

Supporting Information

Chemical components from the seeds of *Catalpa bungei* and their inhibition of soluble epoxide hydrolase, cholinesterase and nuclear factor kappa B activities

Hao-Yu Tang,^a Meng-Meng Bai,^a Jun-Mian Tian,^a Gennaro Pescitelli,^b Trpimir Ivšić,^{b,c} Xiao-Hua Huang,^{a,*} Hyunwoo Lee,^d Ya Nan Son,^d Jang Hoon Kim,^d Young Ho Kim,^d Jin-Ming Gao^{a,*}

^a Shaanxi Key Laboratory of Natural Products & Chemical Biology, Department of Chemistry and Chemical Engineering, College of Science, Northwest A&F University, Yangling 712100, P.R. China

^b Dipartimento di Chimica e Chimica Industriale, Università di Pisa, via Moruzzi 3, I-56124 Pisa, Italy

^c Division of Organic Chemistry and Biochemistry, Ruđer Bošković Institute, 10000 Zagreb, Croatia

^d College of Pharmacy, Chungnam National University, Daejeon 305-764, Republic of Korea

*Corresponding author: ***Prof. Jin-Ming Gao, Ph.D.***

Tel.: +86-29-87092515, E-mail: jinminggao@nwsuaf.edu.cn

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Table S1. NMR data of **1** (CH₃OH-*d*₄)

Number	1				
	¹³ C	¹ H	¹ H- ¹ H COSY	HMBC	NOESY
1	93.1	5.70 d, <i>J</i> = 2.1 Hz	H-9	C-5, C-8	H-6, H-10, H-1'
3	95.9	5.35 d, <i>J</i> = 2.8 Hz	H _α , H _β -4	C-1, C-5	
4	34.4	2.49 dd, <i>J</i> = 13.5, 8.3 Hz	H-5	C-6, C-5	
		2.13 dd, <i>J</i> = 13.9, 3.2 Hz	H-3	C-9, C-6	H-6
5	34.8	2.40, m	H-9, H-6	C-8	H-7
6	87.7	5.05 dd, <i>J</i> = 8.3, 2.7 Hz	H-5, H-7	C-7, C-9, C-5	H-1
7	70.4	4.46 d, <i>J</i> = 8.3 Hz	H-6	C-6, C-8	H-5, H-9
8	79.9				
9	48.3	2.65 br. d, <i>J</i> = 9.9 Hz	H-5, H-1	C-4, C-8	H-7
10	62.1	4.08 d, <i>J</i> = 12.0 Hz		C-3, C-7, C-9	H-1
		3.72 d, <i>J</i> = 11.8 Hz		C-3, C-7	
1'	99.0	4.73 d, <i>J</i> = 8.0 Hz	H-2'	C-1	H-1
2'	74.7	3.19 dd, <i>J</i> = 9.1, 8.1 Hz	H-3', H-2'		
3'	78.2	3.41, m	H-2', H-4'		
4'	71.6	3.31, m	Overlap		
5'	78.1	3.31, m	Overlap		
6'	62.7	3.70, m	H-5'		
		3.90, m	H-5'		
1''	127.6				
2''	111.9	7.25 d, <i>J</i> = 1.8 Hz		C-4''	H-10''
3''	149.4				
4''	150.8				
5''	116.5	6.85 d, <i>J</i> = 8.2 Hz	H-6''	C-3'', C-1''	
6''	124.3	7.13 dd, <i>J</i> = 8.2, 1.9 Hz	H-5''	C-2'', C-4''	
7''	147.5	7.68 d, <i>J</i> = 15.9 Hz	H-7''	C-9'', C-6'', C-2''	
8''	114.9	6.45 d, <i>J</i> = 15.9 Hz	H-8''	C-1''	
9''	168.8				
10''	56.5	3.93, s		C-3''	H-2''

Table S2. NMR data of **2** (CH₃OH-*d*₄)

Number	2				
	¹³ C	¹ H	¹ H- ¹ H COSY	HMBC	NOESY
1	93.1	5.64 d, <i>J</i> = 2.0 Hz	H-9	C-5, C-8	H-6, H-10, H-1'
3	95.9	5.30 d, <i>J</i> = 2.7 Hz	H _α , H _β -4	C-1, C-5	
4	34.4	2.43 dd, <i>J</i> = 13.4, 8.5 Hz	H-5	C-6, C-5	
		2.07 dd, <i>J</i> = 13.9, 3.2 Hz	H-3	C-9, C-6	H-6
5	34.7	2.34 m	H-9, H-6	C-8	H-7
6	87.7	4.99 dd, <i>J</i> = 8.3, 2.7 Hz	H-5, H-7	C-7, C-9, C-5	H-1
7	70.4	4.41 d, <i>J</i> = 8.1 Hz	H-6	C-6, C-8	H-5, H-9
8	79.9				
9	48.3	2.59 br. d, <i>J</i> = 9.9 Hz	H-5, H-1	C-4, C-8	H-7
10	62.1	4.02 d, <i>J</i> = 11.8 Hz		C-3, C-7, C-9	H-1
		3.65 m		C-3, C-7	
1'	98.9	4.67 d, <i>J</i> = 8.0 Hz	H-2'	C-1	H-1
2'	74.7	3.14 t, <i>J</i> = 8.6 Hz	H-3', H-2'		
3'	78.1	3.35, m	H-2', H-4'		
4'	71.6	3.26, m	H-3', H-5'		
5'	78.1	3.28, m	H-4', H-6'		
6'	62.7	3.85, m	H-5'		
		3.65, m	H-5'		
1''	127.0				
2''	131.3	7.46 d, <i>J</i> = 8.6 Hz	H-3''	C-4'', C-7''	
3''	116.9	6.79 d, <i>J</i> = 8.6 Hz	H-2''	C-1'', C-5''	
4''	161.5				
5''	116.9	6.79 d, <i>J</i> = 8.6 Hz	H-6''	C-1'', C-3''	
6''	131.3	7.46 d, <i>J</i> = 8.6 Hz	H-5''	C-2'', C-7''	
7''	147.2	7.62 d, <i>J</i> = 15.8 Hz	H-8''	C-9'', C-2''	
8''	114.5	6.36 d, <i>J</i> = 15.9 Hz	H-7''	C-1''	
9''	168.9				
10''					

Table S3. NMR data of **3** (CH₃OH-*d*₄)

