Supplementary materials

Two new cytochalasins from the endophytic fungus *Xylaria* sp. GDGJ–77B

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Author Contributions

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ABSTRACT: Two new open-chain cytochalasins, xylarchalasins A and B (**1** and **2**), together with six known analogues (**3**–**8**), were isolated from the endophytic fungus *Xylaria* sp. GDGJ–77B from the Chinese medicinal plant *Sophora tonkinensis*. Their structures were elucidated on the basis of comprehensive spectroscopic analysis. Compound **2** displayed moderate antibacterial activities against *Bacillus subtilis* and *Escherichia coli* with MIC values of 25 and 12.5 μg/mL, respectively.
KEYWORDS: *Xylaria* sp.; endophytic fungus; cytochalasins; antibacterial activities

List of supporting information

Table S1. ^{1}H and ^{13}C NMR assignments for compounds **1** and **2** in $CDCl_3$

no.	**1**[a]		**2**[b]	
	δ_C	δ_H (J in Hz)	δ_C	δ_H (J in Hz)
1	171.2		171.0	
3	54.6	3.60, m	54.4	3.64, m
4	49.9	2.56, t (4.4)	50.2	2.59, t (4.3)
5	35.6	2.14, m	35.7	2.15, m
6	57.6		57.6	
7	60.0	2.74, m	60.0	2.73, d (5.0)
8	47.3	2.73, m	47.3	2.76, m
9	85.0		84.9	
10α	43.0	2.81, dd (13.4, 4.7)	44.0	2.88, dd (13.4, 4.4)
10β		2.91, dd (13.4, 9.3)		2.97, dd (13.4, 9.6)
11	14.1	1.12, d (6.9)	14.1	1.14, d (7.8)
12	20.6	1.30, s	20.5	1.31, s
13	127.8	5.92, m	127.9	5.96, m
14	131.5	5.54, m	130.9	5.54, m
15α	36.8	2.14, m	36.4	2.17, m
15β		2.41, m		2.45, m
16	39.8	3.24, m	41.1	3.24, m
17	216.5		206.7	
18	78.1		152.2	
19α	51.4	2.62, d (17.0)	131.8	6.53, dq (7.2, 1.2)
19β		3.06, d (17.0)		
20	202.3	9.74, s	192.9	10.25, d (7.2)
21	154.0		154.0	
22	18.1	1.11, d (6.9)	16.9	1.11, d (6.6)
23	24.7	1.34, s	12.8	2.25, d (1.2)
24	55.0	3.78, s	55.1	3.80, s
1'	129.4		137.5	
2', 6'	130.3	7.11, d (8.4)	129.2	7.20, d (7.2)
3', 5'	114.6	6.86, d (8.4)	129.2	7.35, t (7.2)
4'	158.9		127.4	7.28, t (7.2)
4'-OCH_3	55.4	3.79, s		
18-OH		4.09, s		
-NH		5.87, br s		5.72, br s

[a] ^{1}H NMR measured at 400 MHz; ^{13}C NMR measured at 100 MHz.

[b] ^{1}H NMR measured at 600 MHz; ^{13}C NMR measured at 150 MHz.

Table S2. Antibacterial activities of compounds **1–8** (MIC, $\mu g \cdot mL^{-1}$) [a]

Compounds	MIC (μg/mL)						
	Bacillus paratyphosus B	*Bacillus anthracis*	*Bacillus subtilis*	*Bacillus megaterium*	*Staphylococcus aureus*	*Escherichia coli*	*Shigella dysenteriae*
1	>100	50	100	25	100	50	>100
2	100	50	25	50	50	12.5	100
3	50	25	100	50	>100	50	>100
4	50	100	50	>100	50	25	100
5	>100	25	50	>100	12.5	50	100
6	100	50	25	>100	50	>100	50
7	>100	>100	50	50	>100	100	100
8	50	50	100	100	50	>100	>100
Ampicillin	6.25	3.125	1.56	1.56	3.125	1.56	1.56

[a] MIC-minimum inhibitory concentrations.

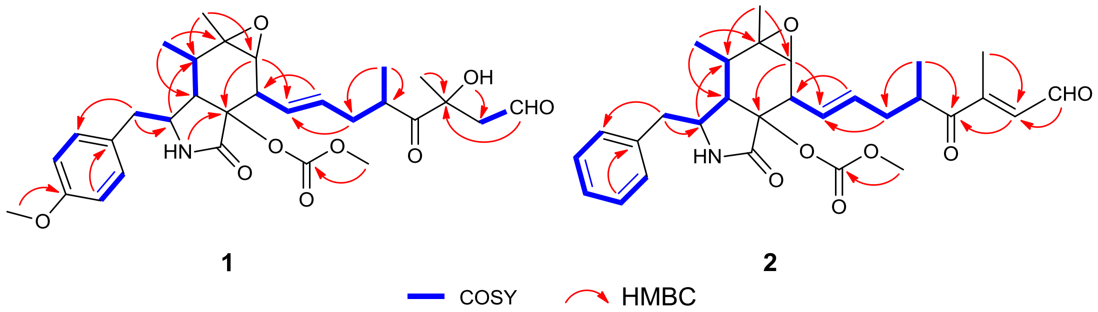

Figure S1. Key HMBC and ^{1}H-^{1}H COSY correlations of compounds **1** and **2**

