

## SUPPLEMENTARY MATERIAL

### A new *ent*-kaurane diterpene derivative from the stems of *Eurya chinensis* R.Br

Jia-Ling Song <sup>a</sup>, Yao Yuan <sup>a</sup>, Ling-Hui Nie <sup>b</sup>, Bai-Lin Li <sup>a</sup>, Xu-Bing Qin <sup>a</sup>, Yan Li <sup>a</sup>,  
Jie-Wei Wu <sup>a\*</sup>, Sheng-Xiang Qiu <sup>a\*</sup>

<sup>a</sup> Program for Natural Product Chemical Biology, Key Laboratory of Plant Resources Conservation and Sustainable Utilization, Guangdong Provincial Key Laboratory of Applied Botany, South China Botanical Garden, Chinese Academy of Sciences, Guangzhou, 510650, People's Republic of China;

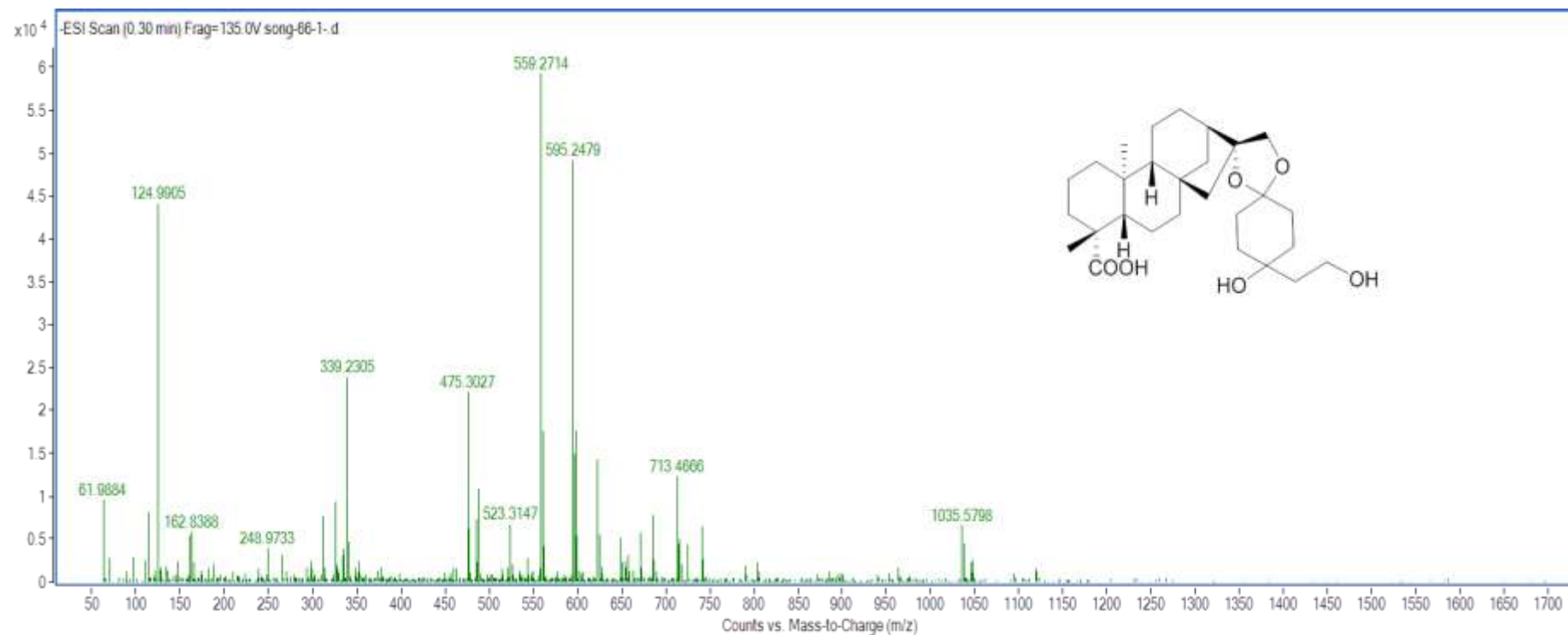
<sup>b</sup> College of Traditional Chinese Medicine, Southern Medical University, Guangzhou 510515, People's Republic of China.

**Abstract:** One new *ent*-kaurane diterpene derivative (**1**), along with four known diterpenes were isolated from the stems of *Eurya chinensis* R.Br. The structure of the new compound was established by extensive analysis of mass spectrometric and 1D and 2D NMR spectroscopic data. Compound **1** showed moderate anti-inflammatory activities with IC<sub>50</sub> value of 8.12  $\mu$ M. This is the first example of diterpenoids with 4-hydroxy-4-(2-hydroxyethyl)-1-hydroxyl-cyclohexanoyl substituent.

**Keywords:** *Eurya chinensis*; diterpene; derivative; anti-inflammatory

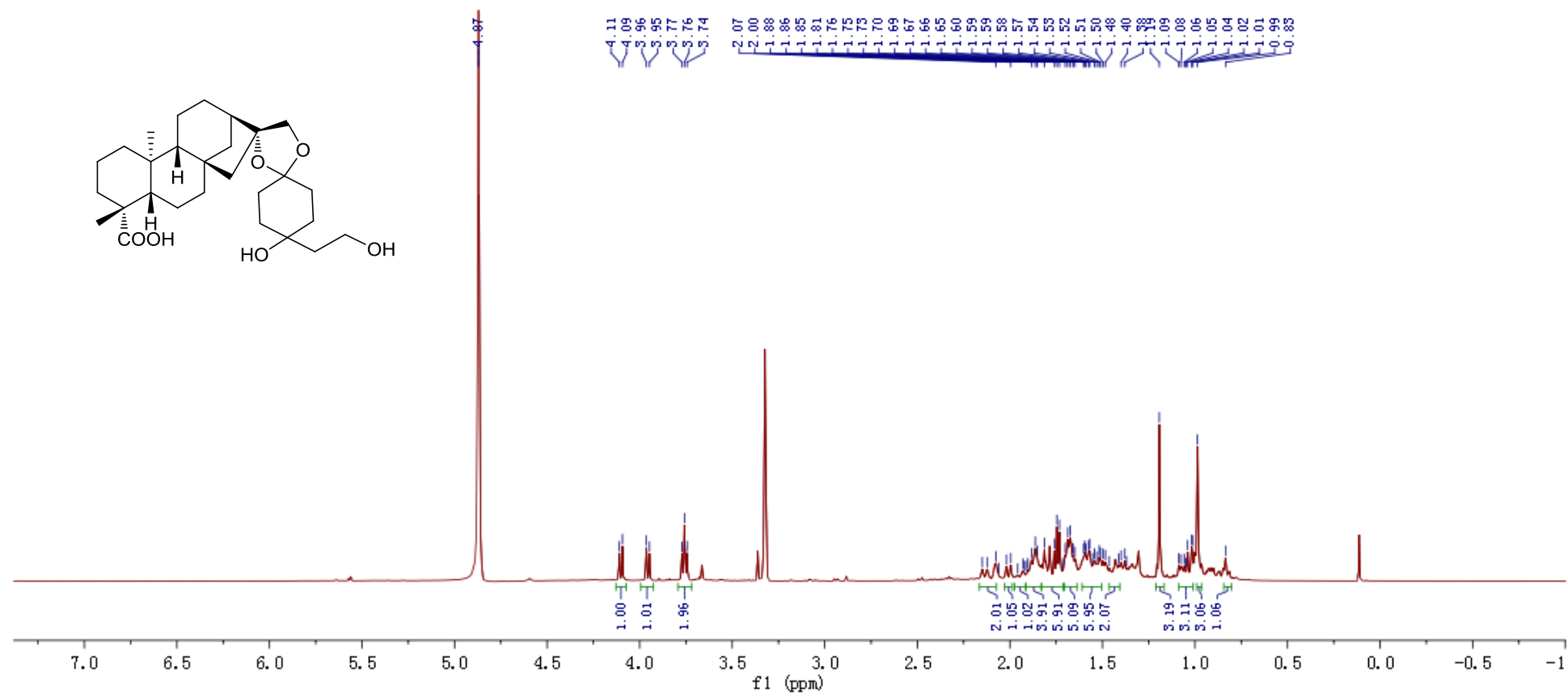
---

\*Corresponding author, Tel/fax: +8620 37081190, Email: wujieweiky@163.com (Wu J.), and sxqiu@scbg.ac.cn

