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Supporting Information

for

Pseudallenes A and B, new sulfur-containing ovalicin sesquiterpenoid derivatives with antimicrobial activity from the deep-sea cold seep sediment-derived fungus *Pseudallescheria boydii* CS-793

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Selected 1D and 2D NMR, and HRESIMS spectra of compounds 1 and 2, and 1D NMR spectra of compounds 3–5

Figure S1. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **1**;

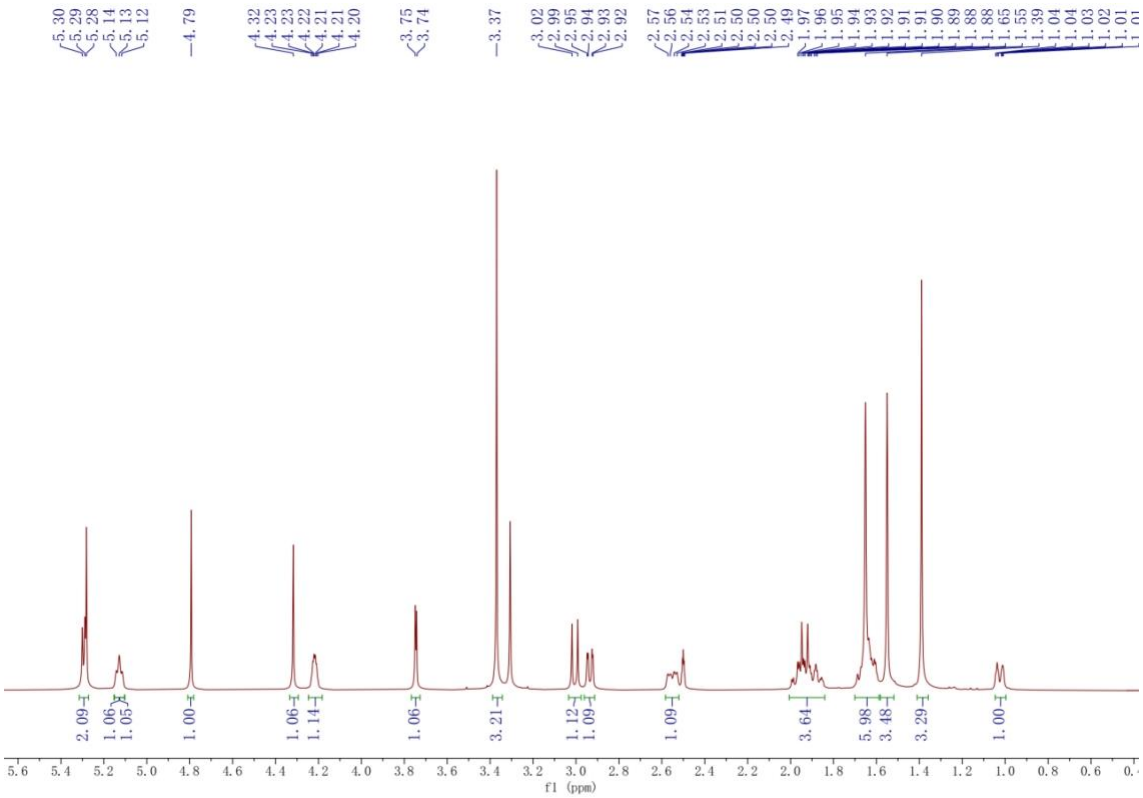

Figure S2. ^{13}C NMR (125 MHz, DMSO-d_6) and DEPT spectra of compound **1**;

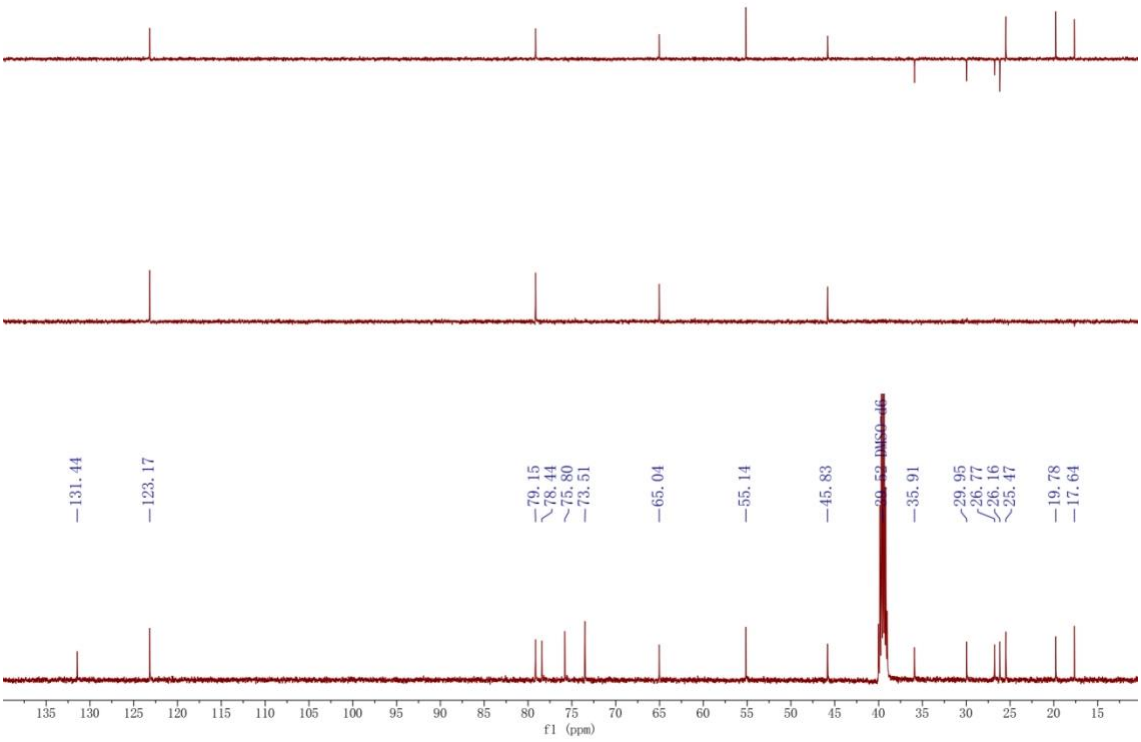

Figure S3. COSY spectrum of compound **1**;.

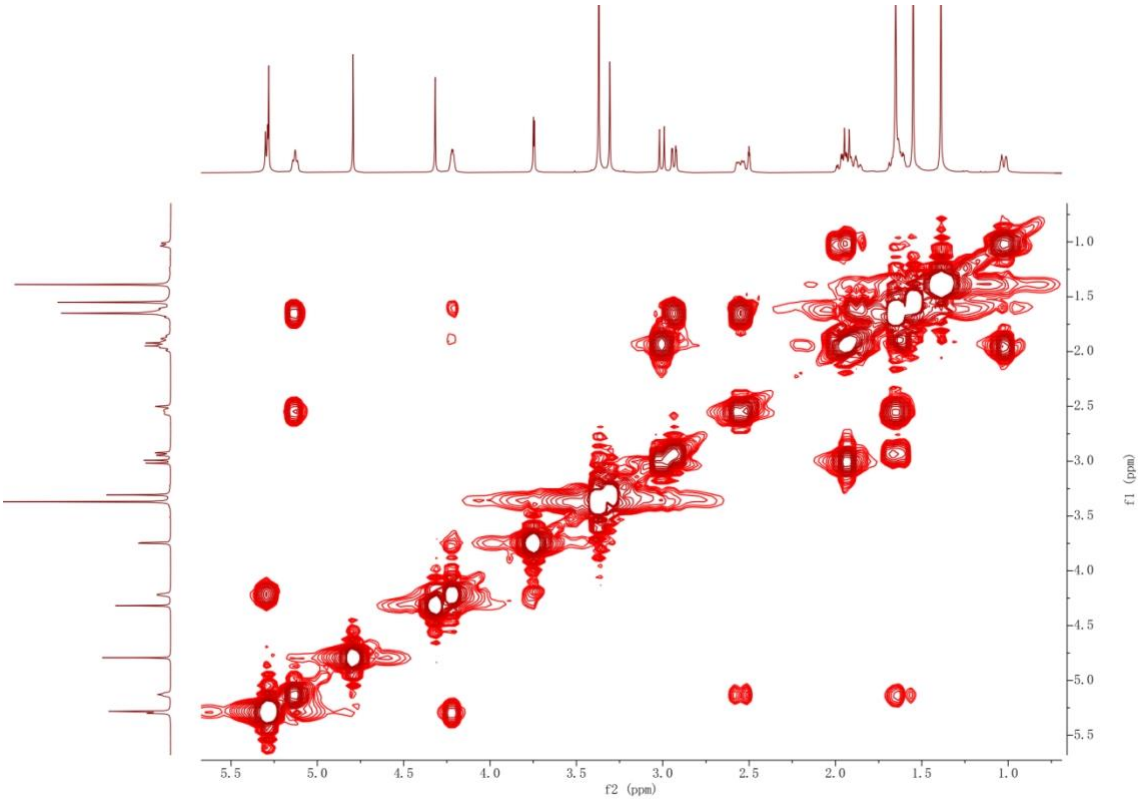

Figure S4. HSQC spectrum of compound **1**;