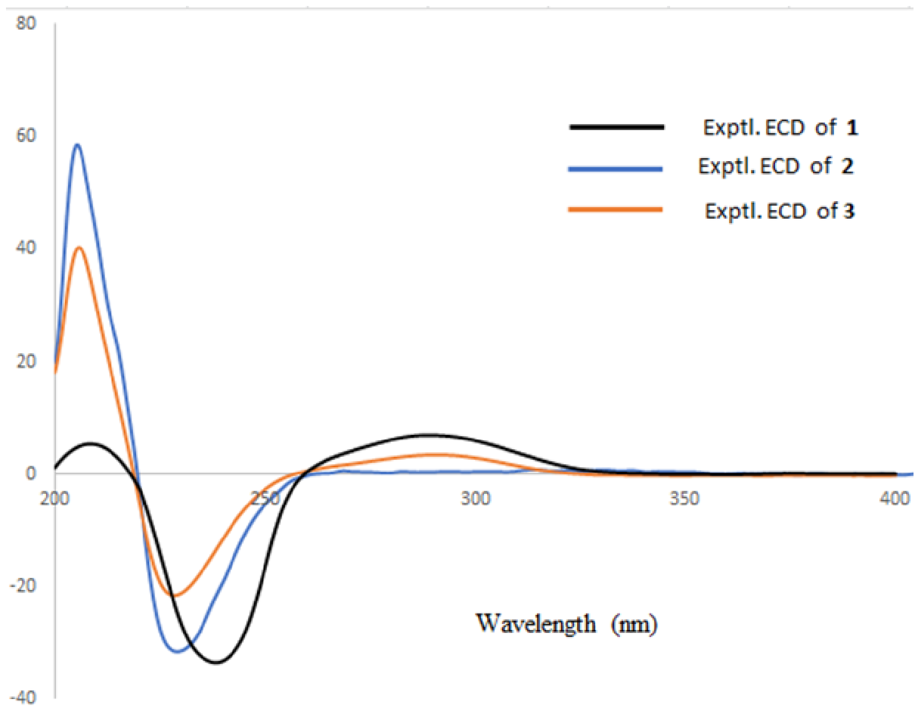

Figure S2. Experimental CD spectra of compounds **1**–**3** in MeOH

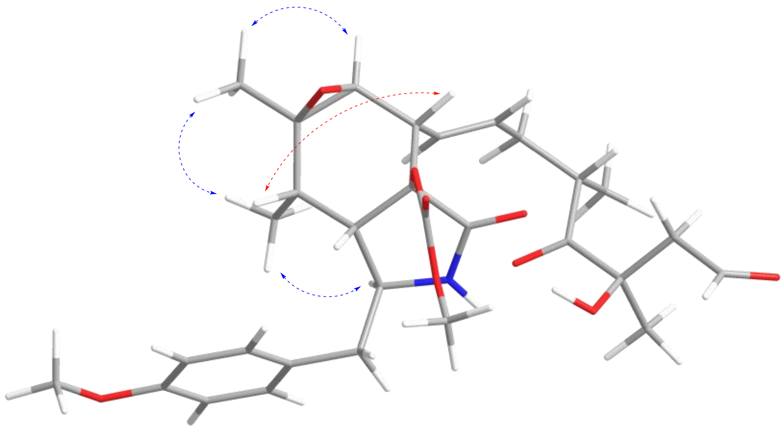

Figure S3. Key NOESY correlations of compound **1**

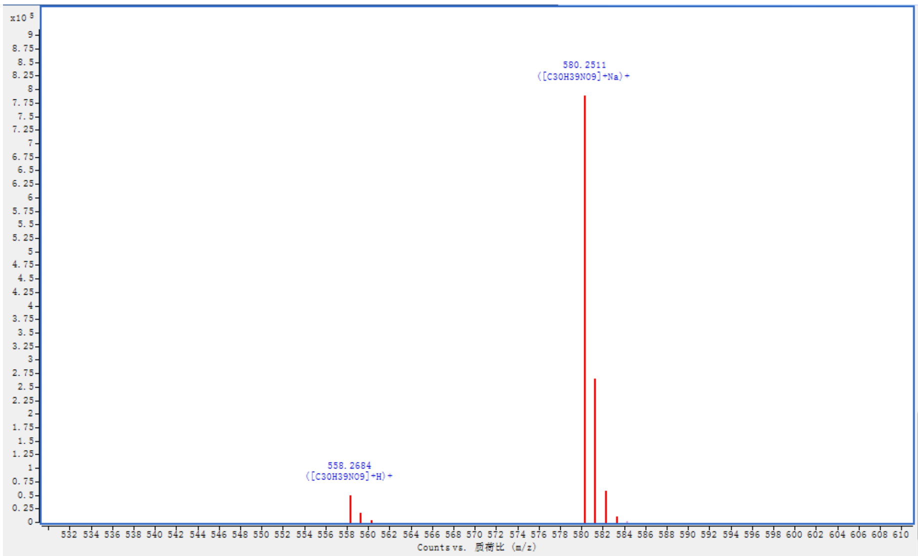

