

Supplementary material for

Title: Antioxidant and Anti-inflammatory Constituents from *Flos populi*

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Abstract:

Investigation of the *n*-butanol extract of *Flos populi* led to the isolation of one new phenolic glycoside, 4'-hydroxybenzyl-2-hydroxybenzoate-1'-*O*- β -D-glucopyranoside (**1**), together with twelve known compounds, which have been determined on the basis of spectroscopic analysis including UV, IR, HR-ESI-MS and 1D/2D NMR. The antioxidant capacity of all compounds were evaluated by ABTS radical-scavenging test and ferric reducing antioxidant power (FRAP) assay. And during a screening procedure for the anti-inflammatory activities among most compounds on lipopolysaccharide (LPS)-stimulated RAW 264.7 macrophage cells, compound **13** exhibited remarkable inhibitory effects on nitric oxide (NO), tumor necrosis factor- α (TNF- α), interleukin (IL)-6 and IL-1 β , suggesting that it might be a promising candidate as an anti-inflammatory agent.

Key words: *Flos populi*; new compound; phenolic glycoside; antioxidant property; anti-inflammatory activity

Table S1. ^1H - and ^{13}C -NMR Data of compound **1** in DMSO

Figure S1. Key HMBC correlations of compound **1**

Figure S2. ^1H -NMR spectrum of compound **1** in DMSO

Figure S3. ^{13}C -NMR spectrum of compound **1** in DMSO

Figure S4. DEPT spectrum of compound **1** in DMSO

Figure S5. HSQC spectrum of compound **1** in DMSO

Figure S6. HMBC spectrum of compound **1** in DMSO

Figure S7. HR-ESI-MS spectrum of compound **1**

Figure S8. IR spectrum of compound **1**

Table S1. ^1H - and ^{13}C -NMR Data of Compound **1** in $\text{DMSO}-d_6$ (δ in ppm, J in Hz)

no.	δ_{H} (J , Hz) ^a	δ_{C} ^b
1		113.5s
2		160.2s
3	7.00 (d, 8.4)	117.9d
4	7.54 (dt, 1.6, 8.0)	136.2d
5	6.96 (t, 8.0)	119.9d
6	7.84 (dd, 1.6, 8.4)	130.6d
7		169.0s
1'		148.4s
2'		126.6s
3'	6.81 (d, 3.1)	115.3d
4'		152.8s
5'	6.69 (dd, 3.1, 8.9)	115.9d
6'	7.04 (d, 8.9)	118.3d
7'	5.40 (s)	62.5t
Glc		
1''	4.65 (d, 7.2)	103.1d
2''	3.23 (m)	73.8d
3''	3.24 (m)	77.0d
4''	3.15 (m)	70.2d
5''	3.16 (m)	77.5d
6''	3.69 (dd, 1.4, 11.8)	61.3t
	3.46 (m)	

^aData measured at 400 MHz. ^bData measured at 100 MHz.

