

## Supporting Information

*Rec. Nat. Prod.* X:X (2021) XX-XX

### Neoflavonoids from the Heartwood of *Dalbergia melanoxylon*

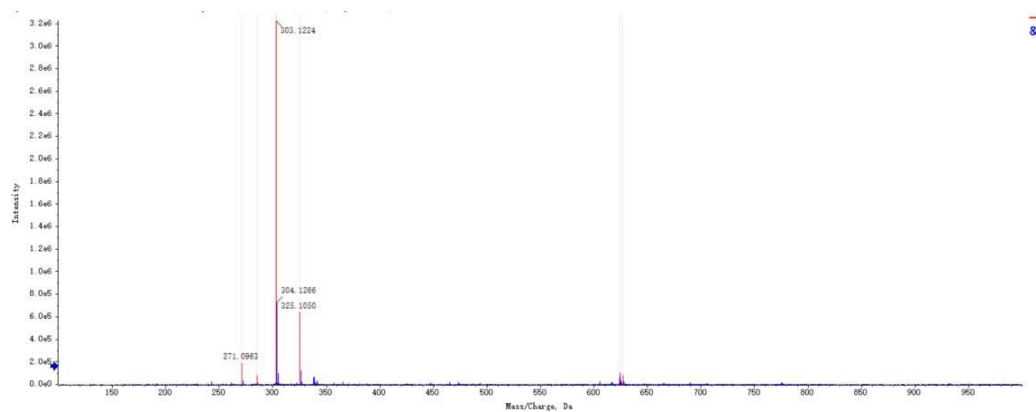
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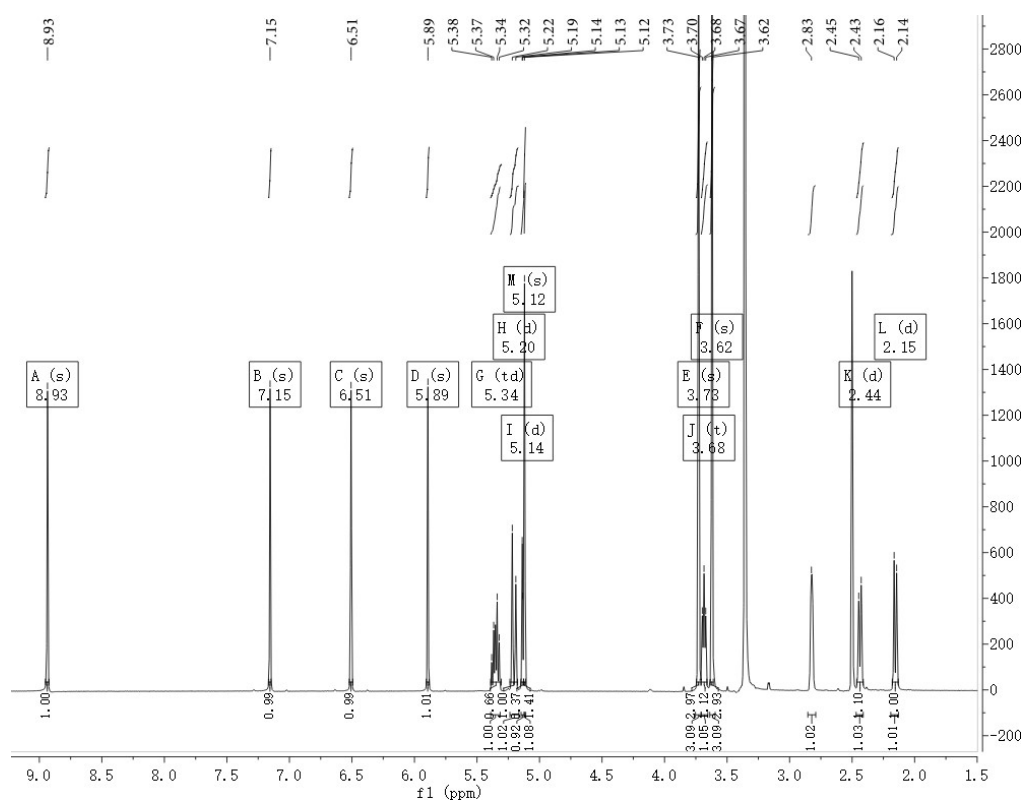
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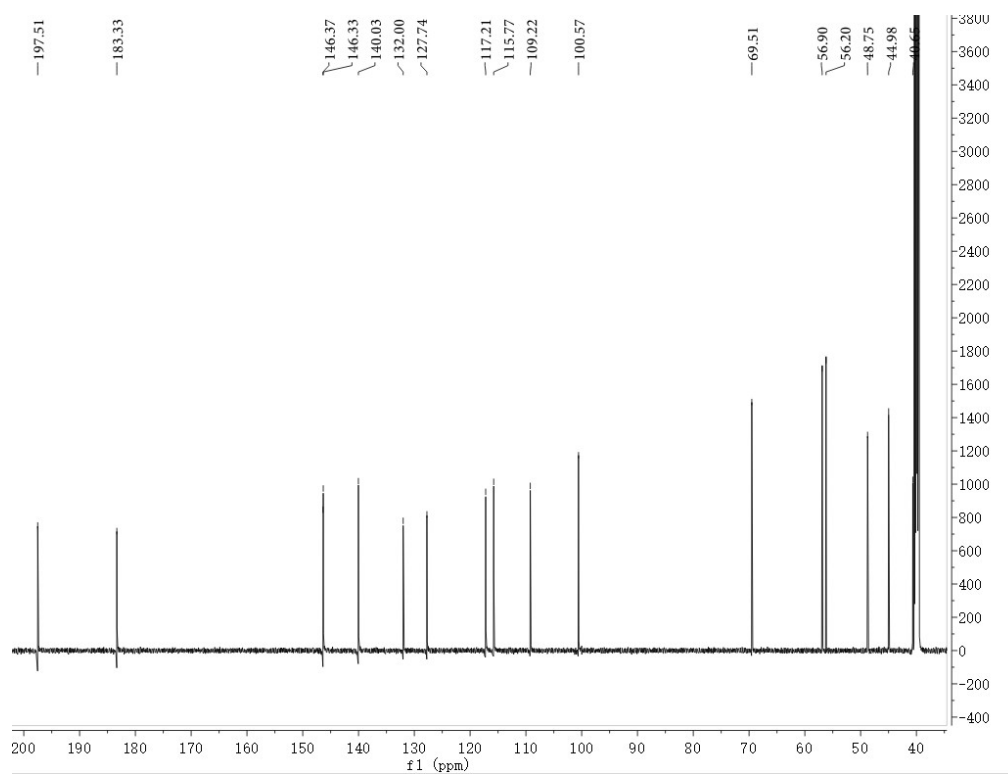
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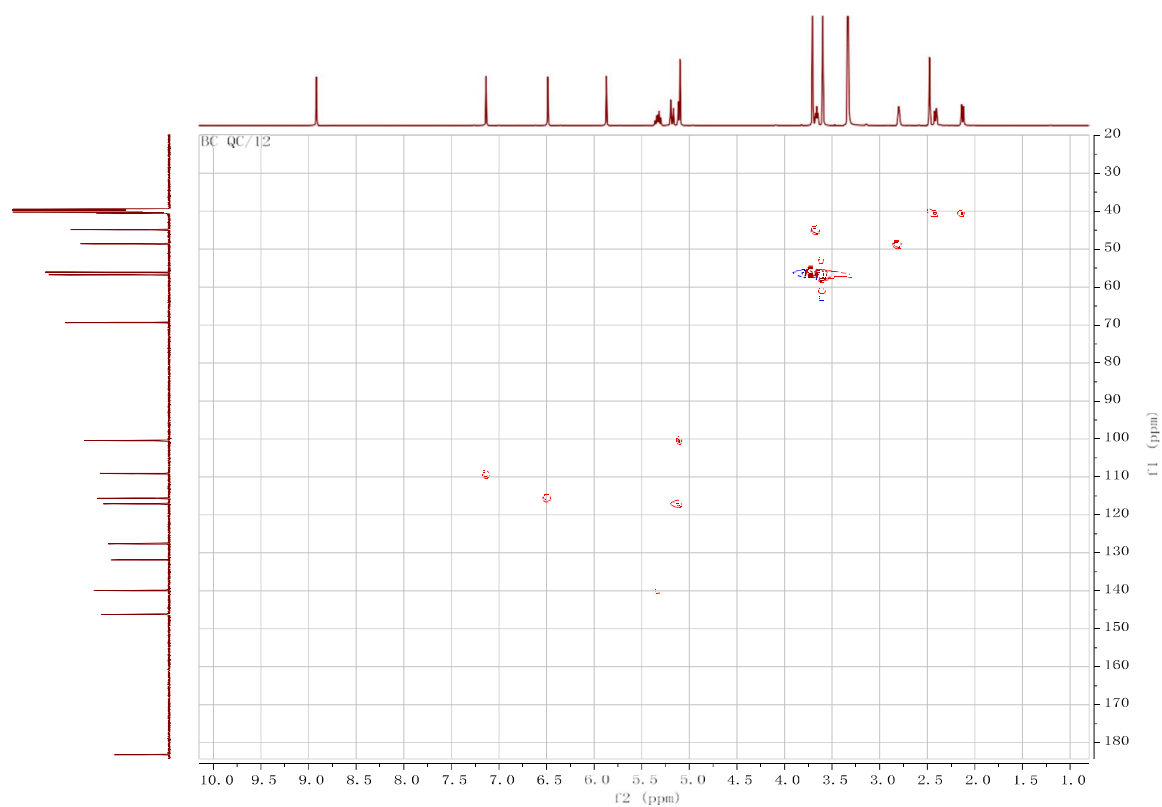
**Figure S1: HR-ESI-MS Spectrum of 1**



