

SUPPLEMENTARY MATERIAL

A Novel Cytotoxic Flavonoid C-Glycoside from *Premna fulva*

Kui-Wu Wang ^{*,a}, Sheng-Nan Yan ^a, Ting-Ting Zhang ^a, Hai-Jiang Zhang ^b, Bin Wu ^c, and Hong Wang ^d

^a*School of Food Science and Biotechnology, Zhejiang Gongshang University, Hangzhou 310018, P. R. China*

^b*Jiangsu Key Laboratory of Regional Resource Exploitation and Medicinal Research, Huaiyin Institute of Technology, Huaian 223003, P. R. China*

^c*Ocean College, Zhejiang University, Hangzhou 310058, P. R. China*

^d*School of Pharmaceutical Science, Zhejiang University of Technology, Hangzhou 310014, P. R. China*

Abstract: *Premna fulva* Craib, locally known as “Zhangu” in China, is a kind of traditional medicinal plant. A phytochemical investigation on this plant led to the isolation of a novel flavonoid glycoside along with three known analogues. The chemical structure of the new compound was determined by spectral and chemical analysis as apigenin 8-C- β -D-xylopyranoside (**1**). Compound **1** showed weak inhibitory activities *in vitro* against to four tumor cell lines (HL-60, Bcap37, SMMC7721, and P388) with IC₅₀ values of 12.58, 19.31, 31.02, and 48.19 μ g/mL, respectively. The result might be helpful to explain the application of *P. fulva* in Traditional Chinese Medicine.

* Corresponding authors: Kui-Wu Wang

Fax: 0086-571-28008900

E-mail: wkwnpc@zjgsu.edu.cn (K.-W. Wang)

- Figure S1. The ^1H NMR (500 MHz, $\text{DMSO-}d_6$) of the new compound **1**
- Figure S2. The ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) of the new compound **1**
- Figure S3. The DEPT 135 spectrum of the new compound **1**
- Figure S4. The ^1H - ^1H COSY spectrum of the new compound **1**
- Figure S5. The HSQC spectrum of the new compound **1**
- Figure S6. The HMBC spectrum of the new compound **1**
- Figure S7. The HRESI-MS spectrum of compound **1**
- Figure S8. The ESI-MS spectrum of compound **1**
- Figure S9. Key ^1H - ^1H COSY and HMBC correlations of compound **1**

Table S1. NMR data of compound **1** ($\text{DMSO-}d_6$)

