Supporting Information

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Neoflavonoids from the Heartwood of *Dalbergia melanoxylon*

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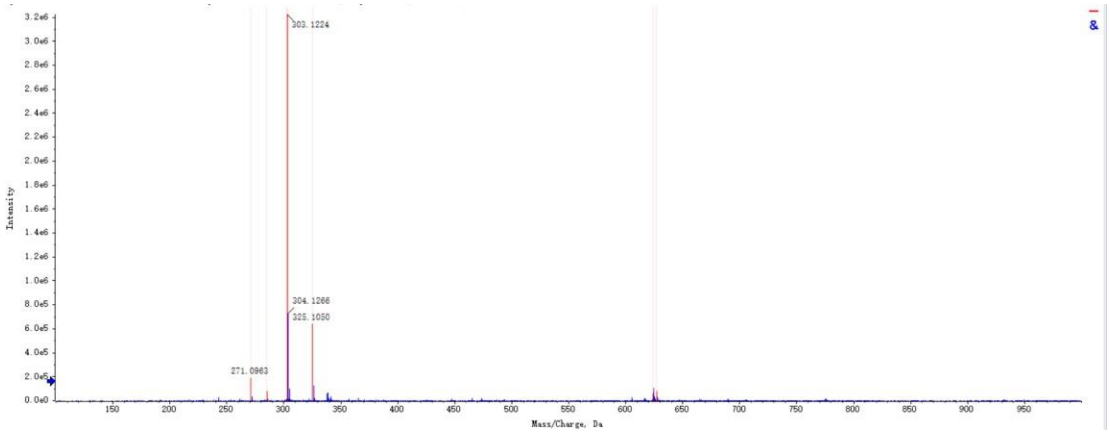


