

SUPPLEMENTARY MATERIAL

A new xanthone glycoside from *Pyrrosia sheareri*

Kang He, Lin-Lin Fan, Tian-Tai Wu and Jiang Du*

The Key Laboratory of Miao Medicine of Guizhou Province, Guiyang College of Traditional Chinese Medicine, Guiyang 550025, Guizhou, China

*Corresponding author. Tel: 86-851-88308057; Email: dujiang2017@sina.com

ABSTRACT

A new xanthone glycoside, 3, 5, 7, 8-tetramethoxyxanthone-1-*O*- β -D-glucopyranoside (**1**), along with five known compounds, mangiferin (**2**), kaempferol (**3**), quercetin (**4**), chlorogenic acid (**5**) and diploptene (**6**), was isolated from the whole plants of *Pyrrosia sheareri* (Bak.) Ching. The structure of compound **1** was established on the basis of extensive spectroscopic analyses and chemical methods.

KEYWORDS: *Pyrrosia sheareri* (Bak.) Ching; xanthone glycoside; 3, 5, 7, 8-tetramethoxyxanthone-1-*O*- β -D-glucopyranoside

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Table S1 ^1H NMR and ^{13}C NMR data of compound **1** (400 MHz, $\text{C}_5\text{D}_5\text{N}$, δ in ppm, J in Hz).

1					
Position	δ_{H}	δ_{C}	Position	δ_{H}	δ_{C}
1	-	161.0 (s)	9	-	175.5 (s)
2	7.27 (1H, d, 2.2)	101.9 (d)	3-OMe	3.71 (3H, s)	56.0 (q)
3	-	164.9 (s)	5-OMe	3.86 (3H, s)	56.6 (q)
4	6.78 (1H, d, 2.2)	95.9 (d)	7-OMe	3.94 (3H, s)	57.7 (q)
4a	-	158.0 (s)	8-OMe	4.10 (3H, s)	62.0 (q)
4b	-	140.1 (s)	1'	5.54 (1H, d, 7.6)	105.2 (d)
5	-	149.4 (s)	2'	4.49 (1H, dd, 8.7, 7.6)	75.1 (d)
6	7.14 (1H, s)	104.8 (d)	3'	4.40 (1H, m)	77.9 (d)
7	-	144.3 (s)	4'	4.31 (1H, t, 9.4)	71.5 (d)
8	-	141.2 (s)	5'	4.19 (1H, m)	79.3 (d)
8a	-	119.0 (s)	6'a	4.63 (1H, brd 11.0)	63.0 (t)
8b	-	108.6 (s)	6'b	4.37 (1H, m)	-