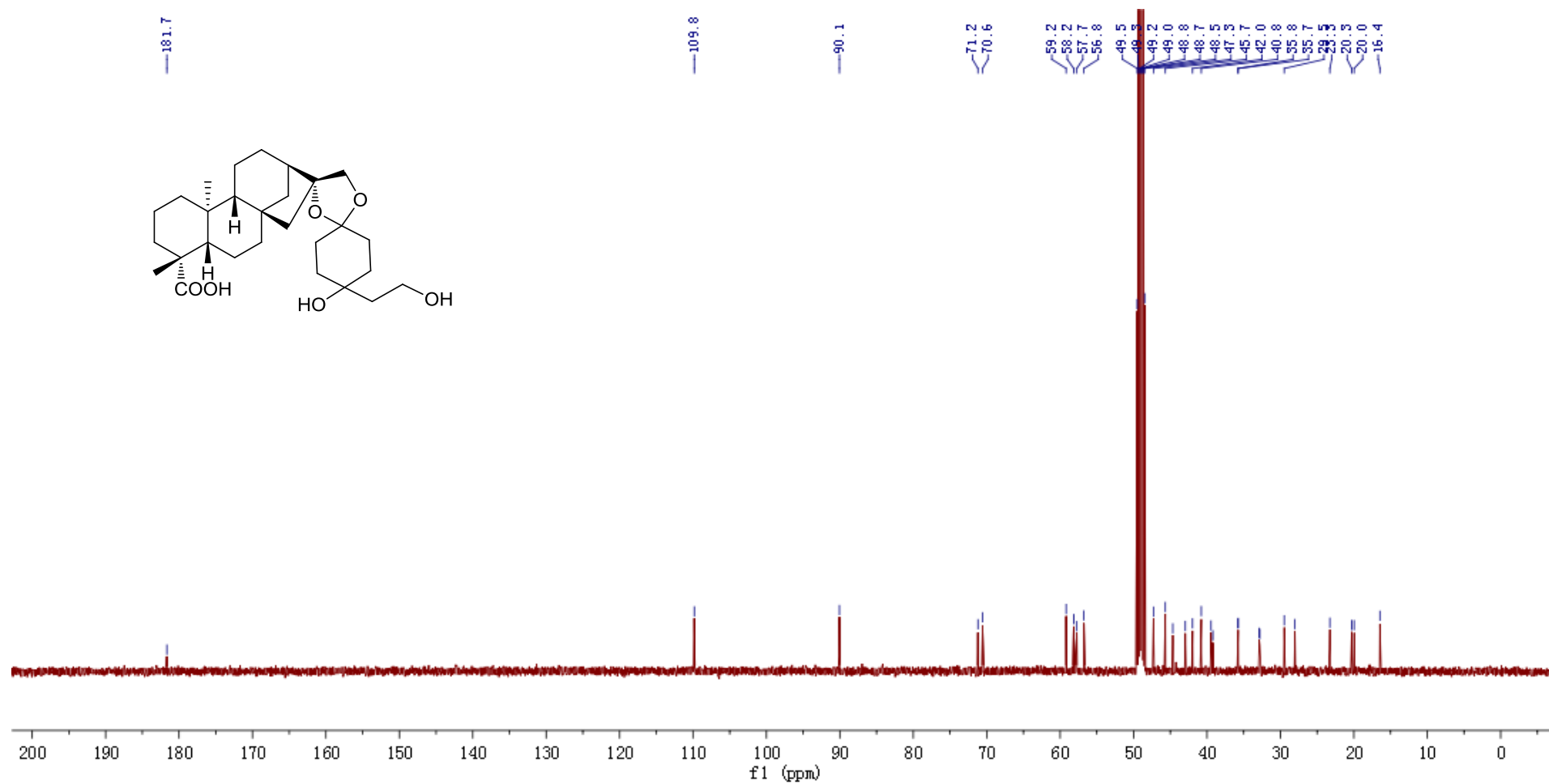


Mass	Calc. Mass	formula
475.3027	475.3060	C <sub>28</sub> H <sub>44</sub> O <sub>6</sub> -H

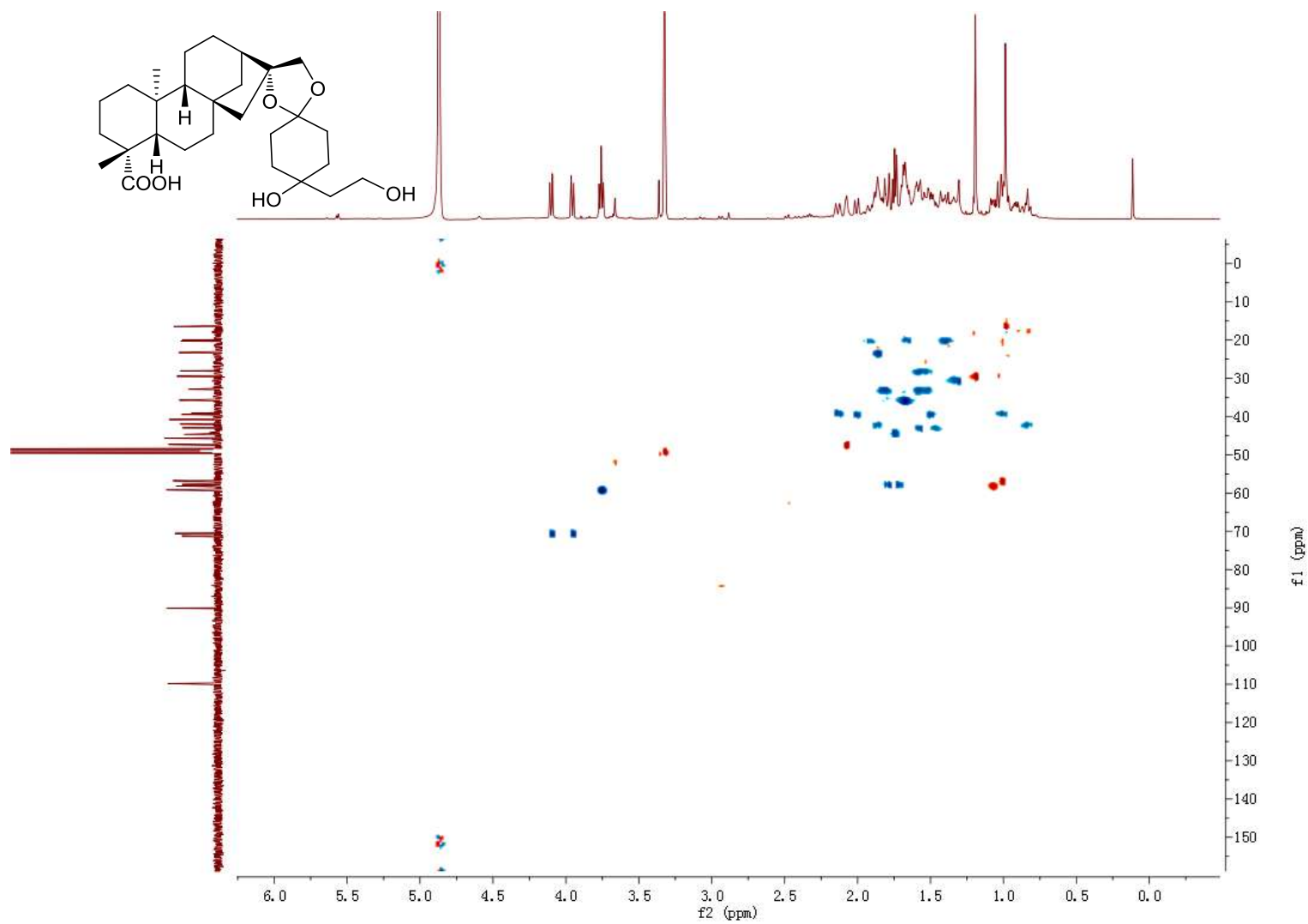
**Figure S1.** HR-ESI-MS spectrum of compound **1**