Figure S4. HR-ESI-MS spectrum of compound **1**

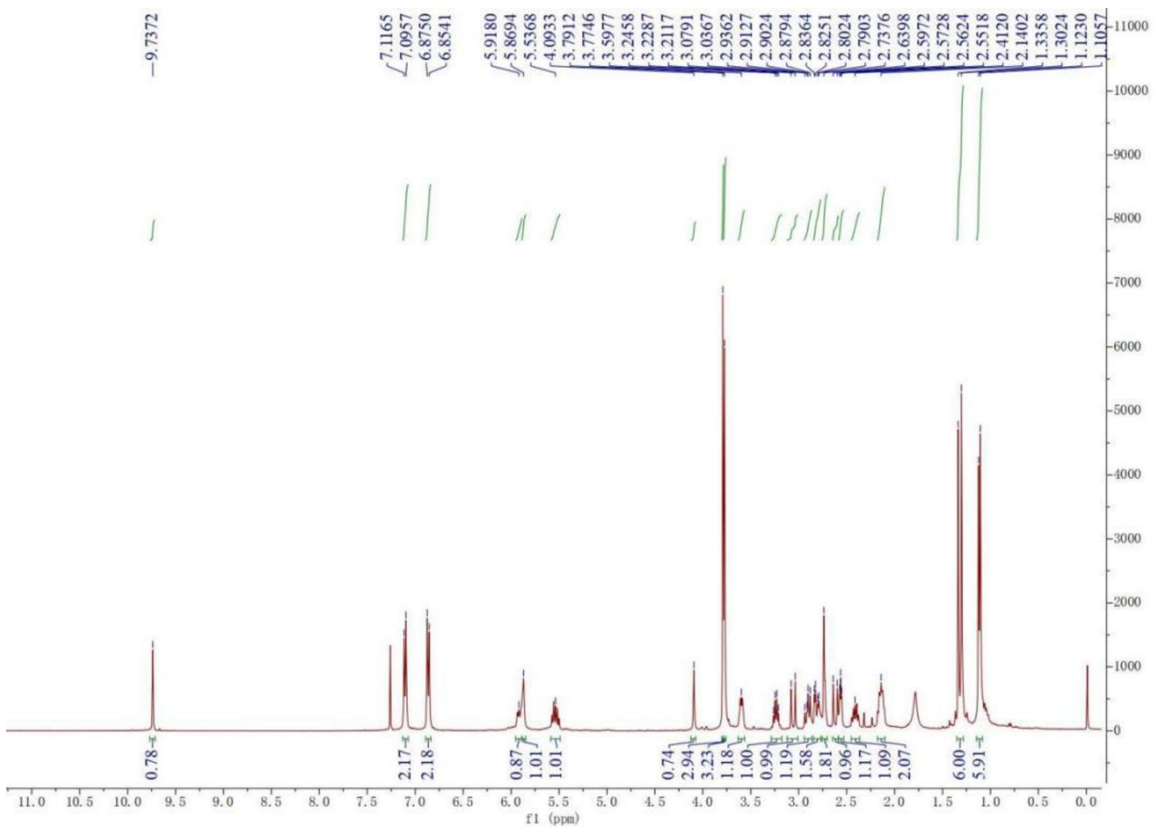

Figure S5. ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **1**

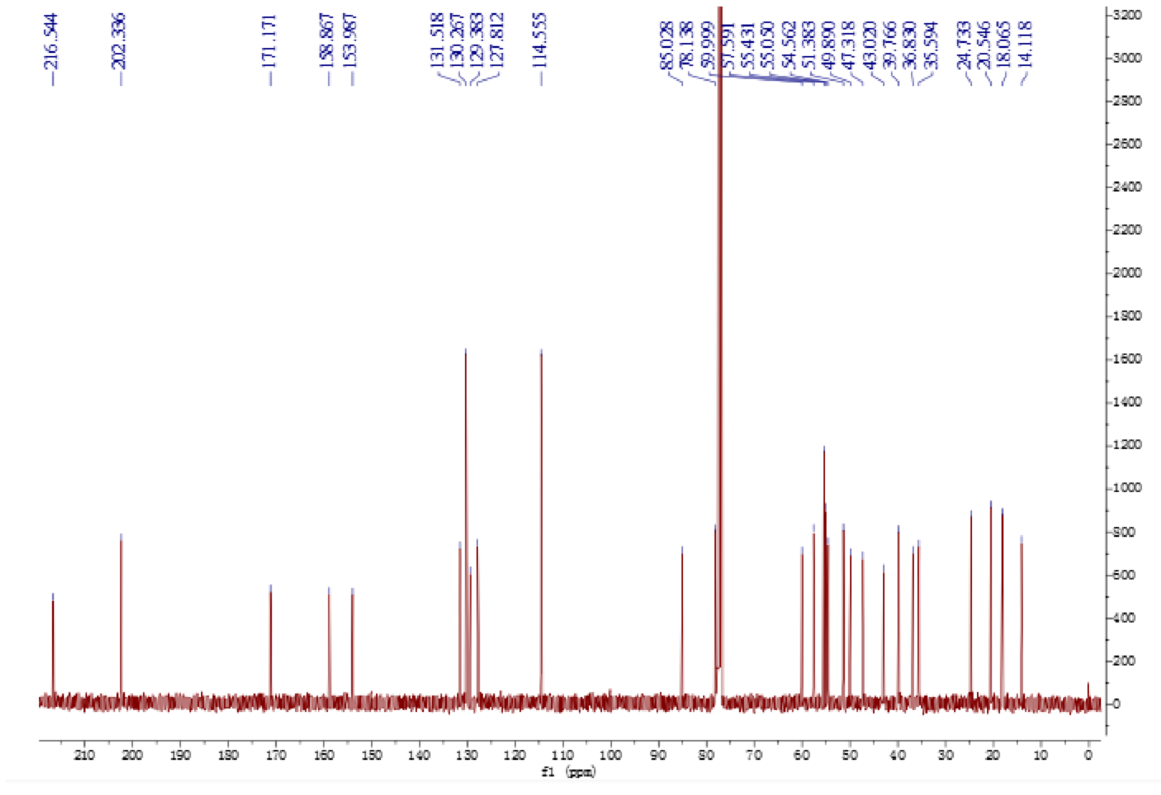

Figure S6. ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **1**