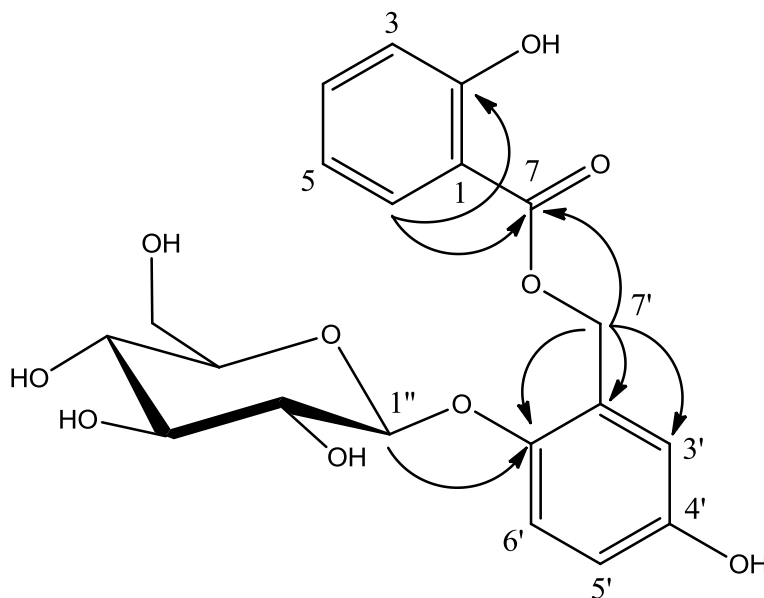


Figure S1. Key HMBC correlations of compound **1**

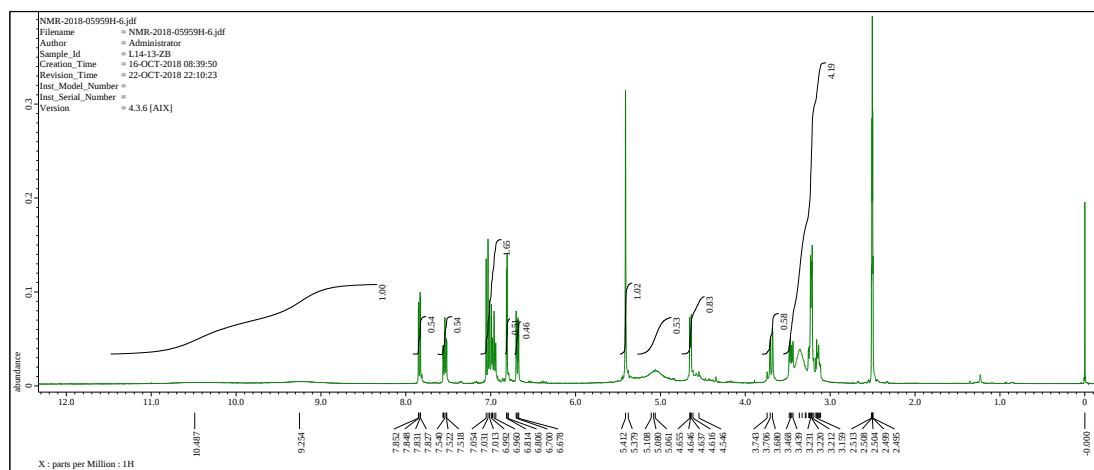


Figure S2. ^1H -NMR spectrum of compound **1** in DMSO

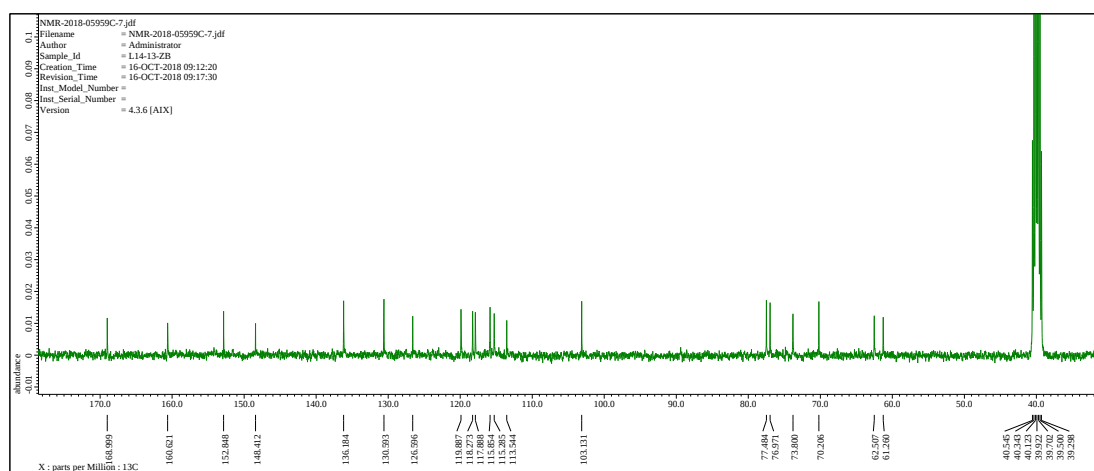


Figure S3. ^{13}C -NMR spectrum of compound **1** in DMSO