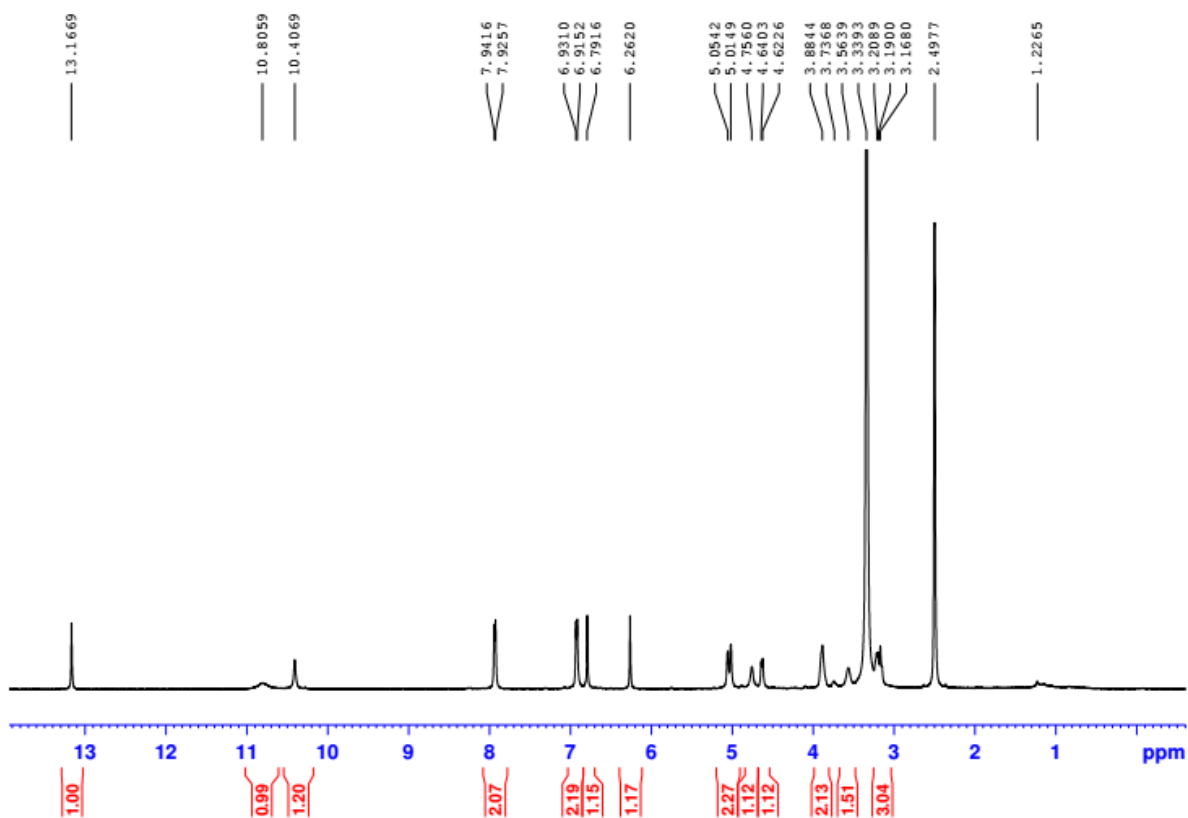


Figure S1. The ¹H NMR (500 MHz, DMSO-*d*₆) of the new compound 1

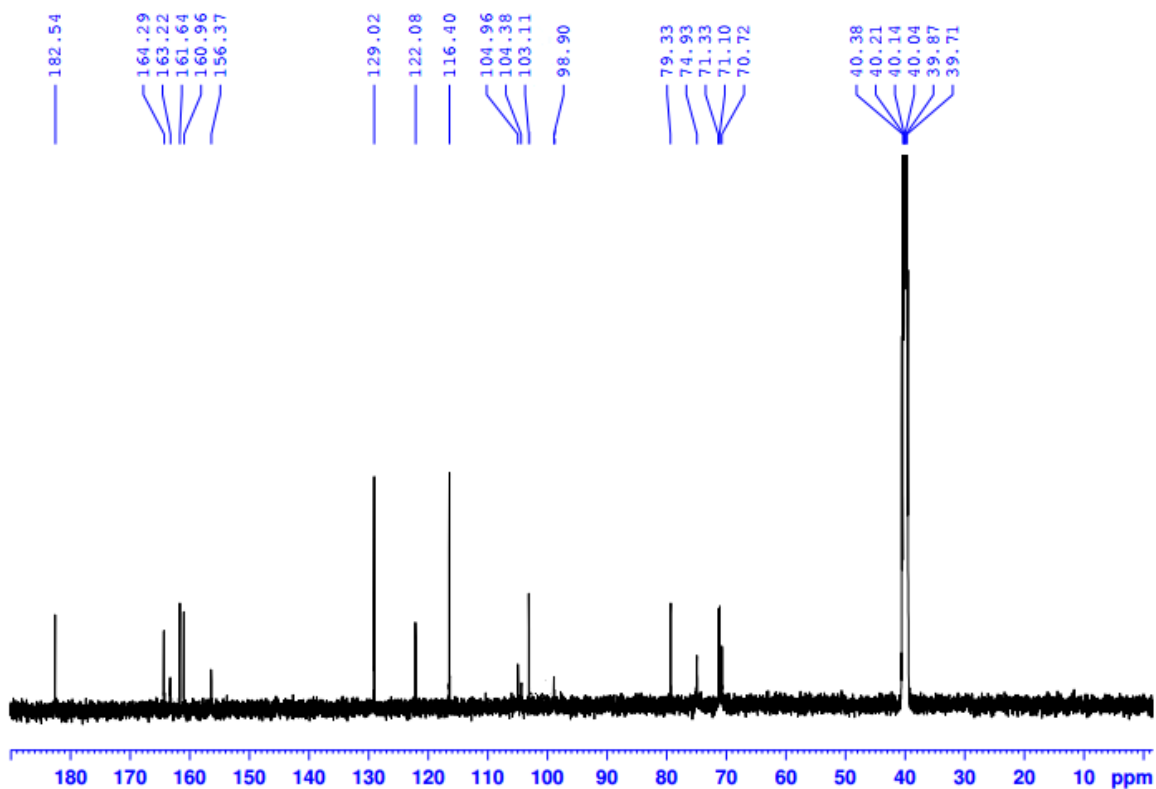