**Figure S2.** <sup>1</sup>H NMR spectrum of compound **1** (CD<sub>3</sub>OD, 500 MHz)



**Figure S3.**  $^{13}\text{C}$  NMR spectrum of compound **1** ( $\text{CD}_3\text{OD}$ , 125 MHz)



**Figure S4.** HQSC spectrum of compound **1**

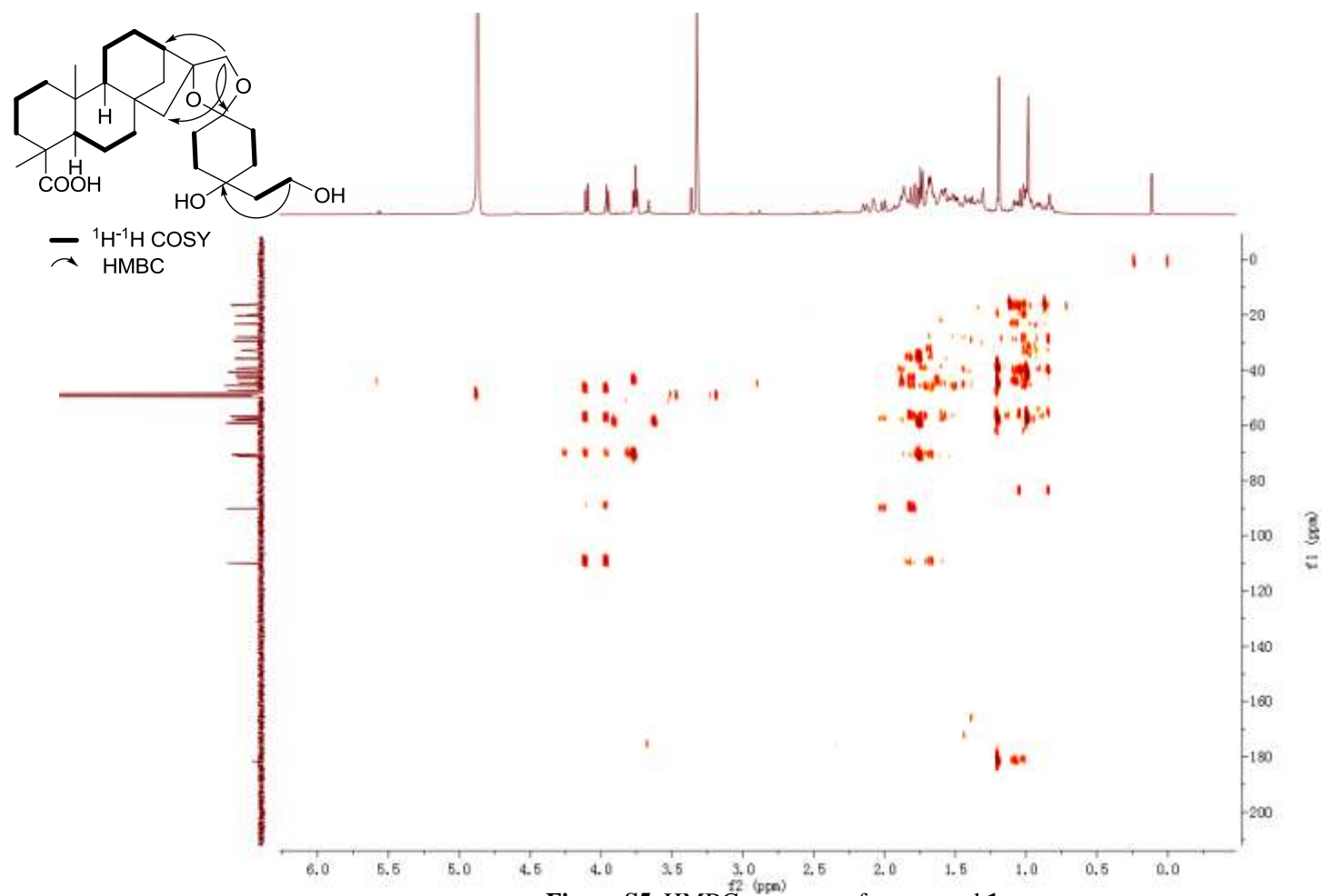
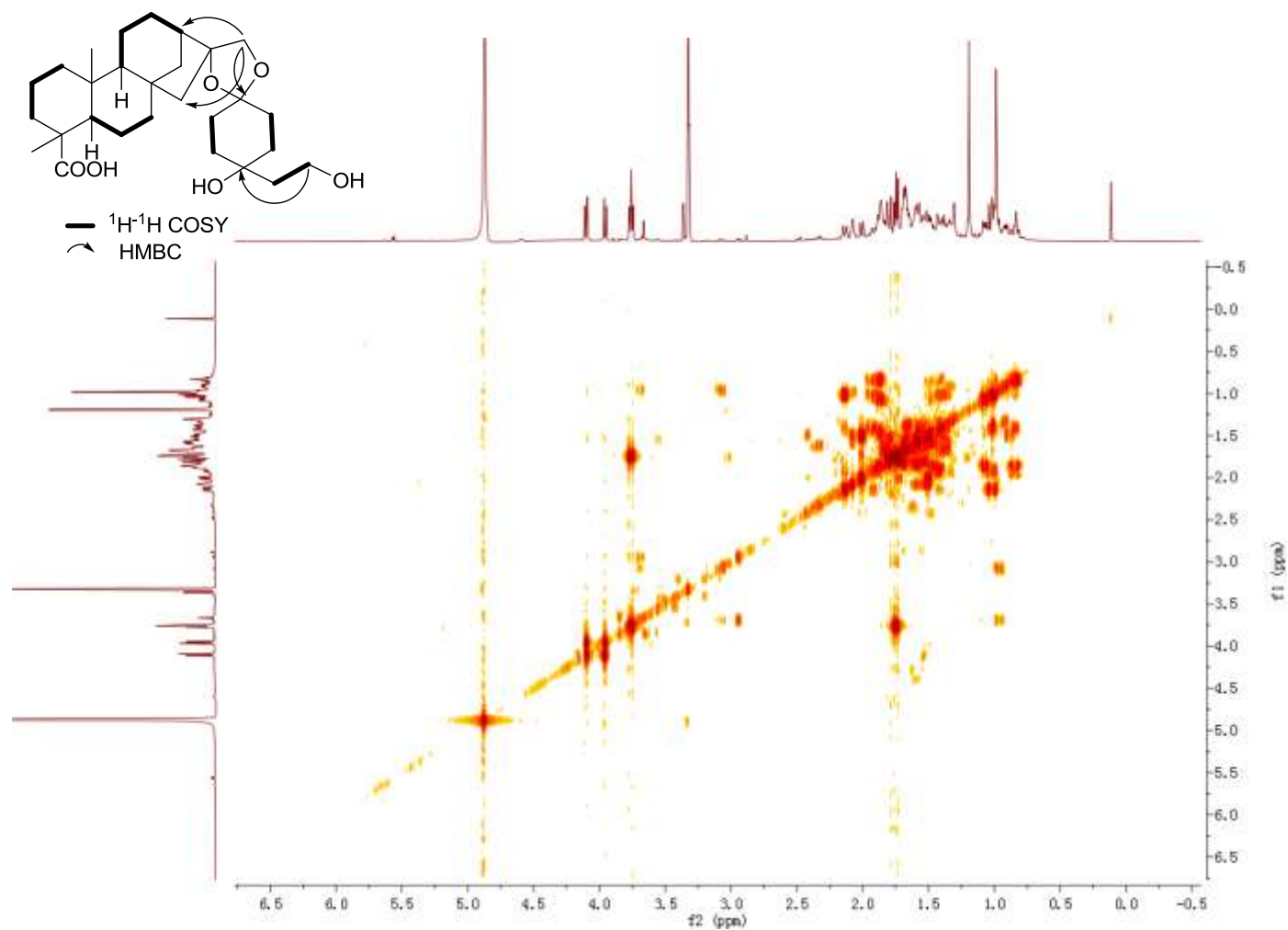
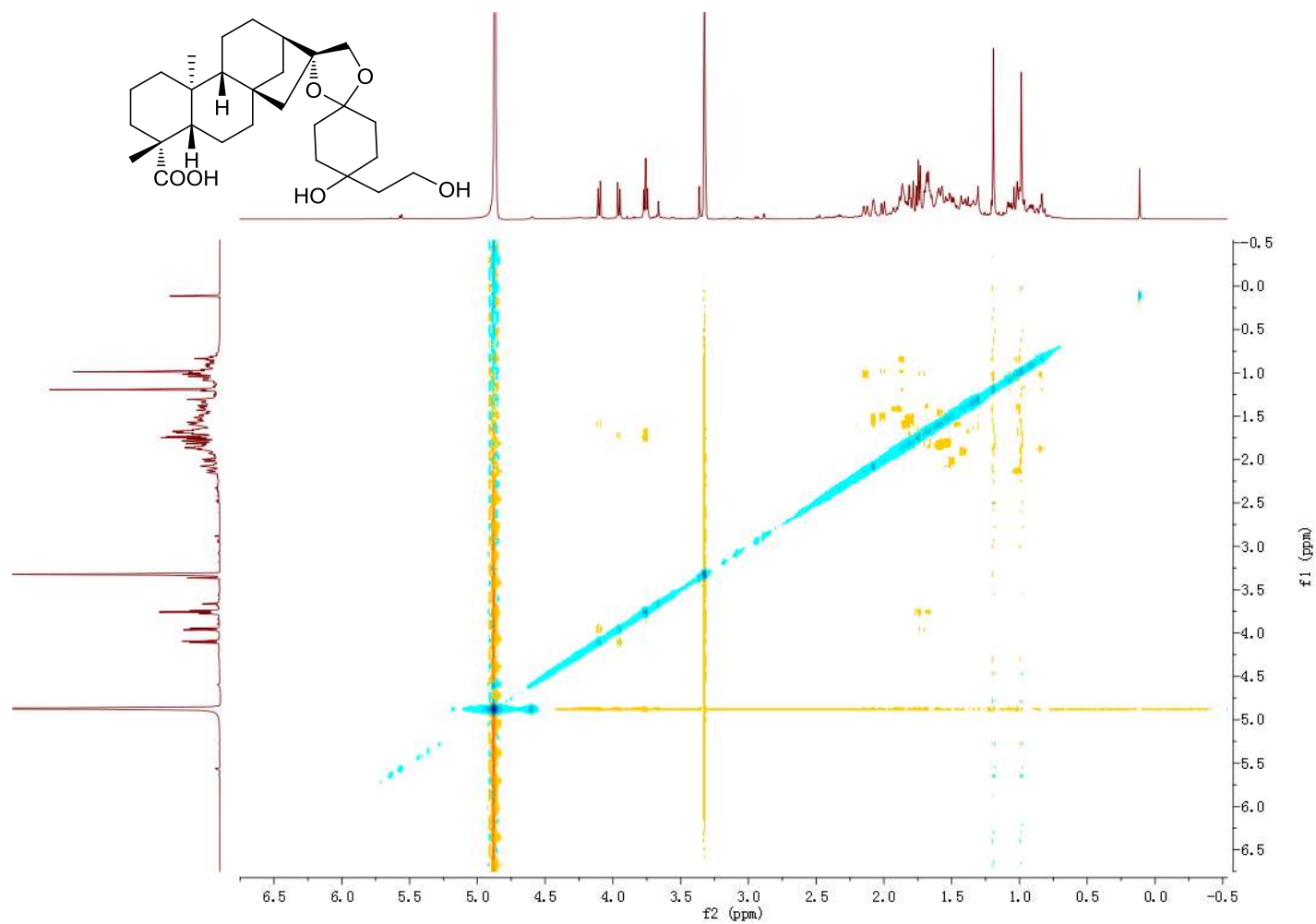