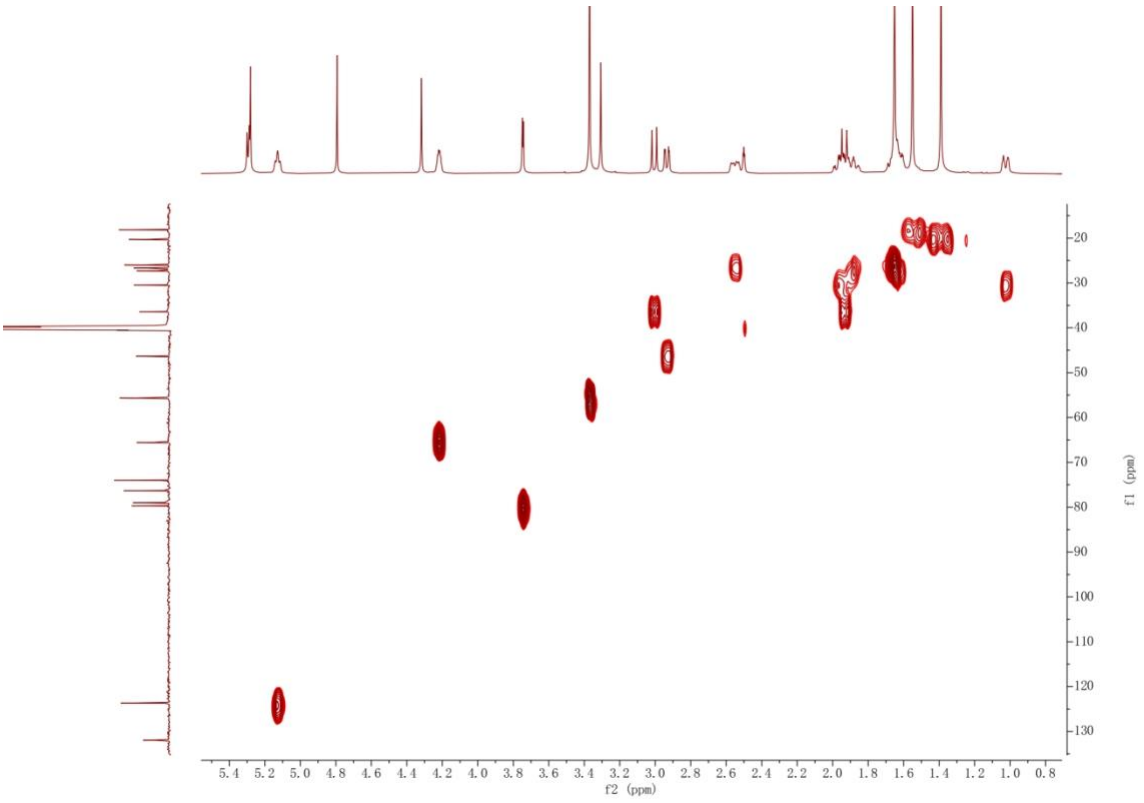

Figure S5. HMBC spectrum of compound **1**;

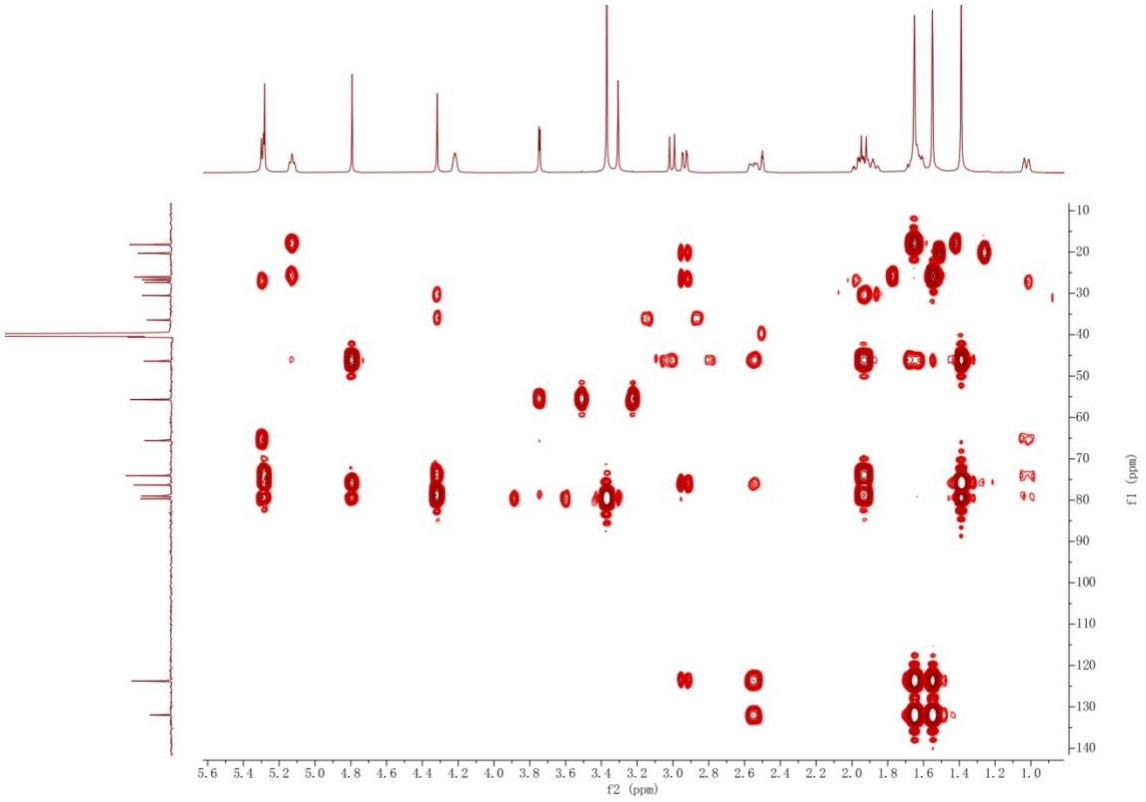

Figure S6. NOESY spectrum of compound **1**;

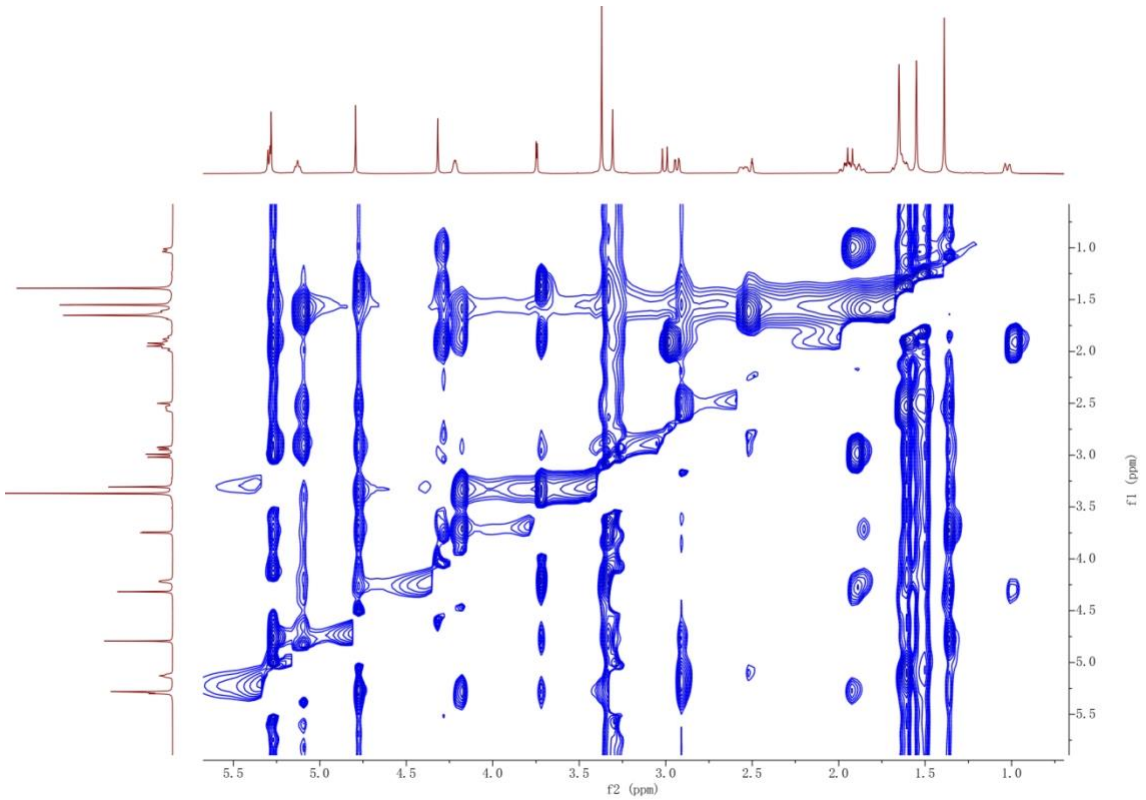

Figure S7. LC-MS spectrum of compound **1**;