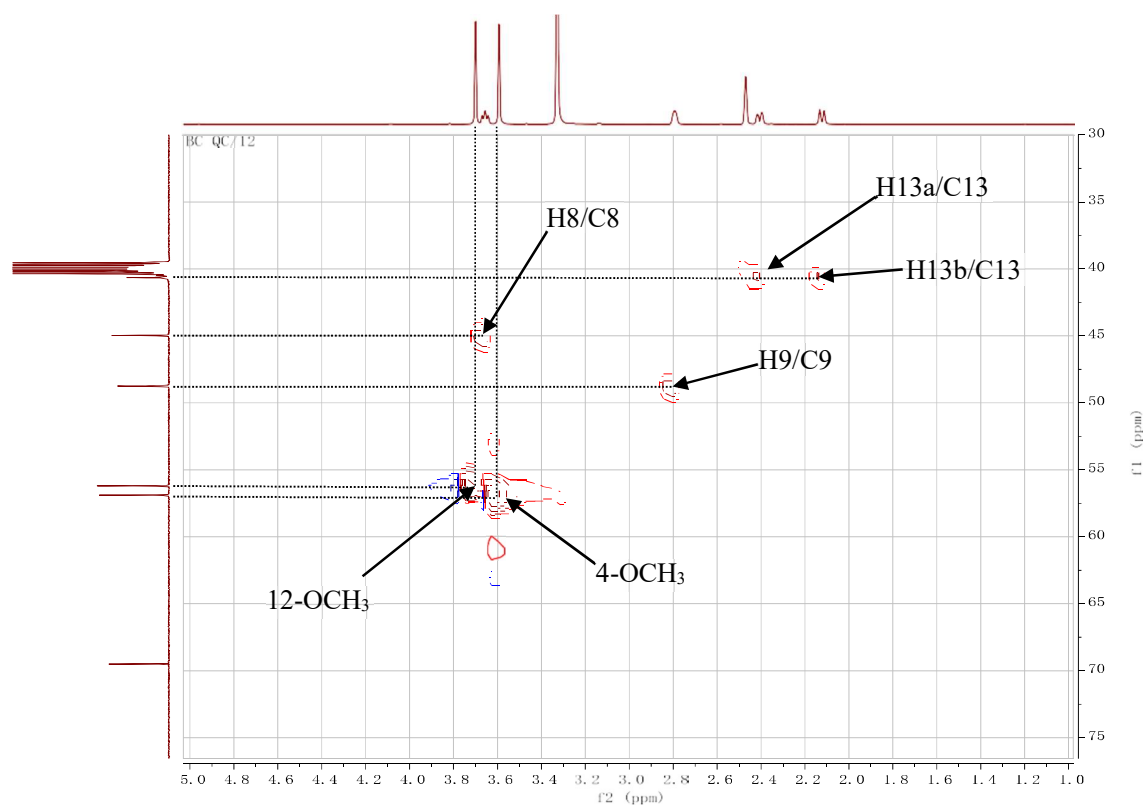
**Figure S2:**  $^1\text{H}$ -NMR (600 MHz,  $\text{DMSO-}d_6$ ) Spectrum of **1**



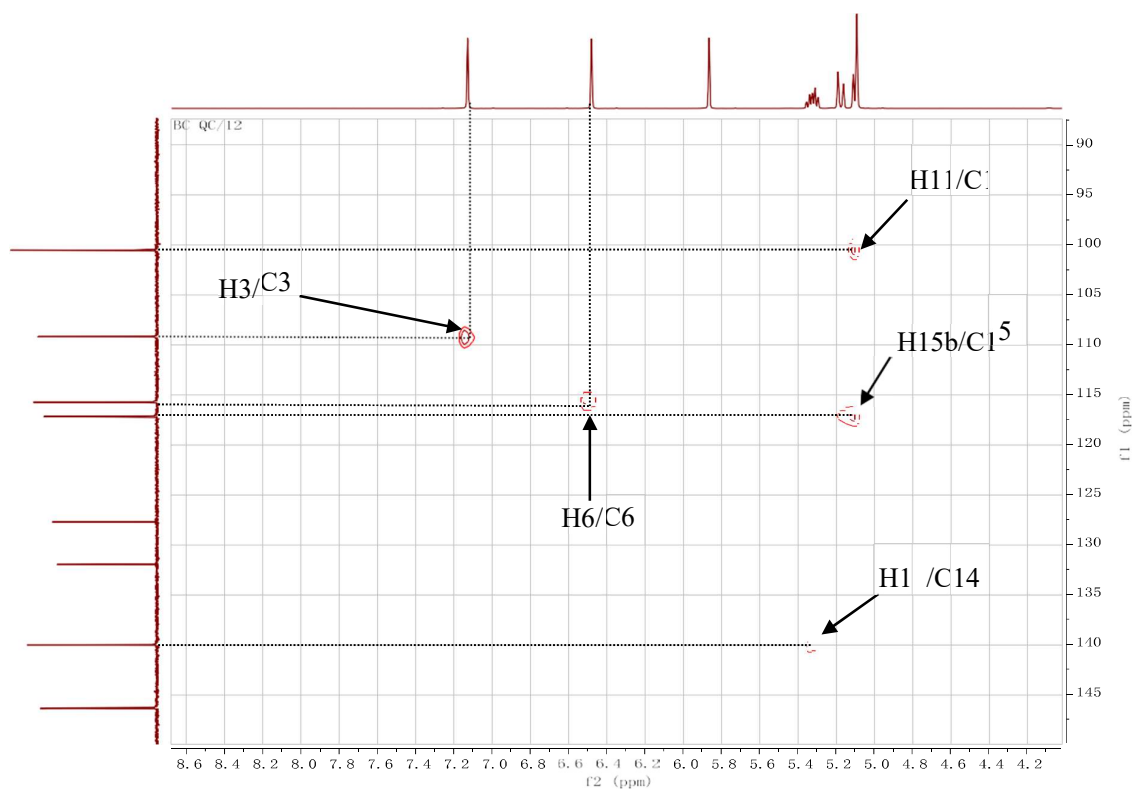
**Figure S3:**  $^{13}\text{C}$ -NMR (150MHz, DMSO- $d_6$ ) Spectrum of **1**