Number	3			
	¹³ C	¹ H	¹ H- ¹ HCOSY	HMBC
1	93.1	5.70 d, <i>J</i> = 2.1 Hz	H-9	C-5, C-8
3	95.9	5.36 d, <i>J</i> = 2.8 Hz	H _α , H _β -4	C-1, C-5
4	34.4	2.49 dd, <i>J</i> = 13.3, 8.5 Hz	H-5	C-6, C-5
		2.16 dd, <i>J</i> = 13.8, 3.2 Hz	H-3	C-9, C-6
5	34.7	2.43, m	H-9, H-6	C-8
6	87.9	5.13 dd, <i>J</i> = 8.3, 2.7 Hz	H-5, H-7	C-7, C-9, C-5
7	70.4	4.54 dd, <i>J</i> = 8.3, 0.9 Hz	H-6	C-6, C-8
8	79.9			
9	48.3	2.67 br. d, <i>J</i> = 9.8 Hz	H-5, H-1	C-4, C-8
10	62.1	4.09 dd, <i>J</i> = 12.1, 0.8 Hz		C-3, C-7, C-9
		3.72 d, <i>J</i> = 12.4 Hz		C-3, C-7
1'	98.9	4.73 d, <i>J</i> = 8.0 Hz	H-2'	C-1
2'	74.2	3.18 dd, <i>J</i> = 9.0, 8.1 Hz	H-3', H-2'	
3'	78.1	3.40, m	H-2', H-4'	
4'	71.6	3.31, m	H-3', H-5'	
5'	78.1	3.30, m	H-4', H-6'	
6'	62.7	3.70, m	H-5'	
		3.91, m	H-5'	
1''	121.4			
2''	132.9	7.92 d, <i>J</i> = 8.8 Hz	H-3''	
3''	116.4	6.87 d, <i>J</i> = 8.8 Hz	H-2''	
4''	164.3			
5''	116.4	6.87 d, <i>J</i> = 8.8 Hz	H-6''	
6''	132.9	7.92 d, <i>J</i> = 8.8 Hz	H-5''	
7''	168.6			

Table S4. Cholinesterase inhibition of compounds

Compounds	cholinesterase inhibition (%)	
	AChE	BChE
1	39.61 ± 3.70 %	35.01 ± 2.55 %
2	41.10 ± 1.03 %	36.77 ± 1.90 %
3	42.34 ± 0.74 %	32.13 ± 1.31 %
4	41.38 ± 4.27 %	34.29 ± 1.60 %
5	37.53 ± 1.78 %	24.18 ± 2.00 %
6	31.31 ± 3.02 %	31.77 ± 1.51 %
7	27.06 ± 4.85 %	27.53 ± 3.34 %
8	37.15 ± 0.44 %	30.05 ± 1.82 %
10	46.49 ± 4.53 %	36.30 ± 3.29 %
11	31.83 ± 3.23 %	19.98 ± 0.87 %
12	25.42 ± 0.44 %	24.85 ± 1.04 %
13	36.85 ± 3.08 %	39.05 ± 2.84 %
14	48.51 ± 0.93 %	50.46 ± 2.89 %
15	34.59 ± 2.06 %	17.06 ± 2.33 %
16	36.09 ± 3.25 %	14.07 ± 0.19 %
17	31.81 ± 3.35 %	24.73 ± 1.53 %
18	35.88 ± 1.36 %	32.22 ± 0.33 %
19	35.72 ± 2.79 %	72.32 ± 0.39 %
20	51.25 ± 4.06 %	31.81 ± 0.33 %
21	56.65 ± 0.79 %	75.90 ± 0.28 %
22	37.72 ± 0.51 %	38.06 ± 1.36 %