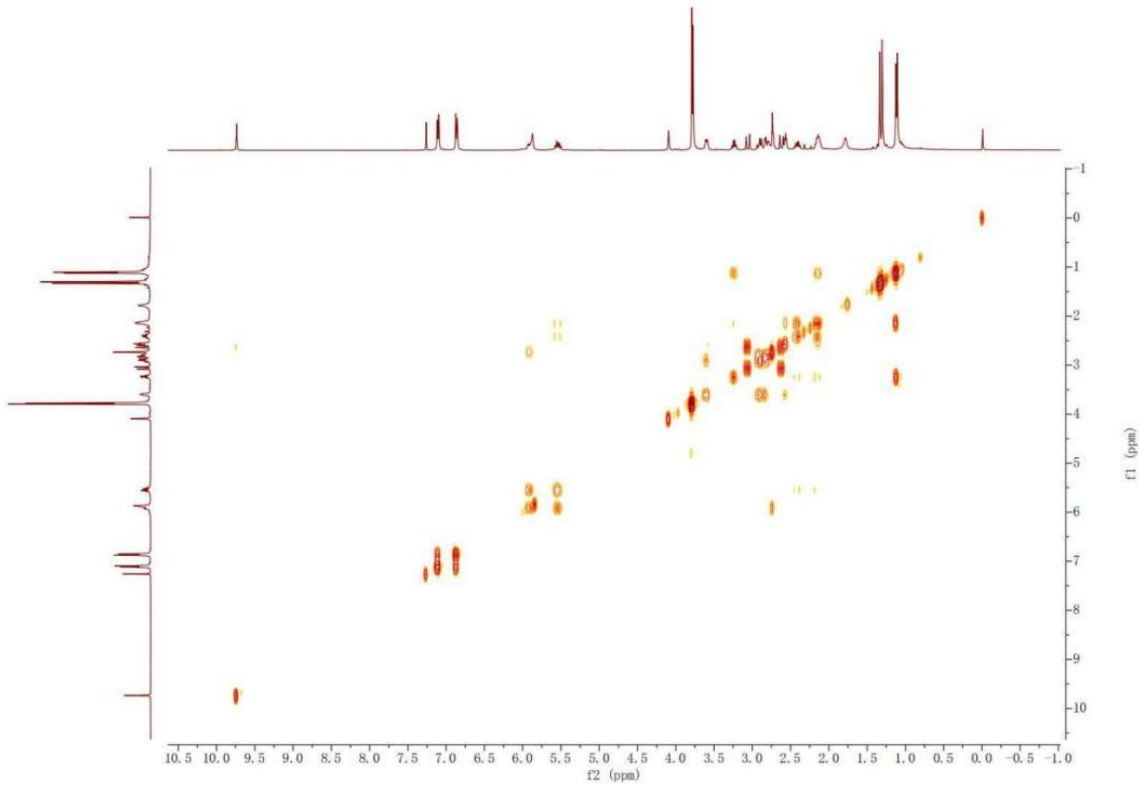

Figure S7. ^{1}H-^{1}H COSY ($CDCl_3$) spectrum of compound **1**

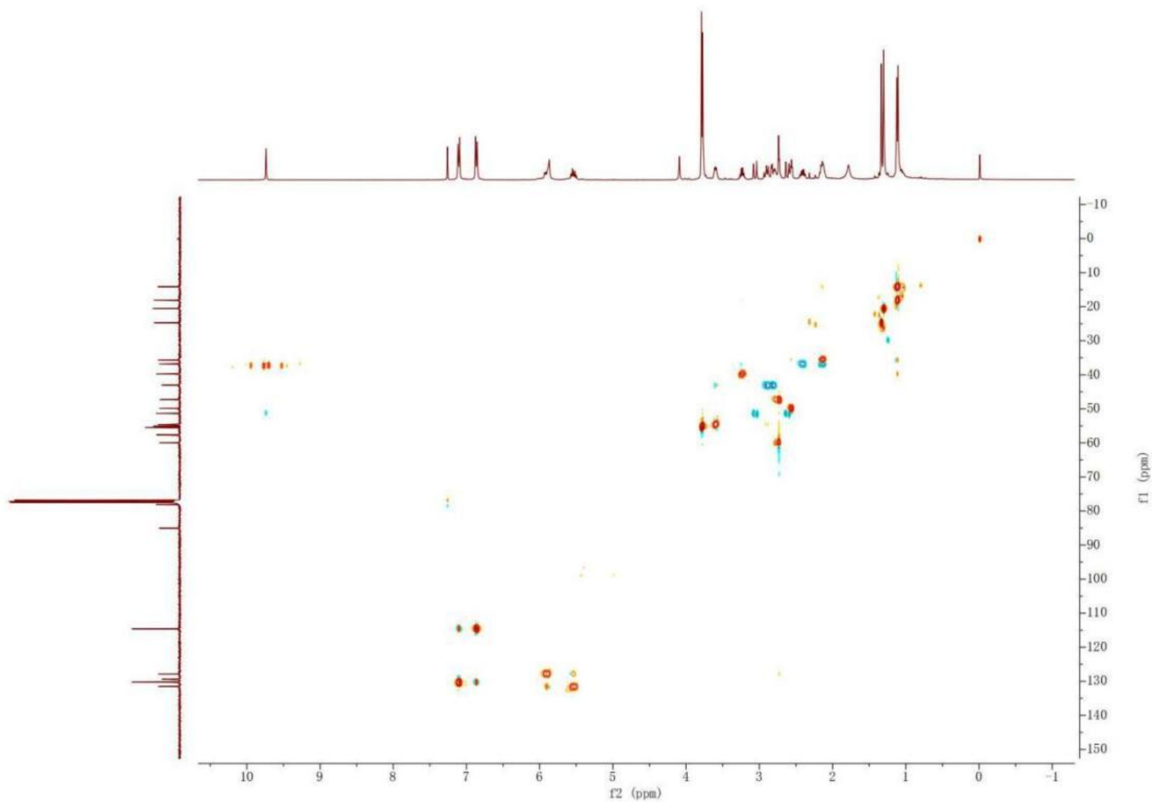

Figure S8. HMQC ($CDCl_3$) spectrum of compound **1**

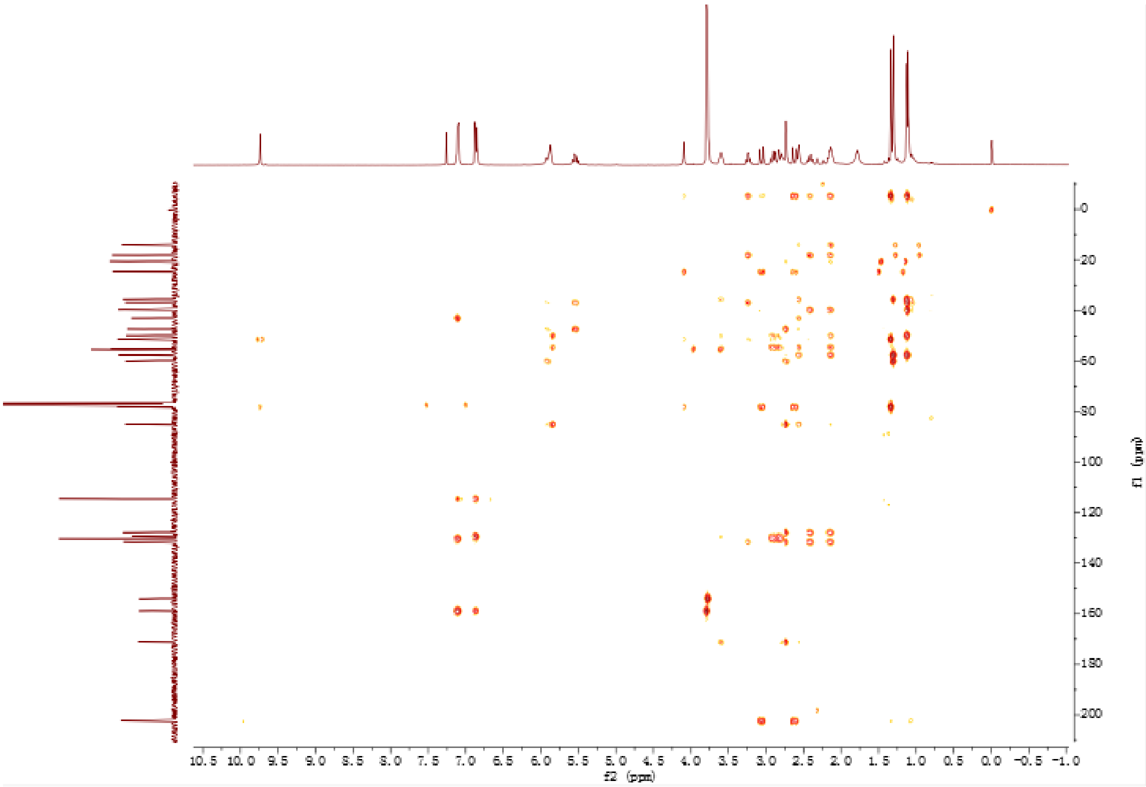