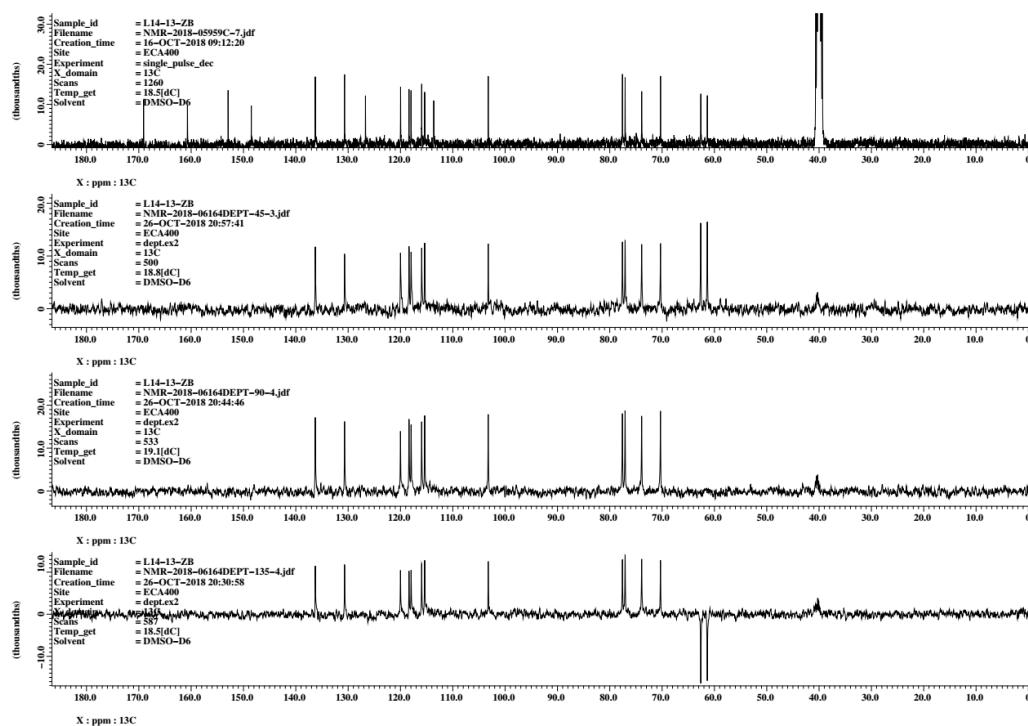


Figure S4. DEPT spectrum of compound **1** in DMSO

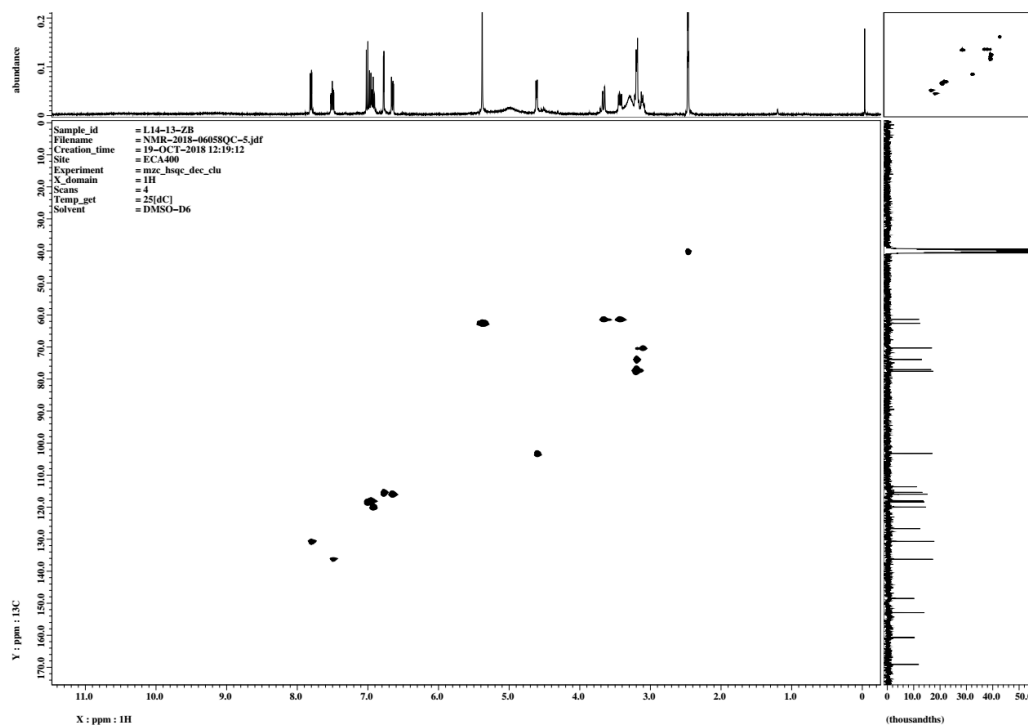


Figure S5. HSQC spectrum of compound **1** in DMSO

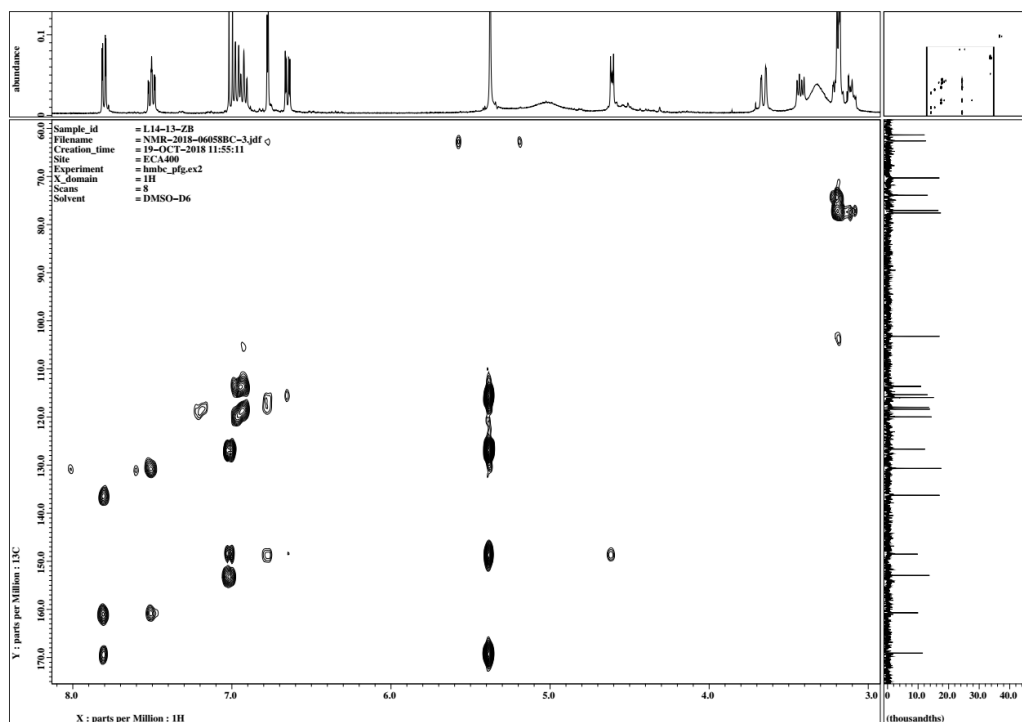


Figure S6. HMBC spectrum of compound **1** in DMSO

Qualitative Analysis Report

Data Filename	5275.d	Sample Name	L14-13-ZB
Instrument Name	TOF G6230A	Acquired Time	2018-10-17
Acq Method	YCL.M	Acquired SW	6200 series TOF/6500 series
IRM Calibration Status	Success		
User Chromatograms			