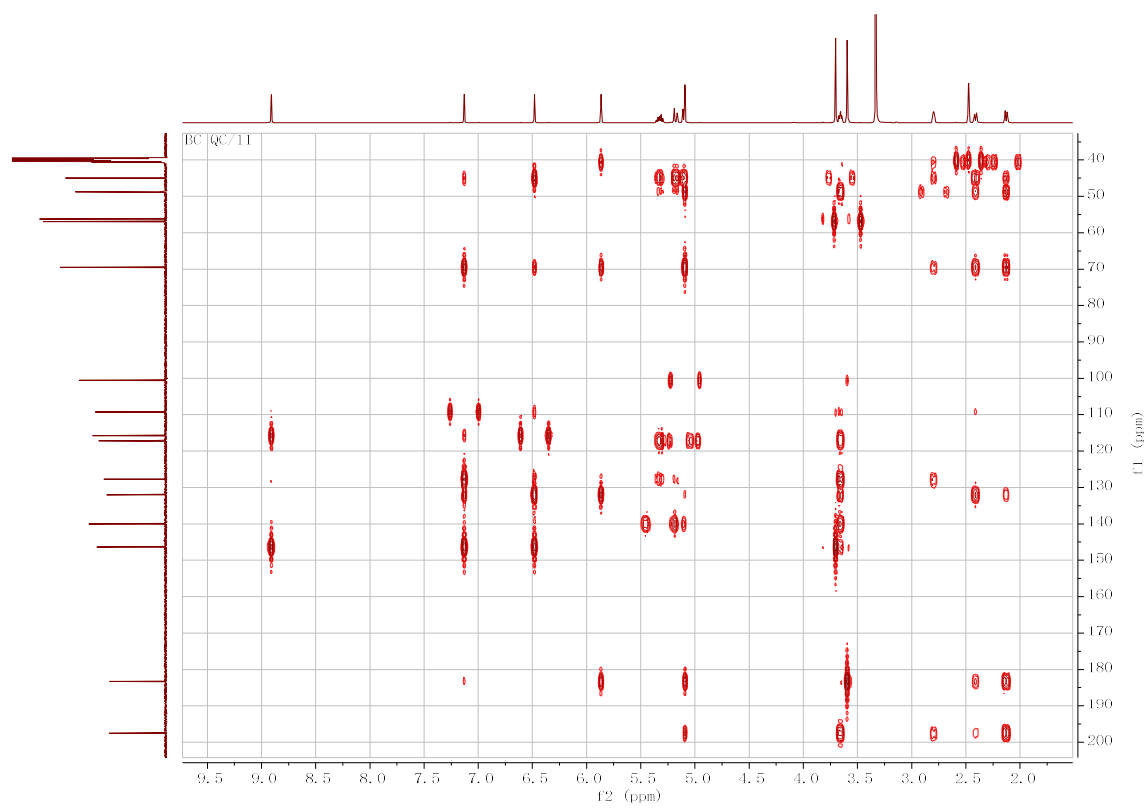
**Figure S4: HSQC Spectrum of 1**



**Figure S5:** HSQC Spectrum of **1** (From  $\delta^1\text{H}$  1.0 ppm to  $\delta^1\text{H}$  5.0ppm )

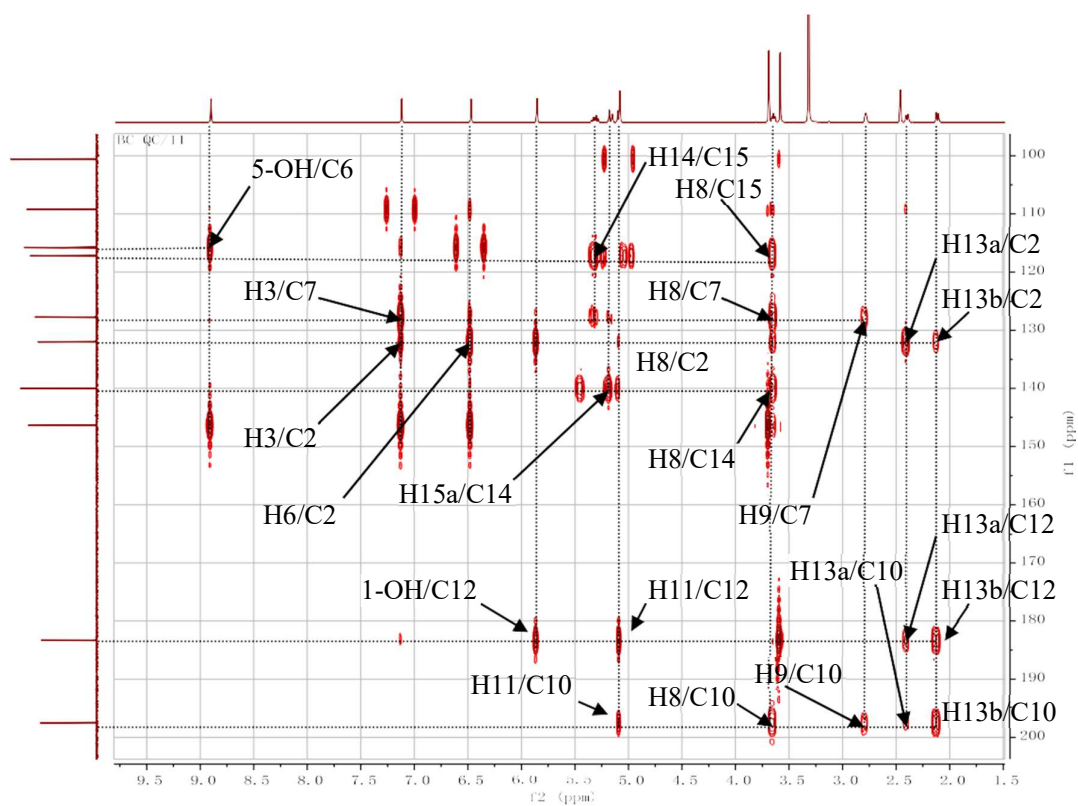


**Figure S6:** HSQC Spectrum of **1** (From  $\delta$ H 4.2 ppm to  $\delta$ H 8.6ppm )

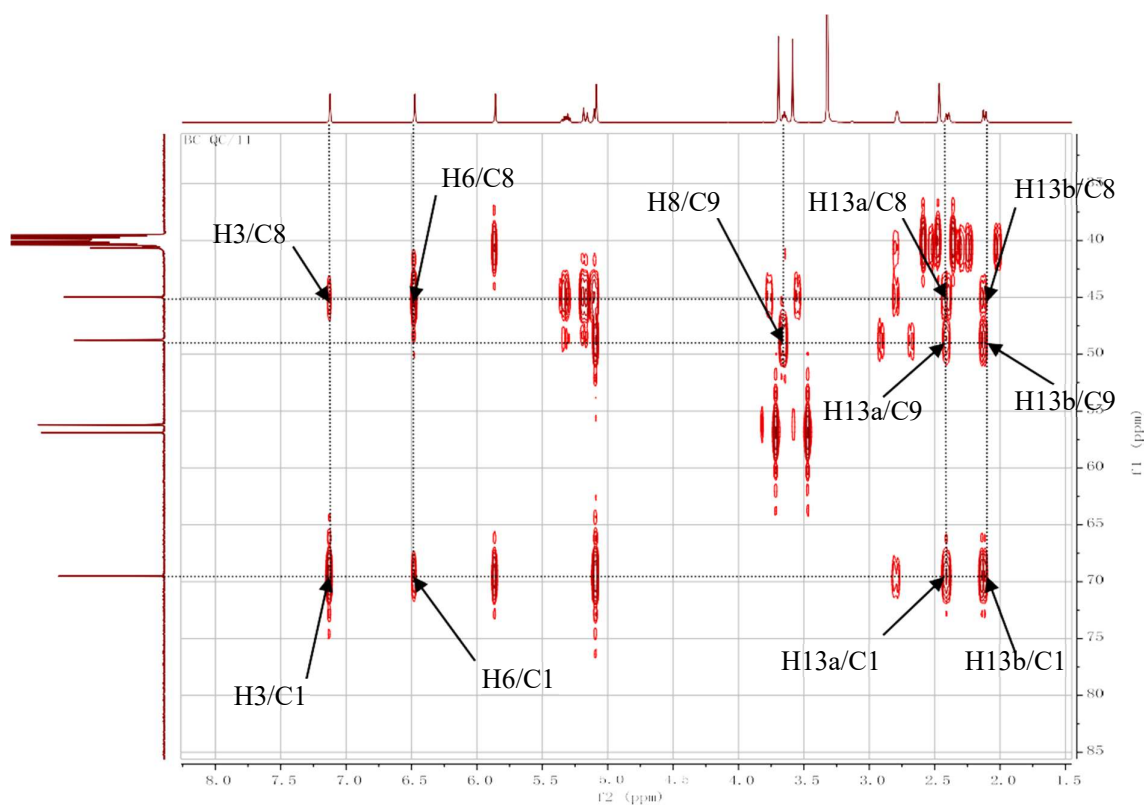


**Figure S7: HMBC Spectrum of 1**

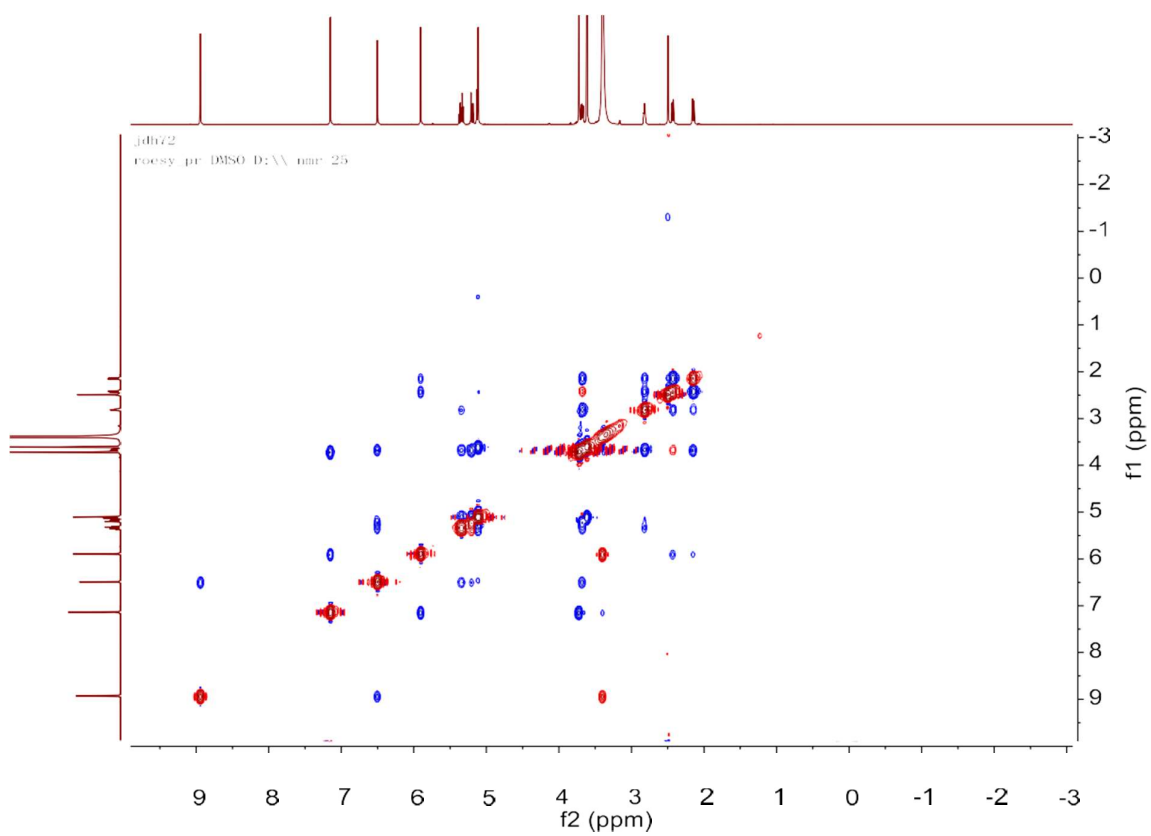




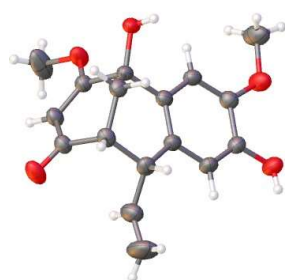
**Figure S8:** HMBC Spectrum of **1** ( From  $\delta_C$  100 ppm to  $\delta_C$  200 ppm )