Figure S9. HMBC ($CDCl_3$) spectrum of compound **1**

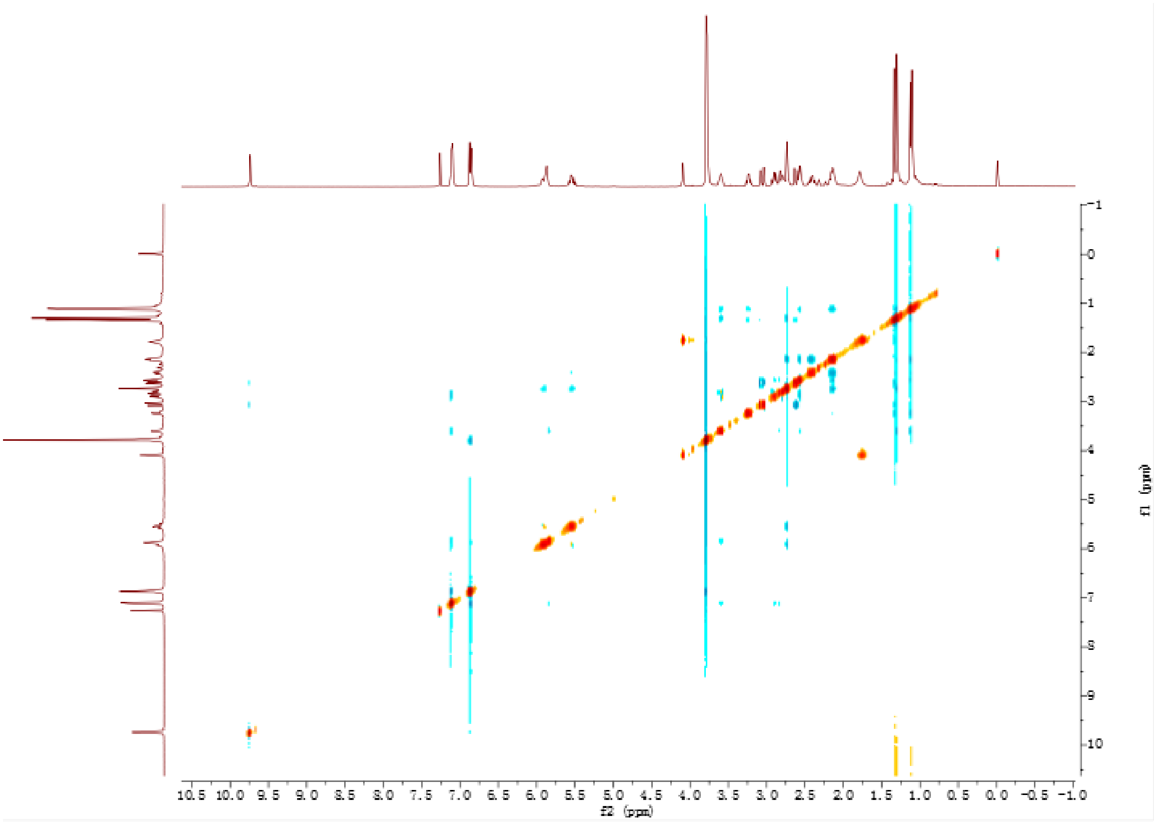

Figure S10. NOESY ($CDCl_3$) spectrum of compound **1**

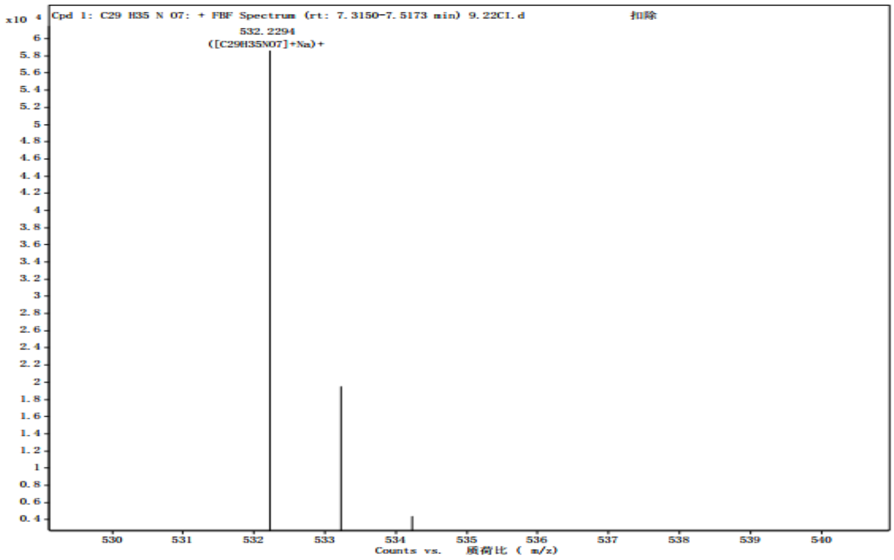

Figure S11. HR-ESI-MS spectrum of compound **2**

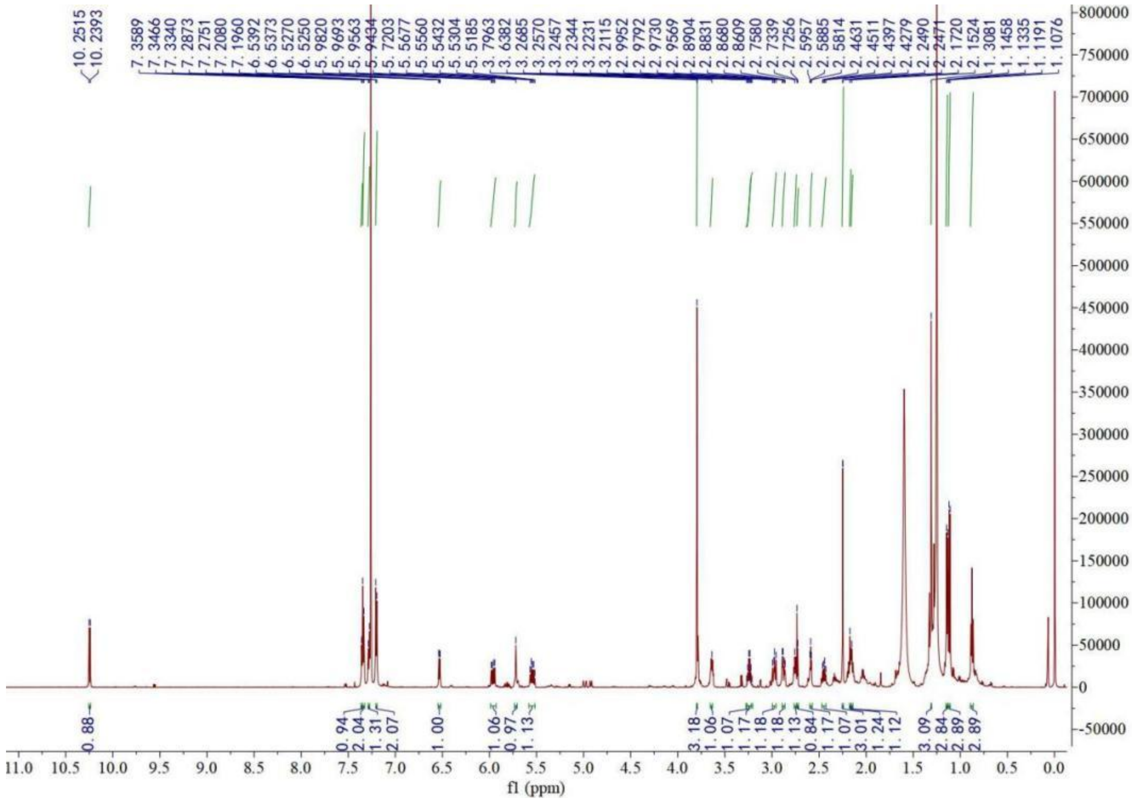