Figure S2. The ¹³C NMR (125 MHz, DMSO-*d*₆) of the new compound 1

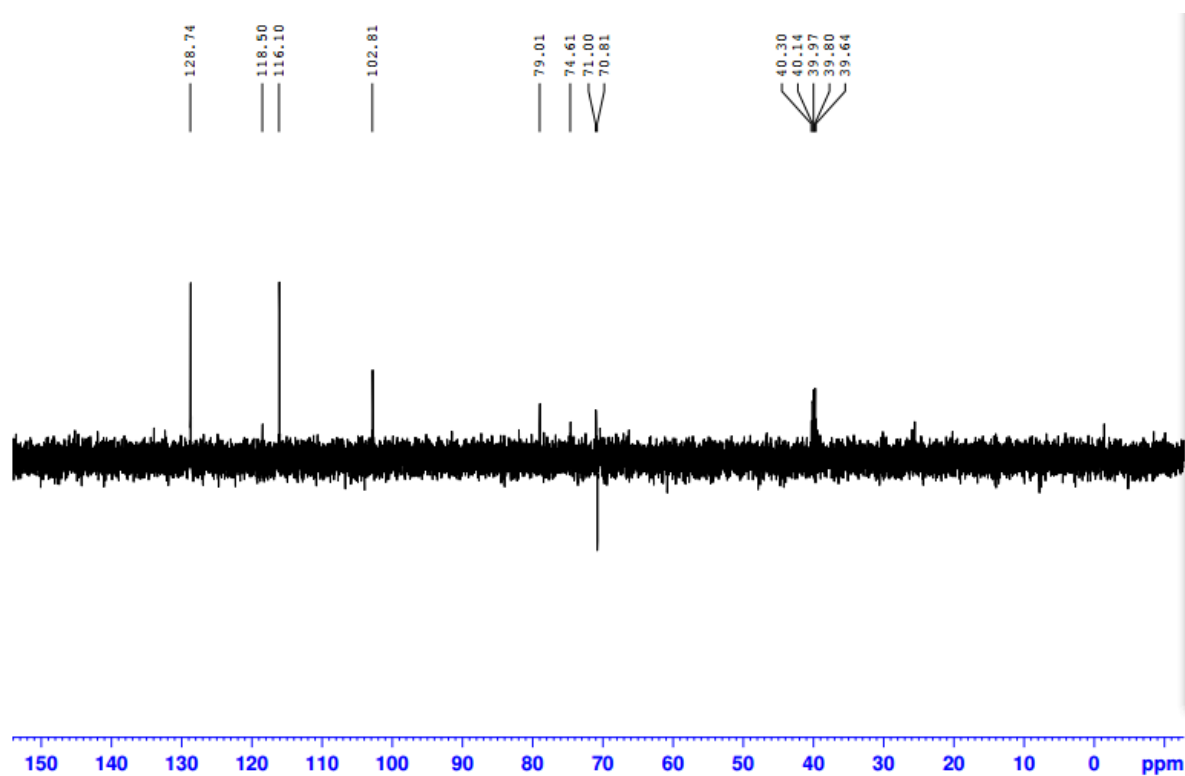


Figure S3. The DEPT 135 spectrum of the new compound **1**