Figure S1: HR-ESI-MS Spectrum of **1**

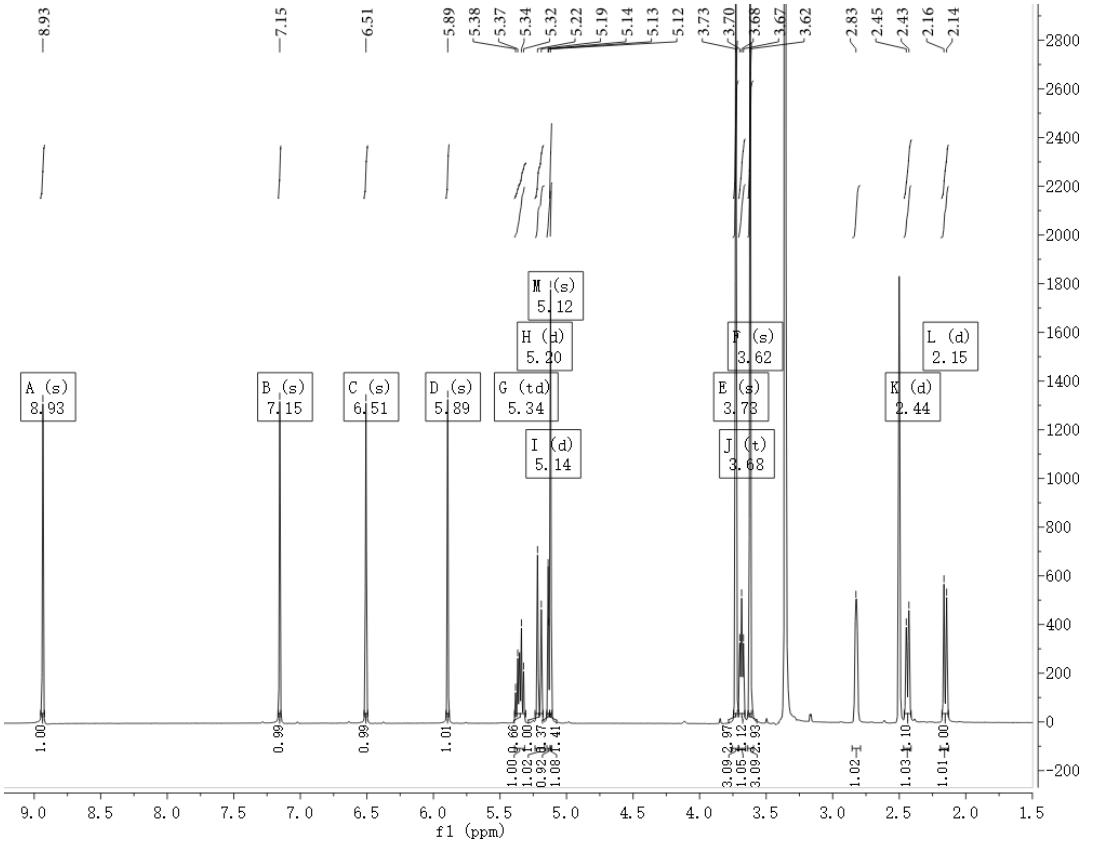


Figure S2: ^{1}H-NMR (600 MHz, DMSO-*d6*) Spectrum of **1**

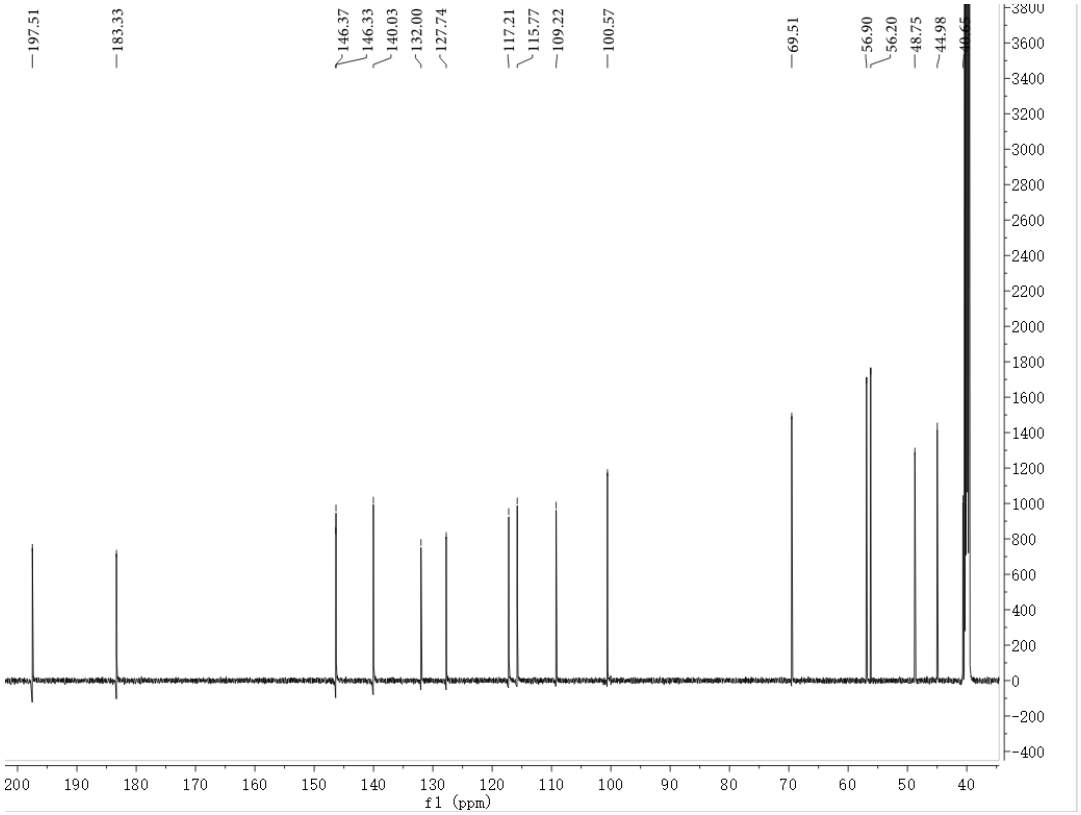


Figure S3: ^{13}C-NMR (150MHz, DMSO-*d6*) Spectrum of **1**

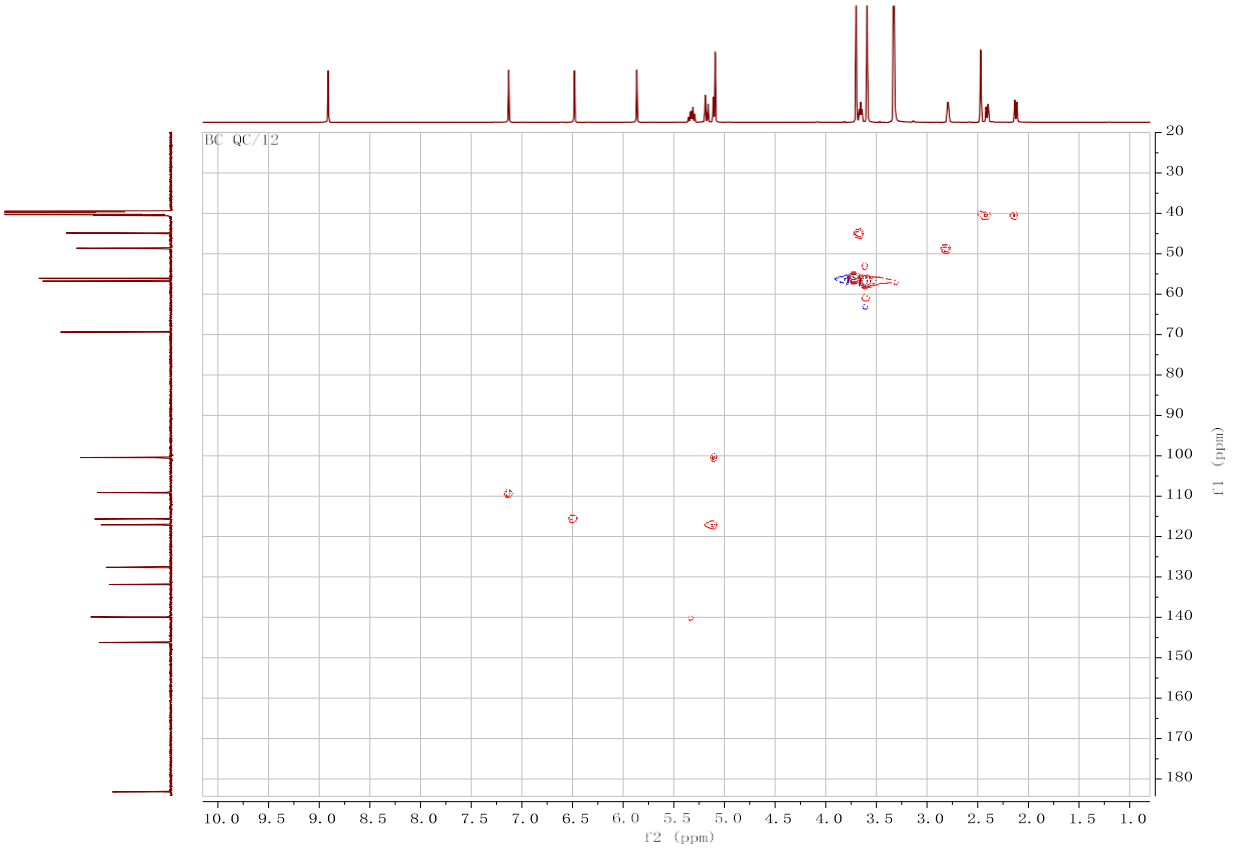


Figure S4: HSQC Spectrum of **1**

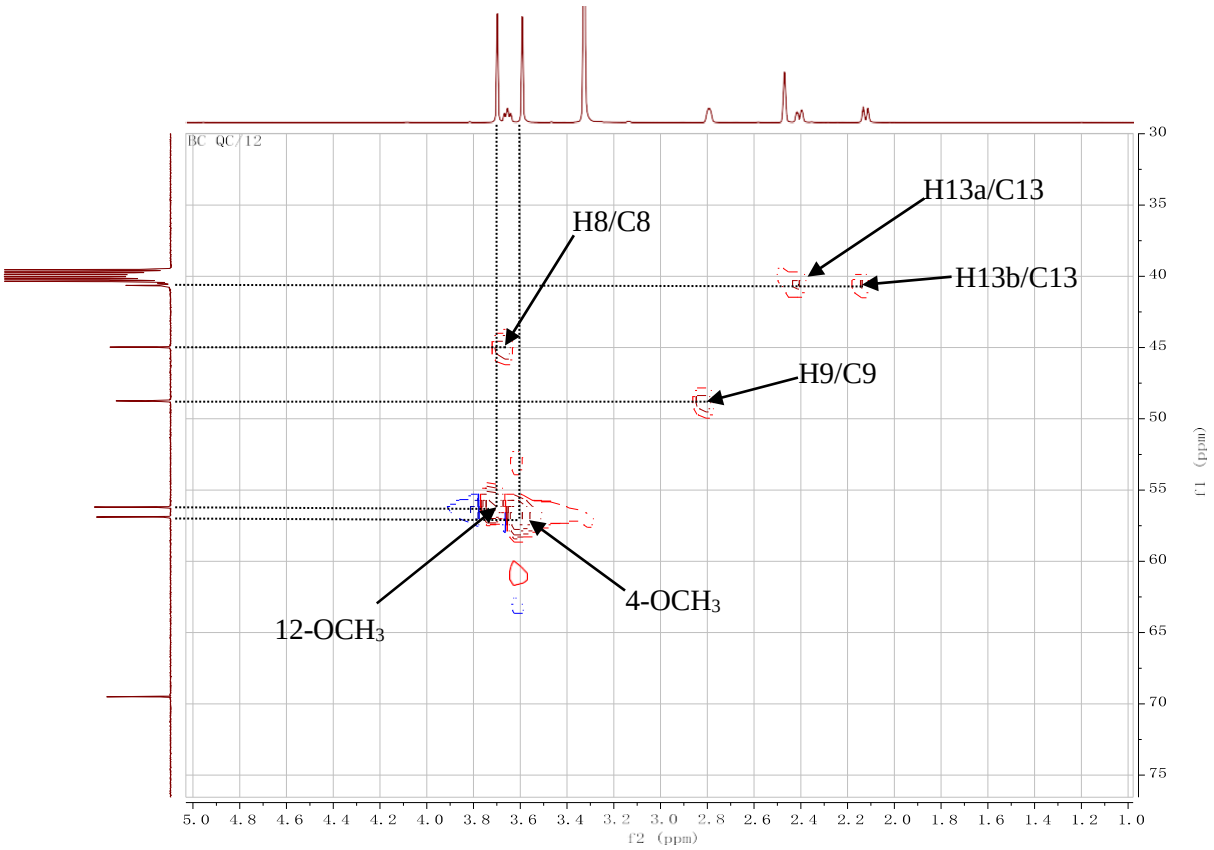


Figure S5: HSQC Spectrum of **1** (From δH 1.0 ppm to δH 5.0ppm)

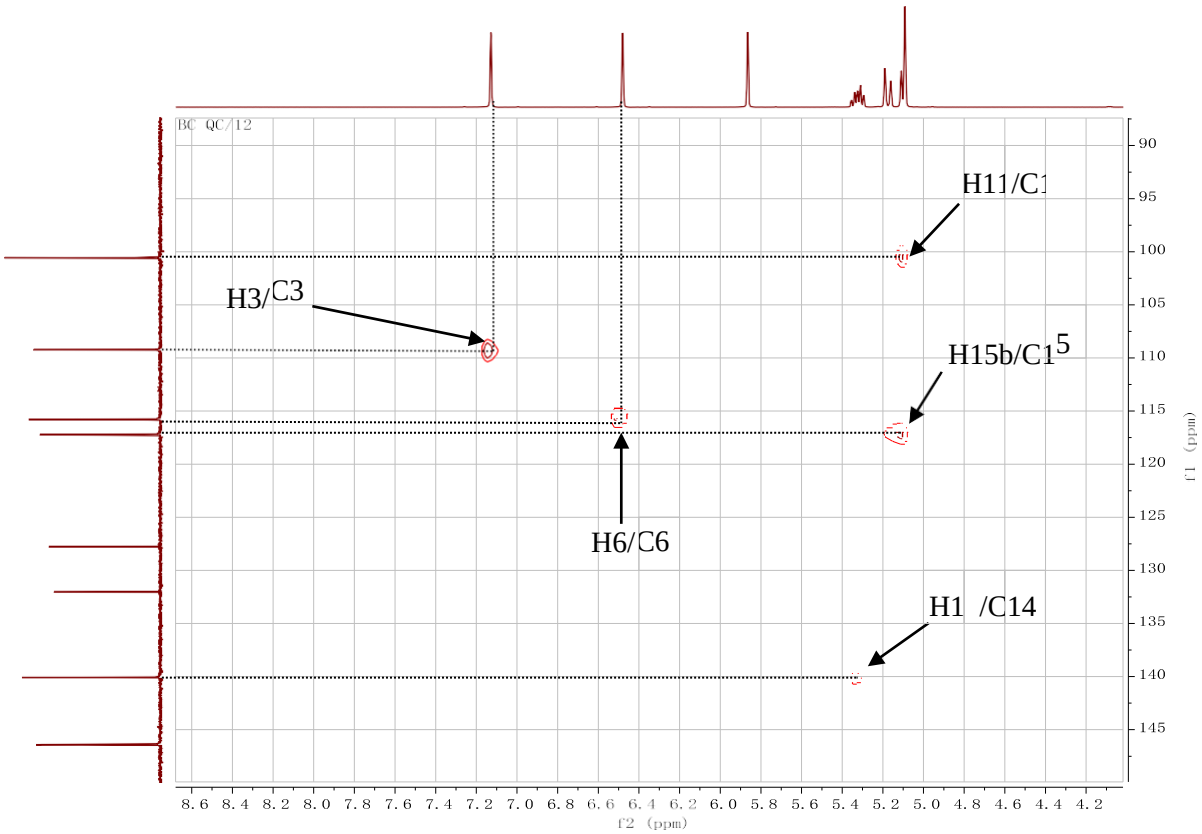


Figure S6: HSQC Spectrum of **1** (From δH 4.2 ppm to δH 8.6ppm)