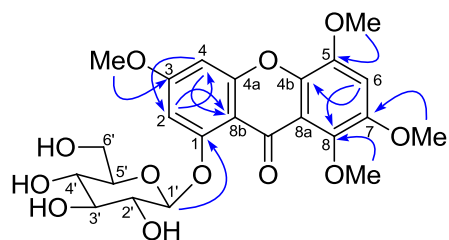


Figure S2. Key HMBC Correlations of Compound **1**

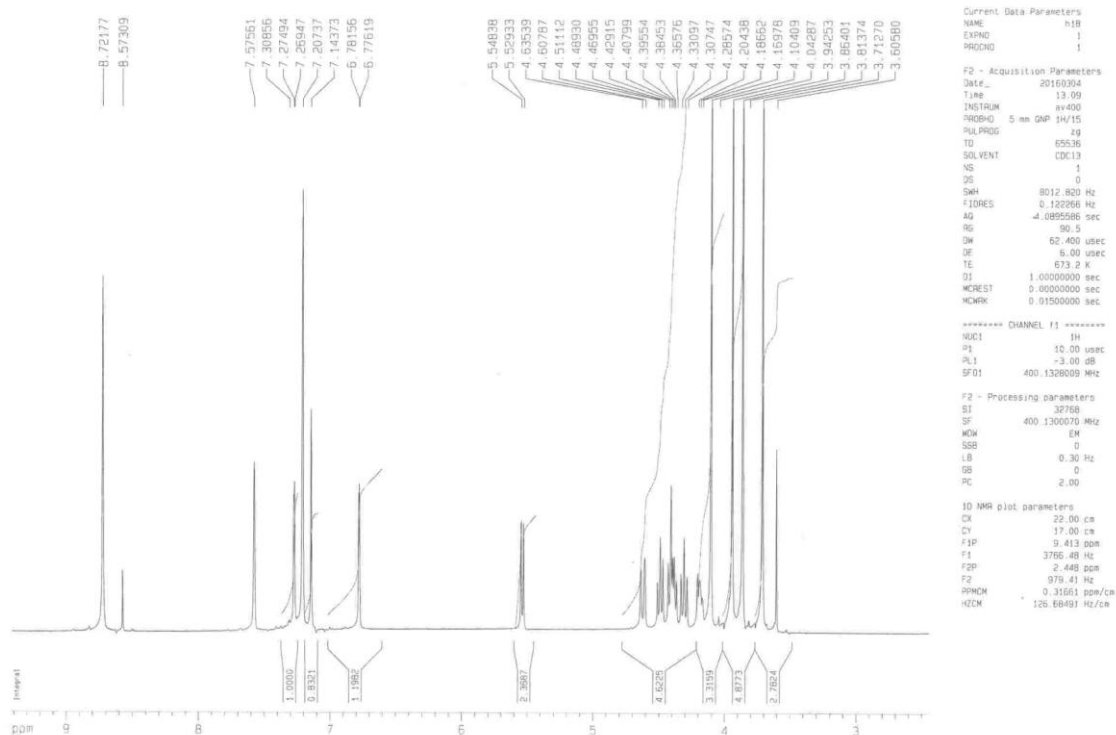


Figure S3. ^1H NMR spectrum of 3, 5, 7, 8-tetramethoxyxanthone-1- O - β -D-glucopyranoside (**1**)