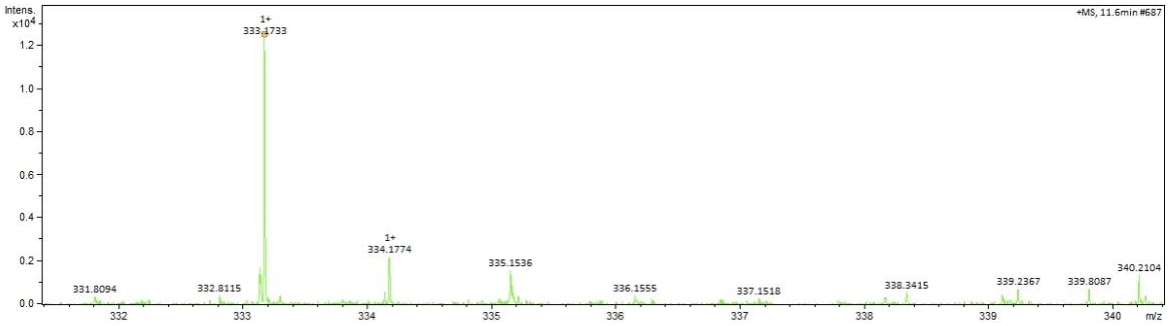

Figure S8. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **2**;

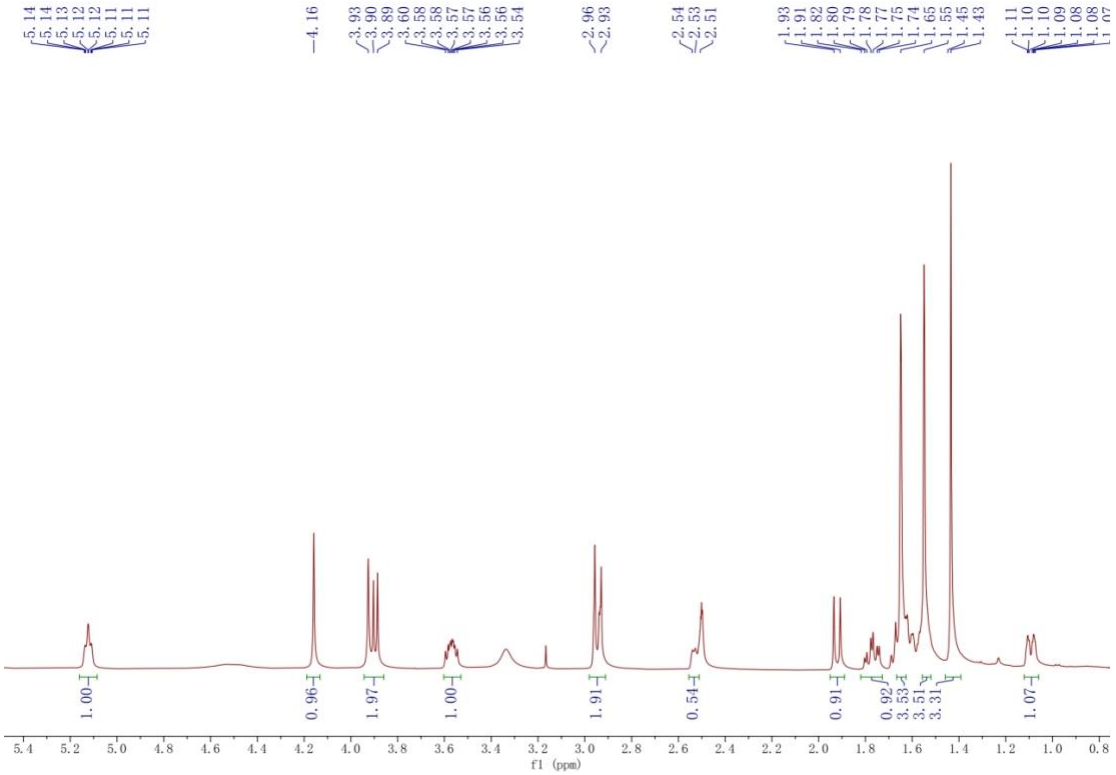

Figure S9. ^{13}C NMR (125 MHz, DMSO-d_6) and DEPT spectra of compound **2**;

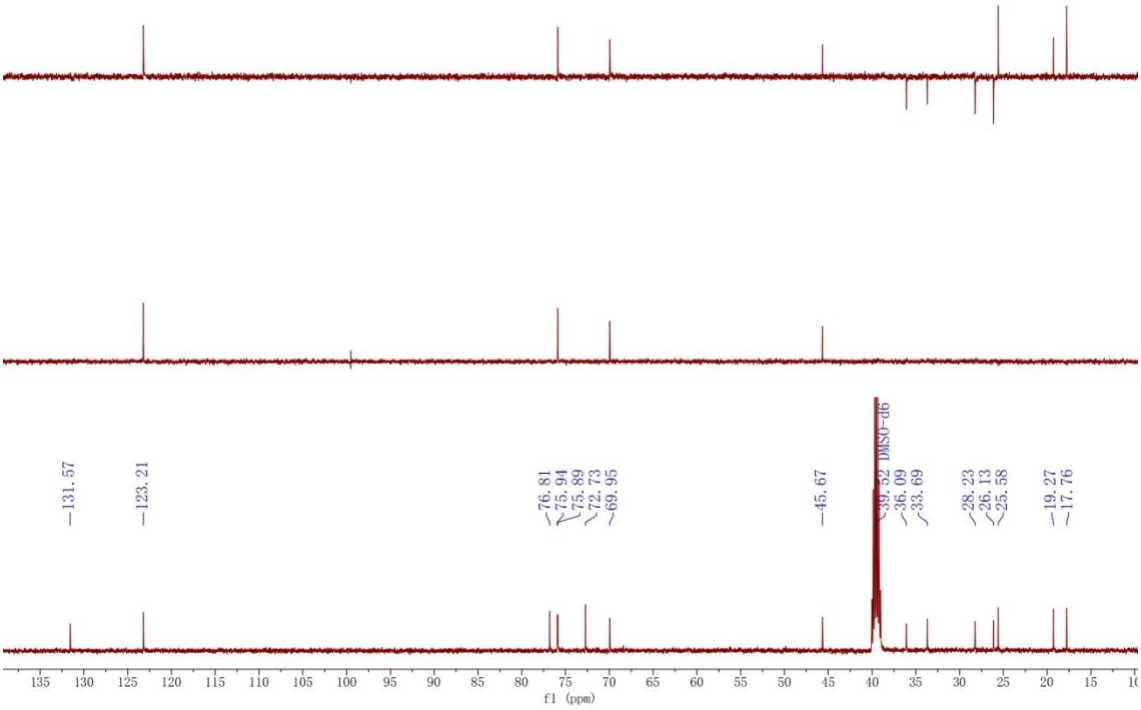

Figure S10. COSY spectrum of compound **2**;.