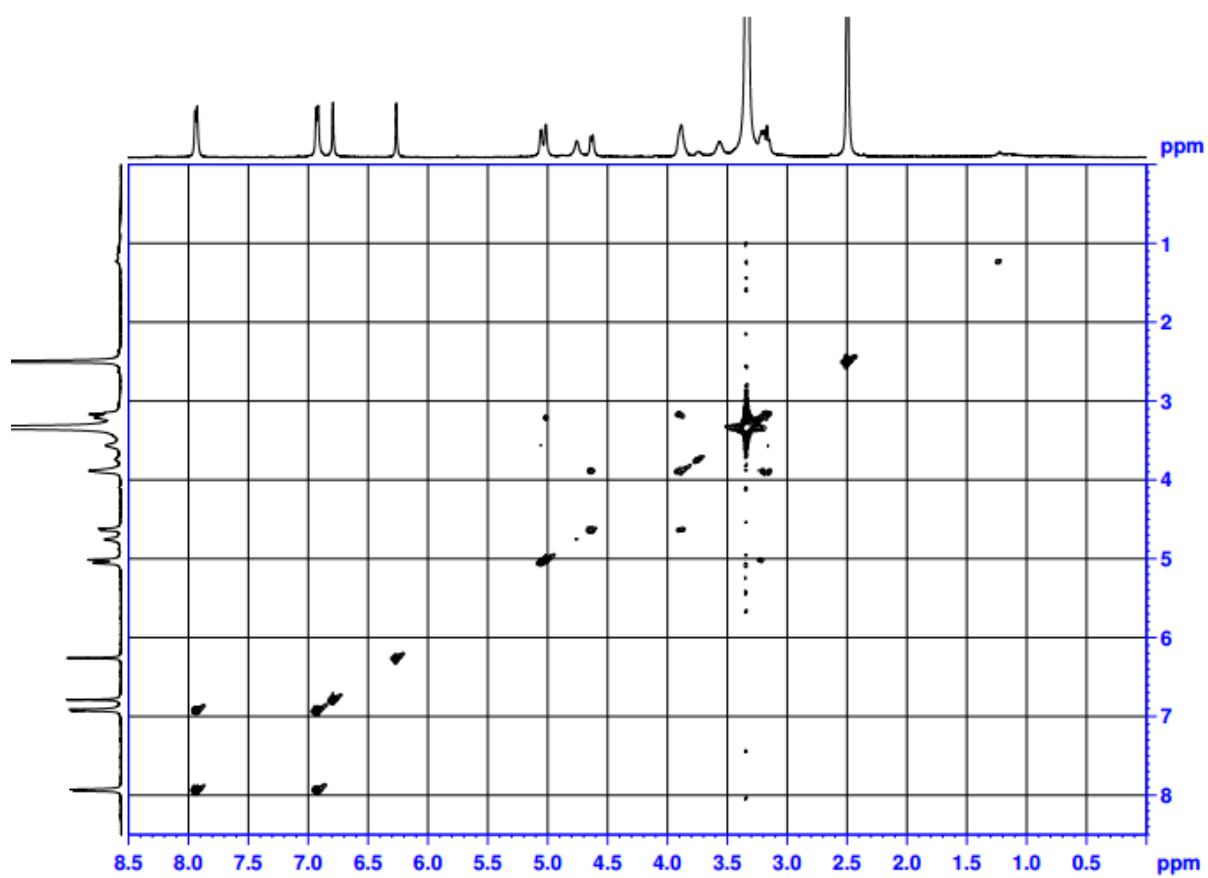


Figure S4. The ^1H - ^1H COSY spectrum of the new compound **1**

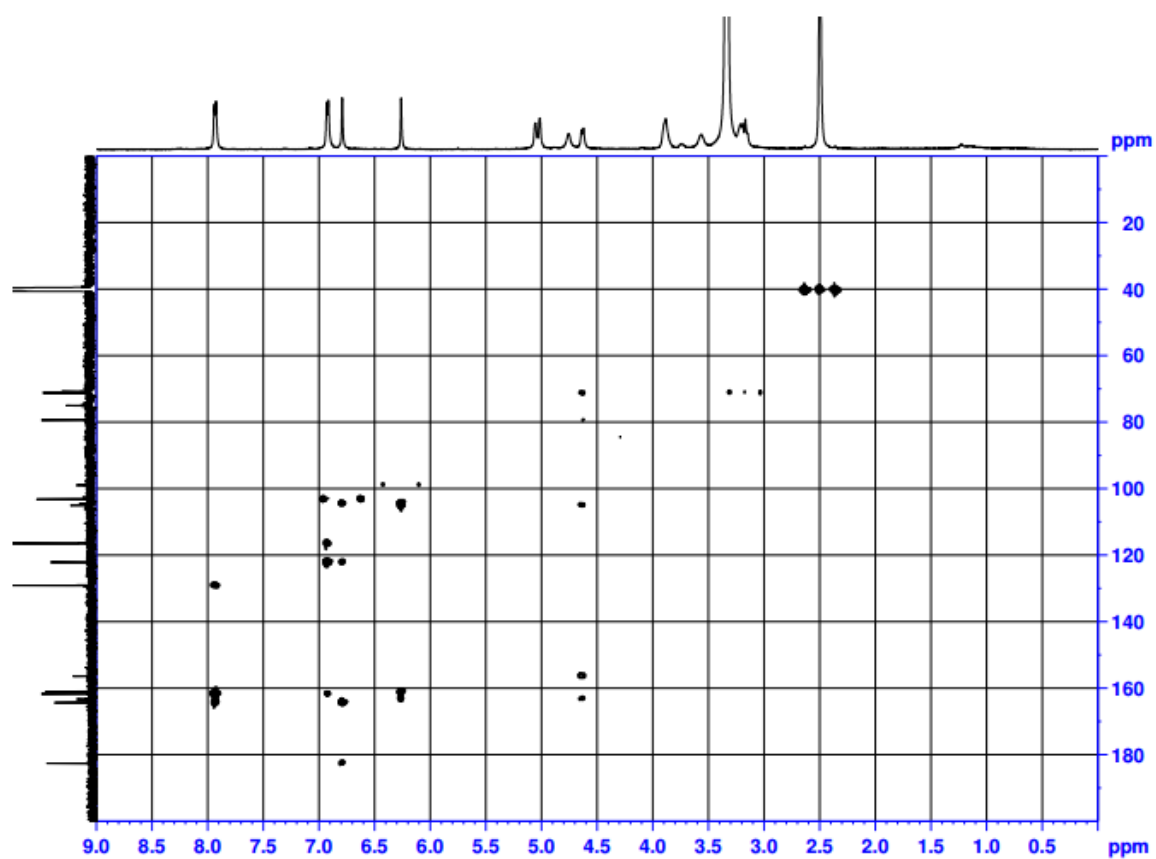