Figure S5. HMBC spectrum of compound **1**

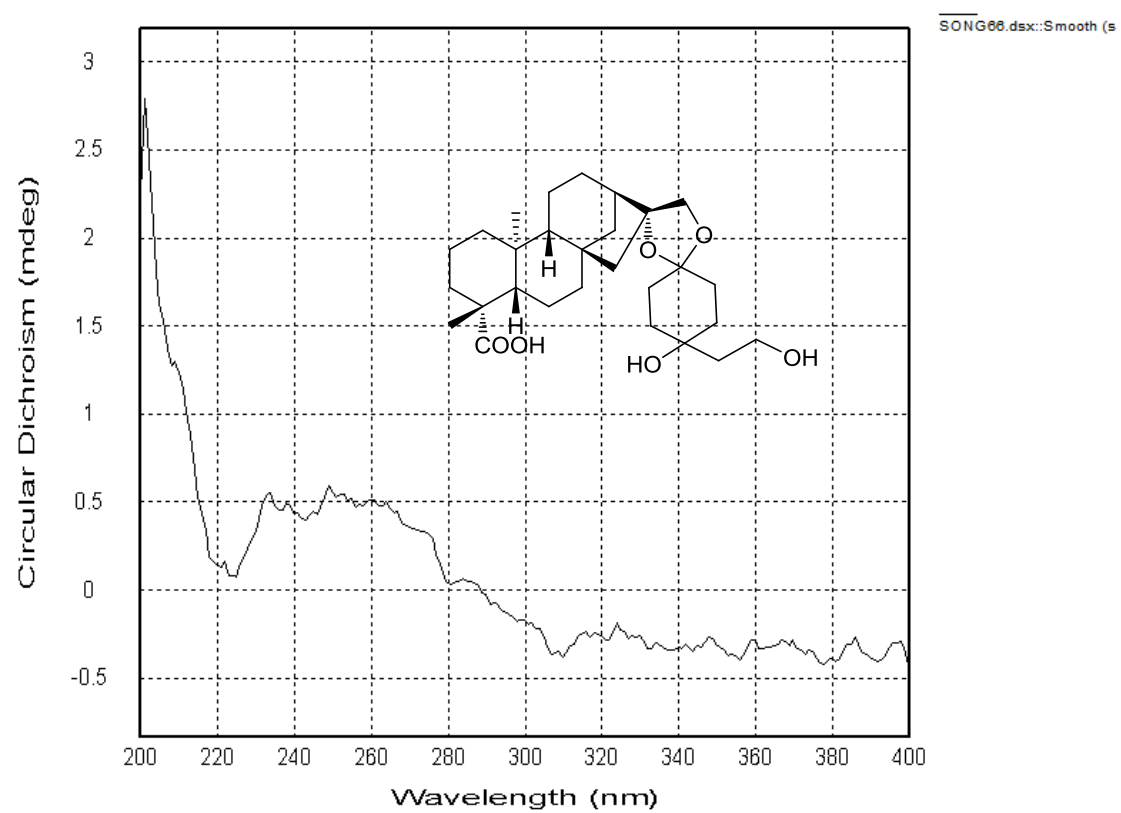
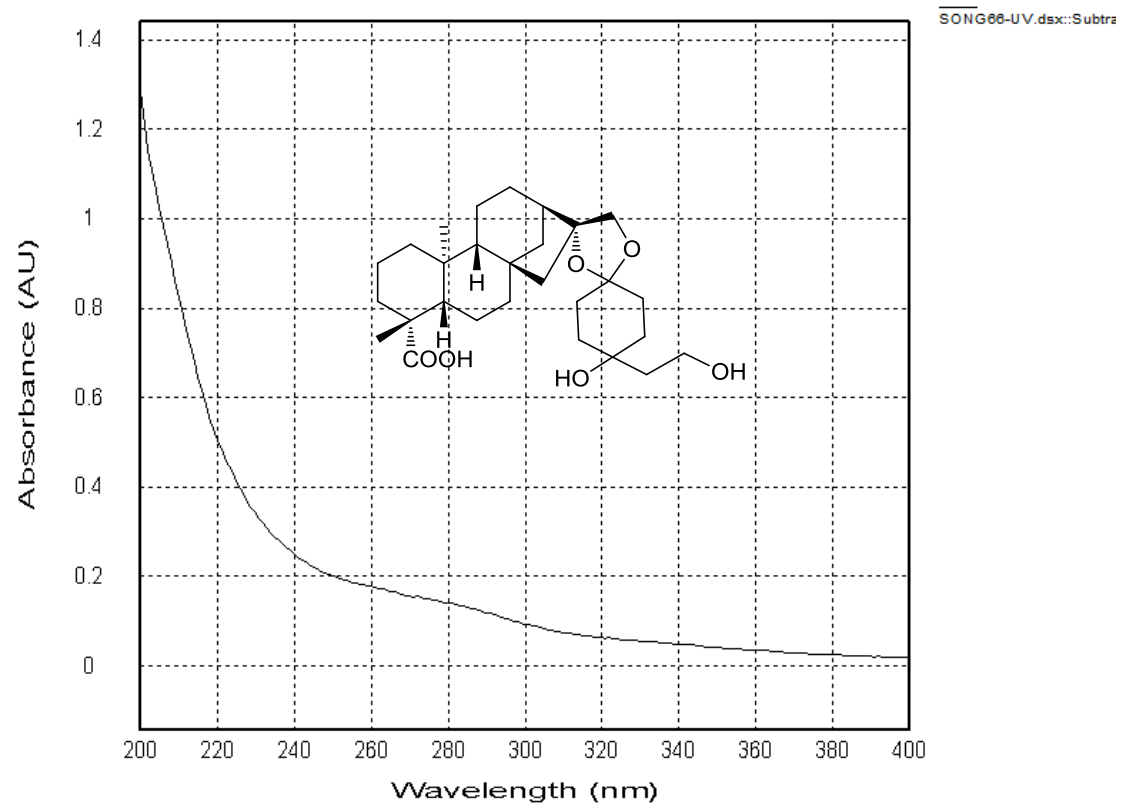