H 18

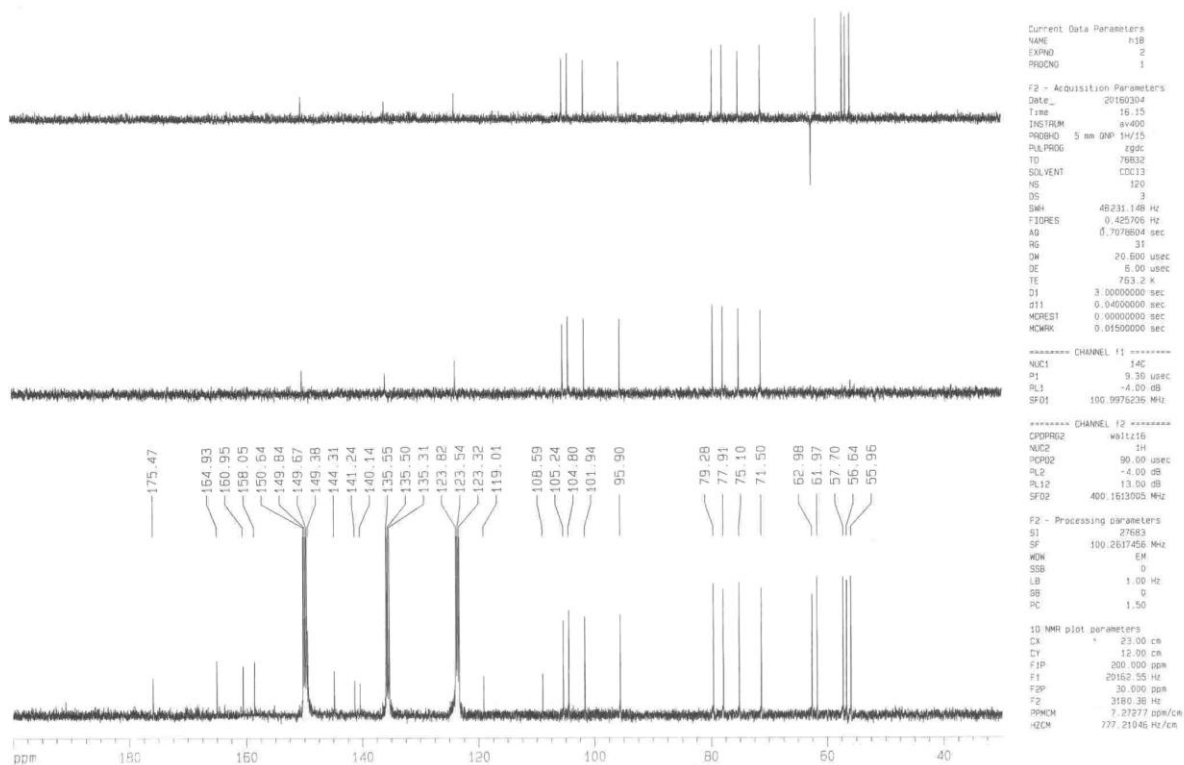


Figure S4. ^{13}C NMR and DEPT spectra of 3, 5, 7, 8-tetramethoxyxanthone-1-*O*- β -D-glucopyranoside (**1**)