Figure S5. The HSQC spectrum of the new compound **1**

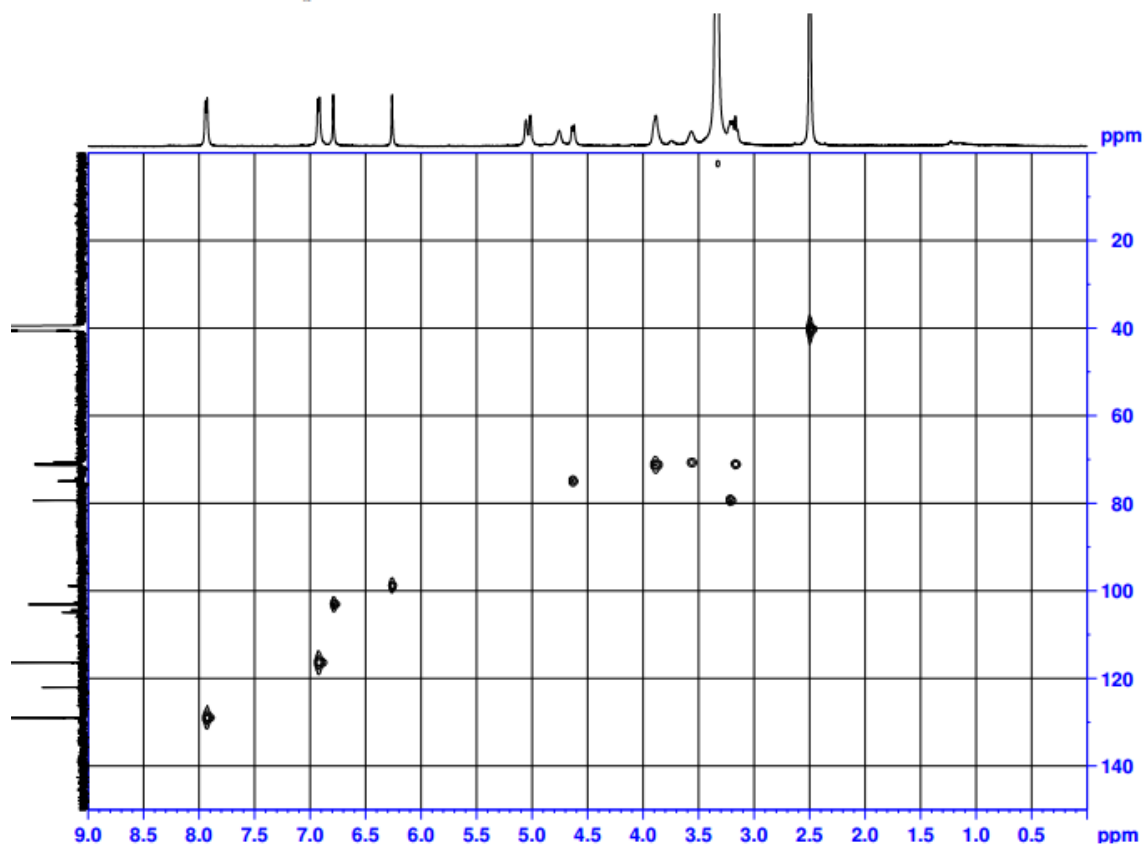


Figure S6. The HMBC spectrum of the new compound **1**

HW-W6

20170721-13 76 (0.956)