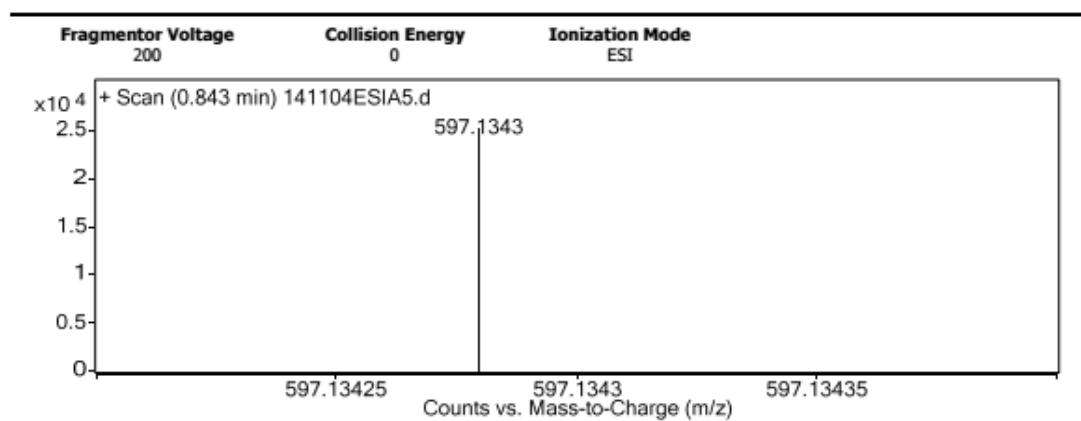


Figure S1. HR ESI MS spectra of compound 1

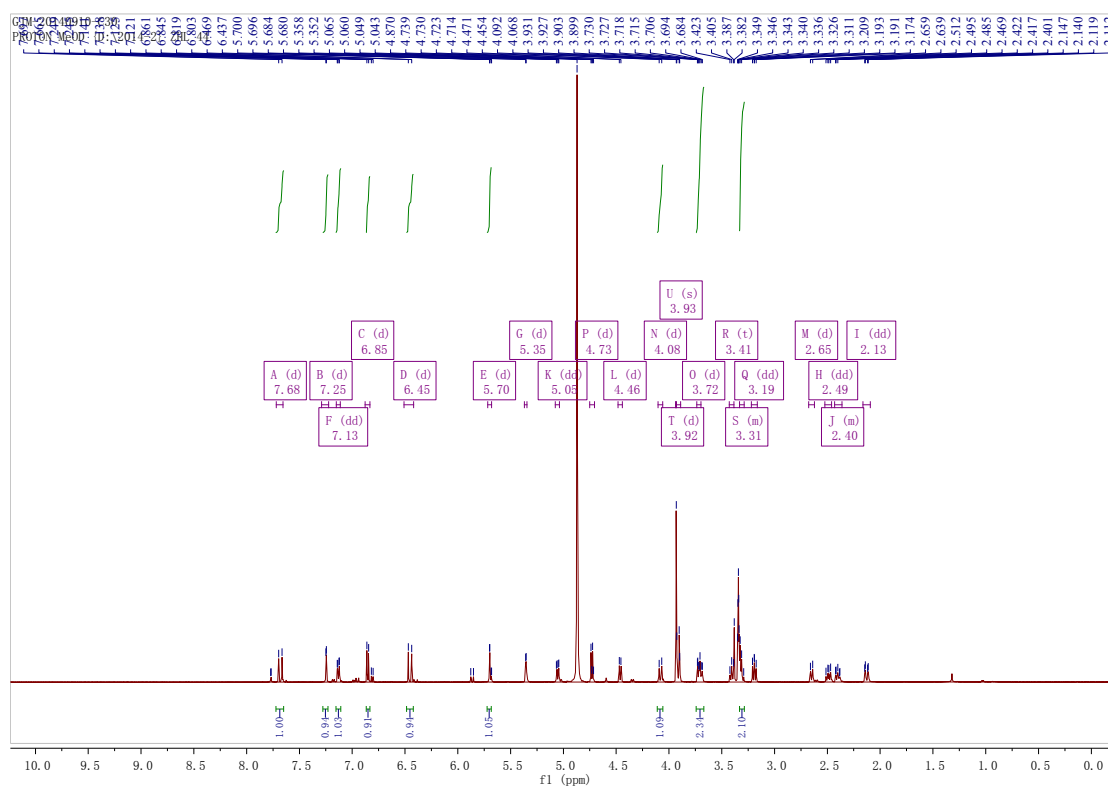


Figure S2. ^1H NMR spectra of compound 1

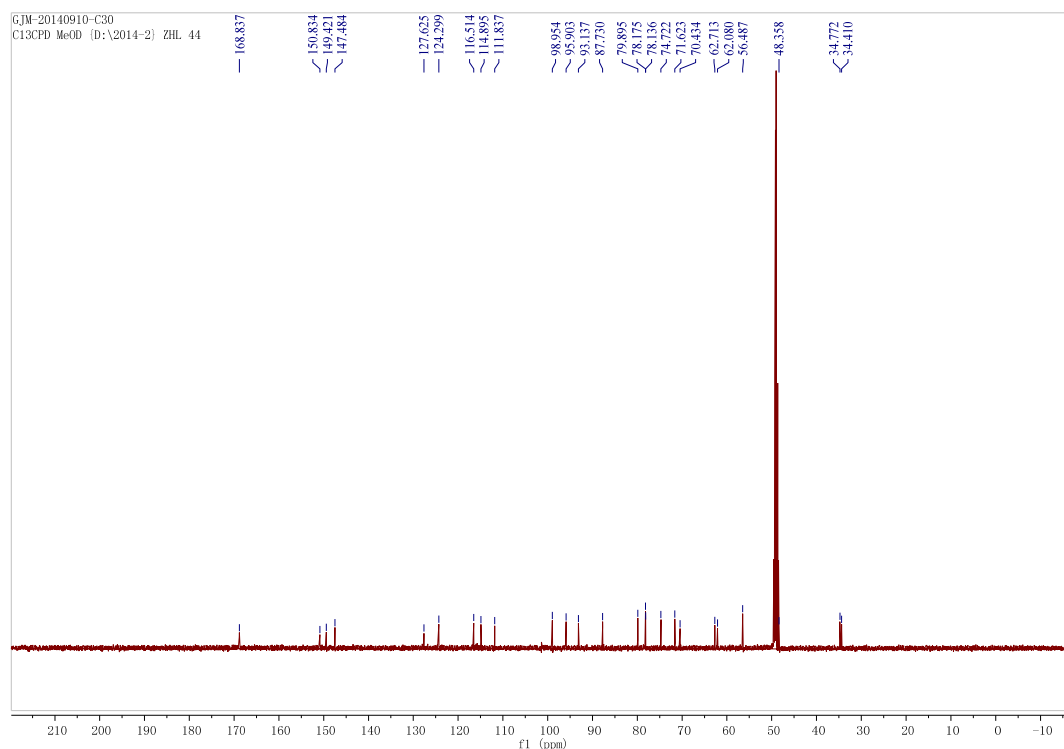


Figure S3. ^{13}C NMR spectra of compound **1**