**Figure S6.**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **1**



**Figure S7.** NOESY spectrum of compound **1**





**Figure S8.** Experimental ECD spectra (in MeOH) spectra of compound **1**

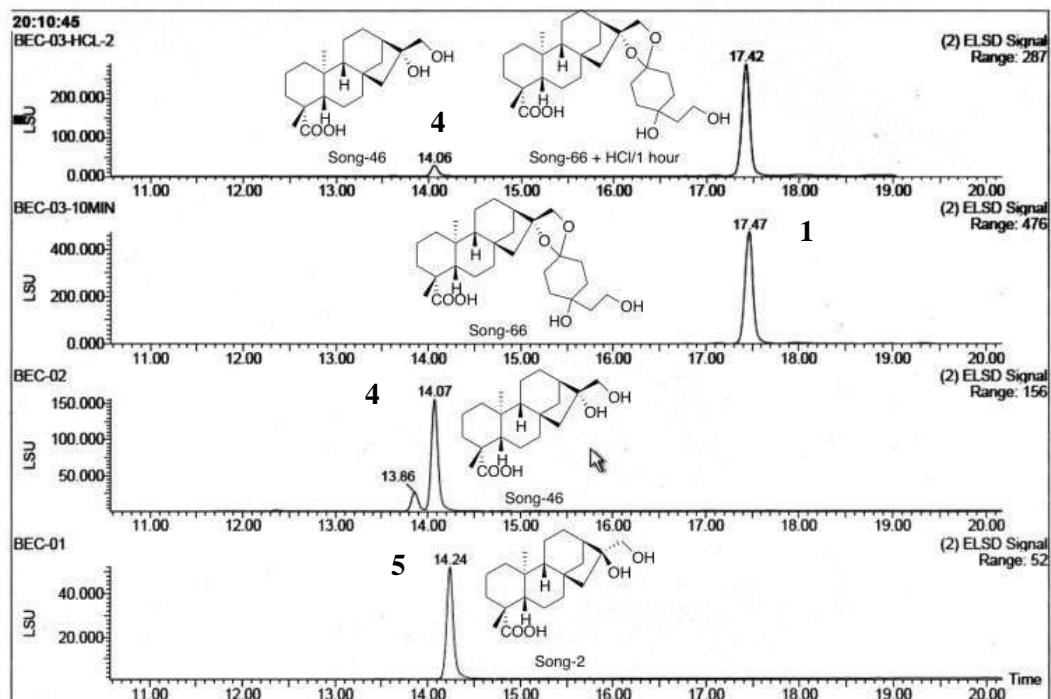


Figure S9 Hydrolysis of **1** analysed by LC-MS.