1: TOF MS ES+
2.82e5

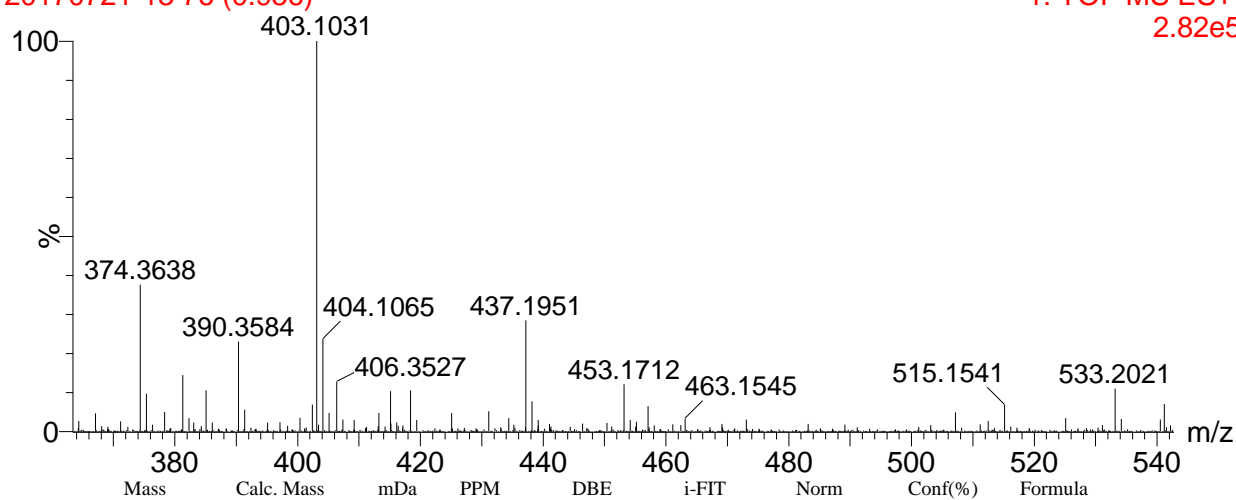


Figure S7. The HRESI-MS spectrum of compound **1**

HM-W-6_170416130932 #722 RT: 5.29 AV: 1 NL: 1.12E4
T: ITMS - c ESI Full ms [110.00-500.00]