Figure S12. ^{1}H NMR (600 MHz, $CDCl_3$) spectrum of compound **2**

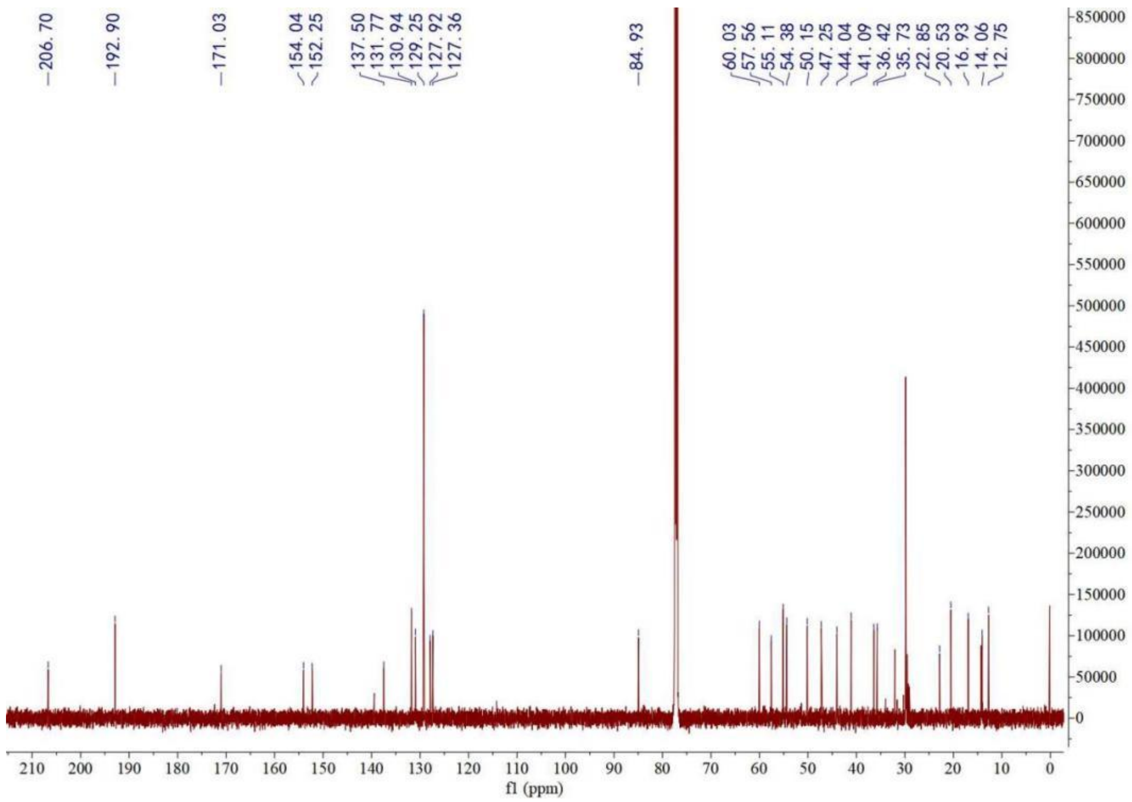

Figure S13. ^{13}C NMR (150 MHz, $CDCl_3$) spectrum of compound **2**

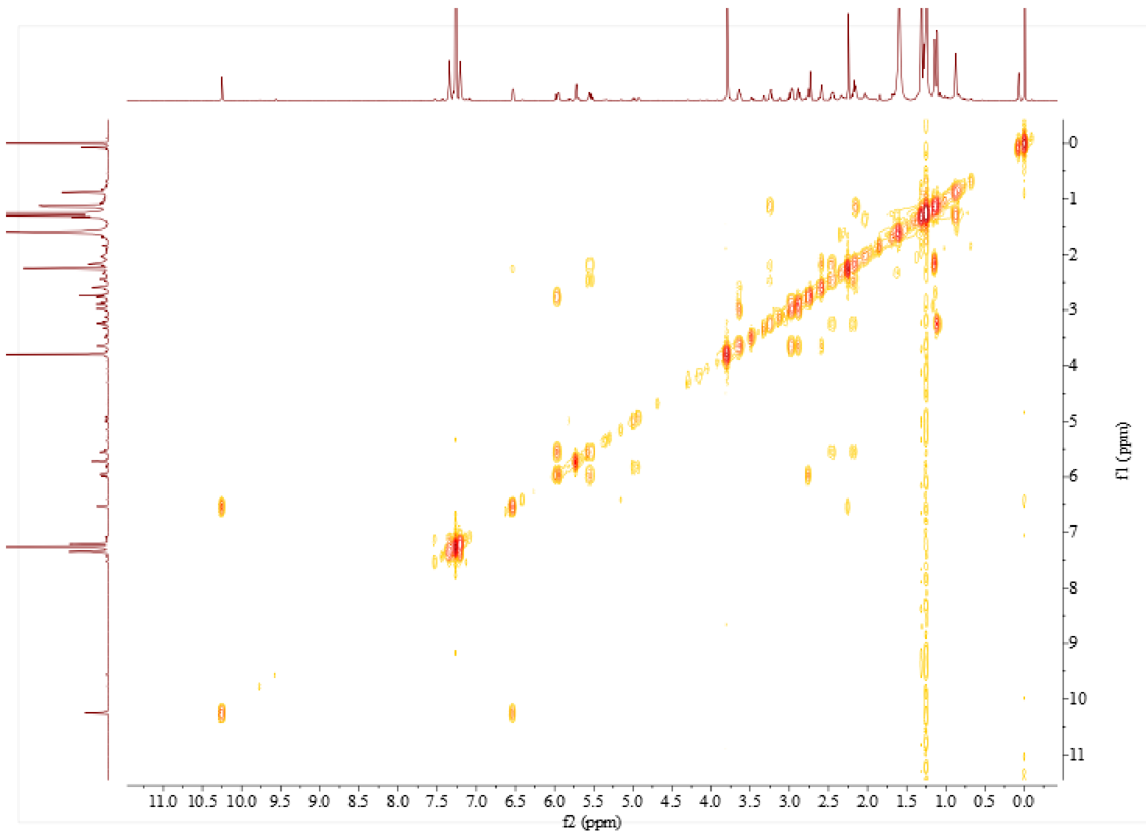

Figure S14. ^1H-^1H COSY ($CDCl_3$) spectrum of compound **2**