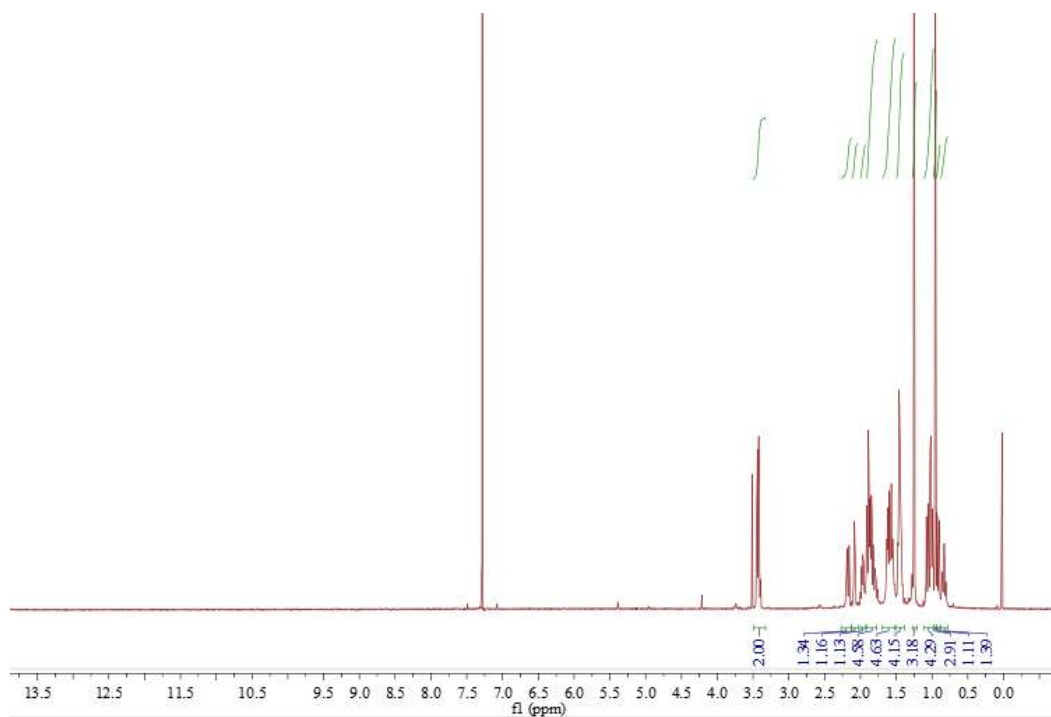
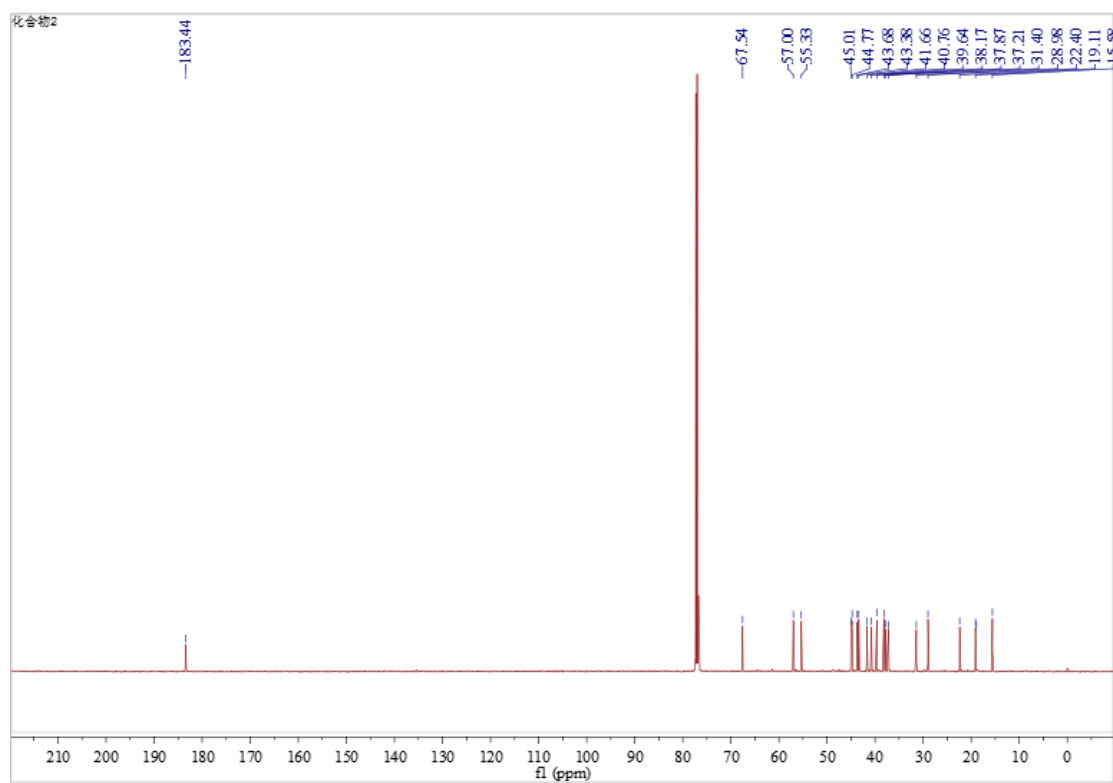
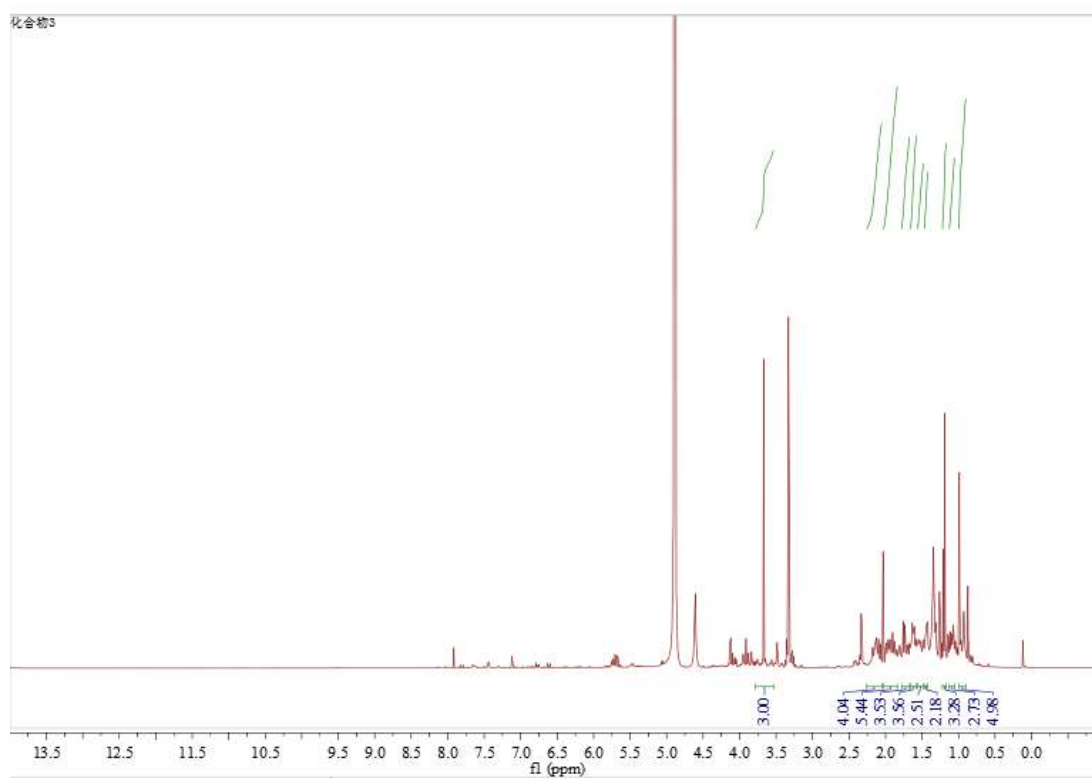


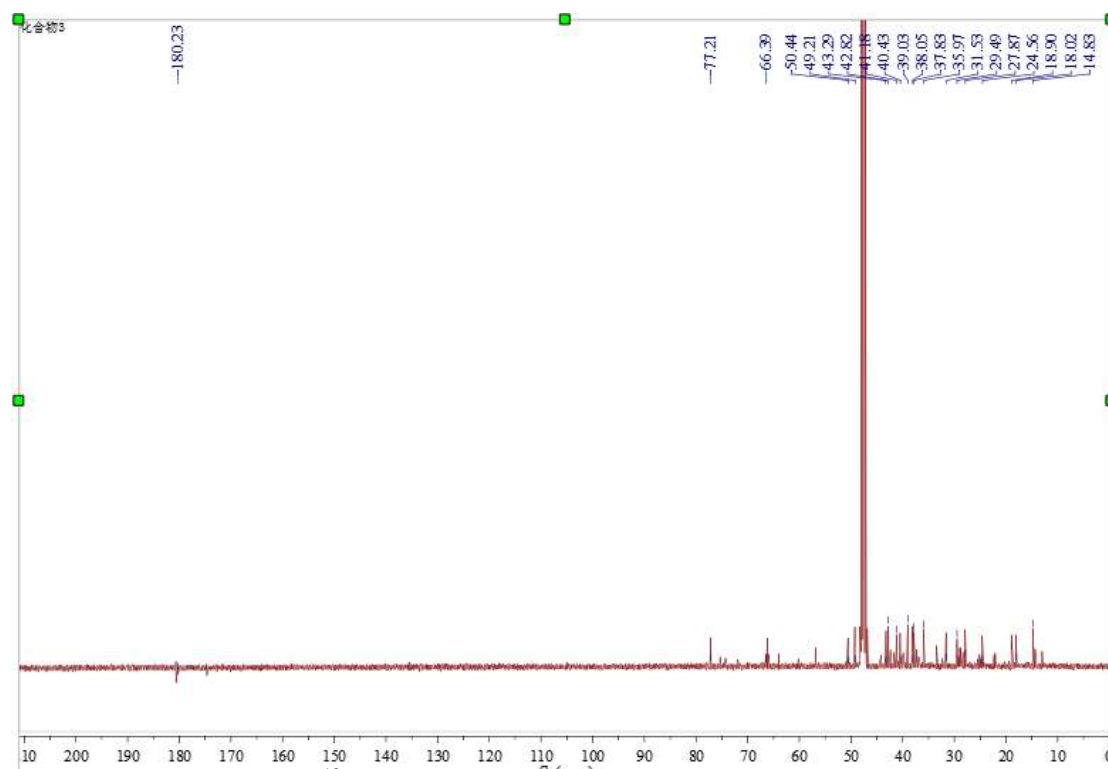
Figure S10.  $^1\text{H}$  NMR spectrum of compound **2** ( $\text{CDCl}_3$ , 500 MHz)