**Figure S9:** HMBC Spectrum of **1** (From  $\delta_C$  35 ppm to  $\delta_C$  85 ppm )



**Figure S10: ROESY Spectrum of 1**

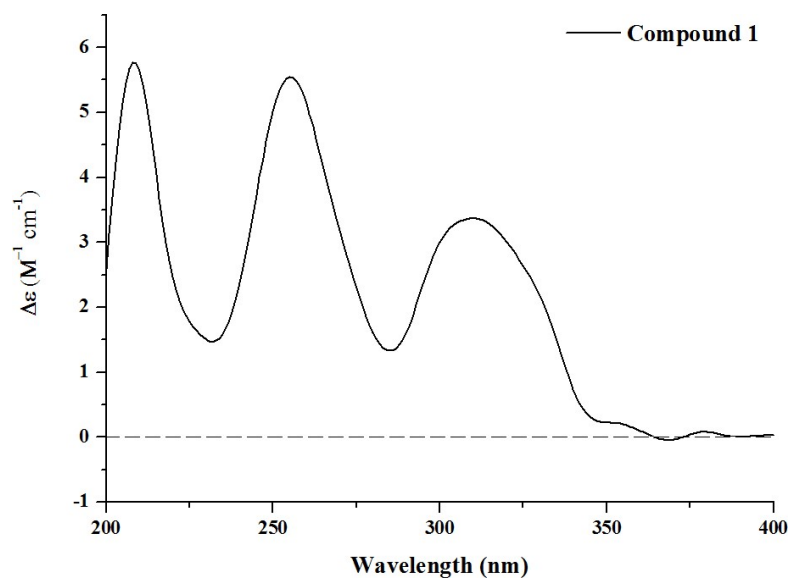


C <sub>17</sub> H <sub>14</sub> O <sub>5</sub>									
a = 7.0084(2)	α = 63.443(3)°	Z = 1							
b = 7.9833(2)	β = 69.141(3)°	Z' = 1							
c = 8.2979(2)	γ = 82.394(2)°	V = 387.87(2)	7.83	R <sub>1</sub>	3.32	%			
				wR <sub>2</sub>	8.99	%			
d min (C <sub>16</sub> )	0.83	[I(1)]	41.0	R <sub>int</sub>	1.64%	Full 134.9	96.1		
Shift	0.000	Max Peak	0.2	Min Peak	-0.1	Goof	1.050	Flack	1(2)
Structure 02A-25 loaded									
Home Work View Tools Info									
Start									
Welcome to Olex2! <a href="#">CHANGELOG</a> <a href="#">Open</a>									
<a href="#">Sacrose</a> <a href="#">THPP</a> <a href="#">Co110</a> <a href="#">ZP2</a> <a href="#">Water</a> <a href="#">Malbac</a> <a href="#">Timmy</a> <a href="#">...</a>									
Documentation: <a href="#">Online</a>   <a href="#">Static PDF</a>   <a href="#">All In-line Help</a>									
Tutorials									
Extension Modules									
Settings									
News									

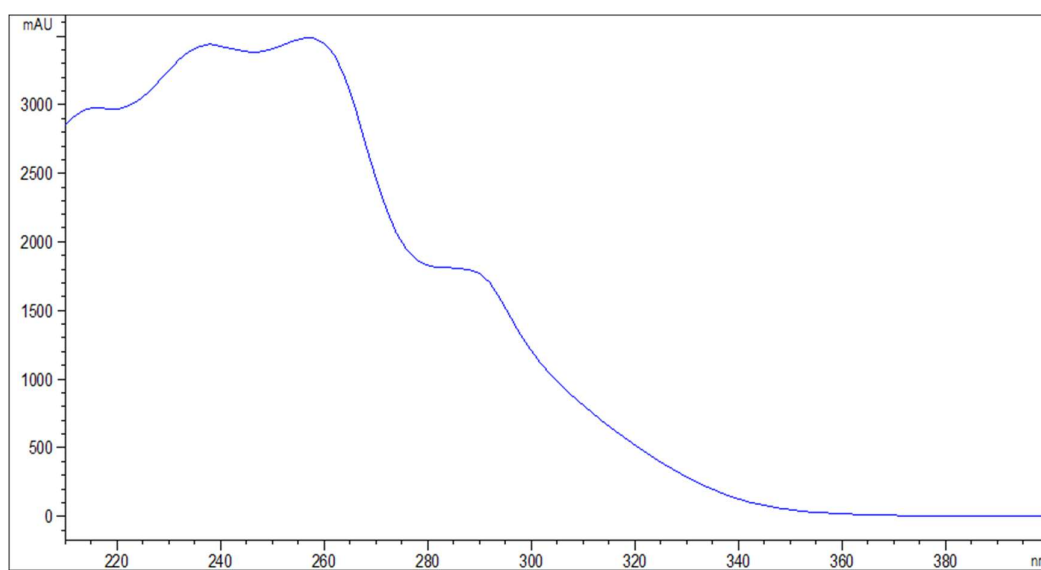
**Figure S11:** ORTEP Spectrum of **1**

[Measurement Information]

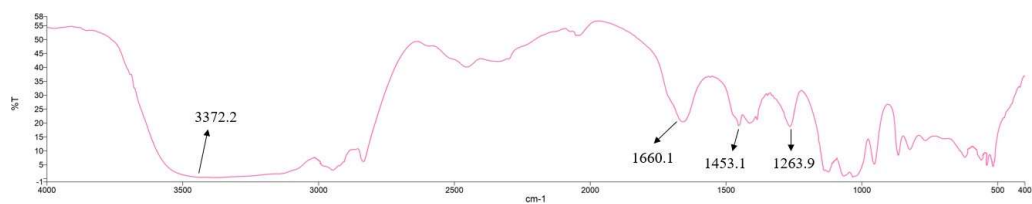
Instrument name J-1500  
Model name J-1500  
Serial No. B049961638  
Photometric mode CD, HT, Abs  
Measure range 400 - 200 nm  
Data pitch 0.5 nm  
CD scale 200 mdeg/0.1 dOD  
FL scale 200 mdeg/0.1 dODD



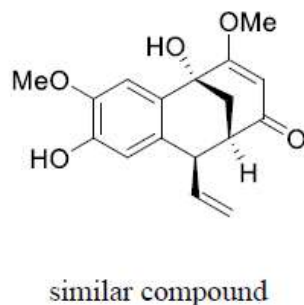
**Figure S12: CD Spectra of 1**



**Figure S13:** UV spectra of compound **1**



**Figure S14:** IR spectra of compound **1**



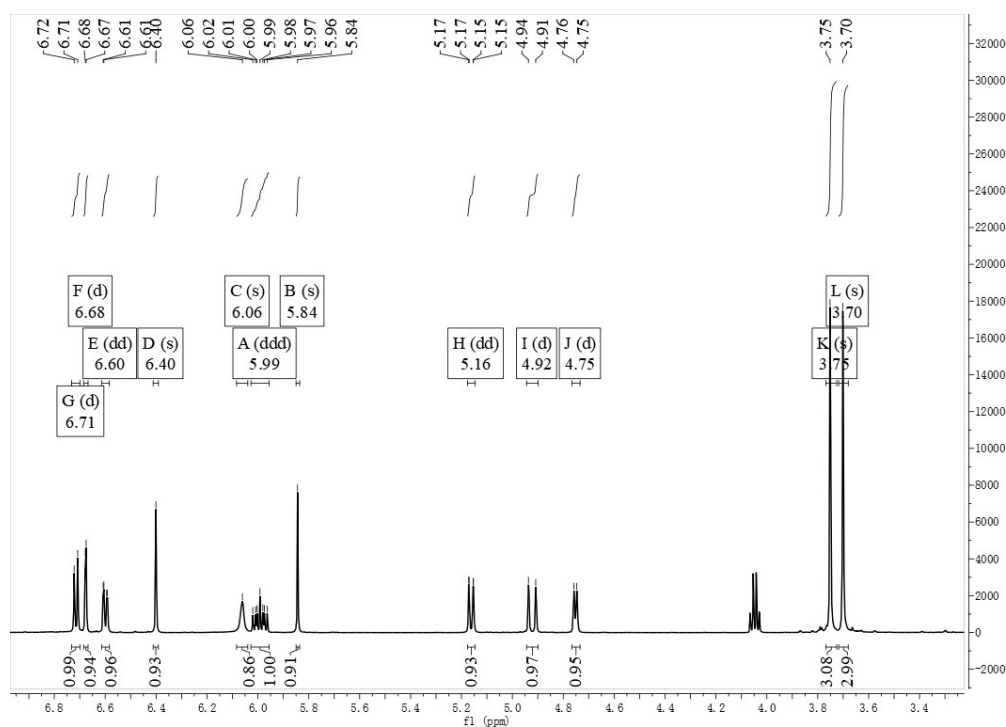
**Table S1.** The most similar compound data to compound 1