Figure S7: HMBC Spectrum of **1**

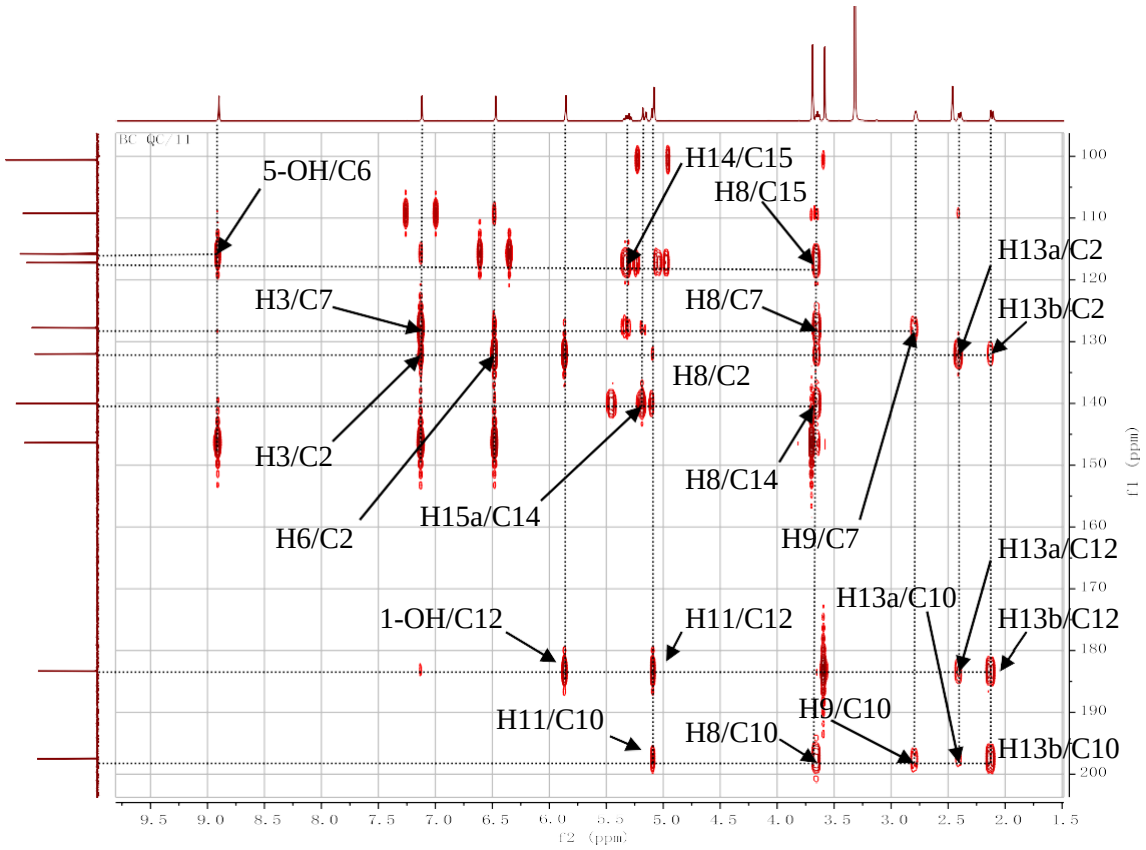


Figure S8: HMBC Spectrum of **1** (From δC 100 ppm to δC 200 ppm)

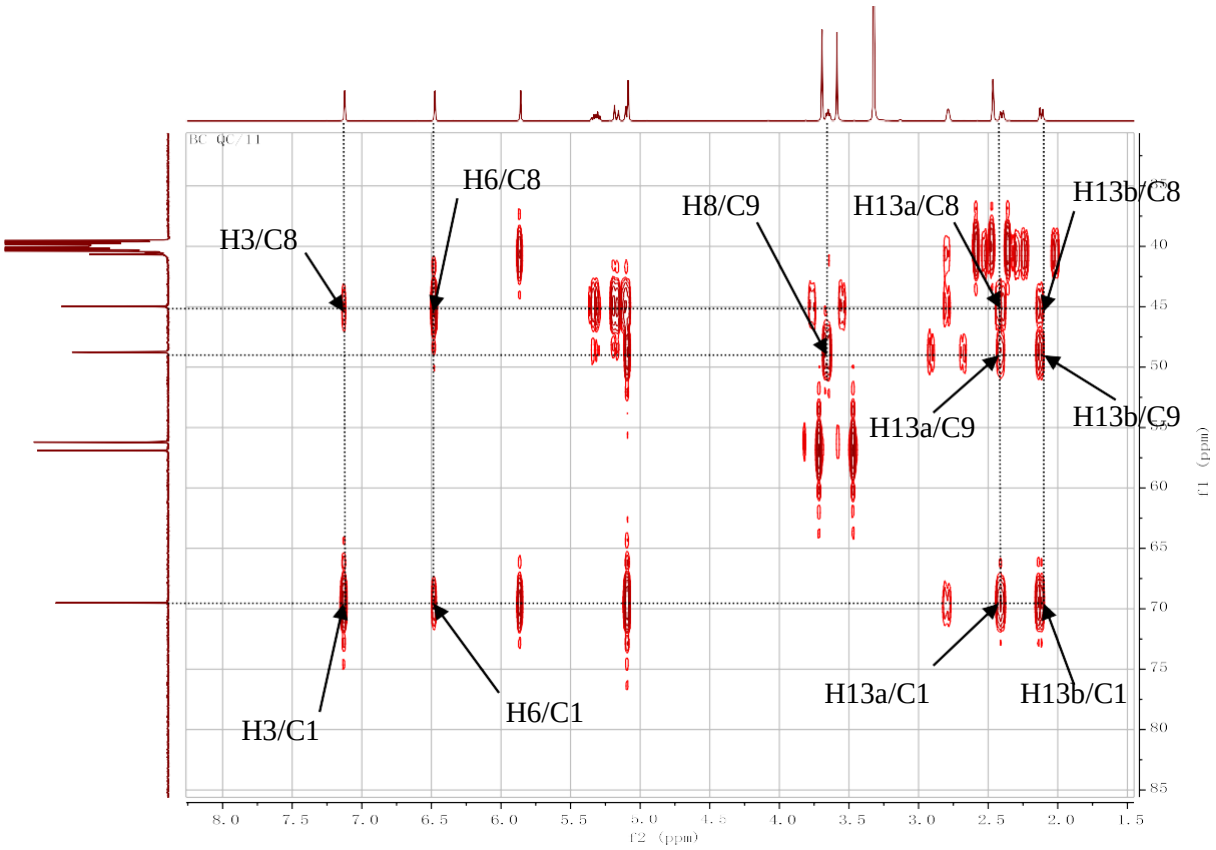


Figure S9: HMBC Spectrum of **1** (From δC 35 ppm to δC 85 ppm)