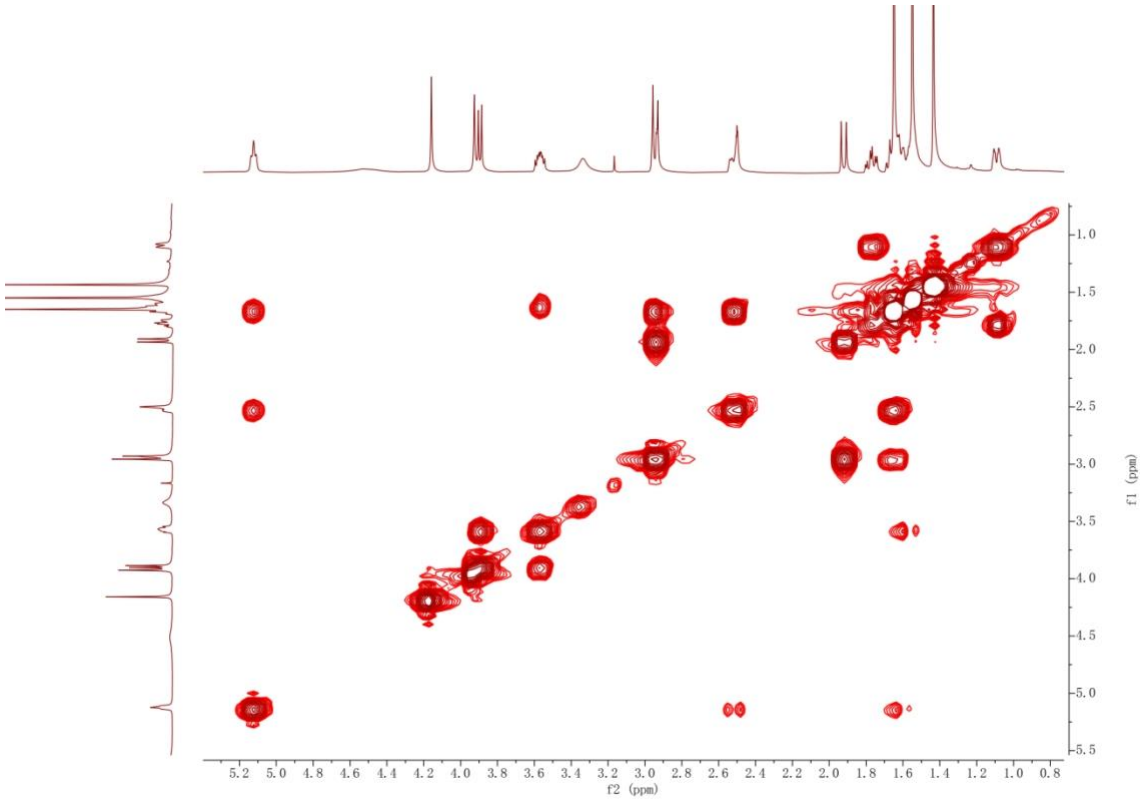

Figure S11. HSQC spectrum of compound **2**;

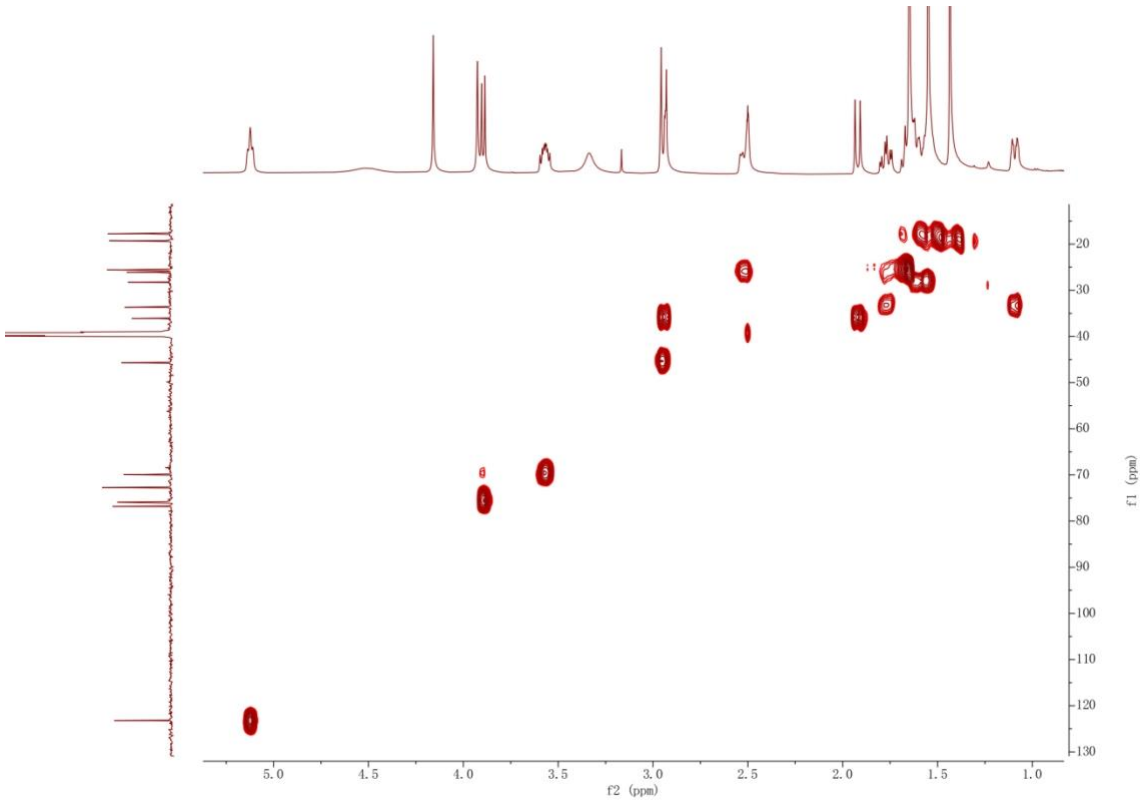

Figure S12. HMBC spectrum of compound **2**;

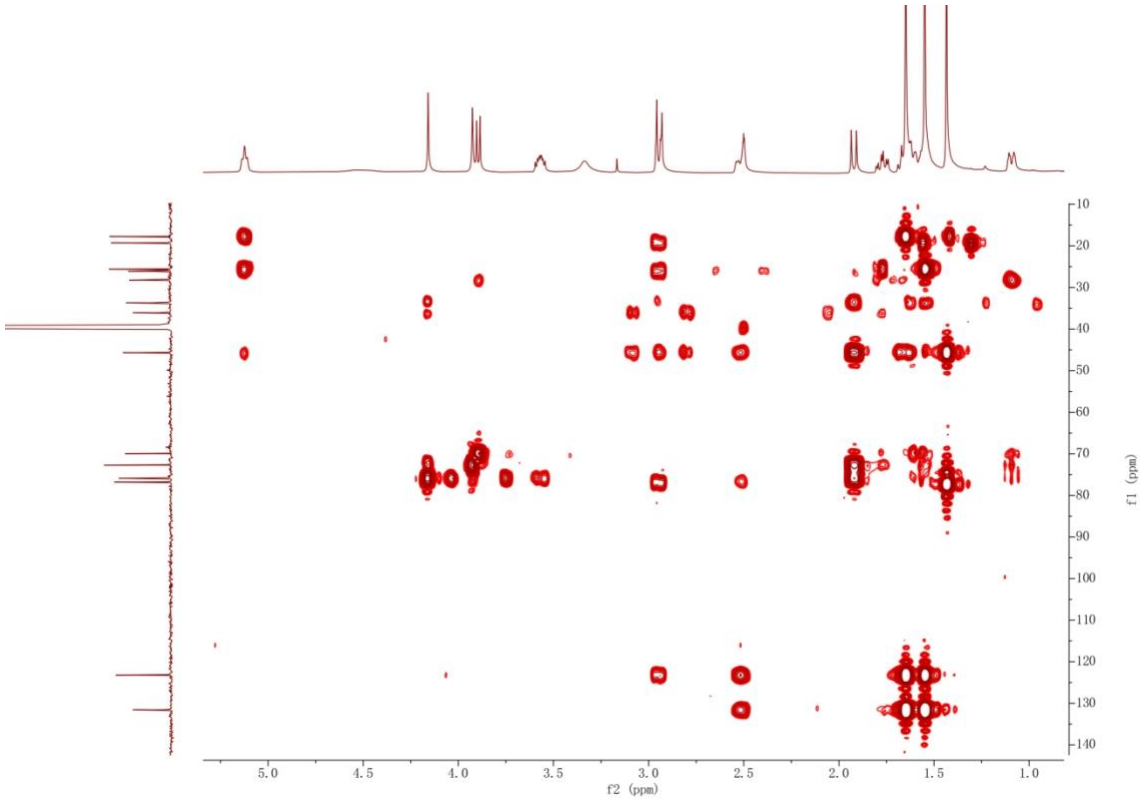

Figure S13. NOESY spectrum of compound **2**;