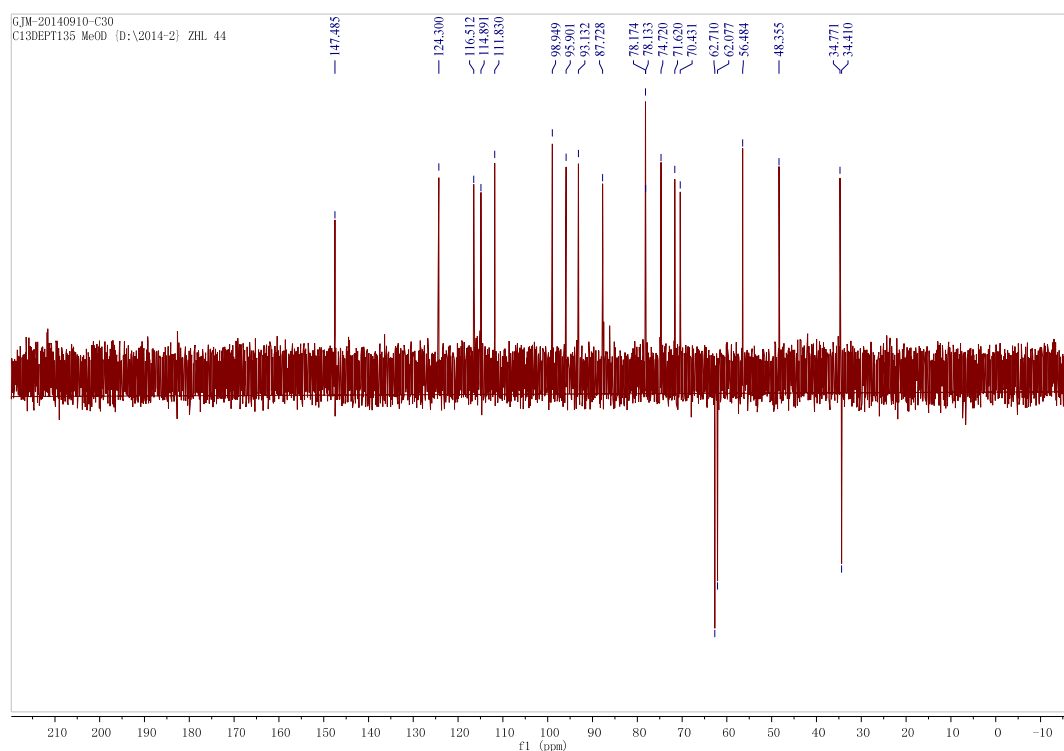


Figure S4. DEPT spectra of compound **1**

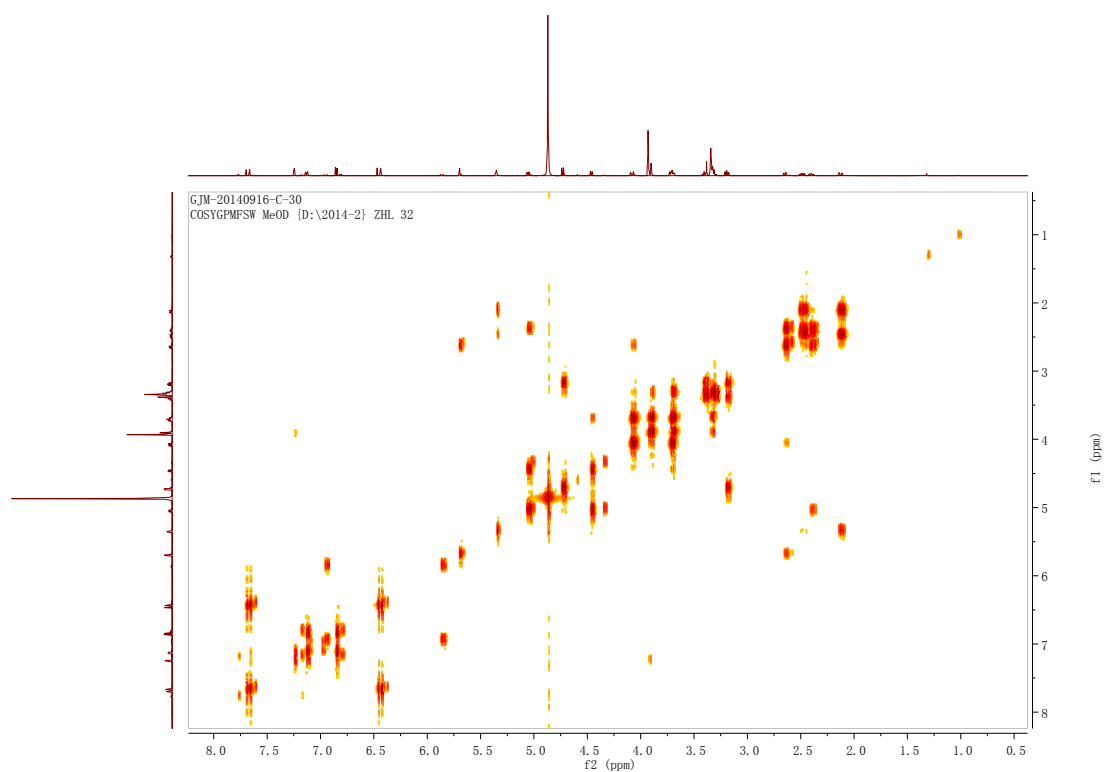


Figure S5. ^1H - ^1H COSY spectra of compound **1**

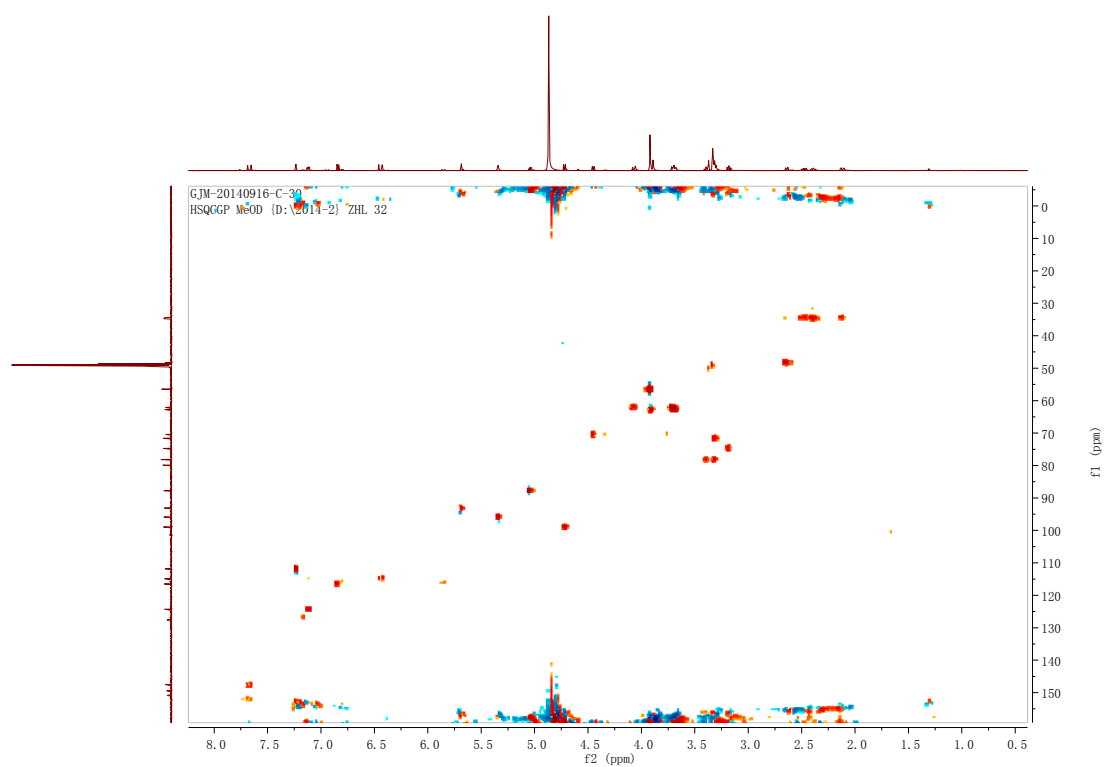


Figure S6. HSQC spectra of compound **1**