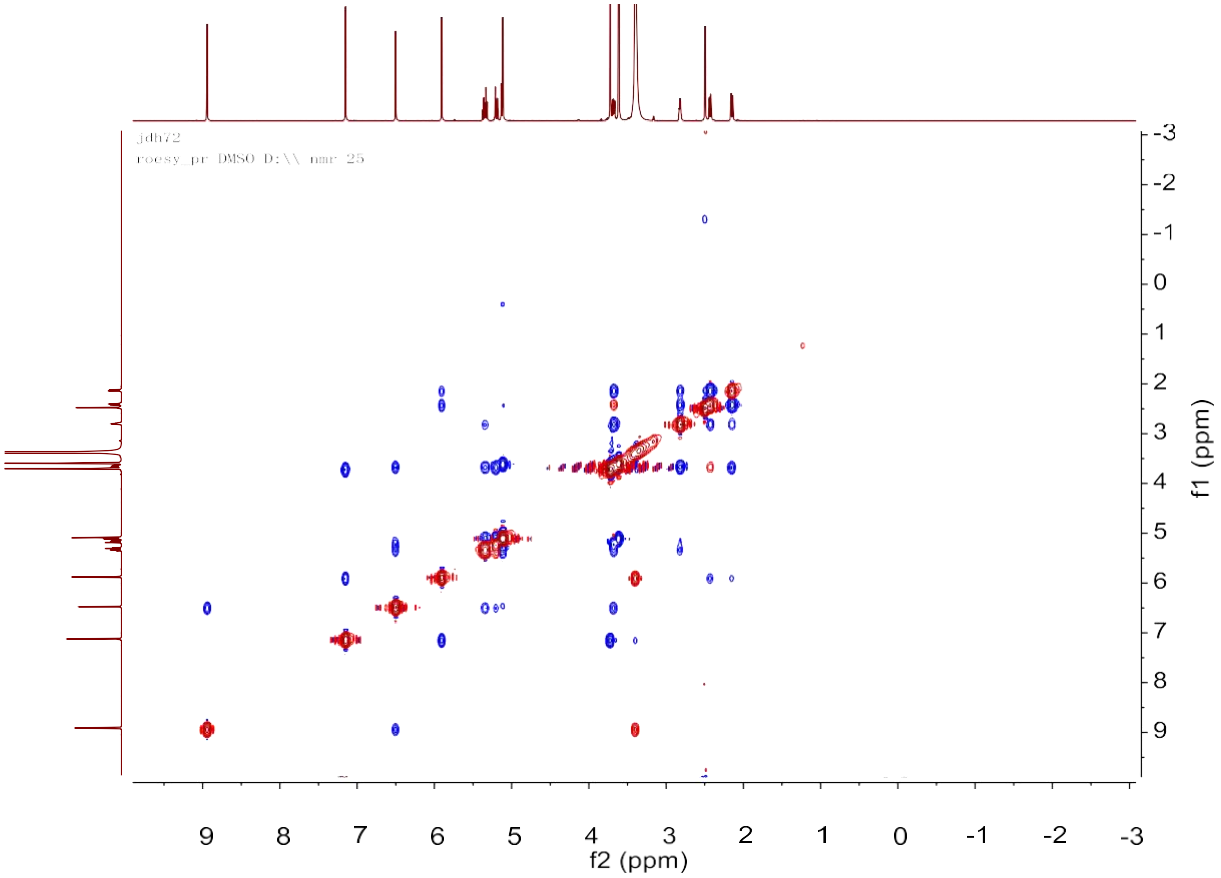


Figure S10: ROESY Spectrum of **1**

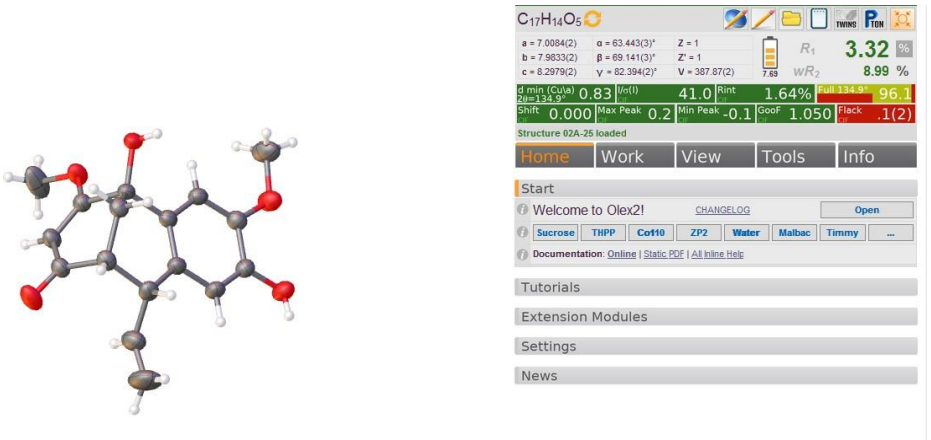


Figure S11: ORTEP Spectrum of **1**

[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

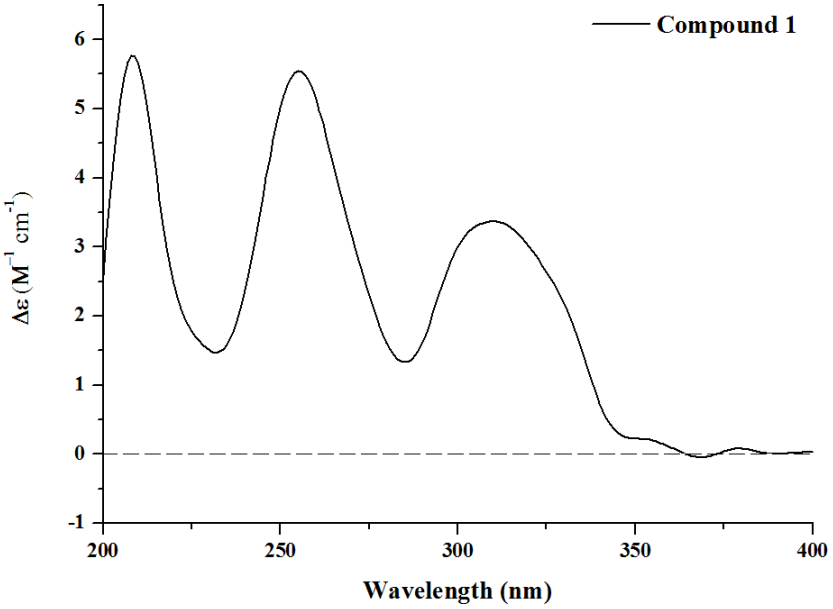


Figure S12: CD Spectra of **1**

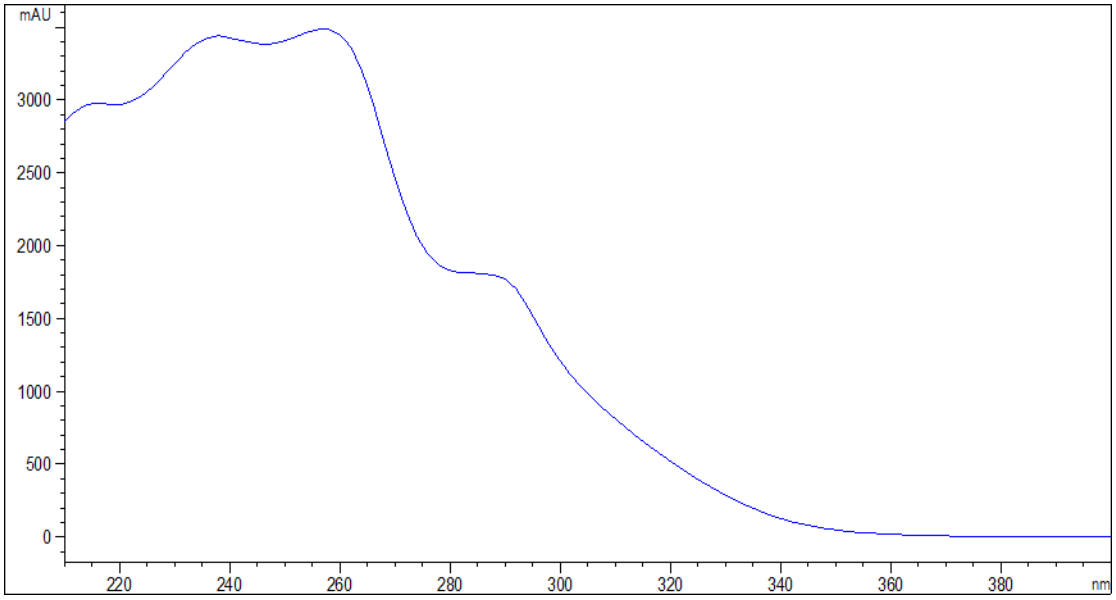


Figure S13: UV spectra of compound **1**

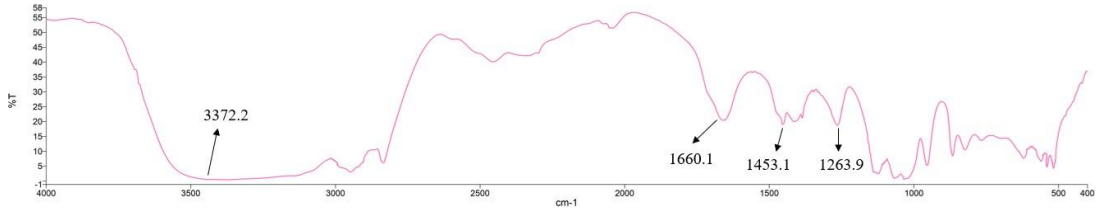
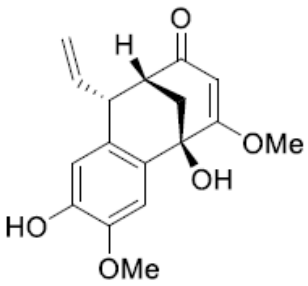
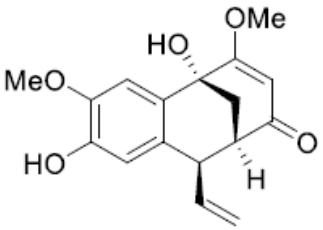


Figure S14: IR spectra of compound **1**



new compound



similar compound

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

No.	compound (1)		similar compound	
	δH, mult. (*J* in Hz)	**δC**	**δH, mult. (*J* in Hz)**	**δC**
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-OCH3	3.73 (3H, s)	56.9	3.90 (3H, s)	56.2
12-OCH3	3.62 (3H, s)	56.2	3.74 (3H, s)	57.0