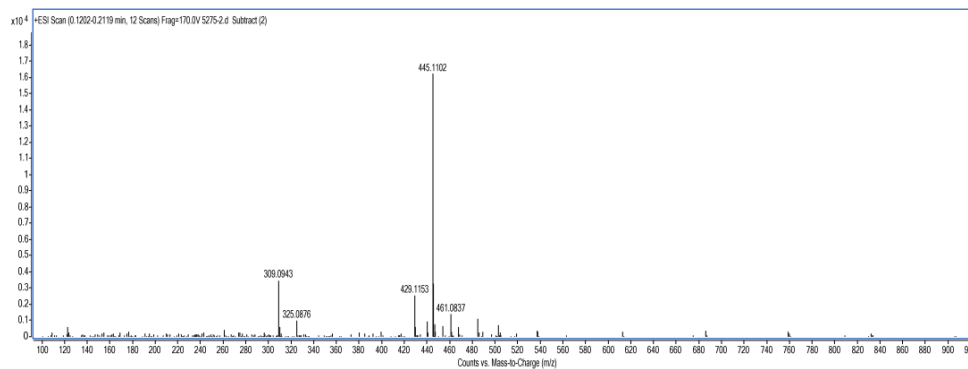


Figure S7. HR-ESI-MS spectrum of compound **1**

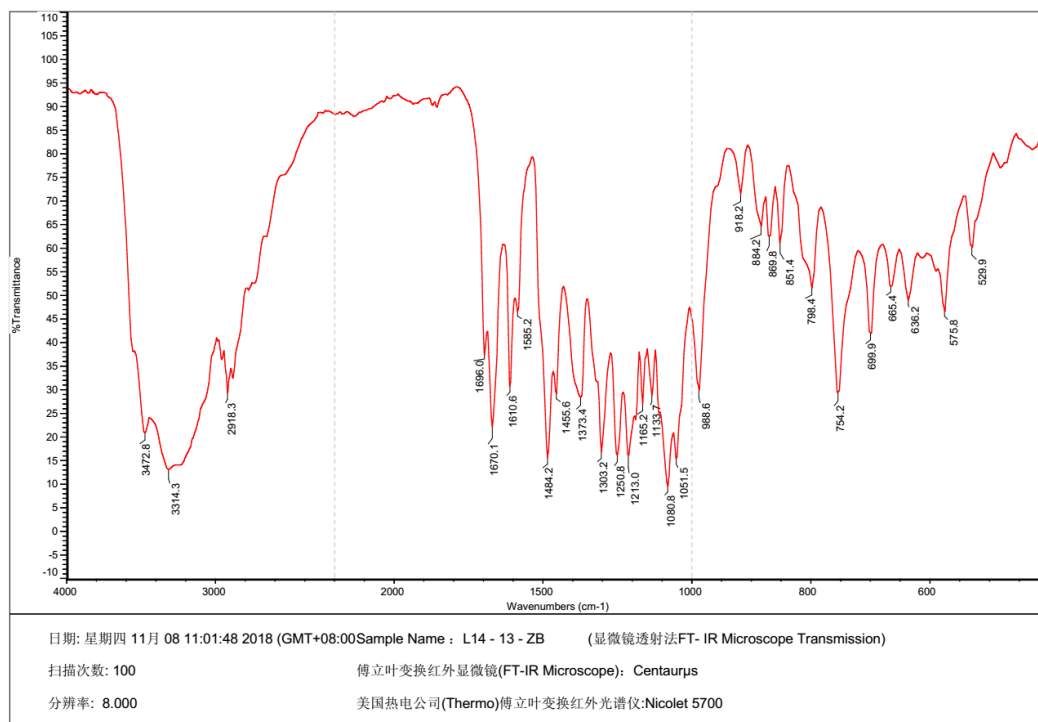


Figure S8. IR spectrum of compound 1