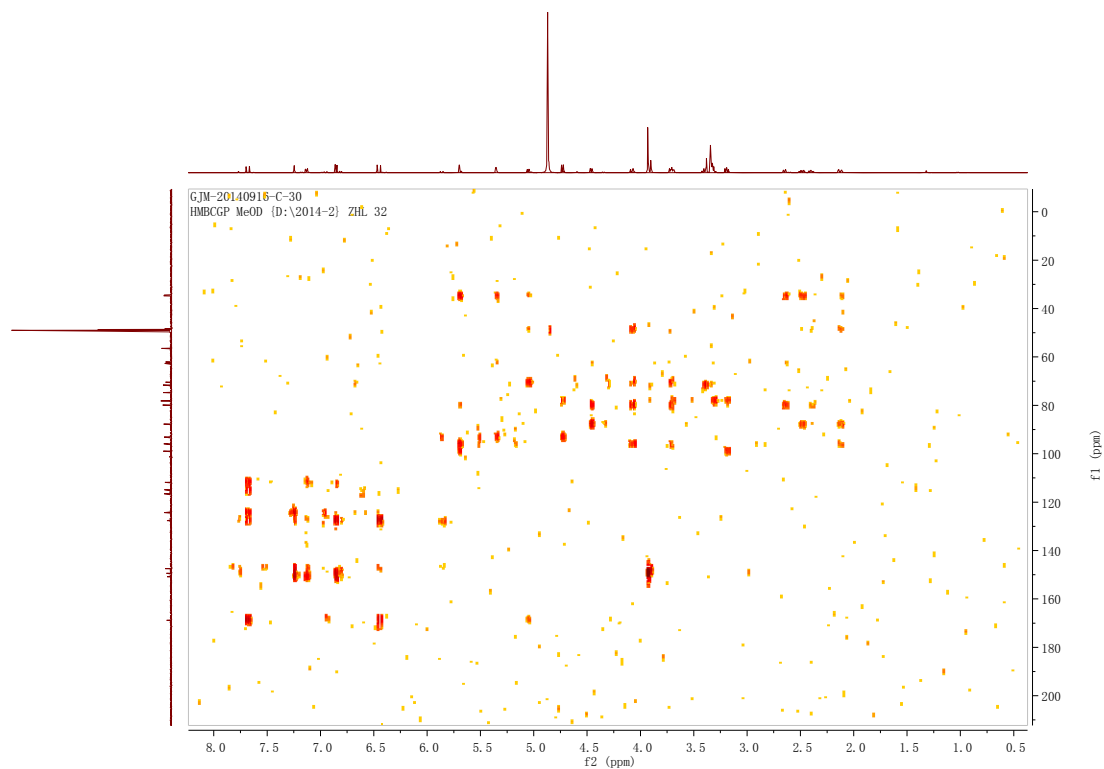


Figure S7. HMBC spectra of compound **1**

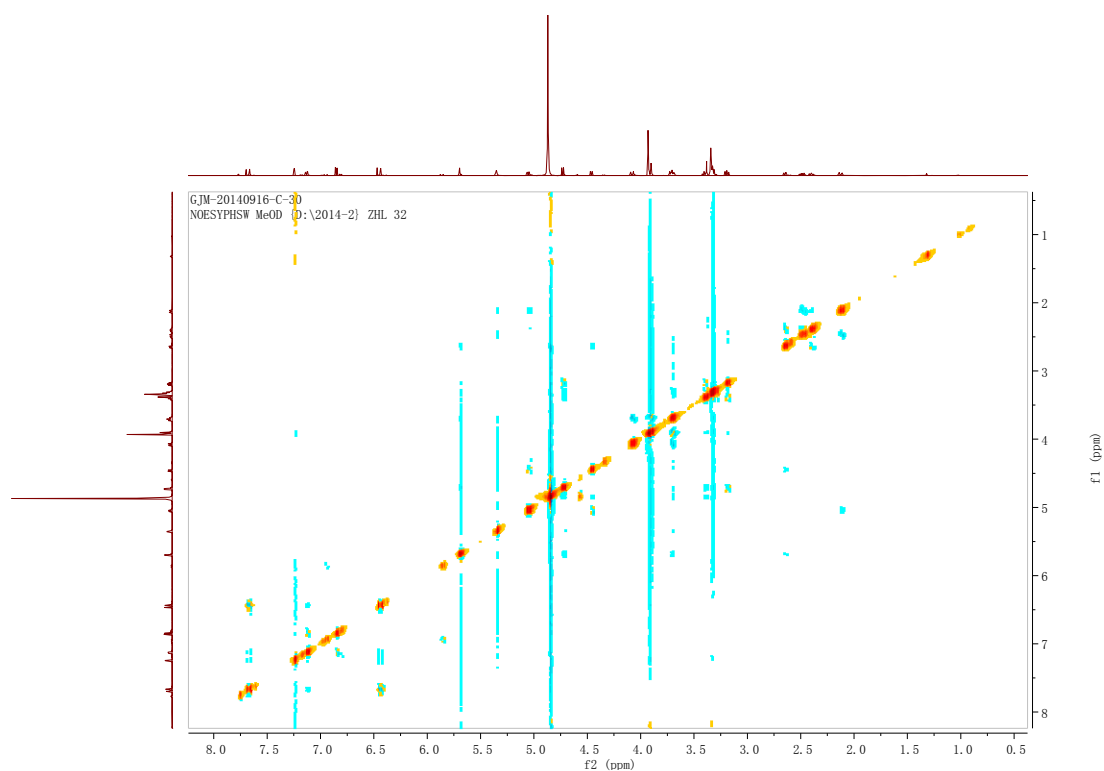


Figure S8. NOESY spectra of compound **1**

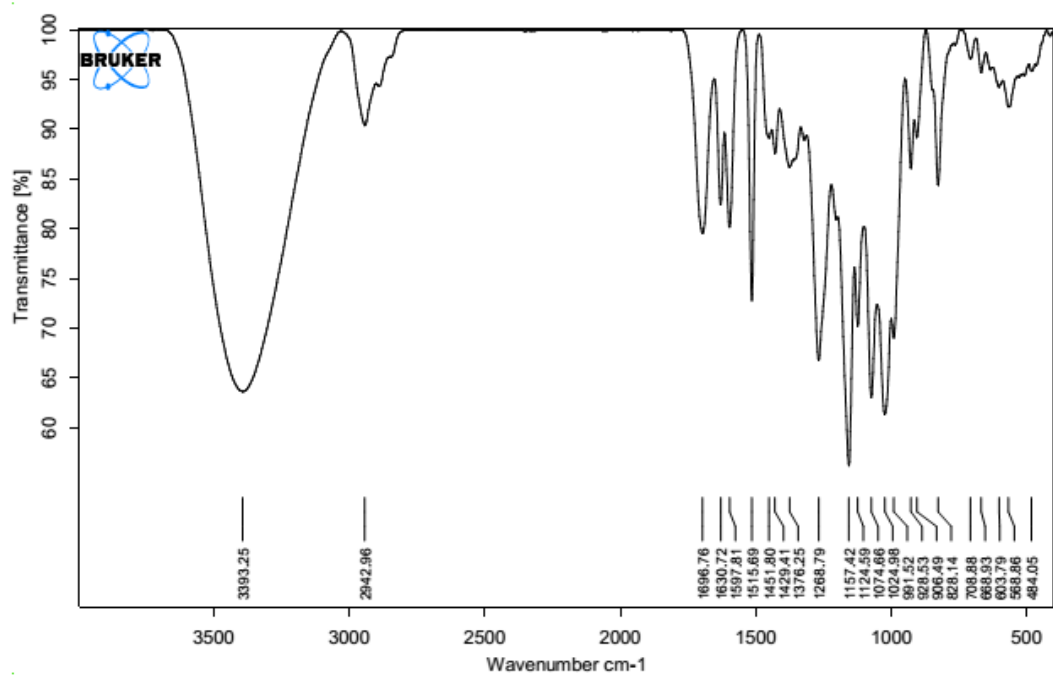


Figure S9. IR spectra of compound 1