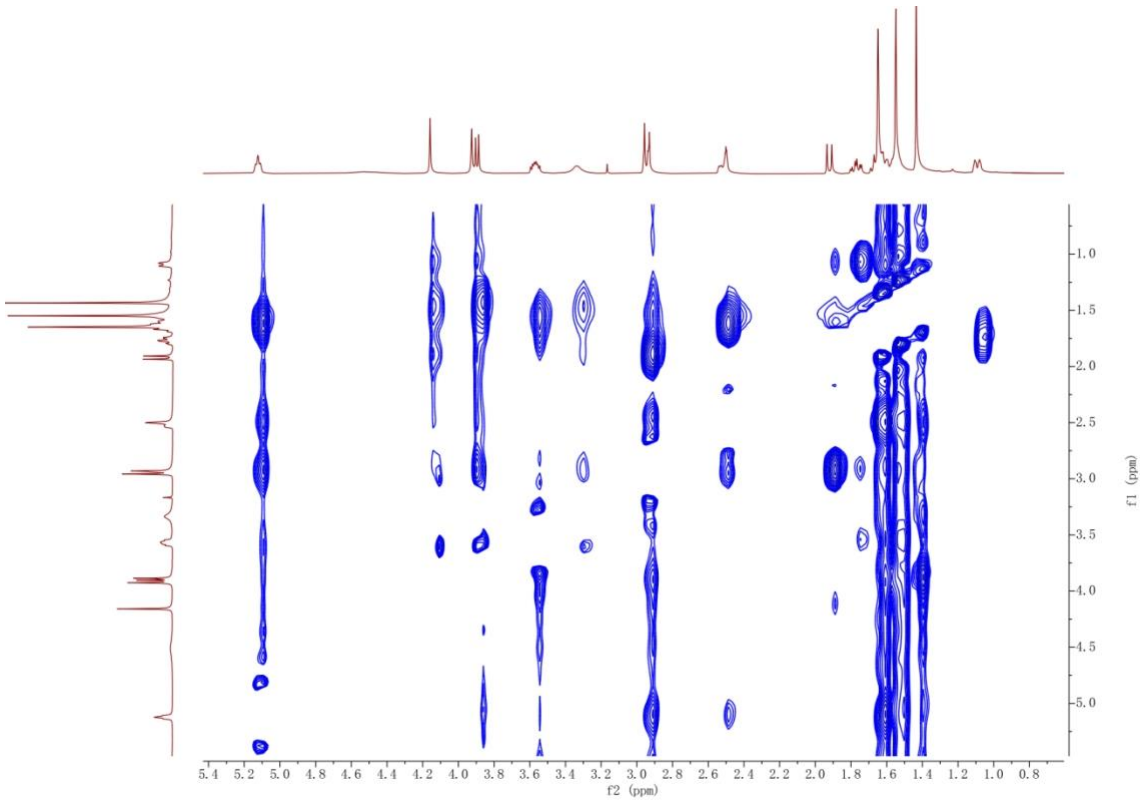

Figure S14. LC-MS spectrum of compound **2**;

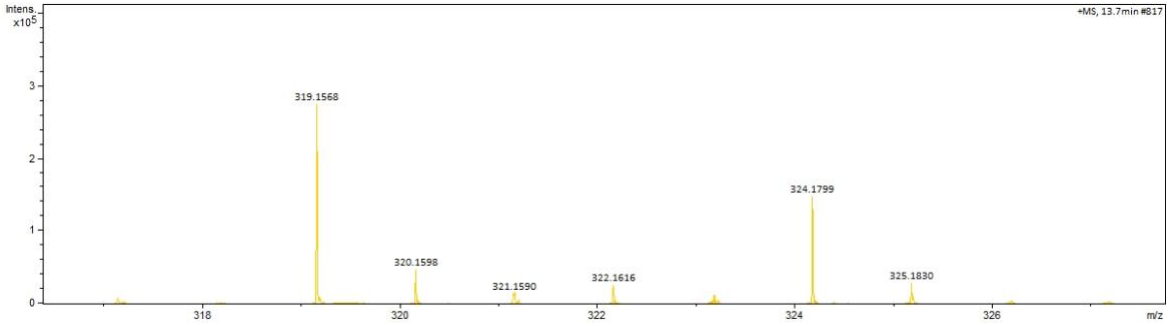

Figure S15. ^{1}H NMR (500 MHz, $CDCl_3$) spectrum of compound **3**;

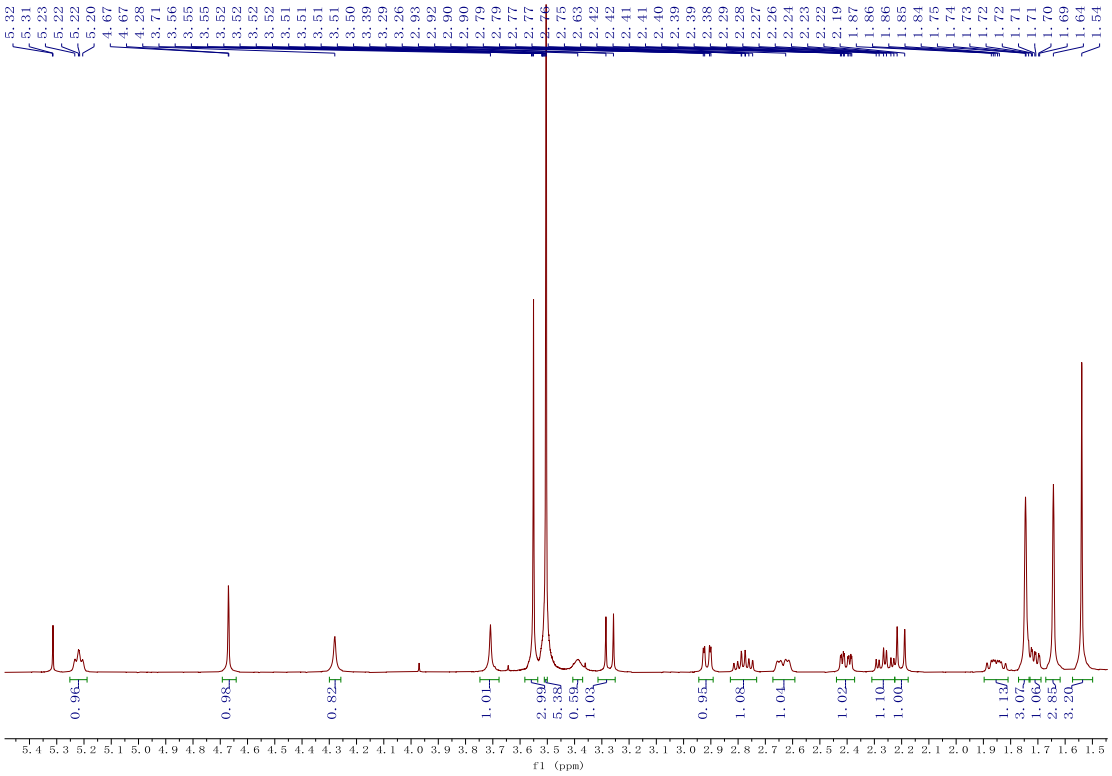

Figure S16. ^{13}C NMR (125 MHz, $CDCl_3$) and DEPT spectra of compound **3**;

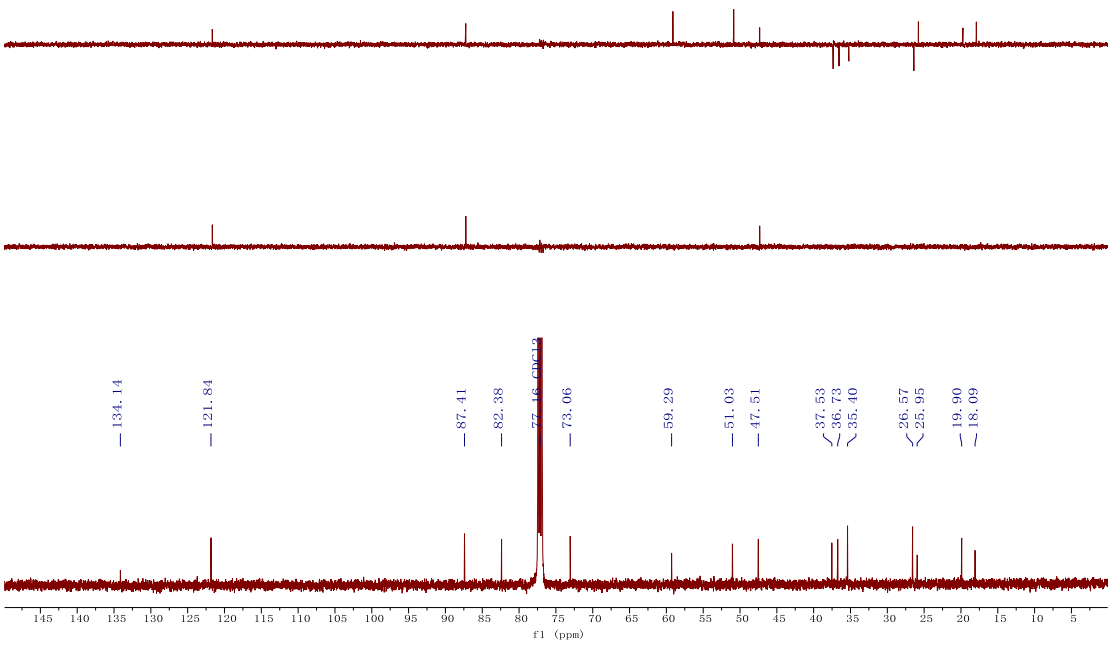

Figure S17. COSY spectrum of compound **3**;