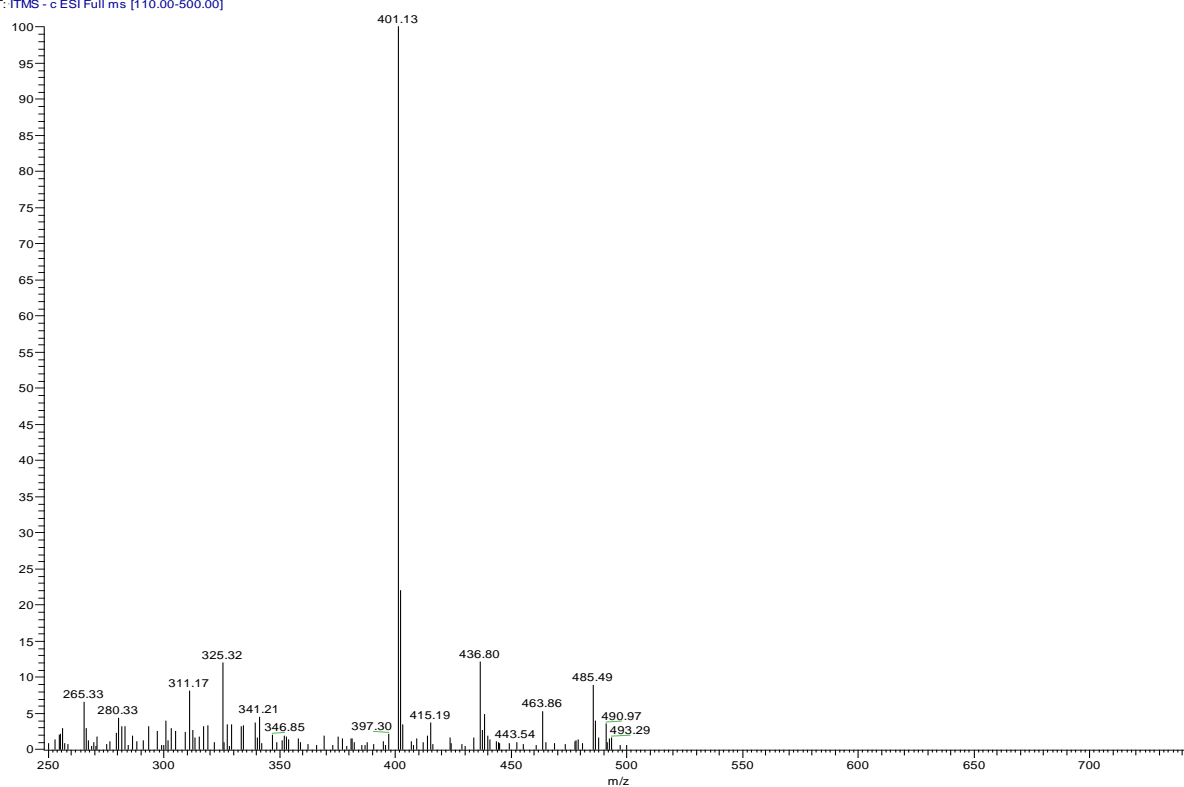
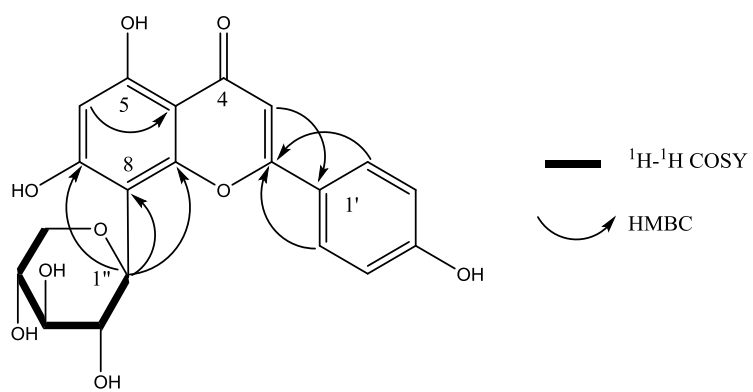


Figure S8. The ESI-MS spectrum of compound **1**



1

Figure S9. Key ^1H - ^1H COSY and HMBC correlations of compound **1**.

Table S1. NMR data of compound **1** (DMSO-*d*₆)

No.	δ_{H} (ppm)	δ_{C} (ppm)	^1H - ^1H COSY	HMBC (H \rightarrow C)
2	-	164.3		
3	6.80 (1H, s)	103.1		C-1', 4', 10
4	-	182.5		
5	-	161.0		
6	6.26 (1H, s)	98.9		C-5, 8, 10
7	-	163.2		
8	-	104.7		
9	-	156.4		
10	-	104.4		
1'	-	122.1		
2', 6'	7.94 (2H, d, $J=8.0$ Hz)	129.0	H-3', 5'	C-2, 4'
3', 5'	6.93 (2H, d, $J=8.0$ Hz)	116.4	H-2', 6'	C-1'
4'	-	161.6		
D-Xyl				
1''	4.64 (1H, d, $J=9.8$ Hz)	74.9	H-2''	C-7, 8, 9, 3''
2''	3.88 (1H, s)	71.3	H-1'', 3''	
3''	3.19 (1H, m)	79.3	H-2'', 4''	
4''	3.60 (1H, s)	70.7	H-3'', 5''	
5''	3.17 (1H, m) 3.88 (1H, s)	71.1	H-4''	
5-OH	13.17 (1H, s)	-	-	
7-OH	10.81 (1H, s)	-	-	
4'-OH	10.41 (1H, s)	-	-	

^1H -NMR and ^{13}C -NMR were measured at 500 MHz and 125 MHz, respectively.