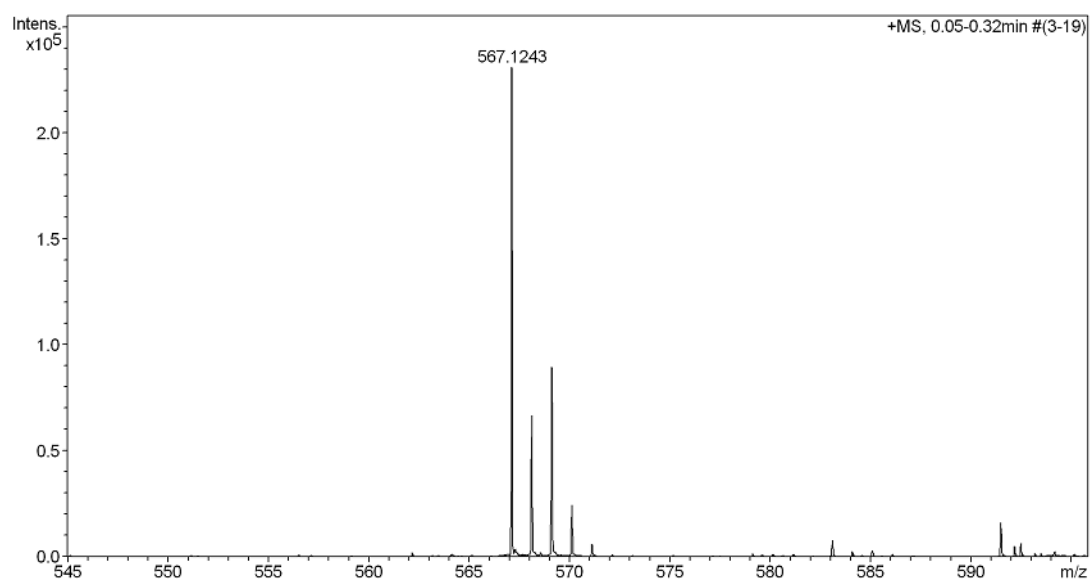


Figure S10. HRESIMS spectra of compound 2

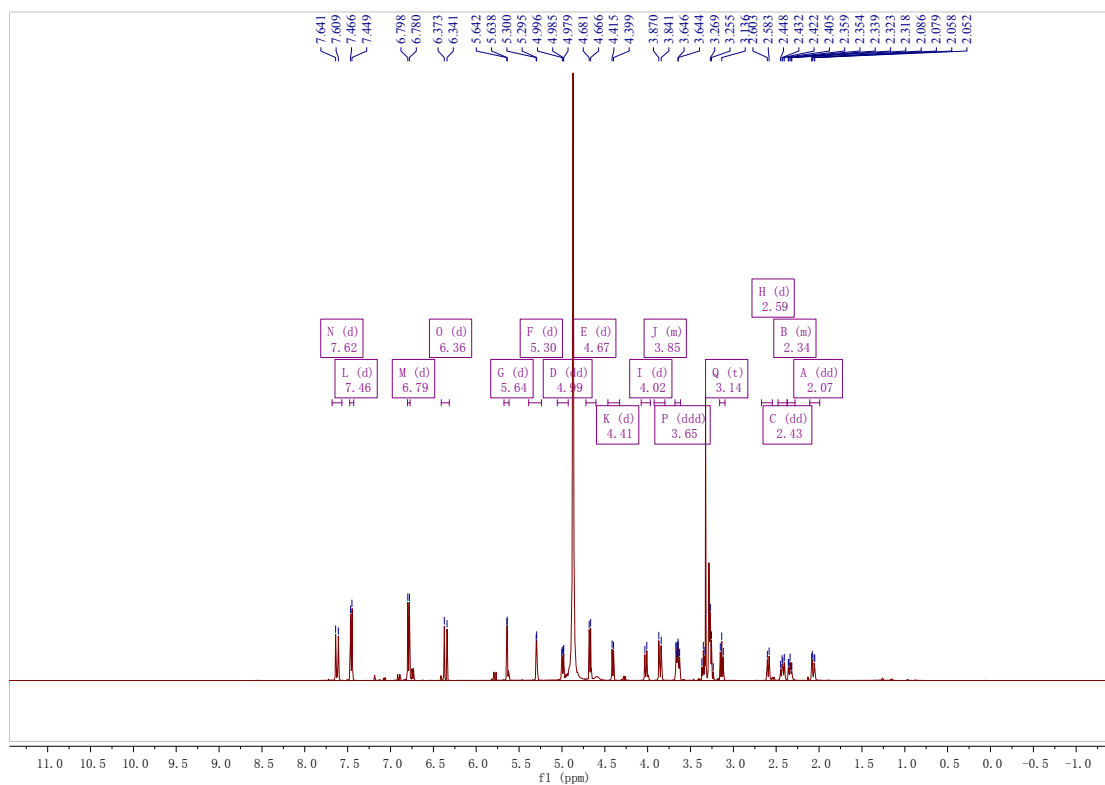


Figure S11. ¹H NMR spectra of compound 2

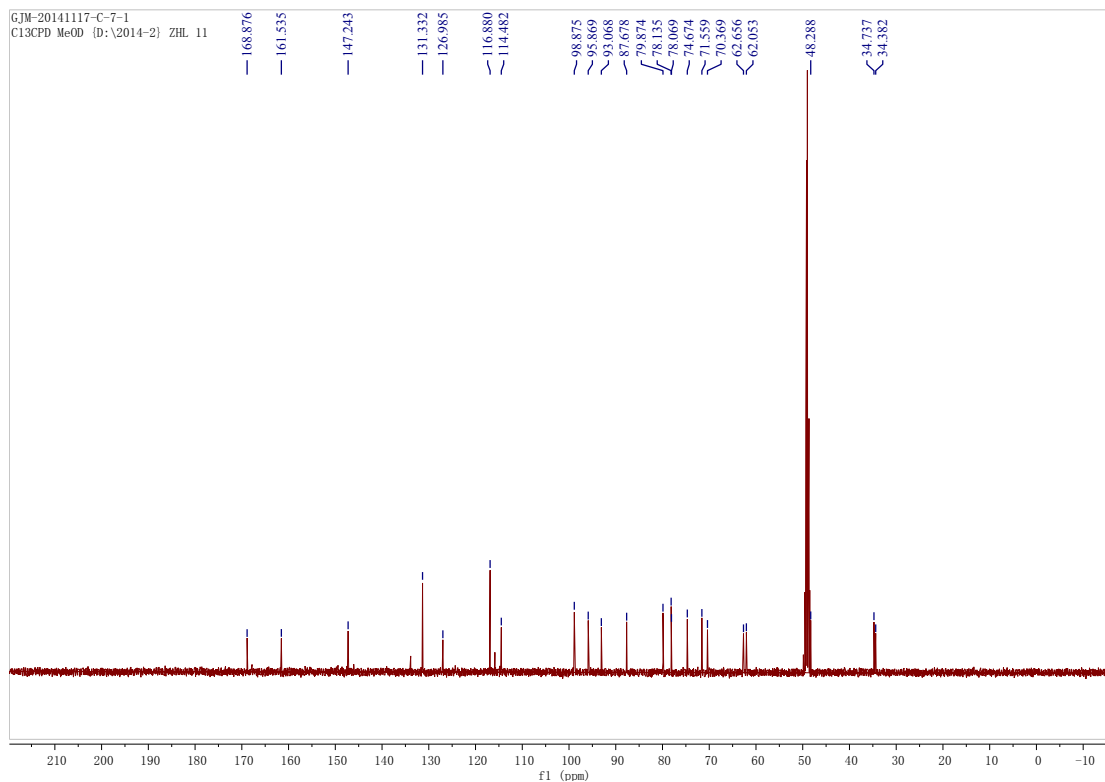


Figure S12. ¹³C NMR spectra of compound 2