No.	compound (1)		similar compound	
	$\delta\text{H}$ , mult. ( $J$ in Hz)	$\delta\text{C}$	$\delta\text{H}$ , mult. ( $J$ in Hz)	$\delta\text{C}$
1	-	69.5	-	70.7
2	-	132.0	-	131.8
3	7.15(1H, s)	109.2	7.02(1H, s)	106.4
4	-	146.4	-	145.5
5	-	146.3	-	145.6
6	6.51 (1H, s)	115.8	6.61 (1H, s)	116.6
7	-	127.7	-	127.7
8	3.68(1H, t, $J = 8.1$ Hz)	45.0	3.51(1H, d, $J = 6.9$ Hz)	44.6
9	2.83(1H, s)	48.8	2.87(1H, s)	48.2
10	-	197.5	-	200.3
11	5.14(H, s)	100.6	5.18(1H, s)	100.0
12	-	183.3	-	181.0
13	2.44 (1H, d, $J = 12.0$ Hz) 2.15(1H, d, $J = 12.0$ Hz)	40.7	2.43 (2H, ddd, $J = 16.2, 12.1, 3.2$ Hz)	35.3
14	5.34(1H, ddd, $J = 16.9, 10.1, 8.1$ Hz)	140.0	6.03(1H, ddd, $J = 17.0, 10.1, 7.0$ Hz)	141.5
15	5.20(1H, d, $J = 16.9$ Hz) 5.14(2H, m)	117.2	4.96(1H, d, $J = 16.9$ Hz) 5.11(1H, d, $J = 10.1$ Hz)	116.3
1-OH	5.89 (1H, s)	-	3.28 (1H, s)	-
5-OH	8.93 (1H, s)	-	5.59 (1H, s)	-
4-OCH <sub>3</sub>	3.73 (3H, s)	56.9	3.90 (3H, s)	56.2
12-OCH <sub>3</sub>	3.62 (3H, s)	56.2	3.74 (3H, s)	57.0

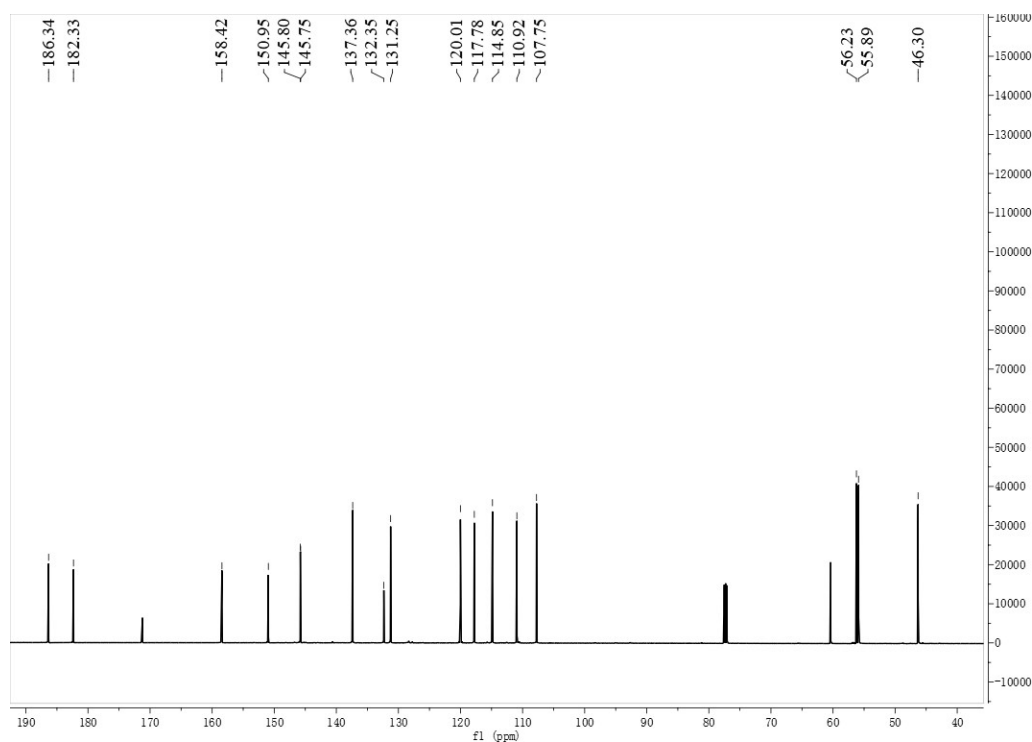


**Table S2.** Crystal data of compound **1**

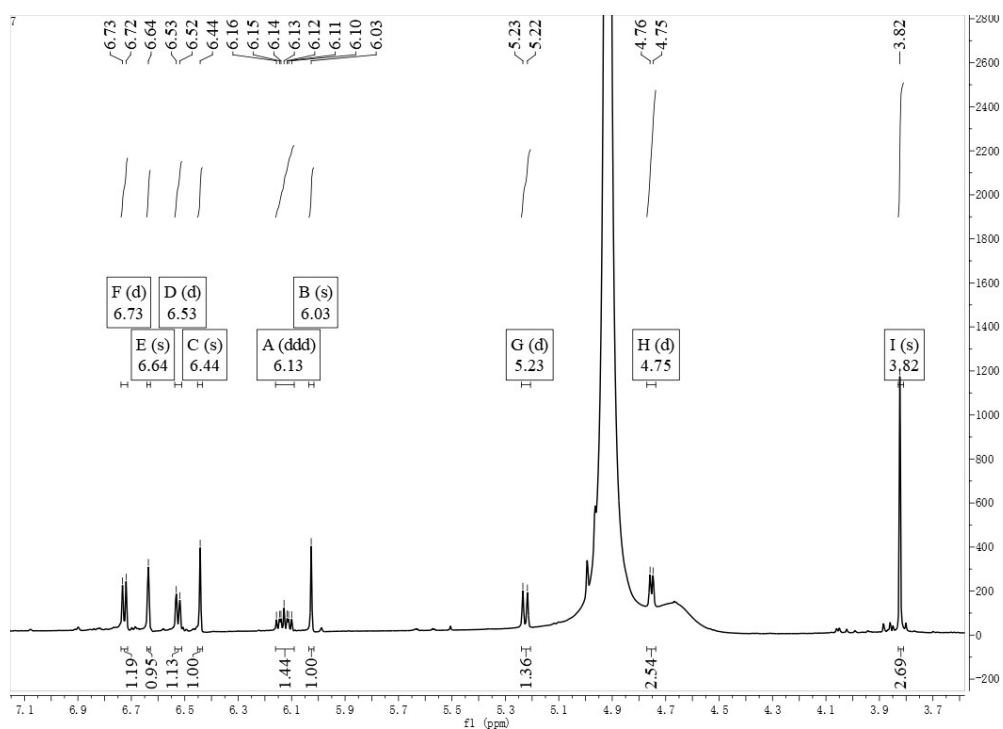
Empirical formula	C <sub>17</sub> H <sub>18</sub> O <sub>5</sub>
Temperature	293(2) K
Formula weight	302.33
Wavelength	1.54184 Å
Triclinic, space group	P1 (no. 1)
Unit cell dimensions	a = 7.0084(2) Å, $\alpha$ = 63.443(3)° b = 7.9833(2) Å, $\beta$ = 69.141(3)° c = 8.2979(2) Å, $\gamma$ = 82.394(2)°
Volume	387.87(2) Å <sup>3</sup>
Z, Calculated density	1, 1.277 g/cm <sup>3</sup>
Absorption coefficient $\mu$	0.788 mm <sup>-1</sup>
F(000)	156.0
2619 reflections	12.402° ≤ 2 $\theta$ ≤ 134.902°
1568 unique	$R_{\text{int}}$ = 0.0164, $R_{\text{sigma}}$ = 0.0244
Max. and min. transmission	1.000 and 0.534
Final $R_1$ indices ( $I > 2\sigma(I)$ )	0.0332
$wR_2$	0.0899
Flack parameter	0.1(2)