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

Empirical formula	$C_{17}H_{18}O_5$
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, α = 63.443(3)° b = 7.9833(2) Å, β = 69.141(3)° c = 8.2979(2) Å, γ = 82.394(2)°
Volume	387.87(2) $Å^3$
Z,Calculated density	1, 1.277 g/cm^3
Absorption coefficient mu	0.788 mm^{-1}
F(000)	156.0
2619 reflections	$12.402° \leq 2\Theta \leq 134.902°$
1568 unique	R_{int} = 0.0164, R_{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)

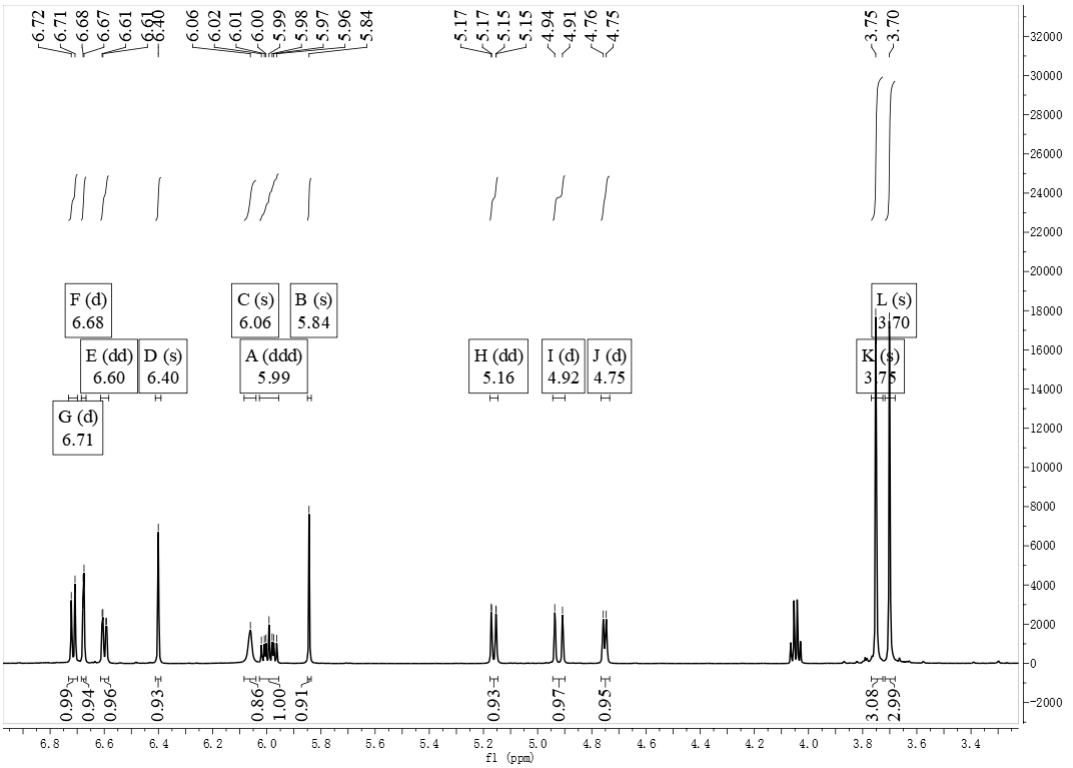


Figure S15: ^{1}H-NMR (600 MHz, Acetone-*d6*) Spectrum of **2**

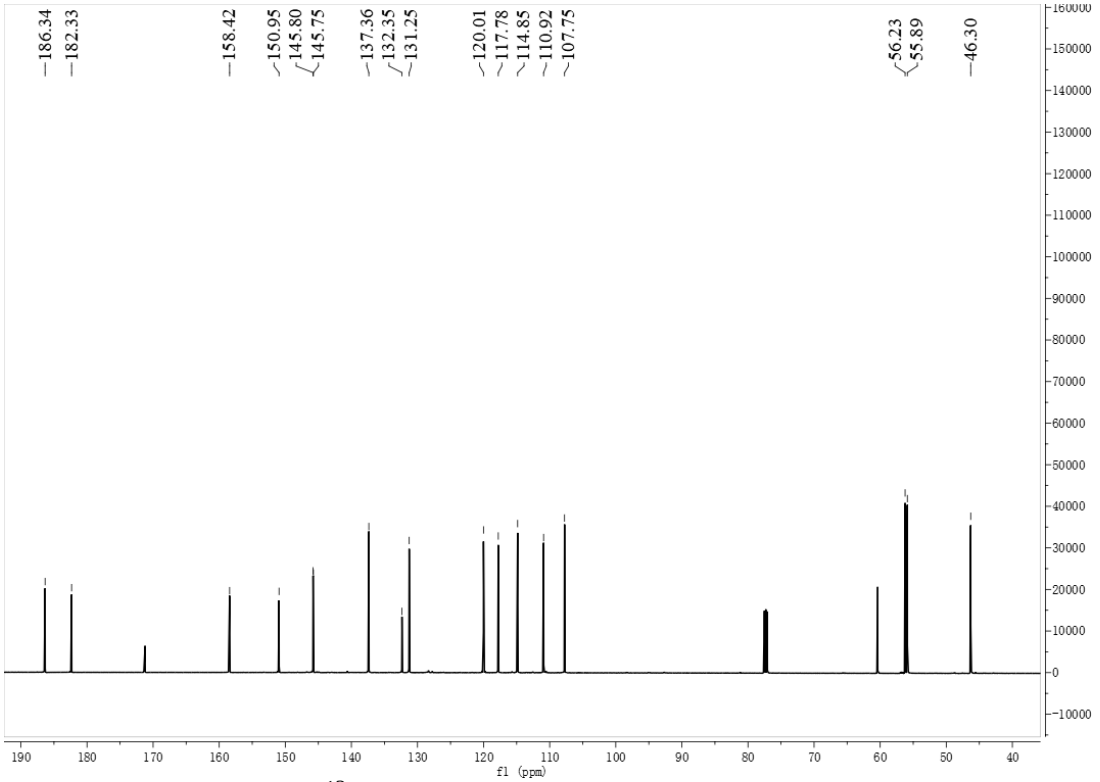