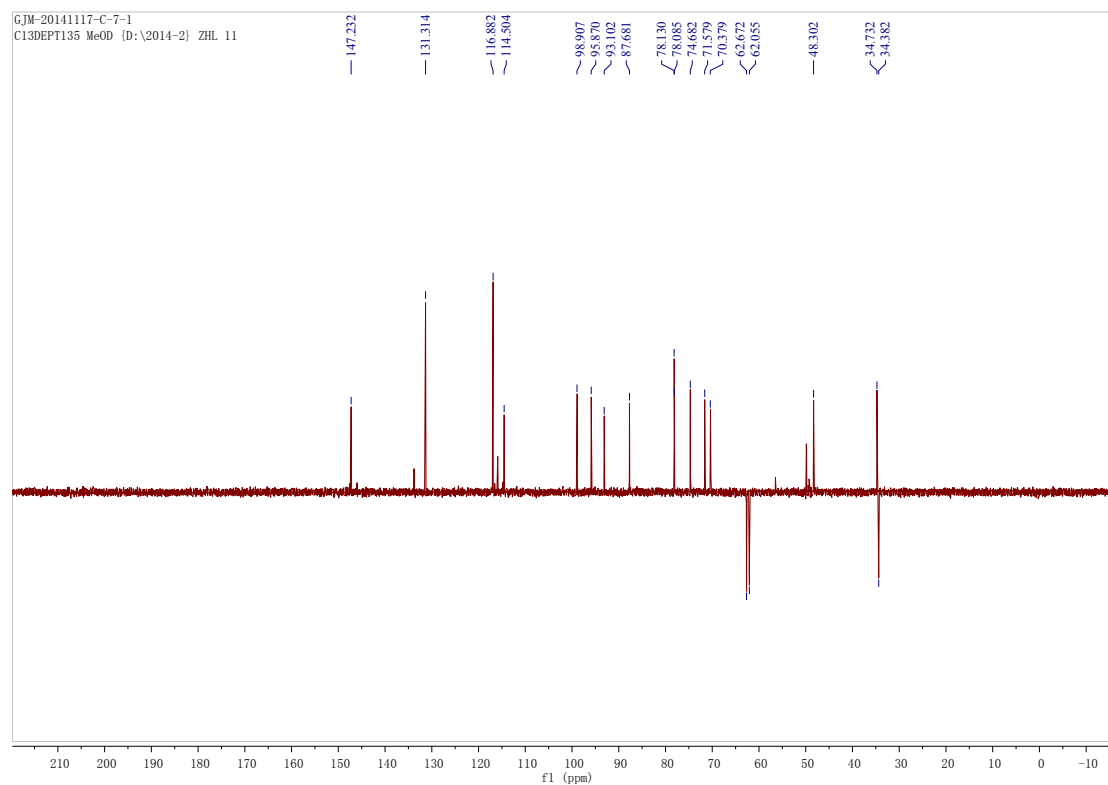


Figure S13. DEPT spectra of compound **2**

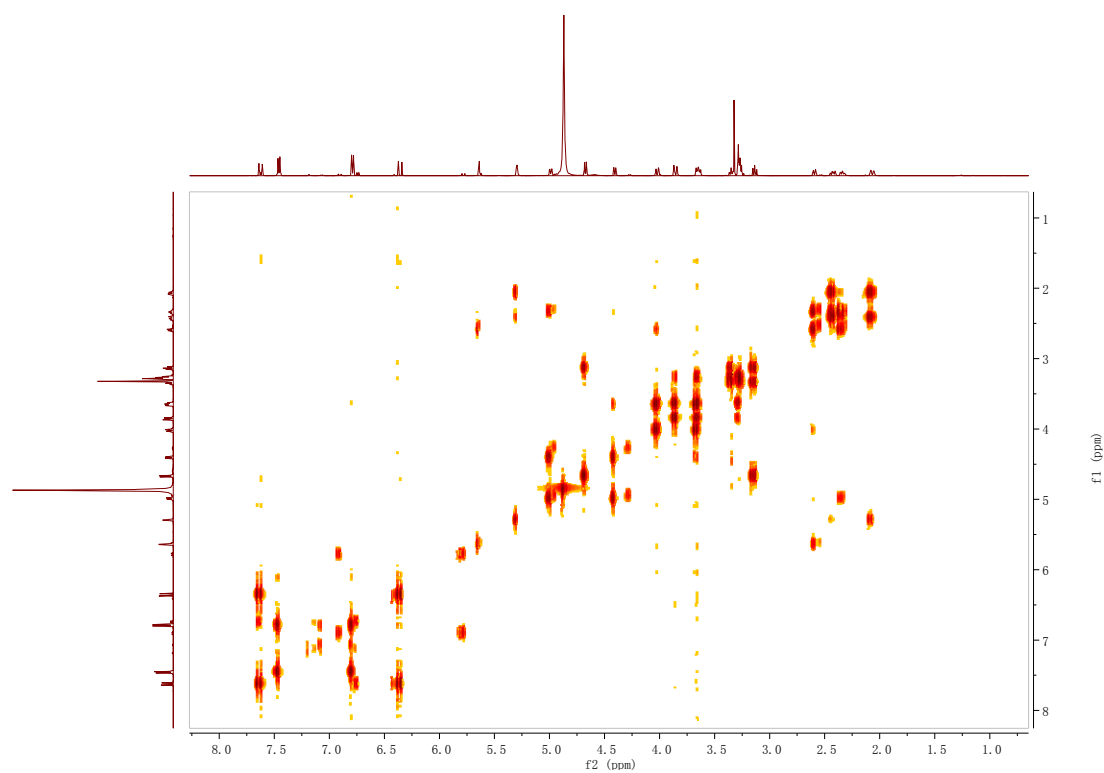


Figure S14. ^1H - ^1H COSY spectra of compound **2**

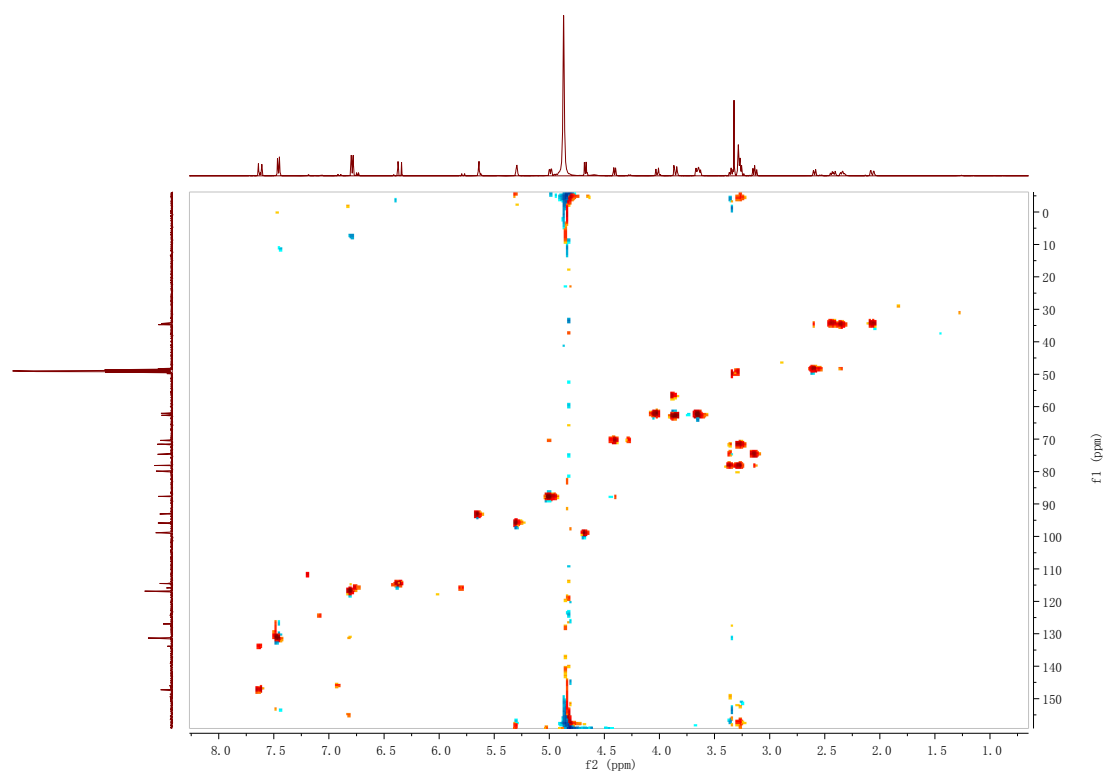


Figure S15. HSQC spectra of compound 2