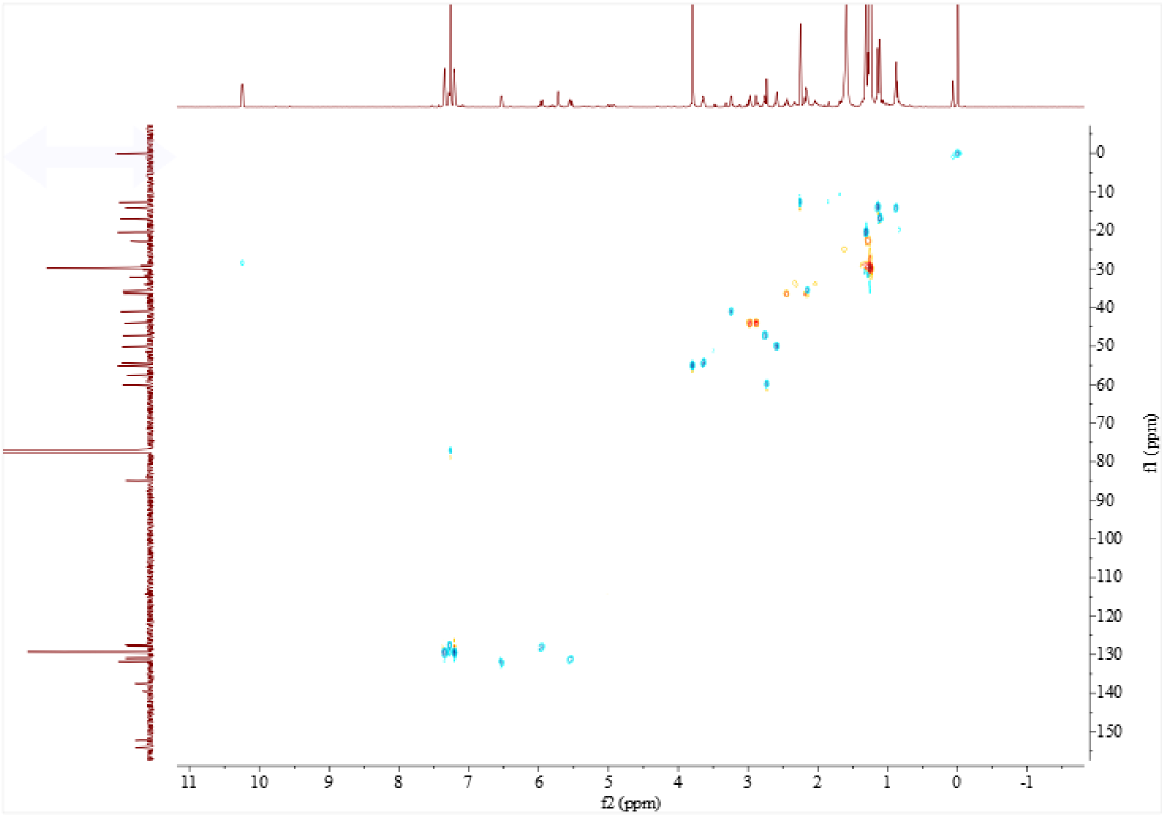

Figure S15. HMQC ($CDCl_3$) spectrum of compound **2**

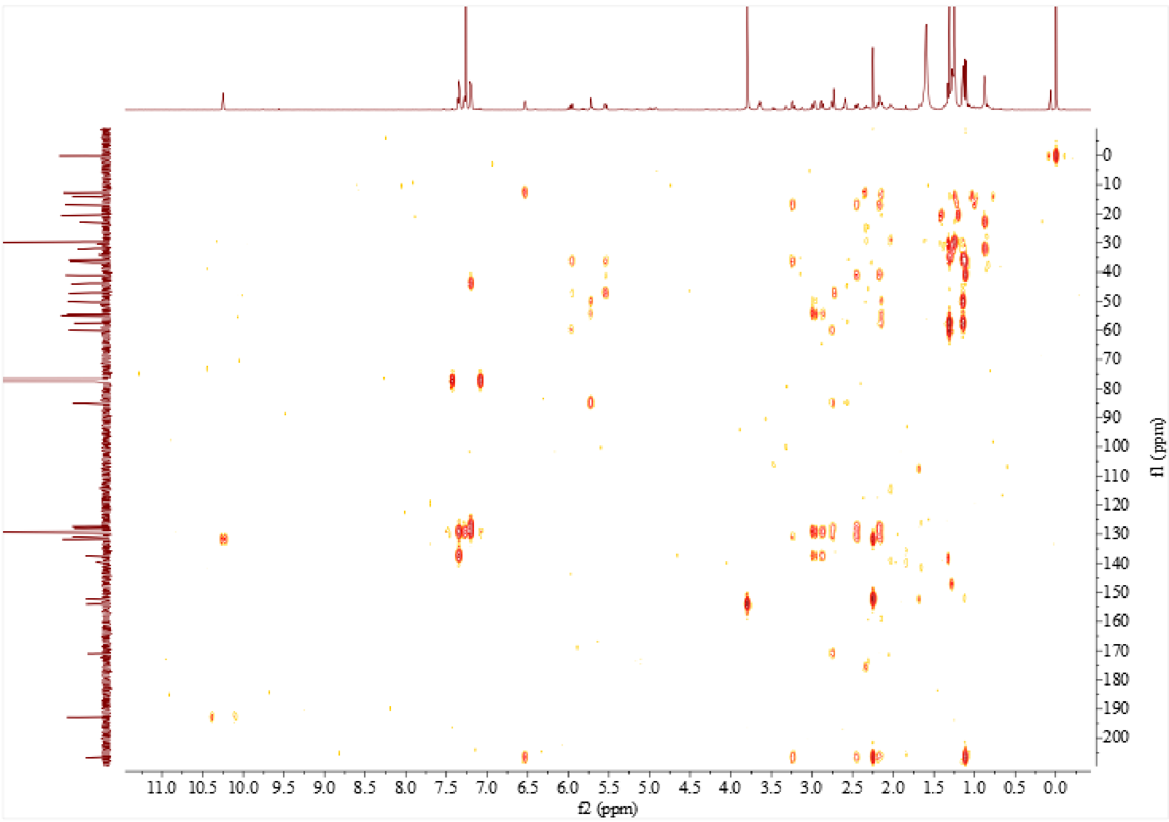

Figure S16. HMBC ($CDCl_3$) spectrum of compound **2**

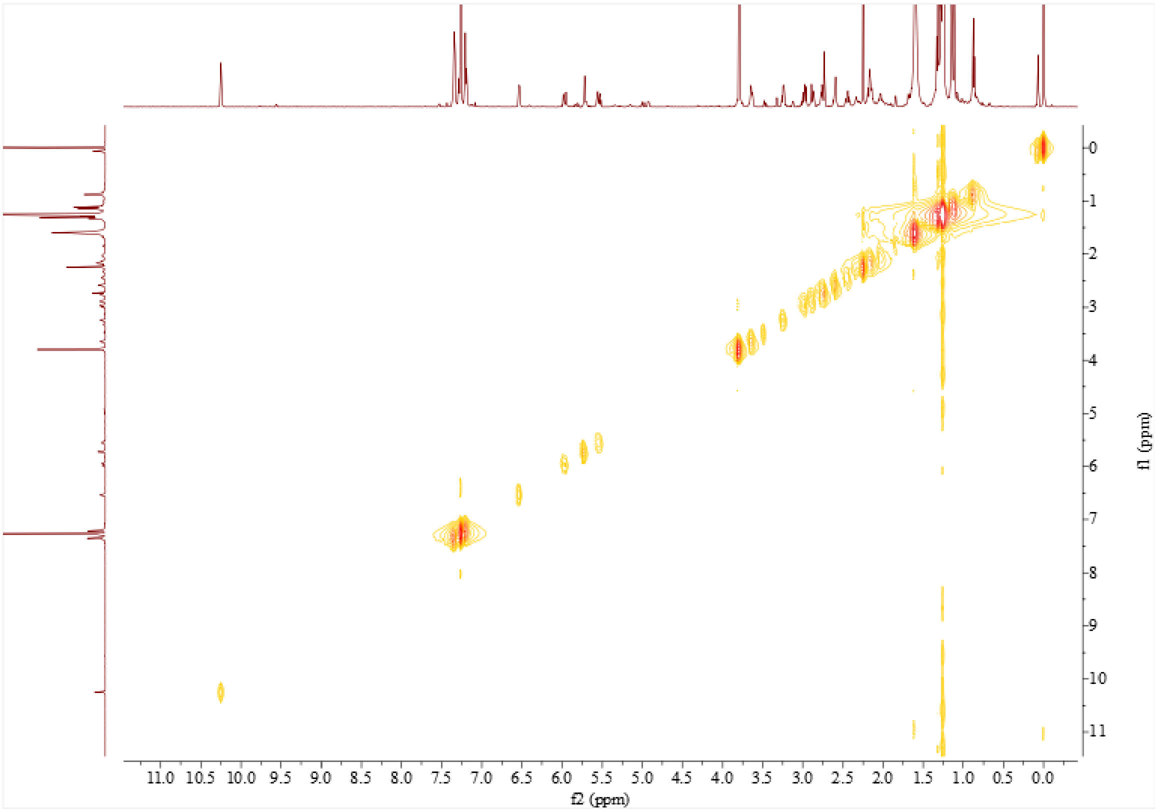