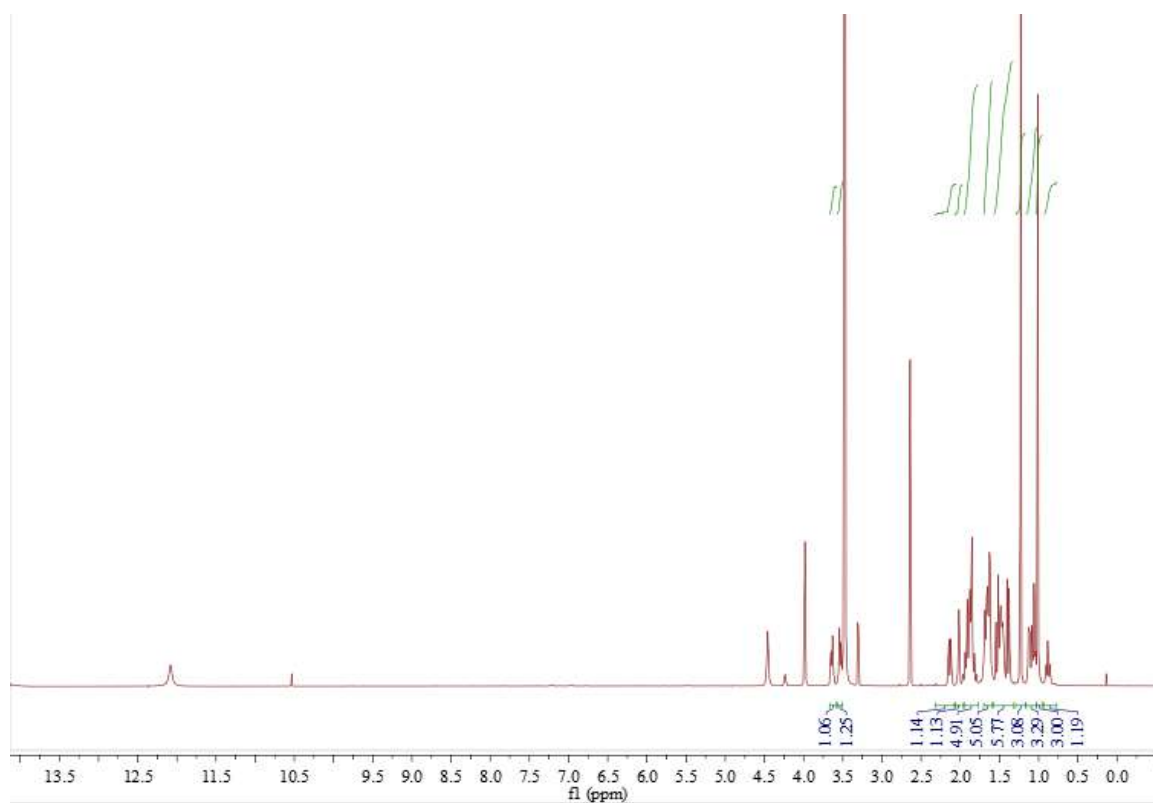
**Figure S11.**  $^{13}\text{C}$  NMR spectrum of compound **2** ( $\text{CDCl}_3$ , 125 MHz)



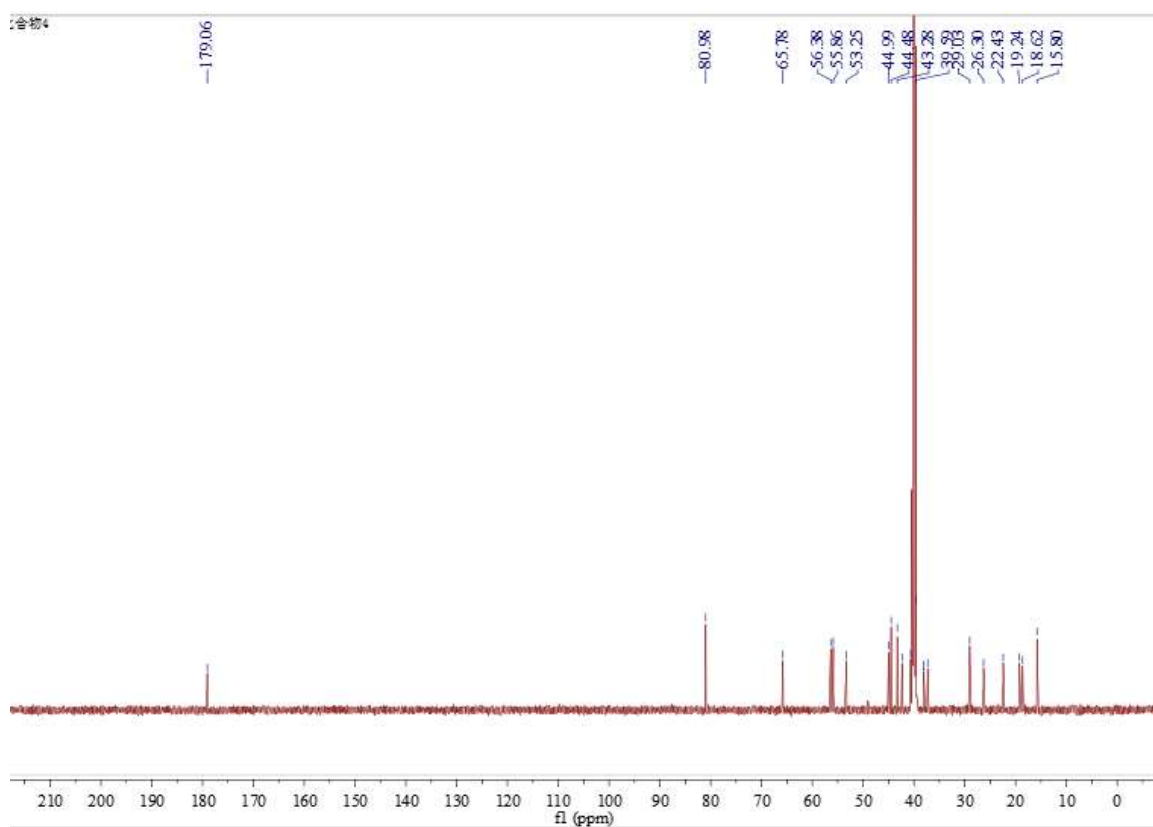
**Figure S12.**  $^1\text{H}$  NMR spectrum of compound **3** ( $\text{CD}_3\text{OD}$ , 500 MHz)



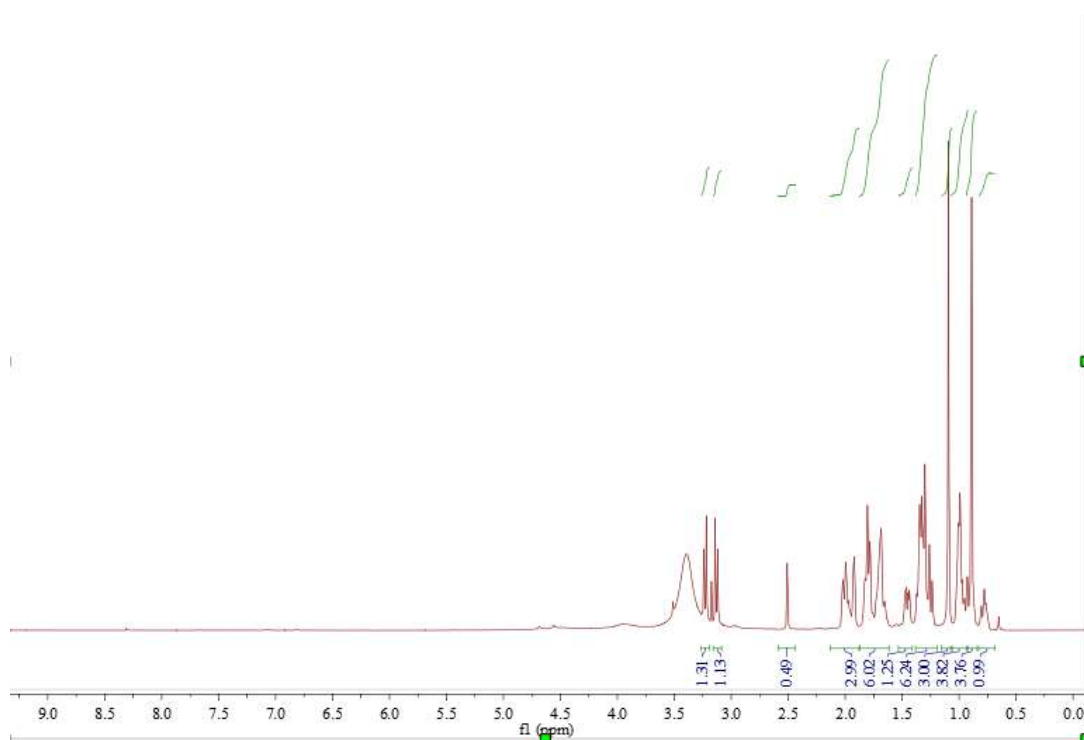
**Figure S13.**  $^{13}\text{C}$  NMR spectrum of compound **3** ( $\text{CD}_3\text{OD}$ , 125 MHz)