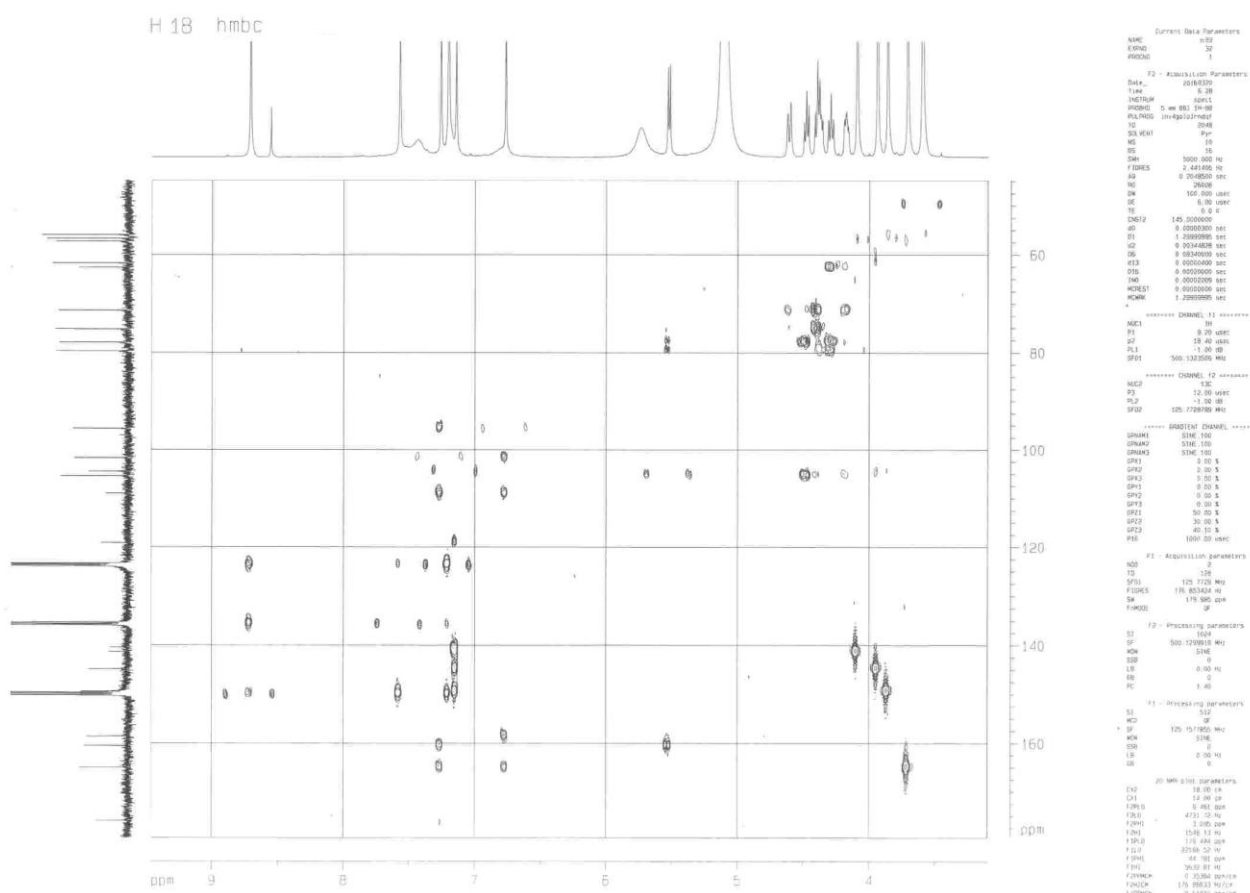


Figure S6. HMBC spectrum of 3, 5, 7, 8-tetramethoxyxanthone-1-*O*- β -D-glucopyranoside (**1**)

Acq. Date: March 23, 2016

Acq. Time: 12:23

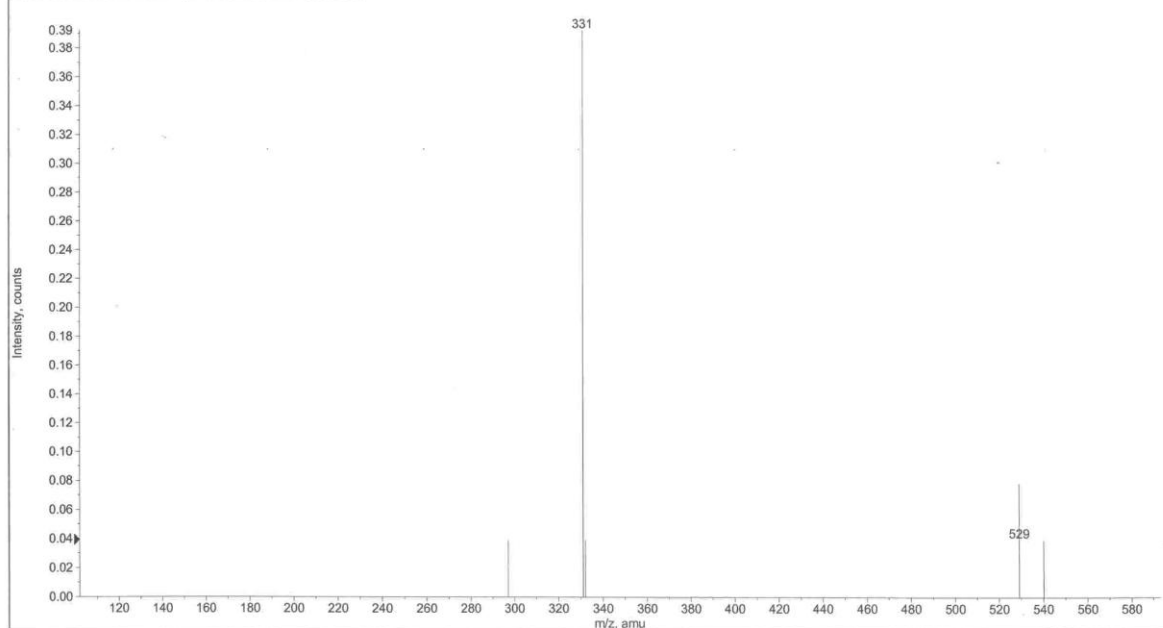
Scan Mode: Zero Width

Sample Name: 326ESIN H 18

Sample Comment:

-TOF MS: 6.127 to 7.050 min from 326ESIN H 18 .wiff
a=3.59528641097214070e-004, t0=9.30623155722676560e+001

Max. 0.4 counts.