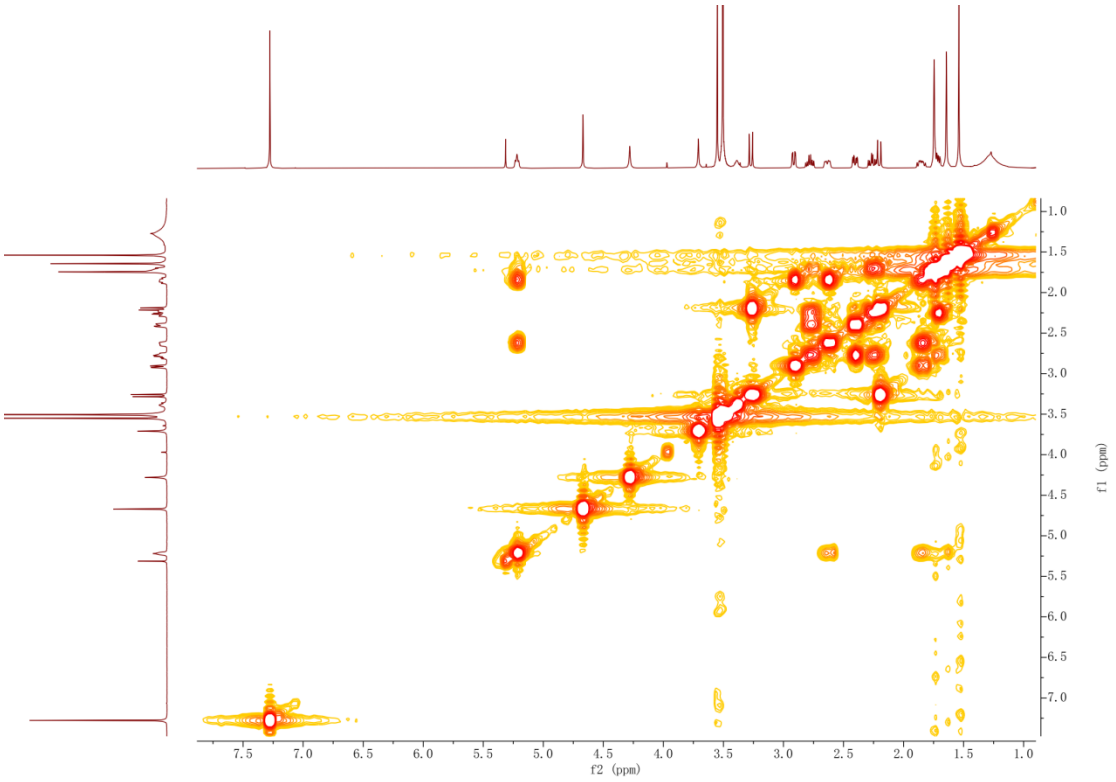

Figure S18. HSQC spectrum of compound **3**;

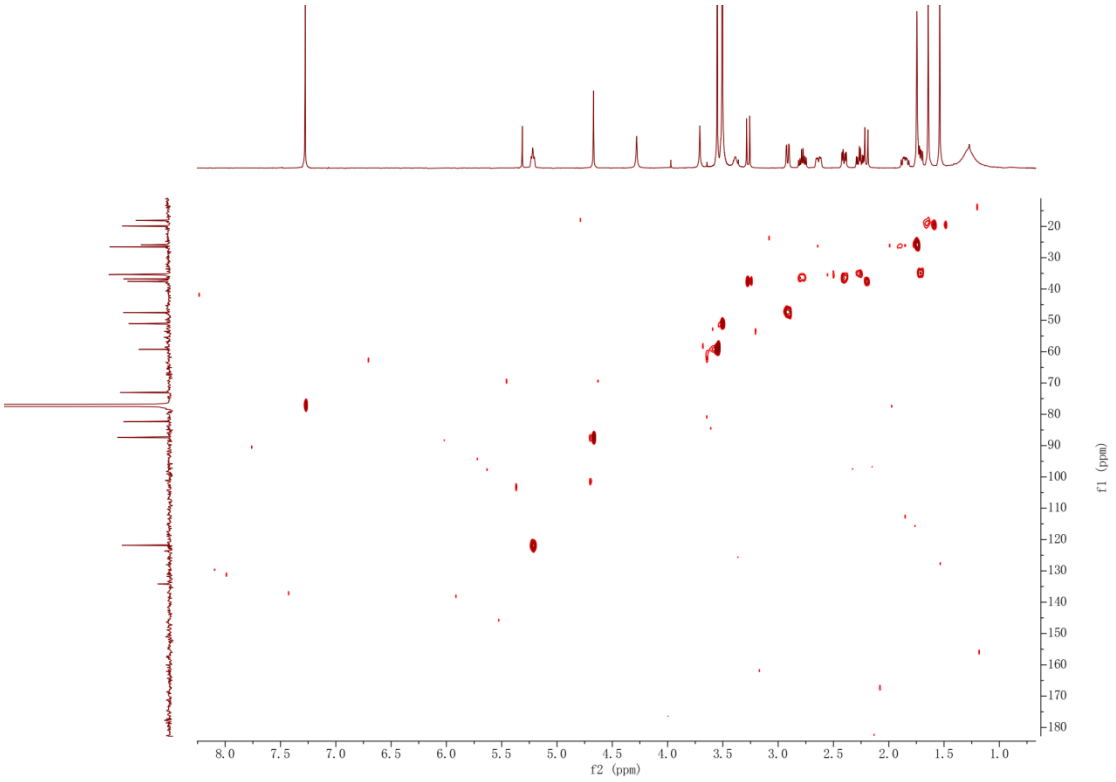

Figure S19. HMBC spectrum of compound **3**;

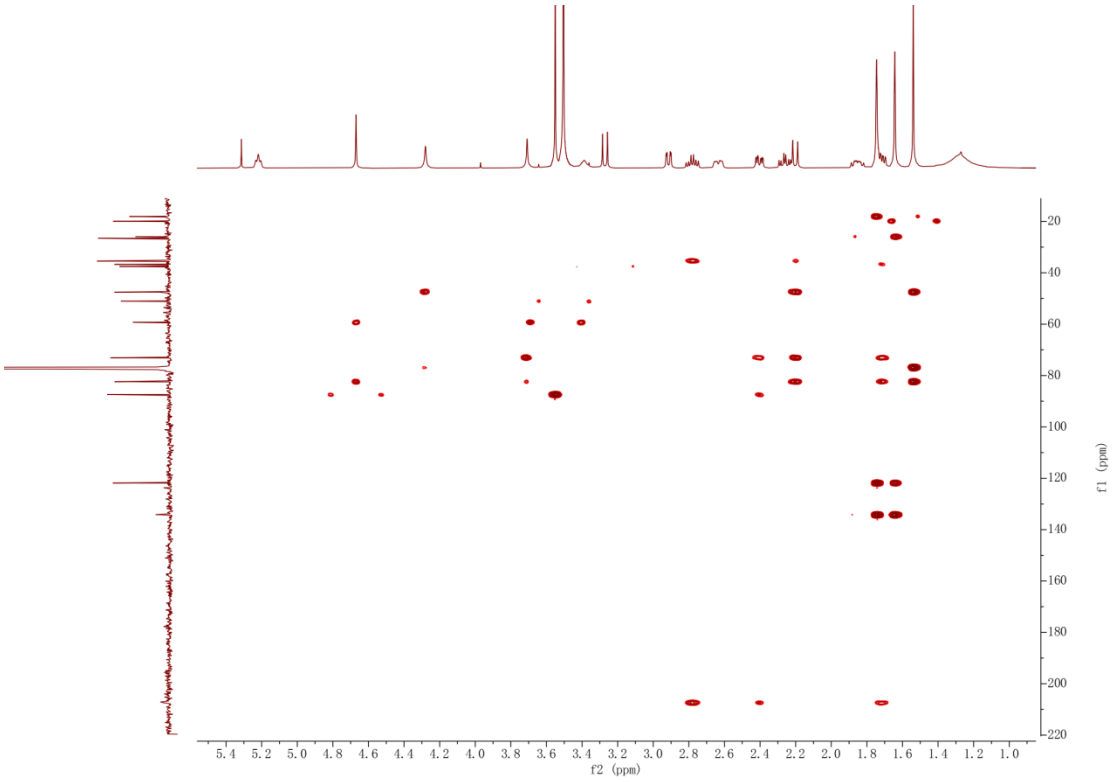

Figure S20. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **4**;