Figure S16: ^{13}C -NMR (150 MHz, Acetone-*d6*) spectrum of **2**

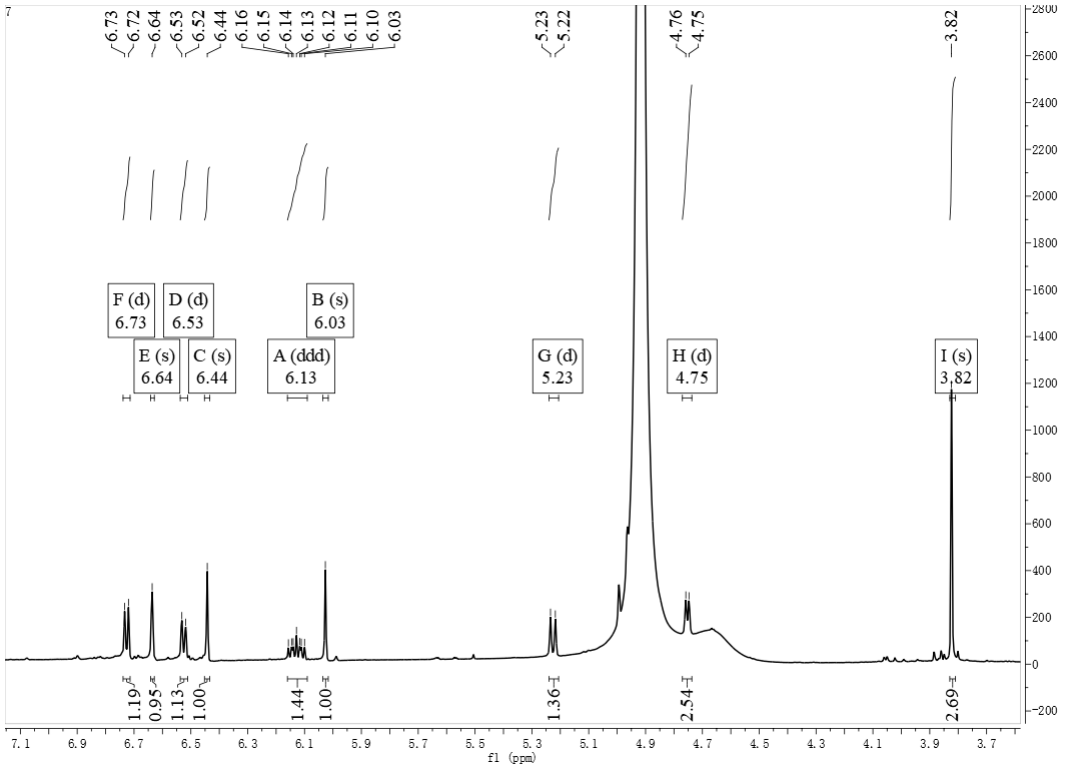


Figure S17: ^{1}H-NMR (600 MHz, Methanol-*d4*) Spectrum of **3**

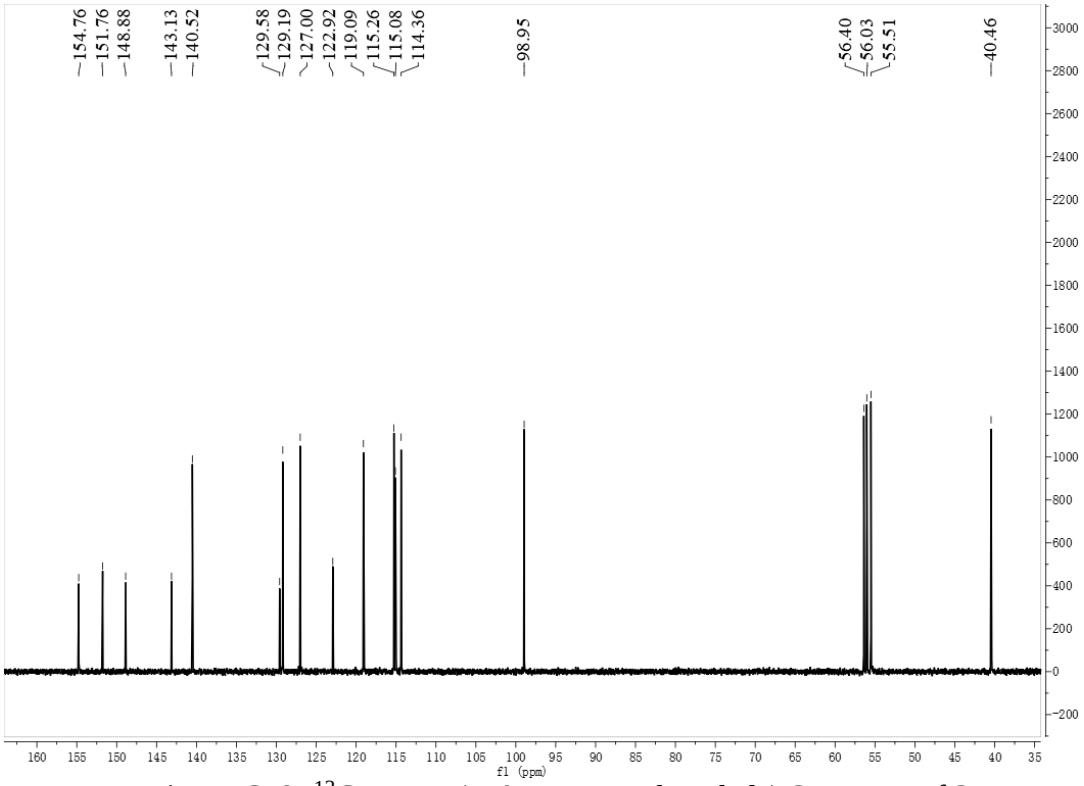


Figure S18: ^{13}C -NMR (150 MHz, Methanol-*d4*) Spectrum of **3**

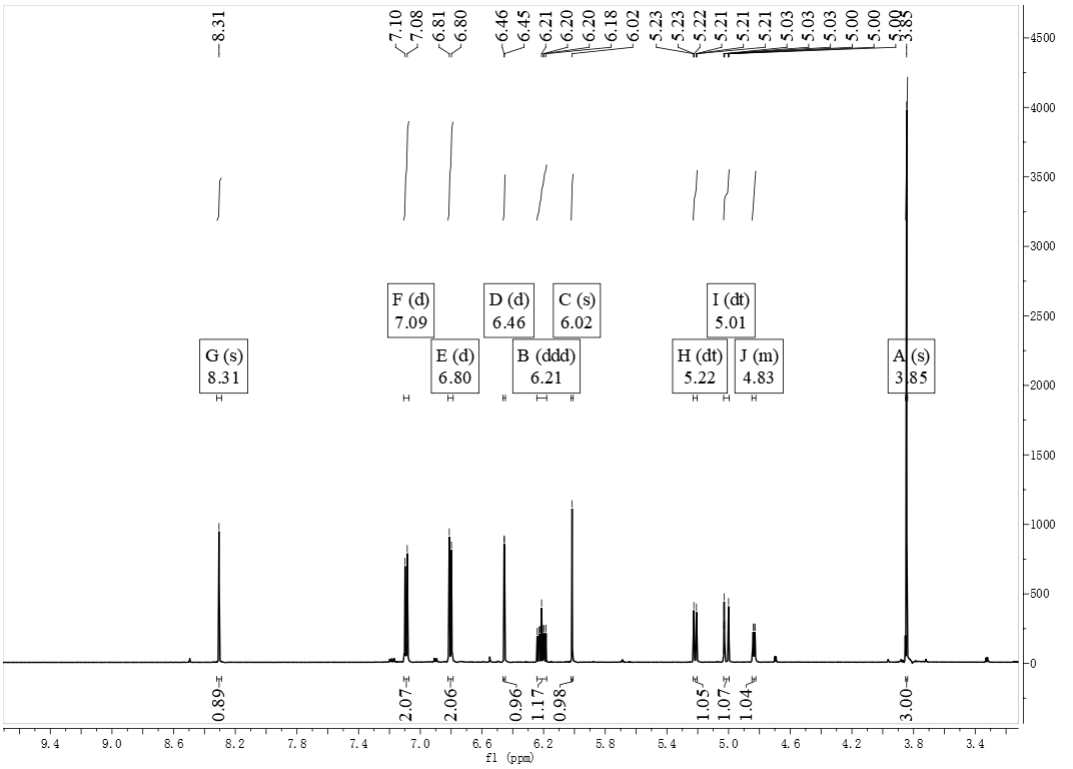


Figure S19: ^{1}H-NMR (600 MHz, Acetone-*d6*) Spectrum of **4**

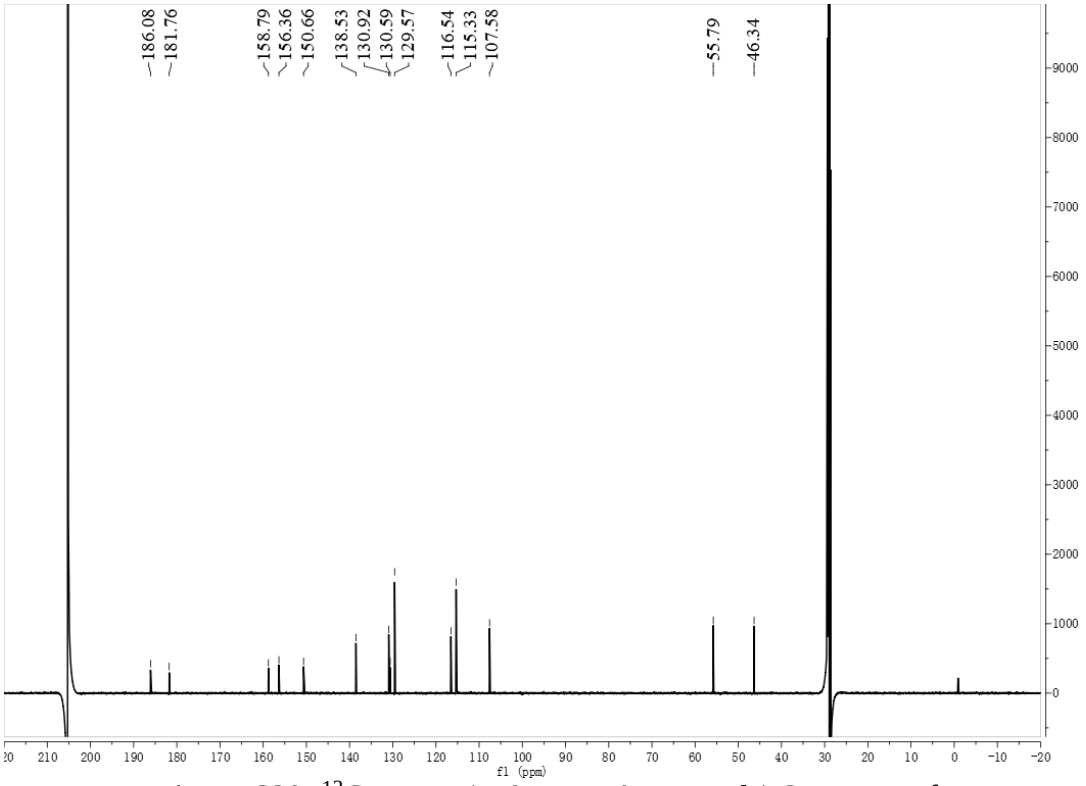


Figure S20: ^{13}C -NMR (150 MHz, Acetone-*d6*) Spectrum of **4**

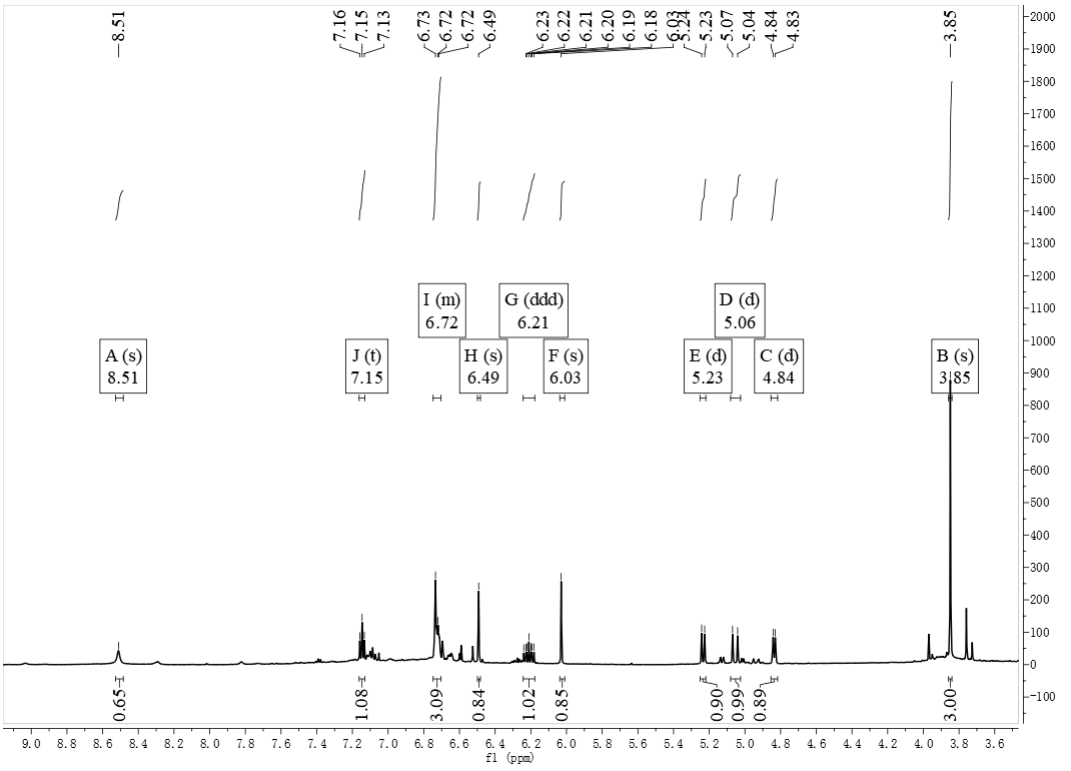


Figure S21: ^{1}H-NMR (600 MHz, Acetone-*d6*) Spectrum of **5**

