

Supplementary Materials

Talaroterpenoids A–F: Six New Seco-Terpenoids from the Marine-Derived Fungus *Talaromyces aurantiacus*

Zi-Hong Peng ^{1,†}, Hui Jia ^{1,†}, Yan-Liang Luo ¹, Li-Jun Zhang ¹, Jia-Tong Zhou ¹, Yuan-Han Xie ¹, Li-Jun Wang ², Jiang-Ke Qin ¹, Jun Li ¹, Guo-Hai Zhang ^{1,*}, Rui-Yun Yang ^{1,*} and Wei-Feng Xu ^{1,*}

¹ State Key Laboratory for Chemistry and Molecular Engineering of Medicinal Resources, Collaborative Innovation Center for Guangxi Ethnic Medicine, School of Chemistry and Pharmaceutical Sciences, Guangxi Normal University, Guilin 541004, China; pengzihong000311@163.com (Z.-H.P.); jiahui18878391665@163.com (H.J.); ly12010927@163.com (Y.-L.L.); ajun840618@mailbox.gxnu.edu.cn (L.-J.Z.); zjt990123@163.com (J.-T.Z.); xieyuanhan0330@163.com (Y.-H.X.); jiangke@sina.com (J.-K.Q.); lijun9593@gxnu.edu.cn (J.L.)

² School of Design, Guangxi Normal University, Guilin 541004, China; gxsd307@126.com

* Correspondence: xuweifeng_u@163.com (W.-F.X.); yang_rui_yun@163.com (R.-Y.Y.); zgh1207@gxnu.edu.cn (G.-H.Z.)

† These authors contributed equally to this work.

List of supporting information

Table S1. The NMR data (400 MHz for ^1H and 100 MHz for ^{13}C in $\text{DMSO-}d_6$) of **1** and **2**

Table S2. The NMR data (400 MHz for ^1H and 100 MHz for ^{13}C in CDCl_3) of **3** and **5**

Table S3. The NMR data (400 MHz for ^1H and 100 MHz for ^{13}C in $\text{DMSO-}d_6$) of **6** and **9**