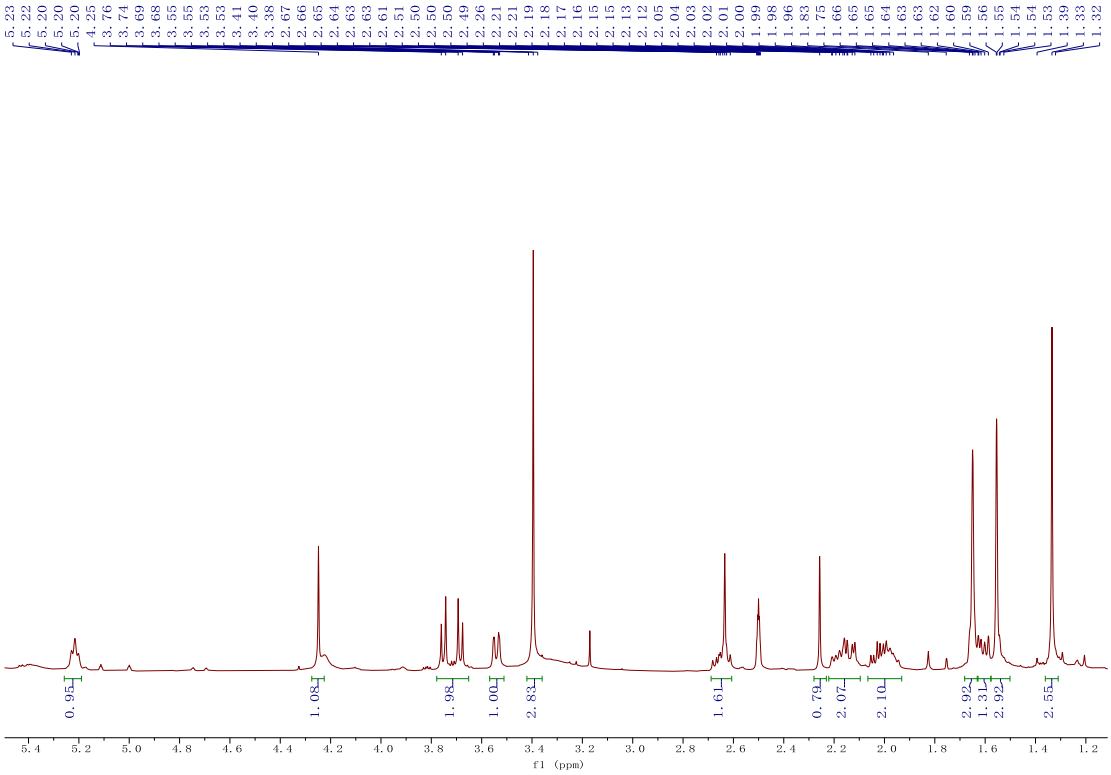

Figure S21. ^{13}C NMR (125 MHz, DMSO-d_6) and DEPT spectra of compound **4**;

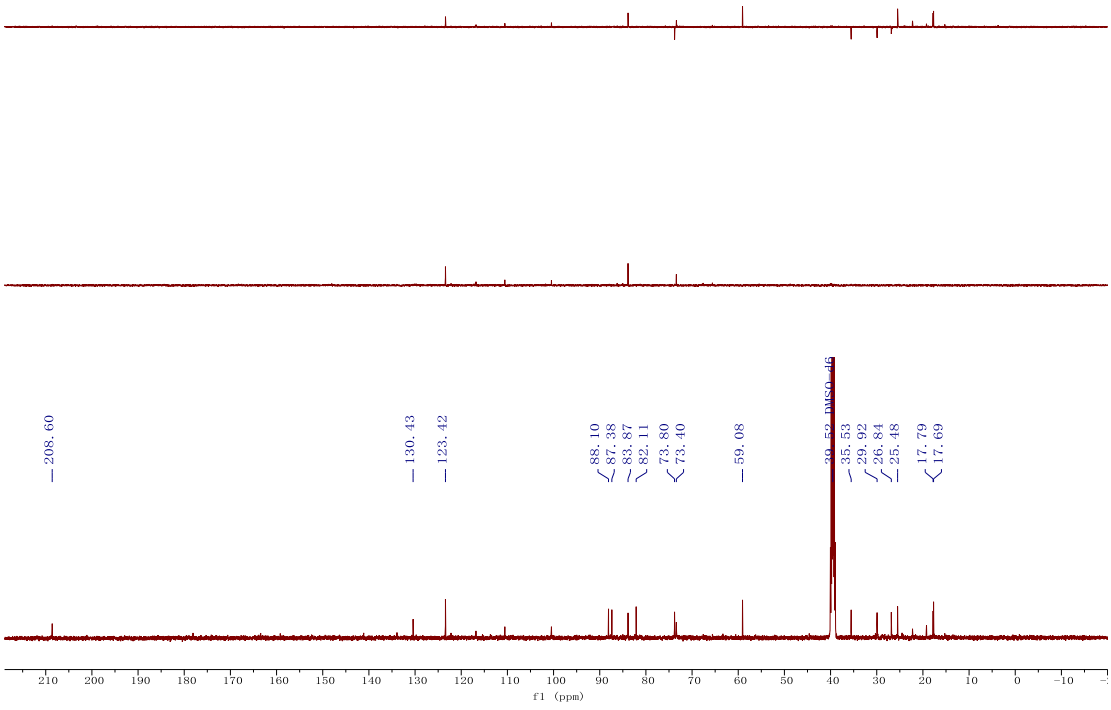

Figure S22. ^{1}H NMR (500 MHz, DMSO-d_6) spectrum of compound **5**;

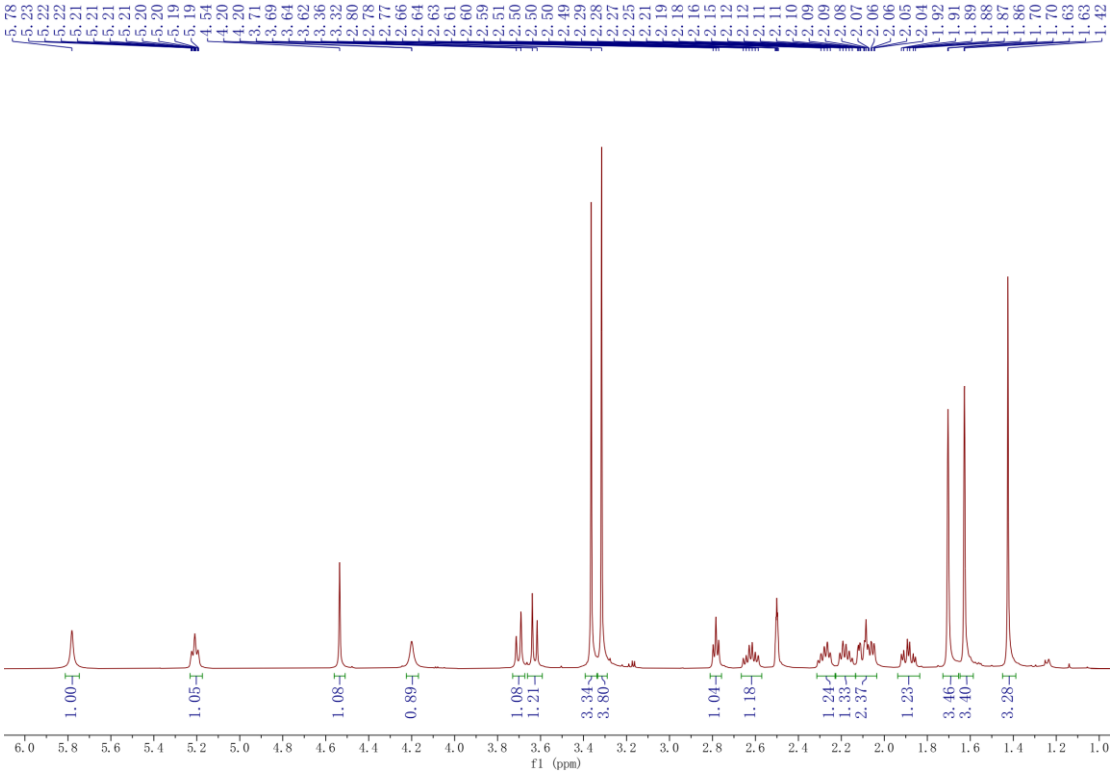

Figure S23. ^{13}C NMR (125 MHz, DMSO-d_6) and DEPT spectra of compound **5**.

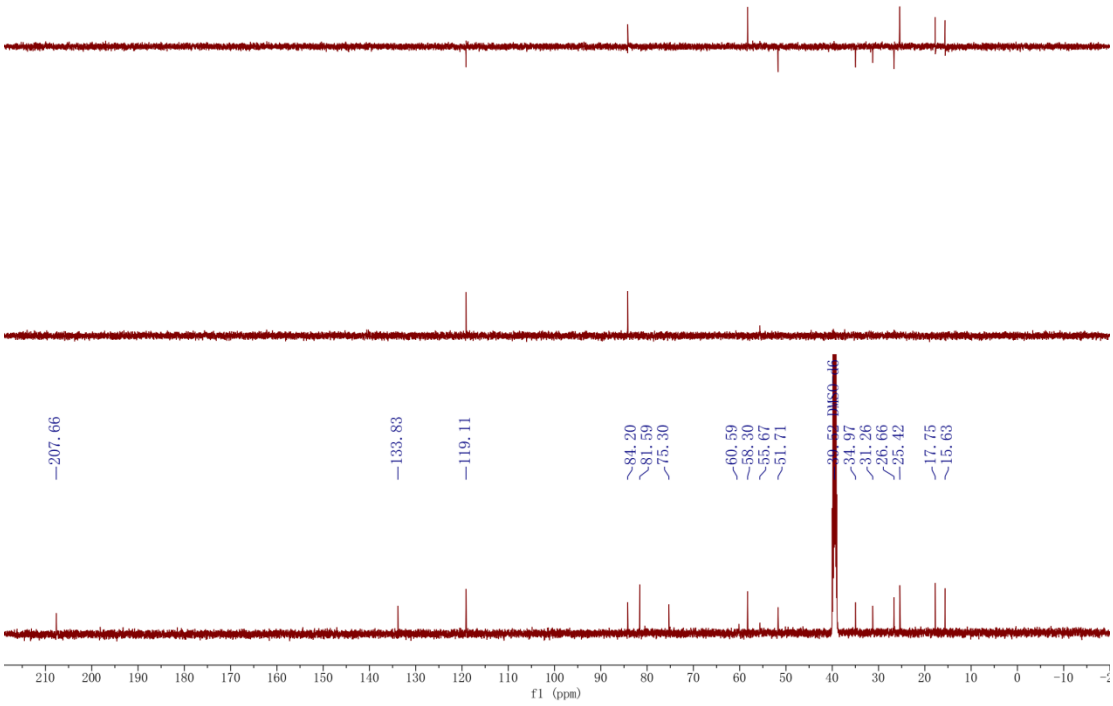

Table S1. Crystal data and structure refinement for compounds **1–3**.