Acq. Date: March 23, 2016

Acq. Time: 13:36

Scan Mode: Zero Width

Sample Name: 326ESINA H 18

Sample Comment:

Elemental composition calculator

Target m/z: +529.1103 amu
Tolerance: +10.0000 ppm
Result type: Elemental
Max num of results: 1000
Min DBE: -10.0000 Max DBE: +60.0000
Electron state: OddAndEven
Num of charges: 0
Add water: N/A
Add proton: N/A
File Name: 326ESINA H 18 .wiff

	Elements	Min Number	Max Number
1	2H	0	0
2	Br	0	0
3	C	0	200
4	Cl	1	1
5	F	0	0
6	H	0	400
7	I	0	0
8	K	0	0
9	N	0	0
10	Na	0	0

Acq. Date: March 23, 2016
Sample Name: 326ESINA H 18

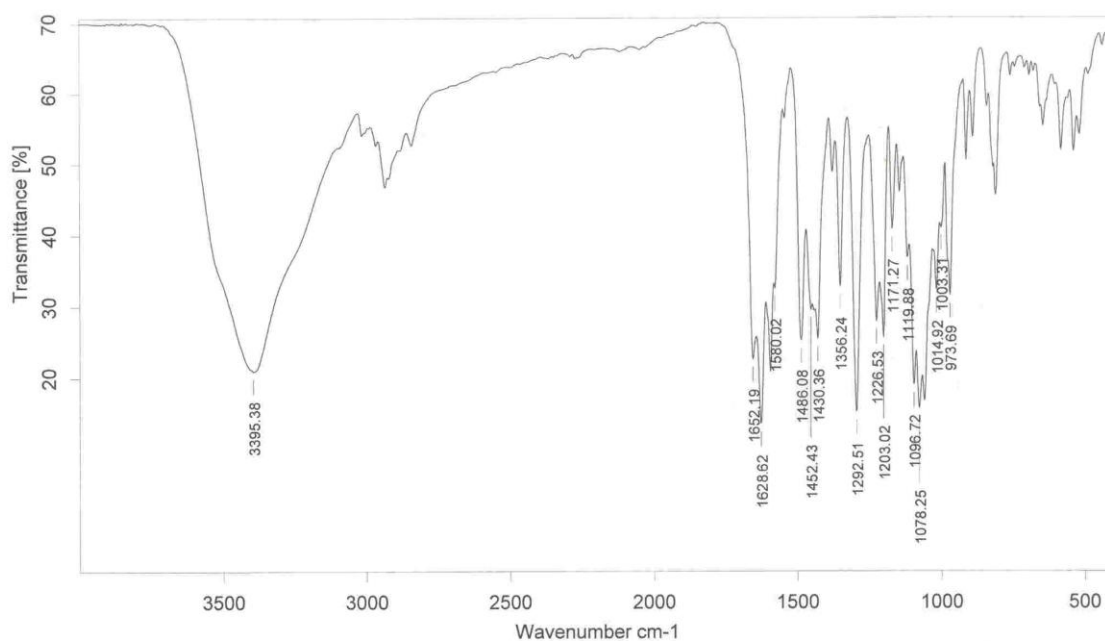
Acq. Time: 13:36
Sample Comment:

Scan Mode: Zero Width

	Elements	Min Number	Max Number
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13	Pt	0	0
14	S	0	0
15	Si	0	0