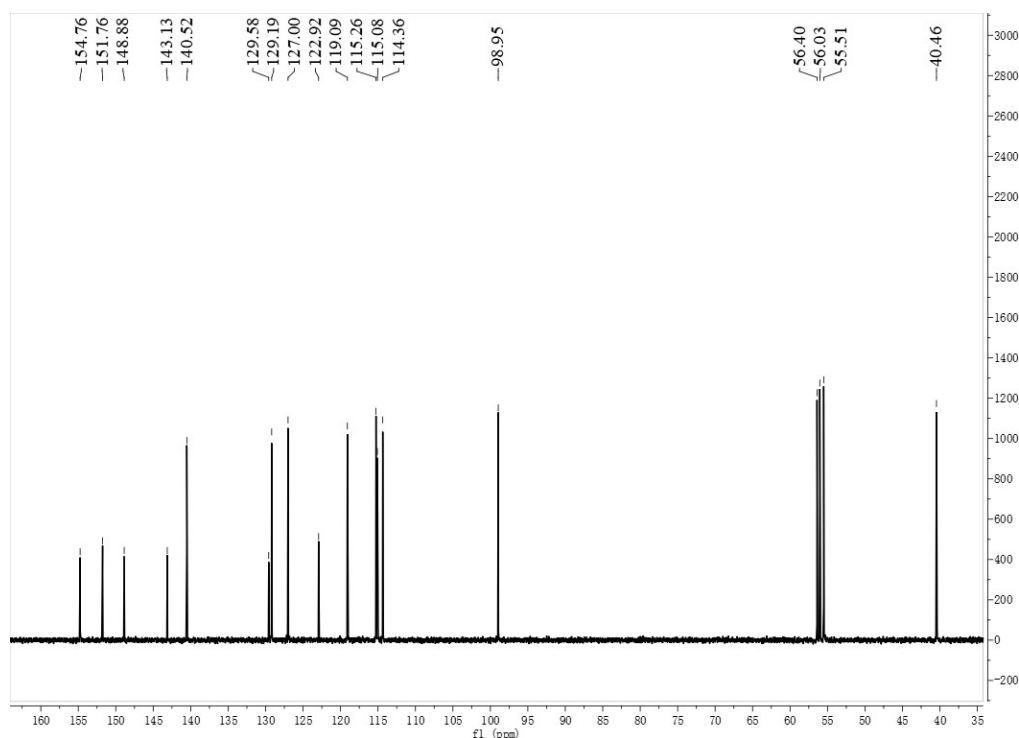
**Figure S15:  $^1\text{H}$ -NMR (600 MHz, Acetone- $d_6$ ) Spectrum of 2**



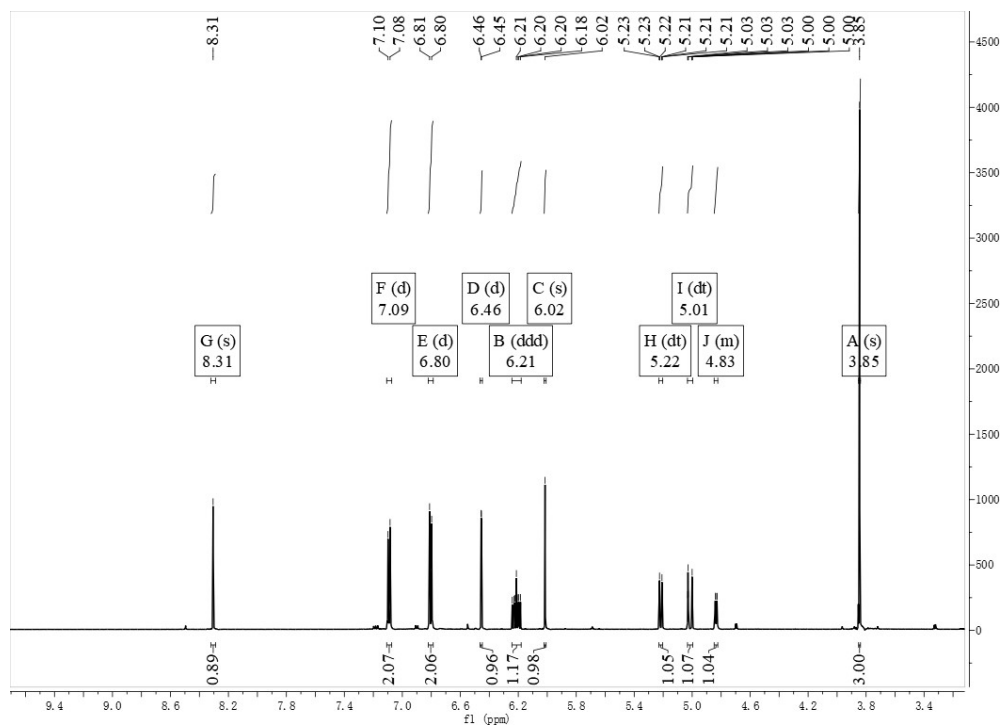
**Figure S16:  $^{13}\text{C}$ -NMR (150 MHz, Acetone- $d_6$ ) spectrum of 2**



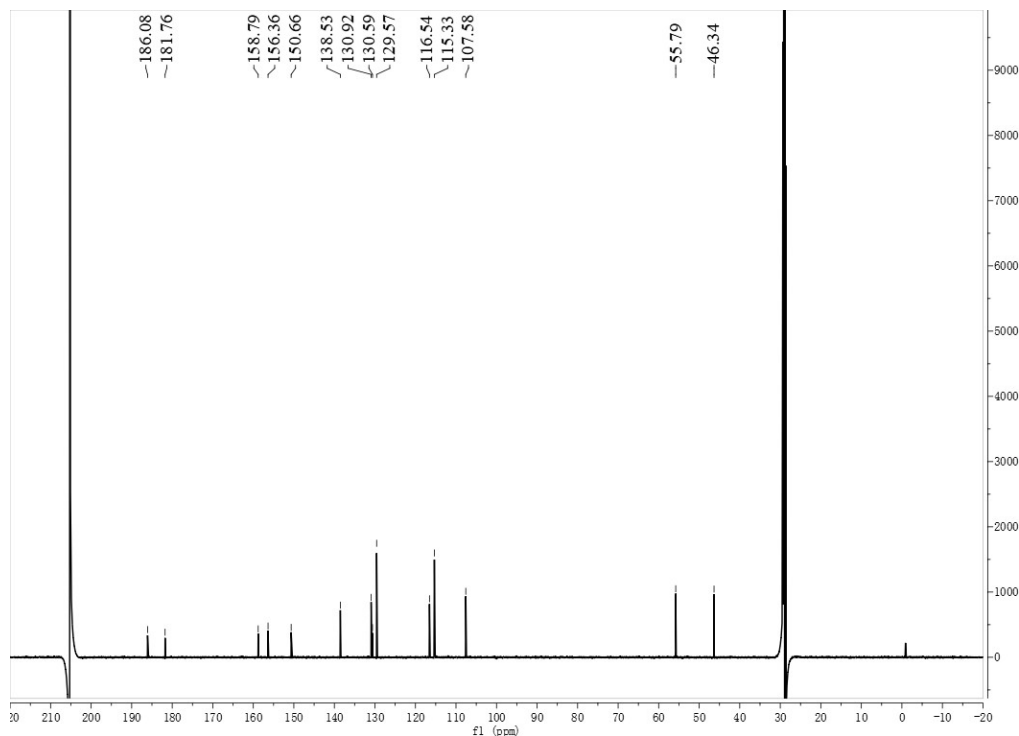
**Figure S17:  $^1\text{H}$ -NMR (600 MHz, Methanol- $d_4$ ) Spectrum of 3**



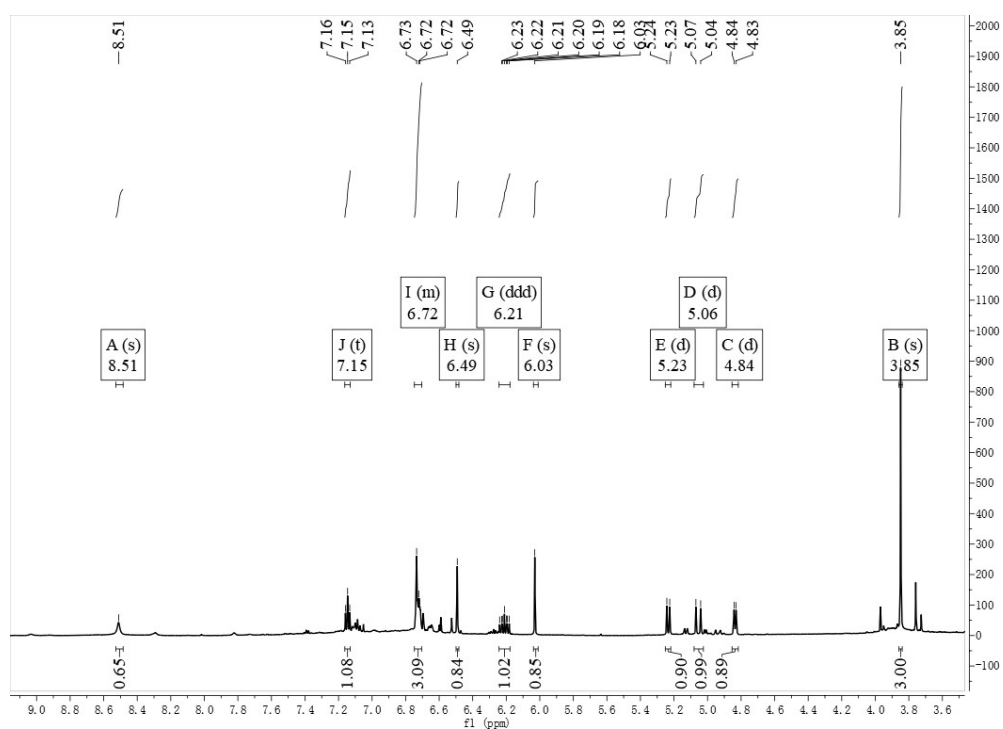
**Figure S18:  $^{13}\text{C}$ -NMR (150 MHz, Methanol- $d_4$ ) Spectrum of 3**