Identification code	Compound **1**	Compound **2**	Compound **3**
Empirical formula	C_{96} H_{166} O_{30} S_6	C_{30} H_{52} O_{10} S_2	C_{16} H_{26} O_5 S
Formular weight	1992.64	636.83	330.43
Temperature	173(2) K	173(2) K	173(2) K
Wavelength	1.54178 A	1.54178 A	1.54178 A
Crytal system, space group	Orthorhombic, P2(1)2(1)2(1)	Triclinic, P1	Hexagonal, P6(1)
Unit cell dimensions	a = 15.0176(3) A alpha = 90 deg. b = 24.2644(4) A beta = 90 deg. c = 29.3542(5) A gamma = 90 deg.	a = 6.50160(10) A alpha = 85.4270(10) deg. b = 7.7295(2) A beta = 81.7990(10) deg. c = 17.5958(4) A gamma = 65.1510(10) deg.	a = 13.99630(10) A alpha = 90 deg. b = 13.99630(10) A beta = 90 deg c = 30.1665(6) A gamma = 120 deg.
Volume	10696.5(3) A^3	794.00(3) A^3	5117.78(13) A^3
Z, Calculated density	4, 1.237 Mg/m^3	1, 1.332 Mg/m^3	12, 1.287 Mg/m^3
Absorption coeffcient	1.783 mm^-1	1.979 mm^-1	1.863 mm^-1
F(000)	4312	344	2136
Crystal size	0.180 x 0.160 x 0.120 mm	0.180 x 0.150 x 0.120 mm	0.160 x 0.140 x 0.120 mm
Theta range for data collection	2.362 to 68.182 deg.	2.538 to 66.525 deg.	3.646 to 68.266 deg
Limiting indices	-17<=h<=17, -21<=k<=29, -33<=l<=35	-7<=h<=7, -9<=k<=9, -20<=l<=20	-16<=h<=16, -16<=k<=16, -36<=l<=36
Reflections collected/unique	67427 / 19396 [R(int) = 0.0550]	18694 / 5468 [R(int) = 0.0381]	65189 / 6250 [R(int) = 0.0627]
Data/restraints/ parameters	19396 / 0 / 1252	5468 / 3 / 415	6250 / 1 / 442
Goodness-of-fit on F^2	1.000	1.033	0.947
Final R indices [I>2sigma(I)]	R1 = 0.0512, wR2 = 0.1339	R1 = 0.0287, wR2 = 0.0714	R1 = 0.0317, wR2 = 0.0848

R indices (all data)	R1 = 0.0605, wR2 = 0.1430	R1 = 0.0322, wR2 = 0.0736	R1 = 0.0361, wR2 = 0.0883
Absolute structure parameter	0.019(6)	0.048(7)	0.024(6)
Extinction coefficient	n/a	n/a	n/a
Largest diff. Peak and hole	0.792 and -0.378 e.A^-3	0.344 and -0.160 e.A^-3	0.175 and -0.189 e.A^-3

Table S2. ^{1}H, ^{13}C, COSY, HMBC Spectroscopic Data for Compound **1** in DMSO-d_6.

no.	**1**		**COSY**	**HMBC**
	δ_C[a]	δ_H[b], mult (*J* in Hz)		
1	78.4, C			
2	79.2, CH	3.75 d (3.1)	H-3	C-8
3	65.0, CH	4.22 dq (6.1, 3.1)	H-2, H-4, 3-OH	
4	26.8, CH_2	*α* 1.61 overlap	H-3, H-5	C-2, C-6
		β 1.87 overlap		
5	30.0, CH_2	*α* 1.03 dt (11.6, 2.7)	H-4	C-1, C-3, C-6
		β 1.97 overlap		
6	73.5, C			
7	75.8, C			
8	45.8, CH	2.93 dd (11.5, 2.4)	H-9	C-10
9	26.2, CH_2	*α* 1.68 overlap	H-8, H-10	C-11
		β 2.55 dd (15.2, 6.3)		
10	123.2, CH	5.14 t (6.9)	H-9	C-12, C-13
11	131.4, C			
12	25.5, CH_3	1.65 s		C-10, C-13
13	17.6, CH_3	1.55 s		C-10, C-12
14	35.9, CH_2	*α* 1.93 d (13.7)		C-1, C-5, C-6, C-8
		β 3.01 d (13.7)		
15	19.8, CH_3	1.39 s		C-1, C-7, C-8
1-OH		5.28 s		C-2, C-6
2-OCH_3/OH	55.1, CH_3	3.37 s		C-2
3-OH		5.29 d (6.0)		C-2, C-4
6-OH		4.32 s		C-5, C-6, C-14
7-OH		4.79 s		C-1, C-7, C-8

Table S3. ^{1}H, ^{13}C, COSY, HMBC Spectroscopic Data for Compound **2** in DMSO-d_6.

no.	**2**		**COSY**	**HMBC**
	δ_C[a]	δ_H[b], mult (*J* in Hz)		
1	76.8, C			
2	75.9, CH	3.89 d (8.7)	H-3	C-4
3	70.0, CH	3.57 ddd (11.1, 8.7, 5.5)	H-2, H-4,	C-1
4	28.2, CH_2	α 1.56 overlap	H-3, H-5	C-6
		β 1.60 overlap		
5	33.7, CH_2	α 1.09 ddd (13.2, 4.3, 2.7)	H-4	C-3, C-6
		β 1.77 td (13.2, 4.8)		
6	72.7, C			
7	76.8, C			
8	45.7, CH	2.94 overlap	H-9	C-7
9	26.1, CH_2	α 1.67 overlap	H-8, H-10	C-11
		β 2.53 overlap		
10	123.2, CH	5.12 t (6.4)	H-9	C-8, C-12, C-13
11	131.6, C			
12	25.6, CH_3	1.65 s		C-10, C-13
13	17.8, CH_3	1.55 s		C-10, C-12
14	36.1, CH_2	α 1.92 d (13.6)		C-1, C-6, C-8
		β 2.95 overlap		
15	19.3, CH_3	1.43 s		C-1, C-8
1-OH		3.93 s		C-6
2-OCH_3/OH		4.50 brs		
3-OH		5.61 brs		
6-OH		4.16 s		C-1, C-5, C-6, C-14
7-OH		3.34		

Table S4. ^{1}H, ^{13}C, COSY, HMBC Spectroscopic Data for Compound **3** in $CDCl_3$.

no.	**3**		**COSY**	**HMBC**
	δ_C[a]	δ_H[b], mult (*J* in Hz)		
1	82.4, C			
2	87.4, CH	4.67, s		
3	207.7, C			
4	36.7, CH_2	*α* 2.78 td (13.7, 6.9)	H-5	C-2, C-3, C-6
		β 2.40 ddd (13.7, 5.4, 1.7)		
5	35.4, CH_2	*α* 1.72 ddd (13.5, 6.9, 1.7)	H-4	C-1, C-3, C-6
		β 2.26 td (13.5, 5.4)		
6	73.1, C			
7	76.8, C			
8	47.5, CH	2.91 dd (11.5, 2.5)	H-9	
9	26.6, CH_2	*α* 1.85 ddd (14.8, 11.5, 7.9)	H-8, H-10	C-11
		β 2.63 dd (15.5, 6.3)		
10	121.8, CH	5.22 t (7.3)	H-9	
11	134.1, C			
12	26.0, CH_3	1.75 s		C-10, C-11, C-13
13	18.1, CH_3	1.64 s,		C-10, C-11, C-12
14	37.5, CH_2	*α* 2.20 d (13.9)		C-1, C-6, C-8
		β 3.27 d (13.9)		
15	19.9, CH_3	1.54 s		C-7, C-8
1-OH				
2-OCH_3/OH	59.3, CH_3	3.55 s		C-2
6-OH		3.71 s		C-1, C-6
7-OH		4.28 s		C-7, C-8