Table S4. X-ray crystallographic data of compound **5**

Table S5. X-ray crystallographic data of compound **6**

Figure S1. The cell viability of BV-2 cells treated with **1–11**

Figure S2. The nitric oxide inhibition of BV-2 cells treated with **1–11**

Figure S3. ^1H NMR (400 MHz, Pyridine- d_5) spectrum of **1**

Figure S4. ^{13}C NMR (100 MHz, Pyridine- d_5) spectrum of **1**

Figure S5. HMQC (Pyridine- d_5) spectrum of **1**

Figure S6. $^1\text{H-}^1\text{H}$ COSY (Pyridine- d_5) spectrum of **1**

Figure S7. HMBC (Pyridine- d_5) spectrum of **1**

Figure S8. J -HMBC (Pyridine- d_5) spectrum of **1**

Figure S9. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of **1**

Figure S10. ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of **1**

Figure S11. HMQC ($\text{DMSO-}d_6$) spectrum of **1**

Figure S12. $^1\text{H-}^1\text{H}$ COSY ($\text{DMSO-}d_6$) spectrum of **1**

Figure S13. HMBC ($\text{DMSO-}d_6$) spectrum of **1**

Figure S14. HRESIMS spectrum of **1**

Figure S15. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of **2**

Figure S16. ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of **2**

Figure S17. HMQC ($\text{DMSO-}d_6$) spectrum of **2**

Figure S18. $^1\text{H-}^1\text{H}$ COSY ($\text{DMSO-}d_6$) spectrum of **2**

Figure S19. HMBC ($\text{DMSO-}d_6$) spectrum of **2**

Figure S20. HRESIMS spectrum of **2**

Figure S21. ^1H NMR (400 MHz, CDCl_3) spectrum of **3**

Figure S22. ^{13}C NMR (100 MHz, CDCl_3) spectrum of **3**

Figure S23. HMQC (CDCl_3) spectrum of **3**

Figure S24. $^1\text{H-}^1\text{H}$ COSY (CDCl_3) spectrum of **3**

Figure S25. HMBC (CDCl_3) spectrum of **3**

Figure S26. NOESY (CDCl_3) spectrum of **3**

Figure S27. HRESIMS spectrum of **3**

Figure S28. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of **6**

Figure S29. ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of **6**

Figure S30. HMQC ($\text{DMSO-}d_6$) spectrum of **6**

Figure S31. $^1\text{H-}^1\text{H}$ COSY ($\text{DMSO-}d_6$) spectrum of **6**

Figure S32. HMBC ($\text{DMSO-}d_6$) spectrum of **6**

Figure S33. NOESY ($\text{DMSO-}d_6$) spectrum of **6**

Figure S34. HRESIMS spectrum of **6**

Figure S35. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of **7**

Figure S36. ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of **7**

Figure S37. ^1H NMR (400 MHz, CDCl_3) spectrum of **7**

Figure S38. ^{13}C NMR (100 MHz, CDCl_3) spectrum of **7**
Figure S39. HMQC (CDCl_3) spectrum of **7**
Figure S40. ^1H - ^1H COSY (CDCl_3) spectrum of **7**
Figure S41. HMBC (CDCl_3) spectrum of **7**
Figure S42. NOESY (CDCl_3) spectrum of **7**
Figure S43. HRESIMS spectrum of **7**
Figure S44. ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of **8**
Figure S45. ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of **8**
Figure S46. HMQC ($\text{DMSO}-d_6$) spectrum of **8**
Figure S47. ^1H - ^1H COSY ($\text{DMSO}-d_6$) spectrum of **8**
Figure S48. HMBC ($\text{DMSO}-d_6$) spectrum of **8**
Figure S49. NOESY ($\text{DMSO}-d_6$) spectrum of **8**
Figure S50. HRESIMS spectrum of **8**
Figure S51. Map of location sites of sea sediment sample used in this study

Table S1. The NMR data (400 MHz for ^1H and 100 MHz for ^{13}C in $\text{DMSO-}d_6$) of **1** and **2**

No.	1		2	
	δ_{C}	δ_{H} (J in Hz)	δ_{C}	δ_{H} (J in Hz)
1	32.3	2.77, overlapped 2.48, overlapped	32.3	2.77, overlapped 2.48, overlapped
2	171.8		171.7	
4	37.4	2.77, overlapped	37.5	2.77, overlapped
5	50.5	2.90, d (2.8)	50.6	2.89, d (3.0)
6	76.9	4.72, t (2.8)	76.6	4.74, t (3.0)
7	40.4	2.64, overlapped 2.51, dd (15.2, 2.4)	39.7	2.64, overlapped 2.54, overlapped
8	142.5		142.4	
9	48.1	2.67, overlapped	48.0	2.67, overlapped
10	49.4		48.8	
11	25.0	1.70, m 1.40, m	24.8	1.70, m 1.40, m
12	38.8	2.25, m 1.96, m	38.8	2.25, m 1.96, m
13	158.5		158.4	
14	116.5	5.54, s	116.5	5.54, s
15	167.6		167.5	
16	18.4	2.05, s	18.3	2.05, s
17	115.4	5.03, s 4.88, s	115.3	5.03, s 4.88, s
18	176.2		174.9	
19	12.8	0.94, d (7.2)	13.0	0.96, d (7.2)
20	177.5		177.2	
21			52.2	3.62, s

Table S2. The NMR data (400 MHz for ^1H and 100 MHz for ^{13}C in CDCl_3) of **3** and **5**

No.	3		5	
	δ_{C}	δ_{H} (J in Hz)	δ_{C}	δ_{H} (J in Hz)
1	37.4	3.12, d (15.0) 2.66, d (15.0)	38.0	2.37, d (15.0) 2.54, d (15.0)
2	170.9		172.5	
4	37.8	2.86, q (7.4)	38.6	2.94, q (7.4)
5	51.7	2.46, dd (11.4, 7.4)	52.1	2.69, dd (11.4, 7.4)
6	77.3	4.93, td (11.4, 4.8)	77.3	4.23, td (11.4, 4.8)
7	42.1	2.23, t (11.8) 3.03, dd (11.8, 4.8)	43.1	2.24, t (11.8) 2.98, dd (11.8, 4.8)
8	141.0		141.6	
9	48.0	2.35, m	47.6	2.30, m
10	50.7		41.9	
11	23.5	1.75, m 1.42, m	22.9	1.77, m 1.62, m
12	39.8	2.35, m 2.07, m	40.0	2.30, m 2.12, m
13	162.1		163.2	
14	115.4	5.67, s	116.5	5.52, s
15	171.2		177.5	
16	19.4	2.18, s	19.9	2.18, s
17	114.0	5.18, s 4.83, s	115.0	5.25, s 4.85, s
18	178.5		179.4	
19	10.1	1.06, d (7.4)	12.5	1.26, d (7.4)
20	171.7		18.4	0.87, s
21	52.2	3.66, s		
22	52.3	3.71, s		

