Chinese Chemical Letters Vol. 13, No. 8, pp 738 – 739, 2002
http://www.imm.ac.cn/journal/ccl/html

A New Chromone Derivative from *Stellera chamaejasme* L.

Bao Min FENG, Yue Hu PEI*, Hui Ming HUA

School of Traditional Chinese Medicines, Shenyang Pharmaceutical University, Shenyang 110016

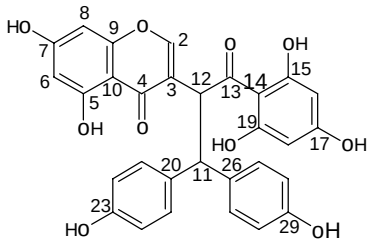
Abstract: A new chromone derivative, 3-[1- (2, 4, 6-trihydroxyphenyl) 3-di-(4-hydroxyphenyl) 1-propanone-2-yl] 5,7-dihydroxy-8-di(4-hydroxyphenyl)methyl-4H-1-benzopyran-4-one, named as isomohsenone was isolated from the roots of *Stellera chamaejasme* L. together with known chamaechromone. Its structure was determined by the analysis of MS and NMR data, especially 2D NMR spectra.

Keywords: *Stellera chamaejasme* L., chromone, 3-[1- (2, 4, 6-trihydroxyphenyl) 3-di-(4-hydroxyphenyl)-1-propanone-2-yl] 5, 7-dihydroxy-8-di-(4-hydroxyphenyl) methyl-4H-1- benzopyran-4-one.

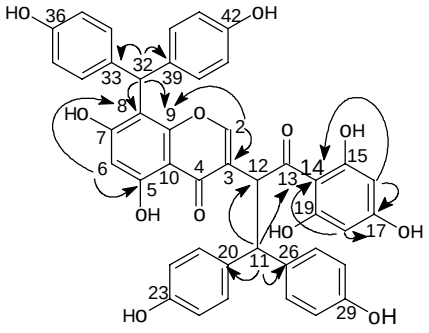
Stellera chamaejasme L., which is widespread in the northern part of China, has been traditionally used as herbal remedy for scabies and tinea. Recently it has been found to possess obvious antitumor and antiviral, especially anti-HIV activities[1-3]. *Stellera chamaejasme* L. is abundant in biflavonoids and so far a few biflavonoids have been isolated from this plant[4-7]. During our investigation of the chemical constituents of the roots of this plant, a new chromone derivative, isomohsenone have been isolated with a known compound, chamaechromone.

Chamaechromone (Compound **1**) was isolated as brown powder and its structure was determined by comparing the NMR data with the literature[8].

Figure 1 Structures of compound **1** and **2** and main HMBC correlations of compound **2**



Compound **1**



Compound **2**

*E-mail: yuehpei@online.ln.cn

Isomohsenone (**2**) was obtained as brown powder with mp 228~230°C (MeOH). It showed positive reaction with $FeCl_3$. Negative ESI-MS suggested its molecular weight was 740 ($[M-H]^-$=739). The ion peak at 541 also indicated the presence of a di (4- hydroxyphenyl) methyl group. Data of ^{1}H NMR δ (in ppm) 7.12 (d, 2H, *J*=8.2Hz), 6.93 (d, 2H, *J*=8.1Hz), 6.52 (d, 2H, *J*=8.2Hz), 6.45 (d, 2H, *J*=8.1Hz), 6.44 (d, 1H, *J*=11.7 Hz), 6.15 (s, 1H), 5.65 (s, 2H) and 4.50 (d, 1H, *J*=11.7Hz) were very similar to those of compound **1** except for the absence of H-8 and the presence of a pair of 4-hydroxyphenyl groups δ_H 6.86 (d, 2H, *J*=8.1Hz), 6.84 (d, 2H, *J*=8.1Hz), 6.62 (d, 2H, *J*=8.1Hz) and 6.60 (d, 2H, *J*=8.1Hz) and a methine proton 5.76 (s, 1H). Thus compound **2** was inferred to be a derivative of chamaechromone with a di-(4-hydroxyphenyl)methyl group at C-8. This result was further confirmed by HMBC spectrum in which δ_H 6.15 (s, 1H, H-6) and 5.76 (s, 1H, H-32) both correlated with δ_C 109.3 (C-8). The assignments of the NMR data were completed by analyzing ^{13}C NMR, ^{1}H-^{1}H COSY and HMBC spectra.

Table 1 ^{1}H NMR and ^{13}C NMR data of compound **2** (DMSO-d_6, δ in ppm)

	$_H$ (*J* Hz)*	δ_C*		$_H$ (*J* Hz)*	C
2	7.97 (s, 1H)	155.2	24	6.52 (d, 1H, 8.2)	114.6
3		120.0	25	7.12 (d, 1H, 8.2)	128.6
4		179.6	26		133.4
5		159.6	27	6.93 (d, 1H, 8.1)	129.5
6	6.15 (s, 1H)	99.2	28	6.45 (d, 1H, 8.1)	114.7
7		164.4	29		155.3
8		109.3	30	6.45 (d, 1H, 8.1)	114.7
9		154.6	31	6.93(d, 1H, 8.1)	129.5
10		103.3	32		42.8
11	4.50 (d, 1H, 11.7)	52.9	33		133.3
12	6.44 (d, 1H, 11.7)	46.4	34	6.86 (d, 1H, 8.1)	129.5
13		202.9	35	6.60 (d, 1H, 8.1)	114.8
14		104.5	36		155.3
15		164.4	37	6.60 (d, 1H, 8.1)	114.8
16	5.65 (s, 1H)	94.8	38	6.86 (d, 1H, 8.1)	129.5
17		165.3	39		133.4
18	5.65 (s, 1H)	94.8	40	6.84(d, 1H, 8.1)	129.5
19		164.4	41	6.62 (d, 1H, 8.1)	114.8
20		134.3	42		155.3
21	7.12 (d, 1H, 8.2)	128.6	43	6.62 (d, 1H, 8.1)	114.8
22	6.52 (d, 1H, 8.2)	114.6	44	6.84 (d, 1H, 8.1)	129.5
23		155.3			
5-OH	12.72 (s, 1H)				

* Recorded at 300 MHz (^{1}HNMR) and 75 MHz (^{13}CNMR)

References

1. T. Ikekawa, A. Ikekawa. *Jpn. Kokai Tokkyo Koho*, **1996**, *26* (11), 08310993.
2. Y. Endo, M. Maruno, N. Miura, M. Baba, T. Ikekewa. *Jpn. Kokai Tokkyo Koho*, **1998**, *27* (10), 10287617.
3. T. Ikekawa, A. Ikekawa. *Jpn. Kokai Tokkyo Koho*, **1996**, *26* (11), 08311056.
4. G. Q. Liu, H. Tatematsu, M. Kurokawa, M. Niwa, Y. Hirata. *Chem. Pharm. Bull.*, **1984**, *32* (1), 362.
5. M. Niwa, H. Tatematsu, G. Q. Liu, Y. Hirata. *Chem. Lett*., **1984**, *148* (4), 539.
6. M. Niwa, X. F. Chen, G. Q. Liu, H. Tatematsu, Y. Hirata. *Chem Letters*, **1984**, *148* (10), 1587.
7. M. Niwa, S. Otsuji, H. Tatematsu, G. Q. Liu, X. F. Chen, Y. Hirata. *Chem. Pharm. Bull*., **1986**, *34* (8), 3249.
8. M. Niwa, G. Q. Liu, H. Tatematsu, Y. Hirata. *Tetra. Lett*., **1984**, *25* (34), 3735.

Received 2 November, 2001