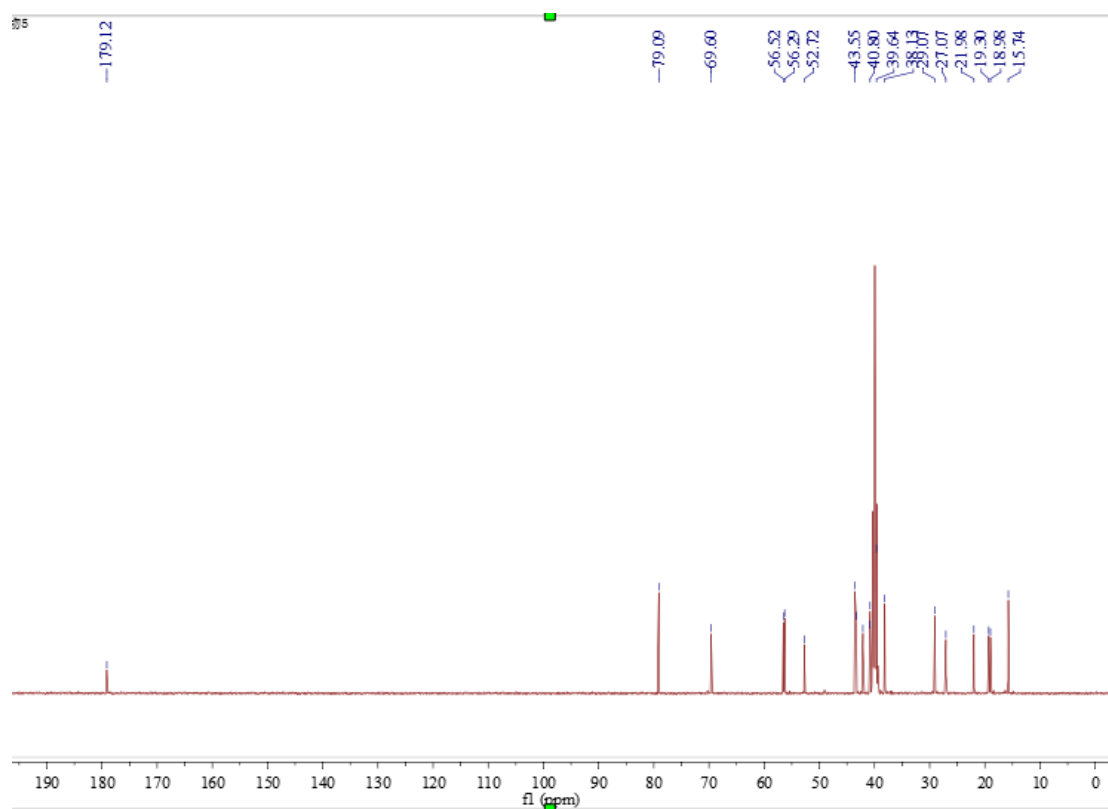
**Figure S14.**  $^1\text{H}$  NMR spectrum of compound **4** ( $\text{CD}_3\text{OD}$ , 500 MHz)



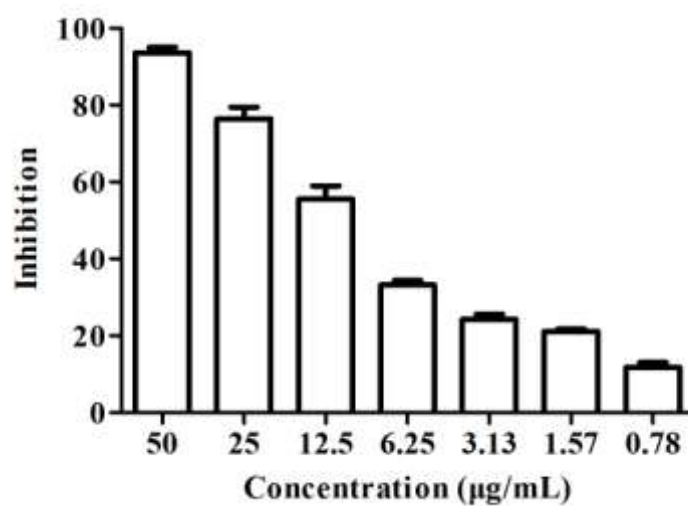
**Figure S15.** <sup>13</sup>C NMR spectrum of compound **4** (CD<sub>3</sub>OD, 125 MHz)



**Figure S16.** <sup>1</sup>H NMR spectrum of compound **5** (DMSO-D<sub>6</sub>, 500 MHz)



**Figure S17.**  $^{13}\text{C}$  NMR spectrum of compound **5** (DMSO- $\text{D}_6$ , 125 MHz)



**Figure S18.** The inhibitory effect of compound **1** on NO production in LPS stimulated RAW264.7 cells

**Table S1.**  $^1\text{H}$  and  $^{13}\text{C}$  NMR Data for **1** and **4** (500 and 125 MHz, respectively) in  $\text{CD}_3\text{OD}$ 

no.	<b>1</b>		<b>4</b>	
	$\delta_{\text{H}}$ (mult., $J$ in Hz)	$\delta_{\text{C}}$	$\delta_{\text{H}}$ (mult., $J$ in Hz)	$\delta_{\text{C}}$
1a	1.88 (m)	42.0	1.89 (m)	40.7
1b	0.84 (m)		0.86 (m)	
2a	1.93 (m)		1.94 (overlapped)	
2b	1.40 (overlapped)	20.0	1.45 (m)	19.2
3a	2.15 (m)		2.15 (m)	
3b	1.03 (m)		1.05 (m)	
4		45.7		43.3
5	1.08 (m)	58.2	1.10 (m)	56.4
6	1.85 (m)	23.3	1.85 (m)	22.4
7a	1.56 (overlapped)	42.9	1.65 (overlapped)	42.4
7b	1.47 (m)		1.49 (overlapped)	
8		44.7		44.5
9	1.01 (brs)	56.8	1.04 (m)	55.9
10		40.8		39.6
11a	1.65 (overlapped)	20.3	1.68 (m)	18.6
11b	1.40 (overlapped)		1.54 (m)	
12	1.56 (overlapped)	28.0	1.62 (overlapped)	26.3
13	2.07 (m)	47.3	2.05 (m)	45.0
14a	2.01 (m)	39.1	1.95 (overlapped)	37.3
14b	1.52 (m)		1.68 (overlapped)	
15a	1.74 (d, $J = 4.2$ Hz)	57.7	1.53 (d, $J = 13.6$ Hz)	53.3
15b	1.79 (d, $J = 4.2$ Hz)		1.39 (d, $J = 14.0$ Hz)	
16		90.1		81.0
17a	4.10 (d, $J = 8.6$ Hz)	70.6	3.63 (d, $J = 11.0$ Hz)	65.8
17b	3.96 (d, $J = 8.6$ Hz)		3.53 (d, $J = 11.0$ Hz)	
18	1.20 (s)	29.5	1.21 (s)	29.0
19		181.7		179.1
20	0.99 (s)	16.4	1.01 (s)	15.8
1'		109.8		
2'	1.68 (overlapped)	35.8		
3'a	1.82 (overlapped)	32.8		
3'b	1.55 (overlapped)			
4'		71.2		
5'a	1.82 (overlapped)	32.9		
5'b	1.55 (overlapped)			
6'	1.68 (overlapped)	35.8		
1''	1.58 (overlapped)	43.0		
2''	3.76 (t, $J = 7.0$ Hz)	59.2		