-H	3'-Н
3'	116.0	6.94 d (8.8)	5'-H, 4'-OH	2'-Н
4'	161.3	OH, 10.40 s	2'6'-H, 4'-OH	-
5'	116.0	6.94 d (8.8)	3'-H, 4'-OH	6′-H
6'	128.6	7.98 d (8.8)	2'-Н	5′-H
1″	98.3	5.34 d (7.0)	2″-Н	2″-Н
2‴	80.8	3.65dd(7.0, 8.2)	1‴-H	1"-Н, 3"-Н
3‴	75.6	3.54*	5"-H, 2"-H	2"-Н, 4"-Н
4‴	68.8	3.50*	3″-Н	3"-Н, 5"-Н
5″	65.6	3.82 brd(ca 7.0)	-	4"-H, 5"-H
		3.47*		5″-H
1‴	104.6	4.52 d (7.5)	2‴-Н, 2‴-Н	2‴-Н
2′′′	74.2	3.00dd (7.5, 8.9)	3‴-Н	1‴-Н, 3‴-Н
3‴	76.1	3.14dd (8.9, 8.4)	2‴-Н	2‴-Н, 4‴-Н
4‴	69.5	3.24 m	3‴-Н	3‴-Н, 5‴-Н
5‴	65.7	3.58dd (5.2, 11.3)	-	4‴-Н, 5‴-Н
		3.04 d (11.3)		5‴-Н
OCH ₃	60.2	3.77 s	-	-

Table I 13 CNMR, 1 HNMR, HMBC and 1 H- 1 HCOSY of mahuangchiside (100 MHz for 13 C and 400 MHz for 1 H in DMSO-d₆, ppm)

*Peaks overlapped.

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