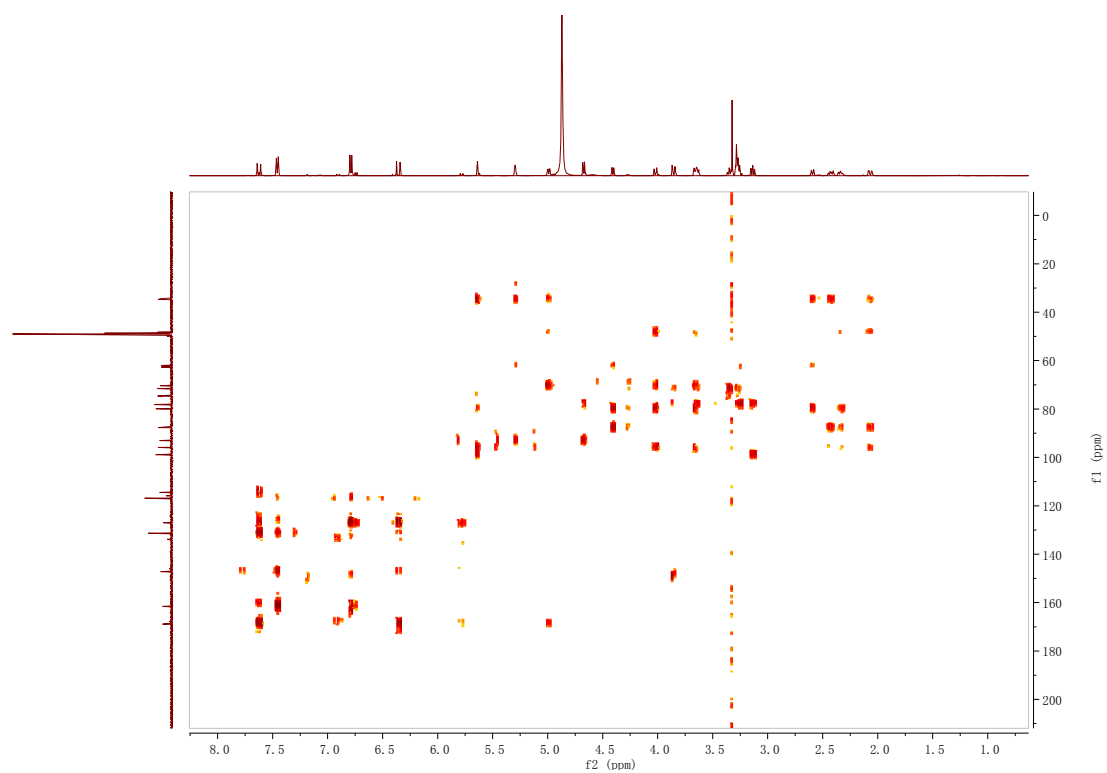


Figure S16. HMBC spectra of compound 2

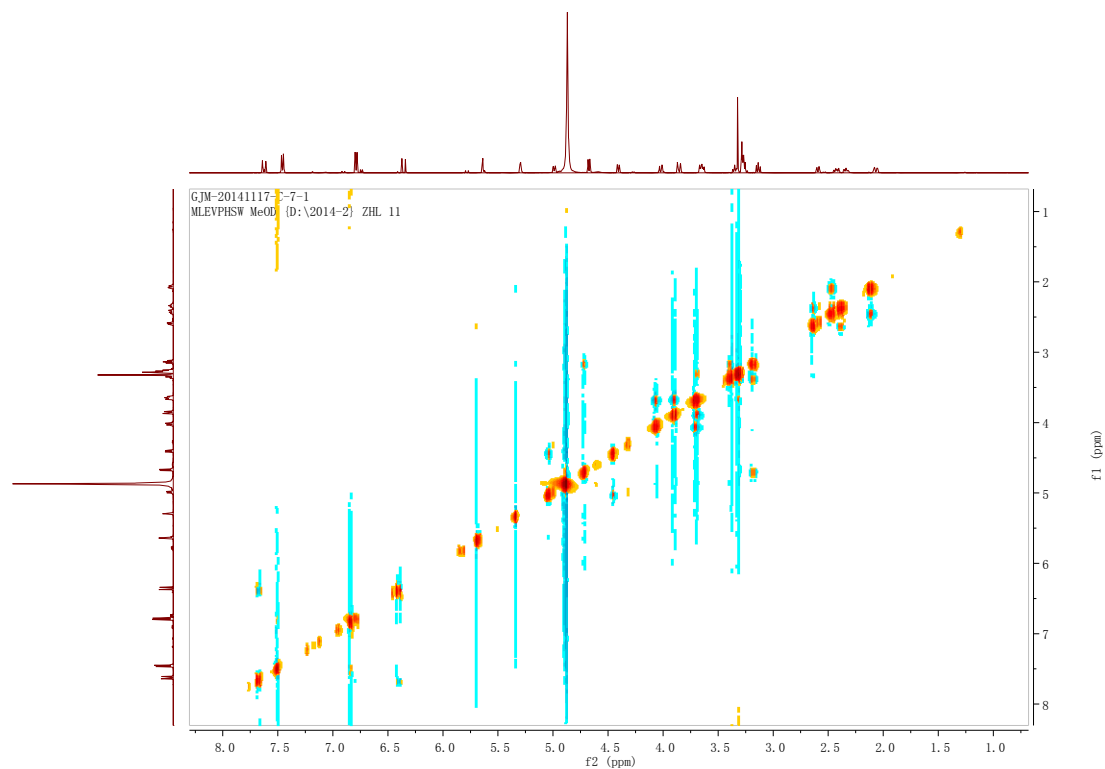


Figure S17. NOESY spectra of compound 2

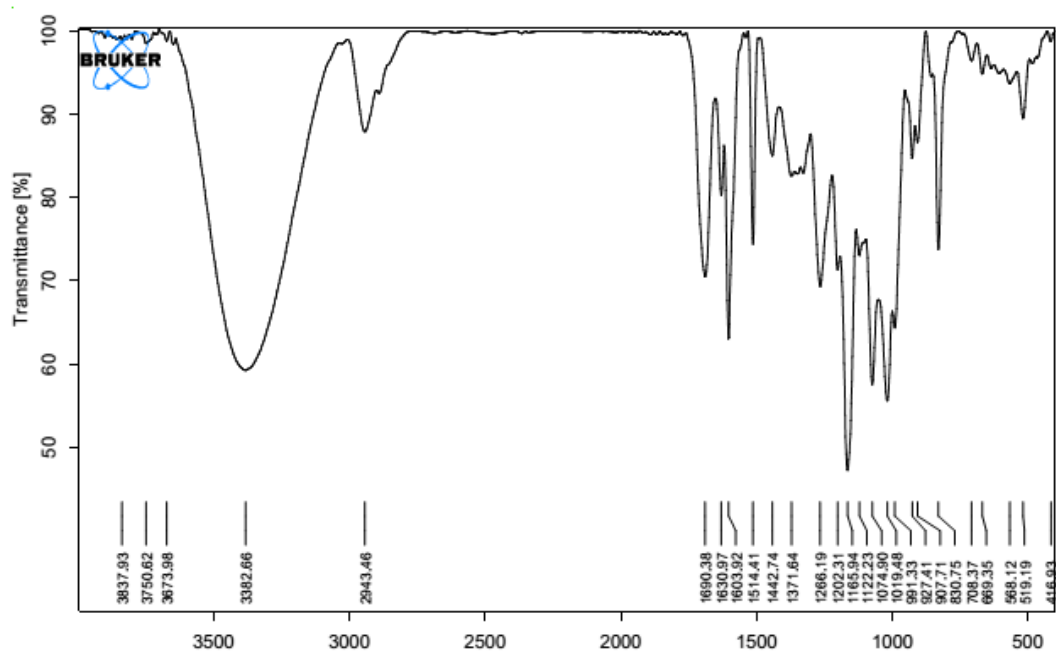


Figure S18. IR spectra of compound 2