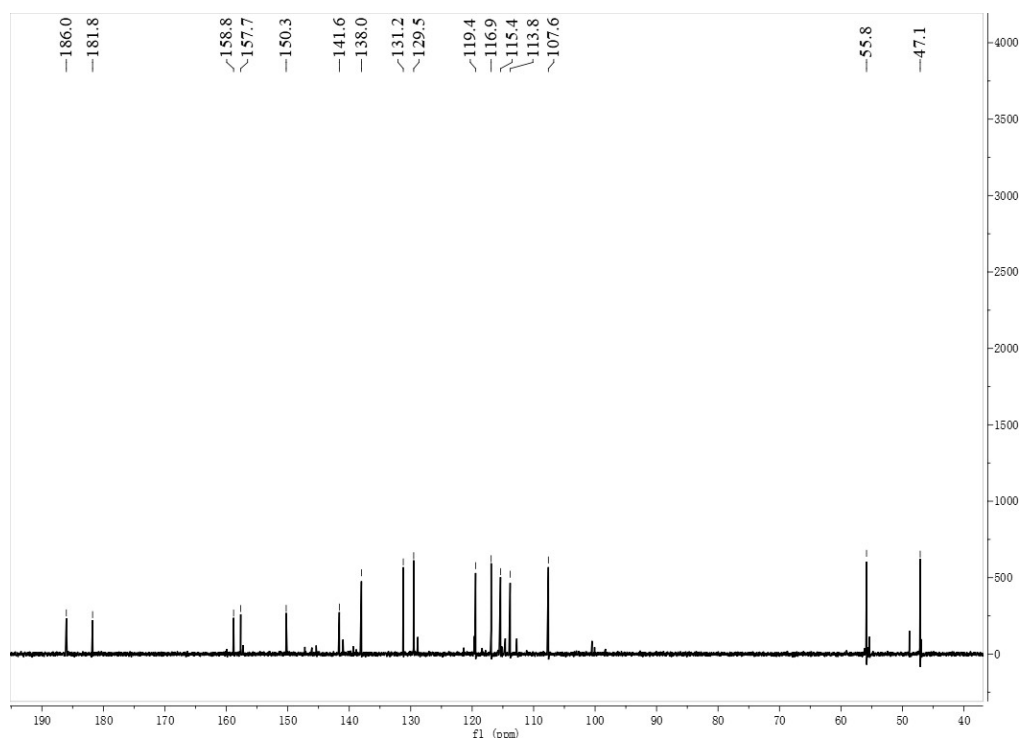
**Figure S19:  $^1\text{H}$ -NMR (600 MHz, Acetone- $d_6$ ) Spectrum of 4**



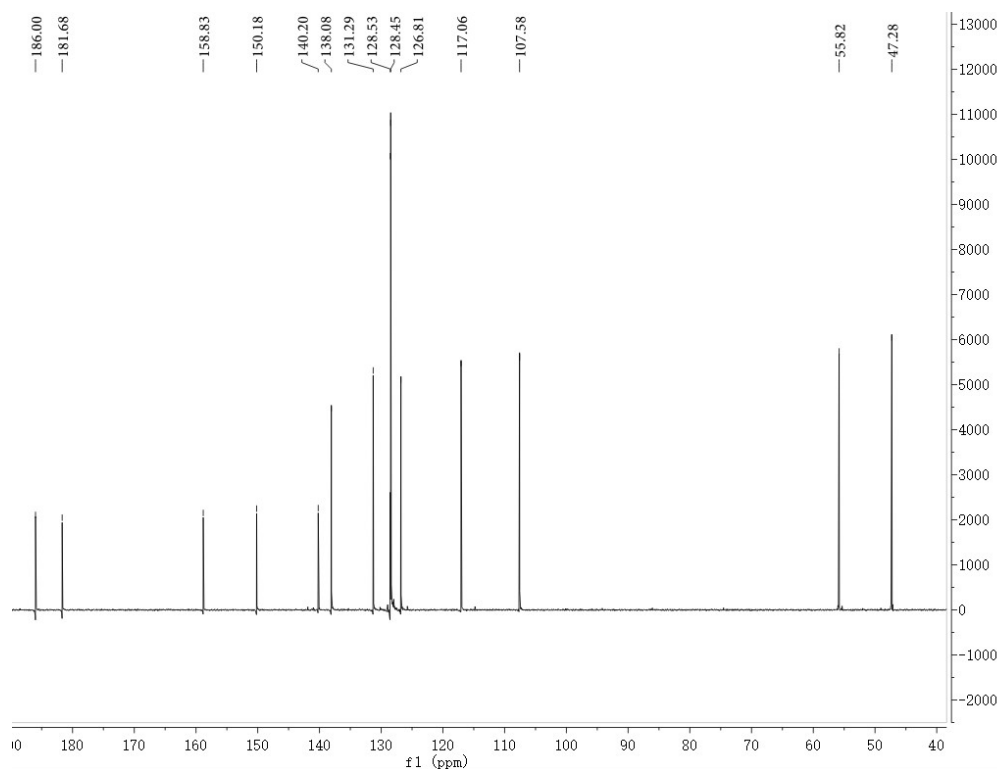
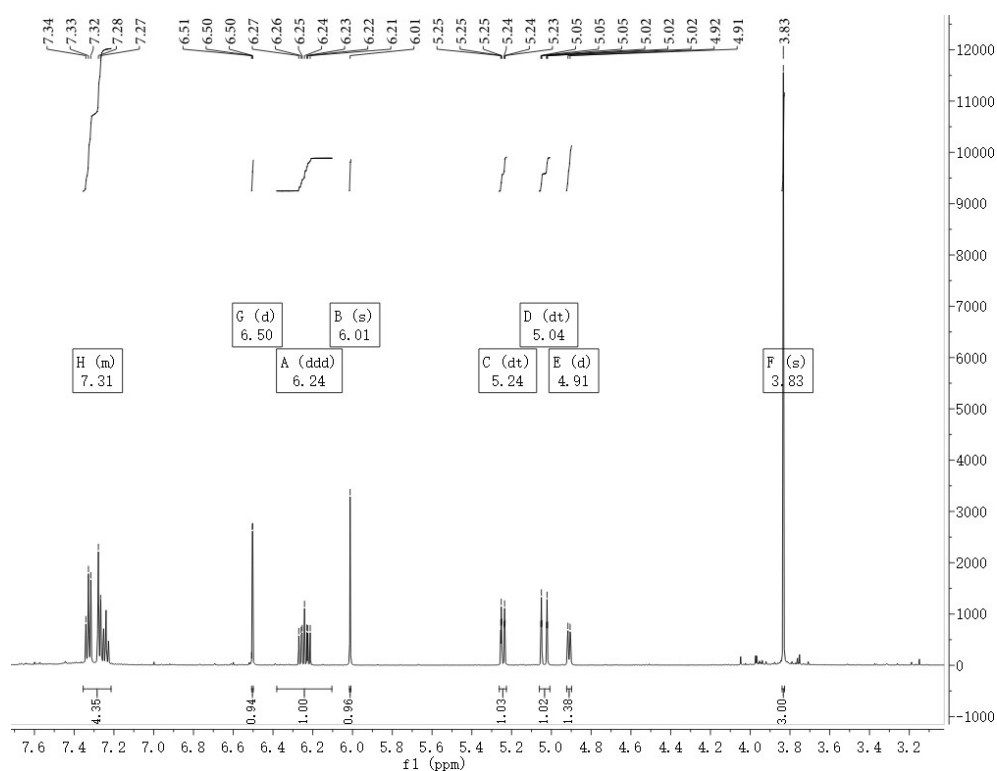
**Figure S20:  $^{13}\text{C}$ -NMR (150 MHz, Acetone- $d_6$ ) Spectrum of 4**



