

A novel flavonoid from the root of *Macrothelypteris torresiana* (Gaud.) Ching

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Abstract

A novel flavonoid was isolated from the root of *Macrothelypteris torresiana* (Gaud.) Ching. The structure of the product was identified as 5, 7-dihydroxy-2-(1, 2-isopropylidioxo-4-oxocyclohex-5-enyl)-chromen-4-one on the ground of chemical and spectroscopic methods.

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Keywords: *Macrothelypteris torresiana* (Gaud.) Ching; Flavonoid; Root

Macrothelypteris torresiana (Gaud.) Ching (*Thelypteridaceae*) is widely distributed in south of China [1]. Some unusual flavonoids were isolated from the species *M. torresiana* and showed significant antitumor activities [2,3]. In our study, a novel flavonoid was isolated for the first time from the root of *M. torresiana*.

The air-dried root of *M. torresiana* was extracted with methanol at room temperature. The methanolic extract was suspended in H₂O and partitioned with CHCl₃, EtOAc, and n-BuOH, successively. The CHCl₃ extract was subjected to column chromatography repeatedly to yield the new compound.

Compound **1** was obtained as yellow amorphous powder with the molecular formula C₁₈H₁₆O₇ determined by HRESIMS ([M+H]⁺ 345.1590). IR (KBr) ν cm⁻¹: 3441 (OH), 1652 (C=O), 1620 (C=O), 1566, 1496, 1446 and 804. UVmax (MeOH): 243 and 300 nm. The ¹H NMR showed the ABX coupling system at δ 4.91 (m, 1H, H-2'), 3.09 (dd, 1H, *J* = 3.6, 17.6 Hz, H-3'a), and 2.75 (dd, 1H, *J* = 1.6, 17.6 Hz, H-3'b) and coupled olefinic protons at δ 6.72 (d, 1H, *J* = 10.0 Hz, H-6'), 6.18 (d, 1H, *J* = 10.0 Hz, H-5'). The location of the H-2' and H-3' was determined by HMBC experiment. In HMBC spectrum, cross signals between H-2' and C-6', between H-3b' and C-5' were observed. These data above suggested the presence of a 1, 2-disubstituted-4-oxocyclohex-5-enyl moiety in compound **1** [2,4]. Two hydroxyl protons at δ 12.54 (s, 1H, OH-5), δ 10.92 (s, 1H, OH-7), meta-coupled aromatic protons at δ 6.41 (d, 1H, *J* = 2.0 Hz, H-8), δ 6.22 (d, 1H, *J* = 2.0 Hz, H-6) and olefinic proton at δ 6.38 (s, 1H, H-3) indicated a 5, 7-dihydroxy-chromone moiety. The location of 1, 2-disubstituted-4-oxo-cyclohex-5-enyl moiety at C-2 was confirmed by the correlation of H-3 and C-1' in HMBC spectrum. Two methyls were located at C-1'' (δ 110.8) by the correlations of H-2'' (δ 1.47, s, 3H, CH₃), H-3'' (δ 1.39, s, 3H, CH₃) and C-1'' (δ 110.8 ppm) in HMBC spectrum. A significant upfield shift for C-1'' (δ 110.8 ppm) suggested that C-1'' disubstituted two hydroxyl protons (C-1' and C-2'). Thus, the

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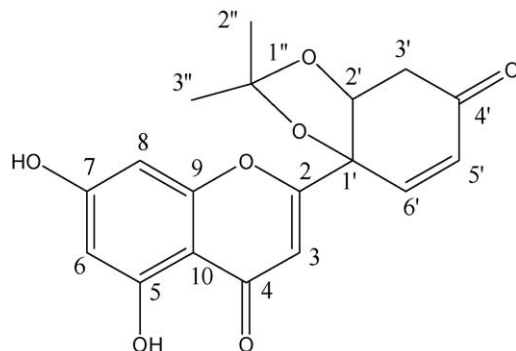


Fig. 1. Chemical structure of compound 1.

Table 1

NMR spectral data of compound **1** (400 MHz for ^1H and 100 MHz for ^{13}C , J (Hz)).

Position	δ_{H}	δ_{C}
2	–	165.7
3	6.38 (s, 1H)	107.0
4	–	182.0
5	–	161.8
6	6.22 (d, 1H, 2.0 Hz)	99.6
7	–	165.0
8	6.41 (d, 1H, 2.0 Hz)	94.7
9	–	158.0
10	–	104.4
1'	–	77.5
2'	4.91 (m, 1H)	77.5
3'a	3.09 (dd, 1H, 3.6, 17.6 Hz)	38.5
3'b	2.75 (dd, 1H, 1.6, 17.6 Hz)	
4'	–	195.3
5'	6.18 (d, 1H, 10.0 Hz)	129.6
6'	6.72 (d, 1H, 10.0 Hz)	144.2
1''	–	110.8
2''	1.47 (s, 3H)	27.7
3''	1.39 (s, 3H)	26.2
5-OH	12.54 (s, 1H)	–
7-OH	10.92 (s, 1H)	–

structure of compound **1** was concluded to be 5, 7-dihydroxy-2-(1, 2-isopropylidioxo-4-oxocyclohex-5-enyl)-chromen-4-one (Fig. 1).

However, the absolute configuration at C-1' and C-2' had not been determined because of the failure of X-ray diffraction. The NMR data of **1** were listed in Table 1.

Acknowledgment

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References

- [1] R.C. Chang, Z.Y. Wu, et al. Flora of China, Editing Committee, 5, Science Publisher, Beijing, 1999, 79.
- [2] S.L. An, R.C. Fang, C.W. Chin, et al. Planta Med. 71 (2005) 867.
- [3] S.L. An, R.C. Fang, Y.F. Hsin, et al. Chem. Pharm. Bull. 55 (2007) 635.
- [4] M.J. Cheng, S.J. Lee, Y.Y. Chang, et al. Phytochemistry 63 (2003) 603.