

A New Xanthone Derivative from *Hypericum Erectum*

Tian Ying AN, Li Hong HU*, Zhong Liang CHEN

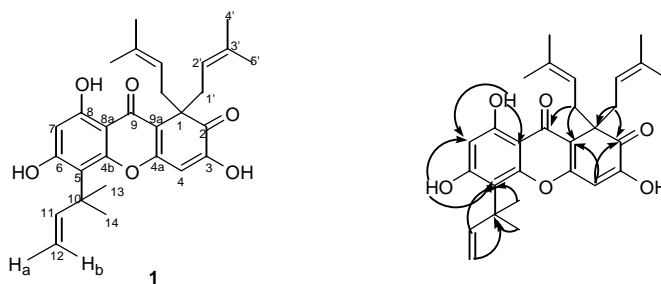
Chinese National Center for Drug Screening, Shanghai Institute of Materia Medica, Shanghai
Institutes for Biological Sciences, Chinese Academy of Sciences, Shanghai 200031

Abstract: A new xanthone, 1,2-dihydro-3,6,8-trihydroxy-1,1-bis (3-methylbut -2-enyl)-5-(1,1-dimethylprop-2-enyl)-xanthen-2,9-dione (**1**), has been isolated from the aerial part of *Hypericum erectum*.

Keyword: Xanthone, *Hypericum erectum*, Guttiferae.

Hypericum erectum (Guttiferae) is an important herb in Chinese medicine as antihemorrhagic agent, astringent and antibiotic agent¹, which has been reported to contain some antiviral prenylated phloroglucinol derivatives² and two antihemorrhagic compounds³. Our phytochemical work on the aerial part of *H. erectum* resulted in the isolation of a new xanthone (**1**), whose structure was elucidated by spectral methods.

Figure 1 Key HMBC correlations of **1**



Compound **1**, isolated as yellow oil, has the molecular formula of $C_{28}H_{32}O_6$, which was established by its HREIMS (found 464.2200; calcd. 464.2199.). The IR spectrum showed the presence of phenolic hydroxyl group (3392 cm^{-1} , br), conjugated carbonyl group (1670 cm^{-1}) and aromatic group ($1558, 1458\text{ cm}^{-1}$). The UV spectrum of **1** (λ_{max} (MeOH) ($\log \epsilon$) 305 (3.56), 417 (3.49) nm) showed the skeleton of xanthone. The NMR data (Table 1) showed the signals of a conjugated hydroxyl (δ 13.40), two free hydroxyl groups (δ 7.04, s, OH-6; δ 6.94, s, OH-3), and two singlet aromatic protons at δ 6.42 (H-4) and δ 6.23 (H-7). They also revealed the presence of two identical isoprenyl substituents (C_1' to C_5'), a 1,1-dimethylprop-2-enyl group (C_{10} to C_{14}). In addition, the

^{13}C NMR data indicated the presence of two carbonyls (δ 201.3, C-2; δ 179.8, C-9), one aliphatic quaternary carbon (δ 55.9, C-1), and ten aromatic carbons. The above data revealed that compound **1** was very similar to patulone, previously isolated from *H. patulum*⁴, except that a singlet aromatic proton (H-5) in patulone was replaced by a 1,1-dimethylprop-2-enyl group in compound **1**. The above speculation was also supported by the HMBC spectrum.

In the HMBC spectrum, cross peaks were observed between the protons of H₃-13/14 and H-11 and the carbon of C-5, indicating that the 1,1-dimethylprop-2-enyl side chain was at C-5. Hence this compound was established as 1,2-dihydro-3,6,8-trihydroxy-1,1-bis(3-methylbut-2-enyl)-5-(1,1-dimethylprop-2-enyl)-xanthen-2,9-dione.

Table 1 ^{13}C NMR (CDCl₃, 100 Hz) and ^1H NMR (CDCl₃, 400 Hz) spectral data of **1**.
(δ ppm, J Hz)

No.	δ_{H}	δ_{C}	No.	δ_{H}	δ_{C}
1		55.9 s	11	6.38 dd (17.8, 10.6)	149.1 d
2		201.3 s	12	a: 5.32 d (10.6)	113.6 t
3		158.7 s		b: 5.40 d (17.8)	
4	6.42 s	108.2 d	13	1.61 s	28.2 q
4a		151.9 s	14	1.61 s	28.2 q
4b		154.9 s	1'	2.78 dd (13.8, 7.9)	37.8 t
5		109.3 s		3.34 dd (13.8, 7.1)	
6		161.4 s	2'	4.58 m	117.8 d
7	6.23 s	101.7 d	3'		135.4 s
8		161.2 s	4'	1.42 s	25.8 q
8a		105.8 s	5'	1.44 s	18.0 q
9		179.8 s	8-OH	13.40 s	
9a		116.3 s	6-OH	7.04 s	
10		41.0 s	3-OH	6.94 s	

Reference

1. Jiangsu New Medical College (ed.), *A Dictionary of the Traditional Chinese Medicines*. Shanghai Scientific Technologic Publisher, Shanghai, **1977**, p.245
2. M. Tada, K. Chiba, H. Yamada, *et al.*, *Phytochemistry*, **1991**, *30*, 2559.
3. T. Kosuge, H. Ishida, T. Satoh, *Chem Pharm. Bull.*, **1985**, *33*, 202.
4. K. Ishiguro, N. Nagareya, A. Suitani, *et al.*, *Phytochemistry*, **1997**, *44*, 1065.

Received 8 August, 2001