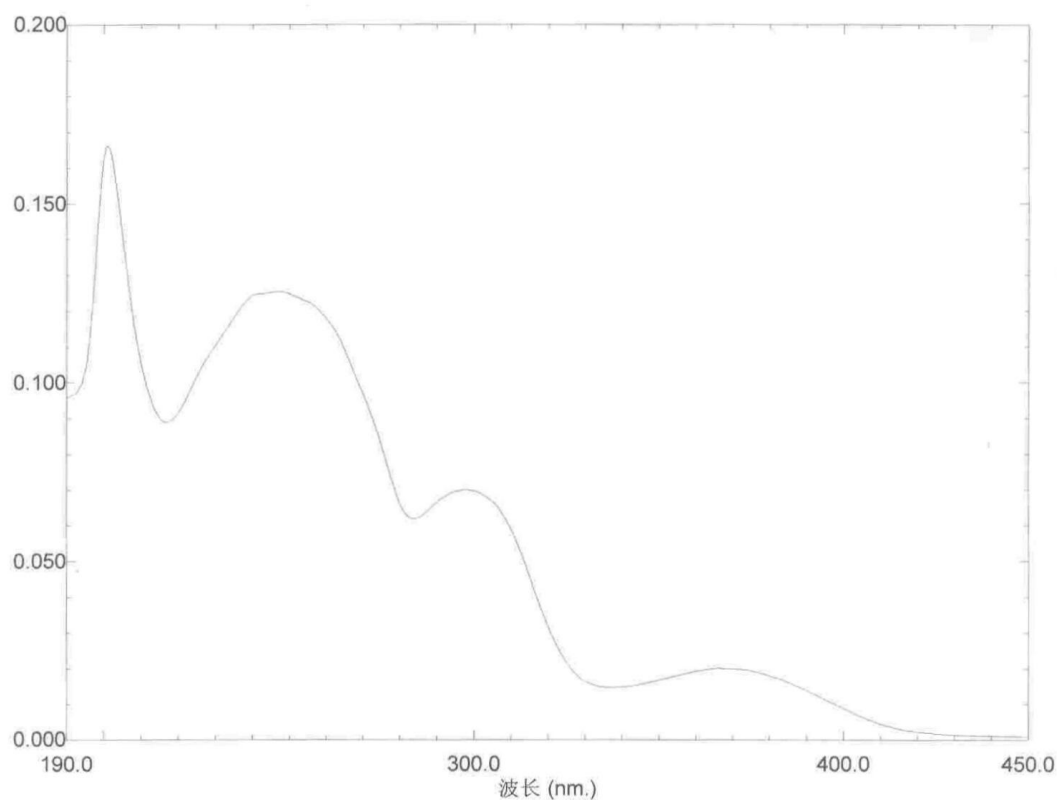
	Formula	Calculated m/z (amu)	mDa Error	PPM Error	DBE
1	C23 H26 O12 Cl	529.1112	-0.9794	-1.8511	10.5

Figure S7. HR-ESI-MS data of 3, 5, 7, 8-tetramethoxyxanthone-1-*O*- β -D-glucopyranoside (**1**)



Sample : H 18		Frequency Range : 399.264 - 3996.23		Measured on : 08/04/2016	
Technique : KBr压片	Resolution : 4	Instrument : Tensor27		Sample Scans : 17	
Customer : 328120IR0	Zerofilling : 2	Acquisition : Double Sided, For			

Figure S8. IR spectrum of 3, 5, 7, 8-tetramethoxyxanthone-1-*O*- β -D-glucopyranoside (**1**)



文件名: H18

创建于: 13:15 16-04-08
数据: 原始

样品浓度: 0.0362毫克/毫升
溶剂: 甲醇

测量模式: Abs.
扫描速度: 中速
狭缝: 5.0
采样间隔: 0.5

否.	波长 (nm.)	Abs.
1	366.50	0.0200
2	298.00	0.0699
3	247.00	0.1254
4	201.00	0.1662

Figure S9. UV spectrum of 3, 5, 7, 8-tetramethoxyxanthone-1-*O*- β -D-glucopyranoside (**1**)