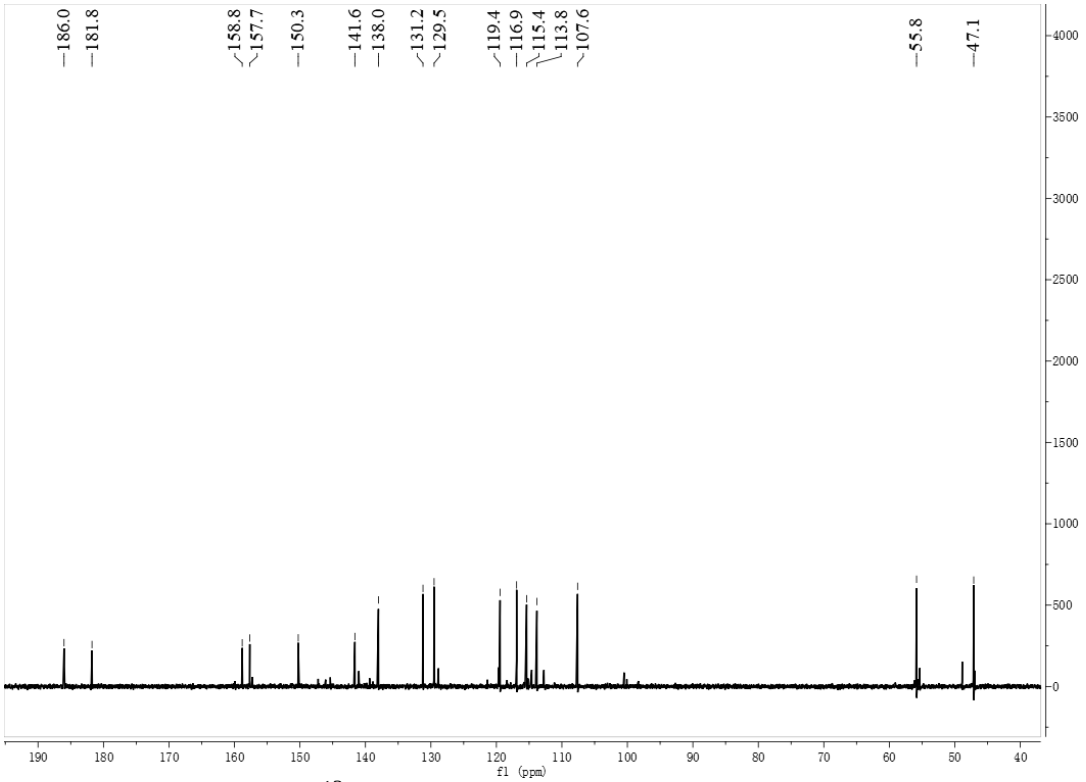


Figure S22: ^{13}C -NMR (150 MHz, Acetone-*d6*) Spectrum of **5**

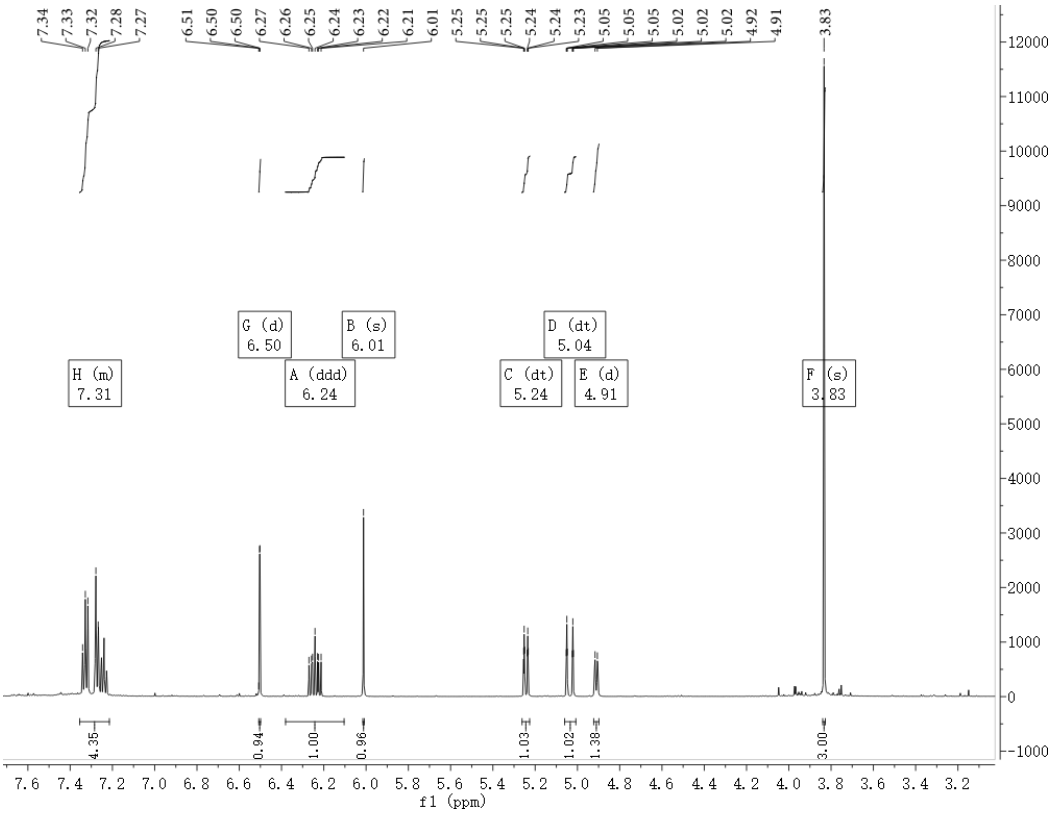


Figure S23: ^{1}H-NMR (600 MHz, Acetone-*d6*) Spectrum of **6**

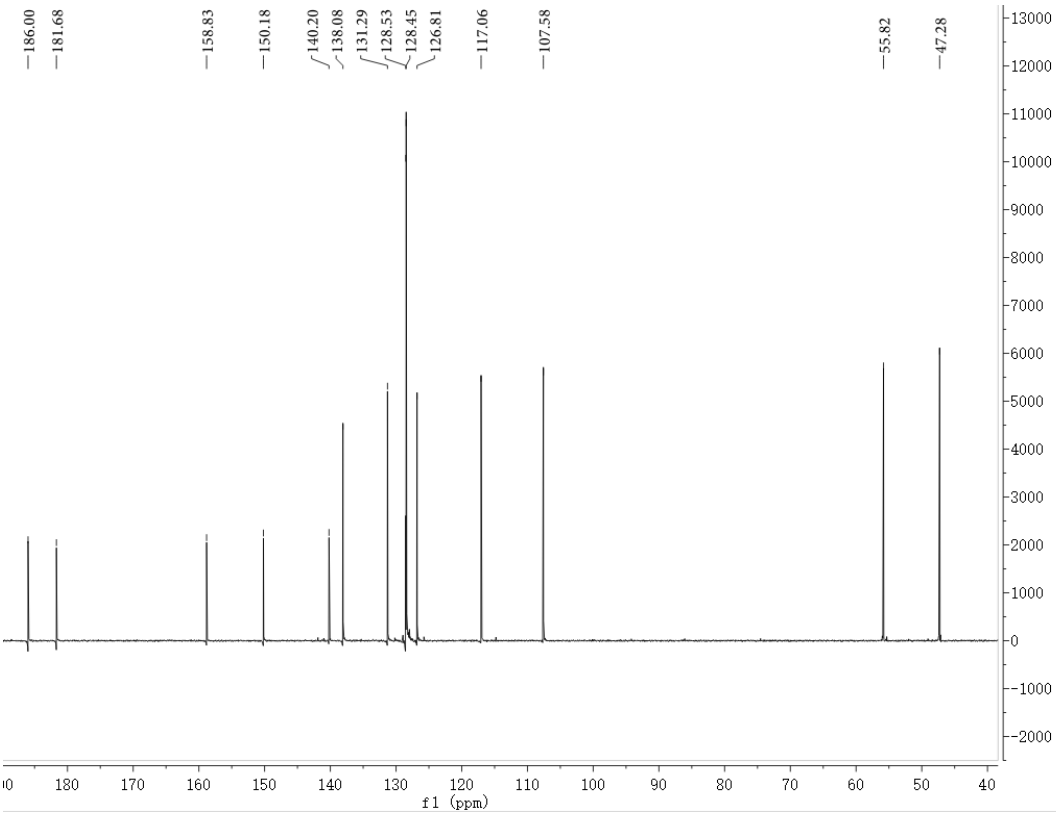


Figure S24: ^{13}C -NMR (150 MHz, Acetone-*d6*) Spectrum of **6**

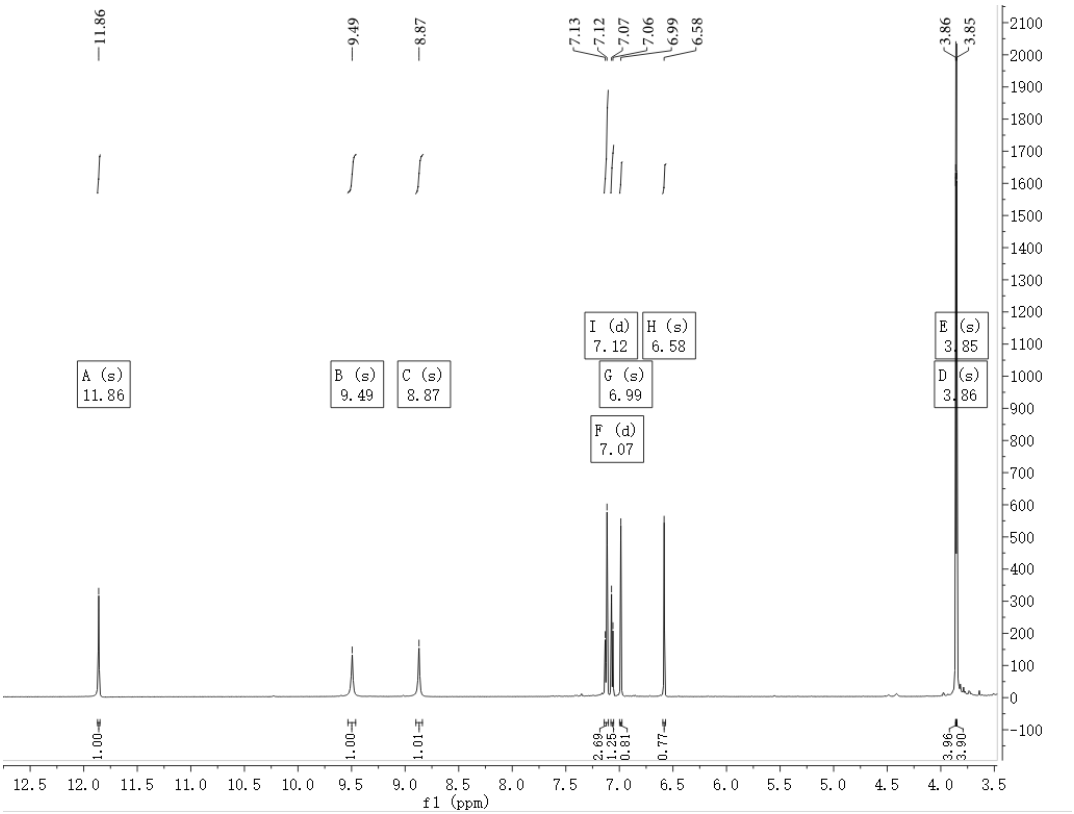


Figure S25: ^{1}H-NMR (600 MHz, DMSO-*d6*) Spectrum of **7**

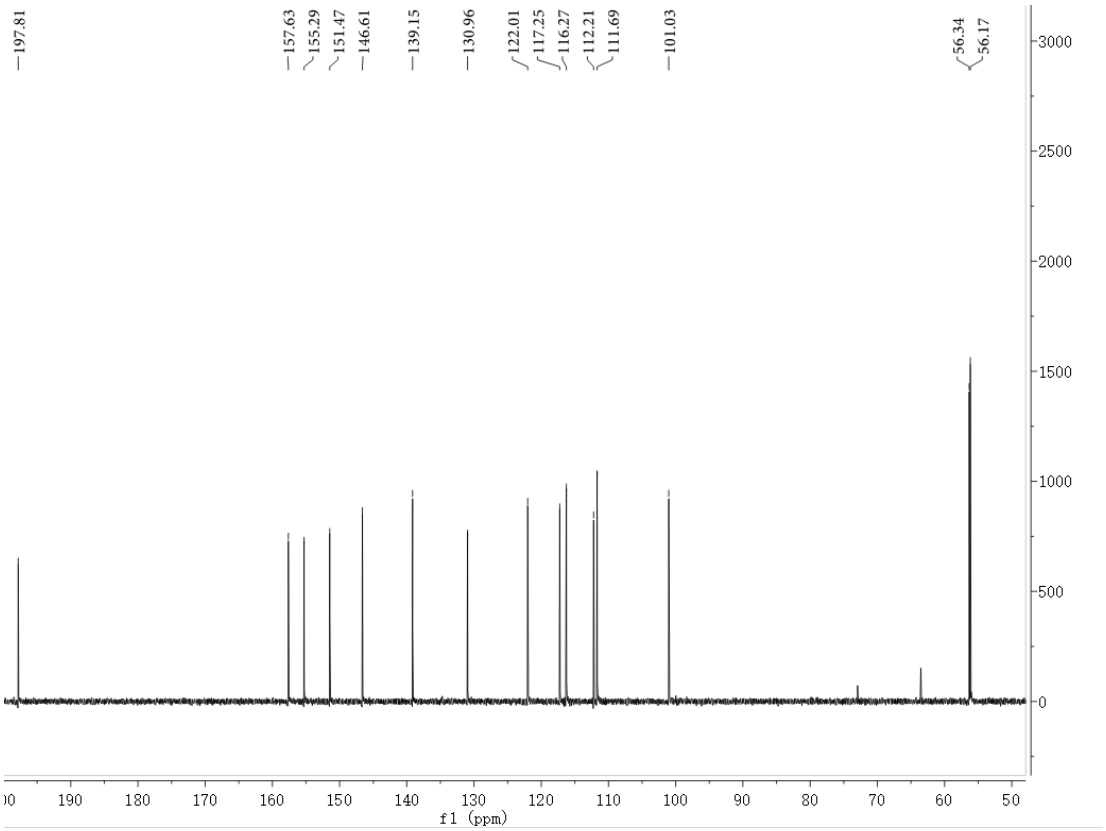


Figure S26: ^{13}C -NMR (150 MHz, DMSO-*d6*) Spectrum of **7**

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 aJASCO 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_{18} 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 5×10^3 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_2 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 5×10^3 cells per well in 96-well microtiter plates in 100 μL of medium and incubated in DMEM containing 10% fetal bovine serum at 37 ℃for 24 h in a 5% CO_2 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 f or 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 1×10^4 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 2 4 h in a 5% CO_2 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.