Figure S17. NOESY ($CDCl_3$) spectrum of compound **2**

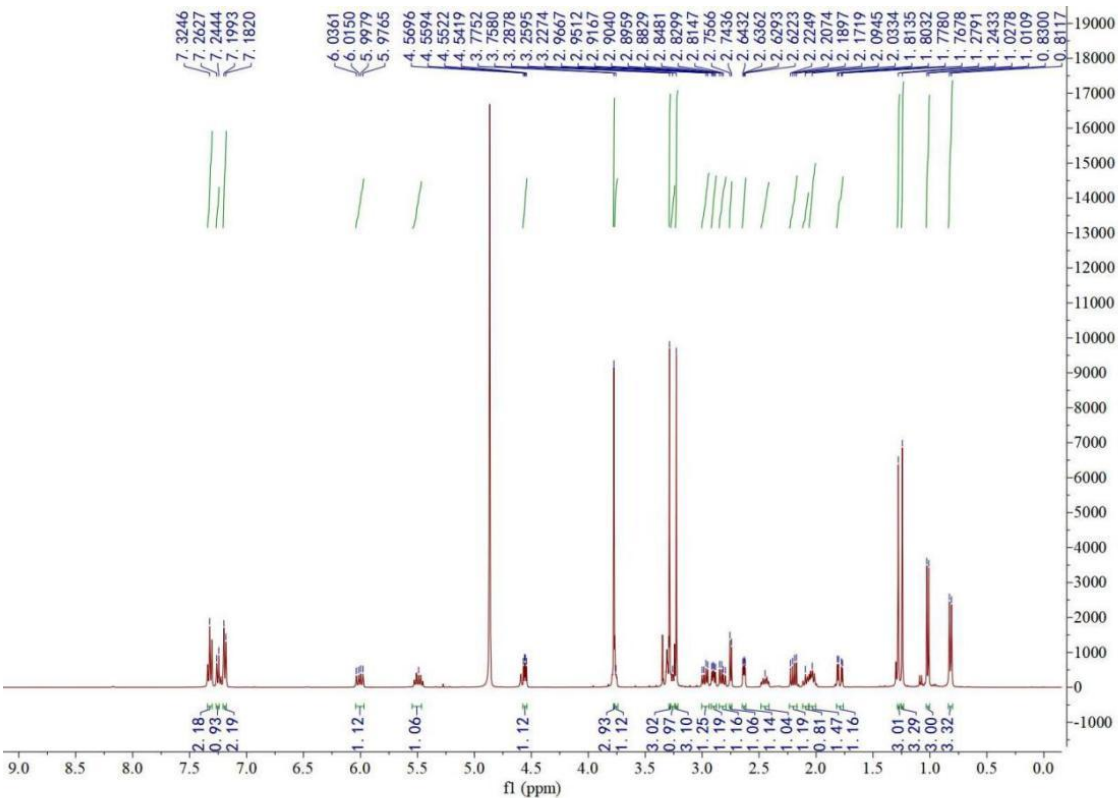

Figure S18. ^{1}H NMR (400 MHz, CD_3OD) spectrum of compound **3**

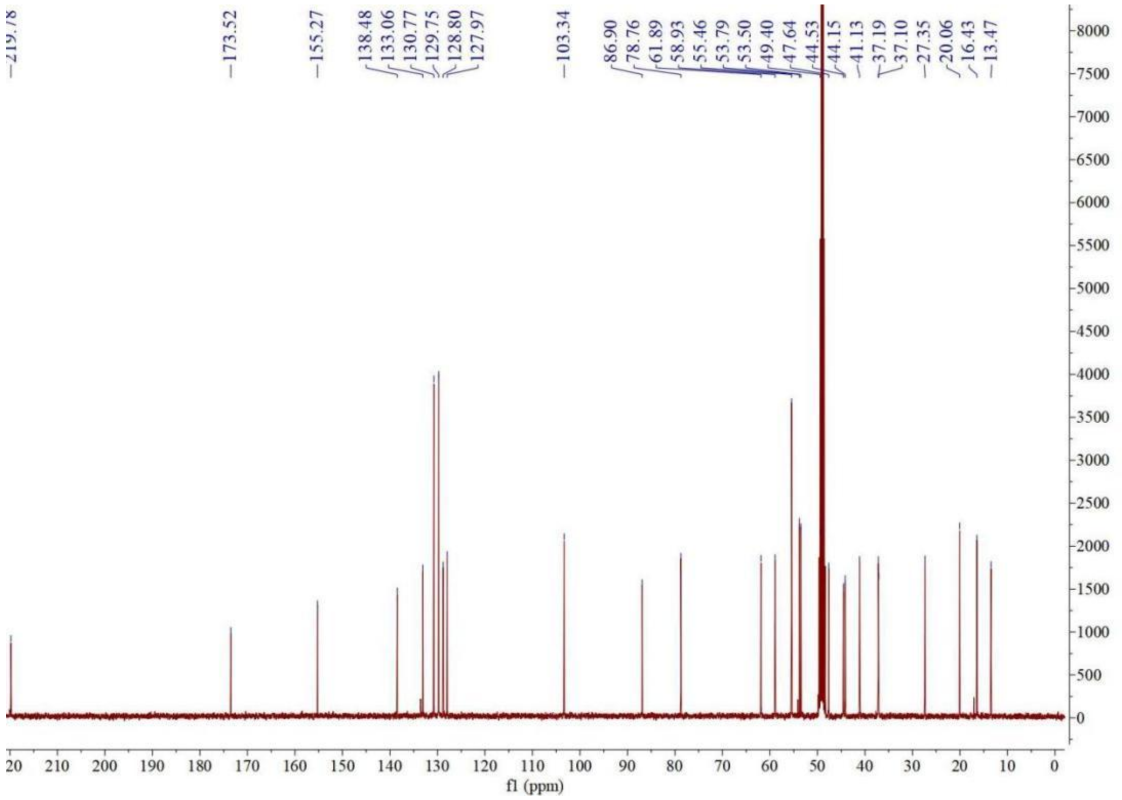

Figure S19. ^{13}C NMR (100 MHz, CD_3OD) spectrum of compound **3**