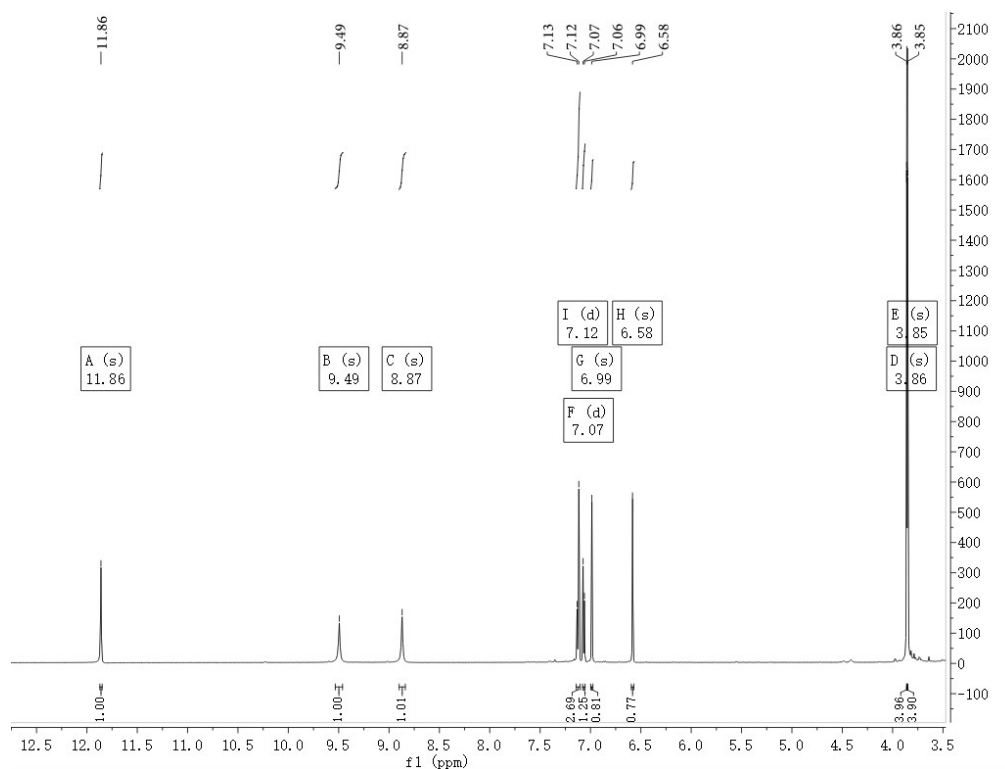
**Figure S21:  $^1\text{H}$ -NMR (600 MHz, Acetone- $d_6$ ) Spectrum of 5**



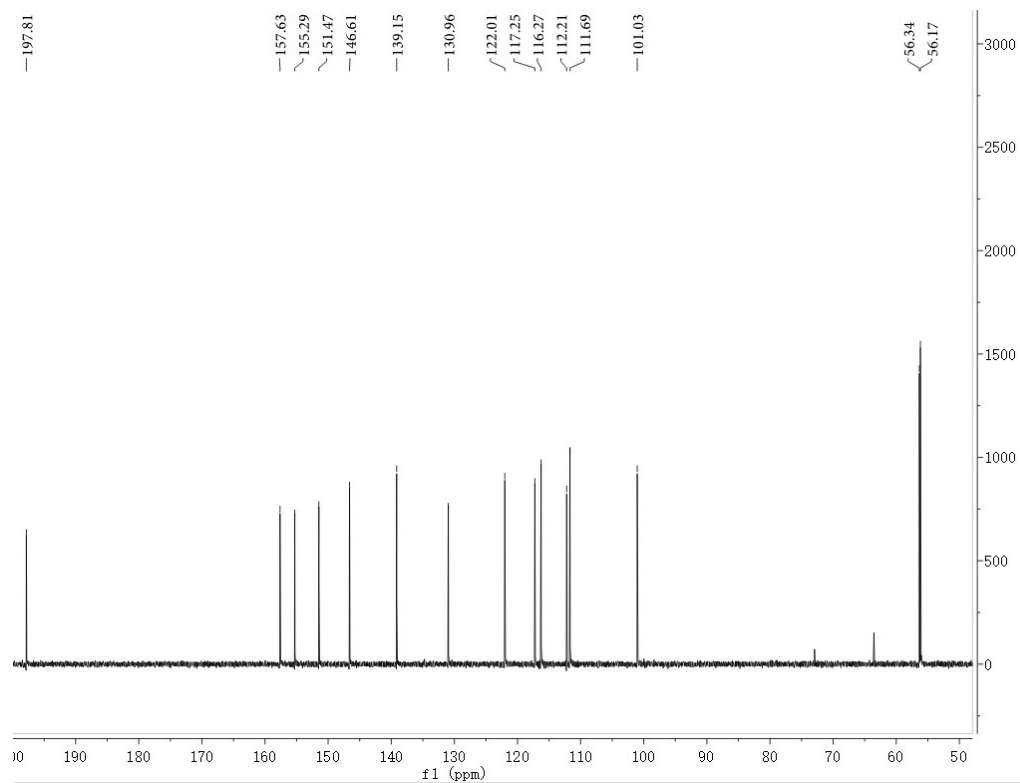
**Figure S22:  $^{13}\text{C}$  -NMR (150 MHz, Acetone- $d_6$ ) Spectrum of 5**



**Figure S24:  $^{13}\text{C}$ -NMR (150 MHz, Acetone- $d_6$ ) Spectrum of 6**



**Figure S25:  $^1\text{H}$ -NMR (600 MHz,  $\text{DMSO-}d_6$ ) Spectrum of 7**



**Figure S26:  $^{13}\text{C}$ -NMR (150 MHz,  $\text{DMSO-}d_6$ ) Spectrum of 7**

## Experimental

### *General Experimental Procedures*

UV spectra were obtained on a 210A doublebeam spectrophotometer (Shimadzu, Japan). MS data were obtained on a Triple TOF 5600 + MS (AB SCIEX, USA). 1D and 2D NMR spectra were recorded on a Bruker AV 600 spectrometer (Bruker Corporation, Fallanden, Switzerland). CD spectra were recorded using a JASCO J-1500 spectropolarimeter (CA, USA). Semipreparative HPLC was performed on an LC 3000 (Beijing Tong Heng Innovation Technology Co., Ltd., China) with a semipreparative C<sub>18</sub> column (250 × 10 mm, 10 μM, Phenomenex, USA). Optical rotations were measured using a JASCO P-1020 polarimeter (JASCO Corporation, Tokyo, Japan). Sephadex LH-20 (25, 100 mm, Pharmacia Fine Chemical Co Ltd, Uppsala, Sweden) was used for column chromatography. Analytical thin layer chromatography plates (GF 254 Silica gel) and column chromatography silica gel (100- 200 mesh, 200-300 mesh) were purchased from Qingdao Haiyang Chemical Co, Ltd. (Qingdao, China). The value of optical density was measured by Absorbance Microplate Reader (SpectraMax 190, Molecular Devices Corporation, USA).

### *Bioactivity Test-Anti-inflammatory Assays*

The cytotoxicities of compounds **1-7** and the positive control quercetin, were evaluated against RAW 264.7 cells. Cells were seeded at a density of  $5 \times 10^3$  cells per well in 96-well microtiter plates in 100 μL of medium and incubated in dulbecco's modified eagle medium (DMEM) containing 10% fetal bovine serum at 37 °C for 24 h in a 5% CO<sub>2</sub> atmosphere. The test compounds were undergone five different concentrations (1, 5, 10, 20, 40 μM) and was added to each well in a final volume of 200 μL. After the incubation period, 20 μL MTT solution and 180 μL nutrient solution was added to each well and incubated for an additional 4 h at 37 °C. The absorbance was measured at 490 nm using a microplate spectrophotometer.

The inhibition of NO production activities: RAW264.7 Cells were seeded at a density of  $5 \times 10^3$  cells per well in 96-well microtiter plates in 100 μL of medium and incubated in DMEM containing 10% fetal bovine serum at 37 °C for 24 h in a 5% CO<sub>2</sub> atmosphere. These cells were pretreated with various concentrations (1, 5, 10, 20, 40 μM) of compounds **1-7** and quercetin extract for 1 h. Cells were then treated with 1 μg/mL of LPS. After 24h, the supernatant in each well was collected for nitric oxide (NO) determination. Concentrations of NO in supernatants were measured with Griess Reagent, according to each manufacturer's instructions.

### *Bioactivity Test- Antitumor Assays*

The antitumor activities of compounds **1-7** and the positive control Fluorouracil (5-FU), were evaluated against Caco-2, MDA-MB-468, MDA-MB-231 and CT26 cell lines. Cells were seeded at a density of  $1 \times 10^4$  cells per well in 96-well microtiter plates in 100 μL of medium and incubated in RPMI 1640 Medium containing 10% fetal bovine serum at 37 °C for 24 h in a 5% CO<sub>2</sub> atmosphere. The test compounds were undergone five different concentrations (1, 10, 20, 40, 80 μM) and was added to each well in a final volume of 200 μL. After the incubation period, 20 μL MTT solution and 180 μL nutrient solution was added to each well and incubated for an additional 4 h at 37 °C. The absorbance was measured at 490 nm using a microplate spectrophotometer.