Table S3. The NMR data (400 MHz for ^1H and 100 MHz for ^{13}C in $\text{DMSO-}d_6$) of **6** and **9**

NO.	6		9	
	δ_{C}	δ_{H} , (J in Hz)	δ_{C}	δ_{H} , (J in Hz)
1	74.7	4.16, d (4.2)	75.0	4.16, d (4.2)
2	35.2	2.56, m	29.0	2.42, m
		2.68, dd (15.8, 4.2)		2.70, dd (15.8, 4.2)
3	170.0		170.1	
4	79.6		80.0	
5	50.5	1.57, d (8.2)	50.5	1.67, m
6	25.2	1.52, m	22.5	1.69, m
7	69.2	3.69, m	72.9	4.76, dt, (10.8, 5.2)
8	49.1	2.19, m	49.3	2.53, m
9	86.9		86.6	
10	49.5		49.9	
11	48.8	1.86, d (14.2)	49.1	1.88, d (14.2)
		2.41, d (14.2)		2.55, d (14.2)
12	10.3	0.87, d (7.4)	10.8	0.91, d (7.4)
13	65.5	4.45, d (13.0)	65.6	4.45, d (13.0)
		4.52, d (13.0)		4.65, d (13.0)
14	21.9	0.98, s	21.3	1.00, s
15	30.9	1.18, s	30.7	1.20, s
16			170.2	
17			21.2	2.01, s
1'	46.8		47.0	
2'	127.8		128.1	
3'	107.3		107.7	
4'	78.2	5.04, d (8.4)	78.6	5.04, d (8.4)
5'	41.3	2.83, dd (8.4, 6.2)	41.6	2.84, dd (8.4, 6.2)
6'	38.9	2.07, m	39.3	2.05, m
7'	18.4	0.74, s	18.6	0.75, s
8'	21.9	1.62, s	22.2	1.62, s
9'	175.1		175.3	
10'	11.8	1.04, d (7.4)	12.2	1.05, d (7.4)

Table S4. X-ray crystallographic data of compound **5**

Identification code	5
Empirical formula	C ₁₉ H ₂₃ O ₆
Formula weight	347.37
Temperature [K]	297.0 (2)
Crystal system	monoclinic
Space group (number)	C2y
<i>a</i> [Å]	28.1075(12)
<i>b</i> [Å]	6.8034(2)
<i>c</i> [Å]	9.8758(4)
α [°]	90
β [°]	96.987(4)
γ [°]	90
Volume [Å ³]	1874.49(12)
<i>Z</i>	4
ρ_{calc} [gcm ⁻³]	1.231
μ [mm ⁻¹]	0.757
<i>F</i> (000)	742.7
Radiation	CuK α (λ =1.54184)
2 θ range [°]	6.34 to 154.17
Index ranges	$-34 \leq h \leq 34$, $-5 \leq k \leq 8$, $-12 \leq l \leq 12$
Reflections collected	6689
Independent reflections	2694 [$R_{\text{int}} = 0.0292$, $R_{\text{sigma}} = 0.0257$]
Completeness to $\theta = 67.684^\circ$	99.9 %
Data / Restraints / Parameters	2694/1/239
Goodness-of-fit on F^2	1.049
Final <i>R</i> indexes [$I \geq 2\sigma(I)$]	$R_1 = 0.0418$, $wR_2 = 0.1231$
Final <i>R</i> indexes [all data]	$R_1 = 0.0484$, $wR_2 = 0.1297$
Flack parameter	0.12(17)

Table S5. X-ray crystallographic data of compound **6**

Identification code	6
Empirical formula	C ₂₅ H ₃₄ O ₉
Formula weight	478.22
Temperature [K]	297.2(6)
Crystal system	orthorhombic
Space group (number)	<i>P</i>2₁2₁2₁
<i>a</i> [Å]	10.86785(12)
<i>b</i> [Å]	14.38306(19)
<i>c</i> [Å]	30.5354(4)
α [°]	90.0
β [°]	90.0
γ [°]	90.0
Volume [Å ³]	4773.07(11)
<i>Z</i>	4
ρ_{calc} [gcm ⁻³]	1.332
μ [mm ⁻¹]	0.84
<i>F</i> (000)	2048.0
Radiation	Cu K α (λ =1.54184)
2 θ range [°]	6.79 to 154.99
Index ranges	-6 \leq h \leq 13, -18 \leq k \leq 16, -38 \leq l \leq 23
Reflections collected	19923
Independent reflections	5177 [<i>R</i> _{int} = 0.0357, <i>R</i> _{sigma} = 0.0413]
Completeness to θ = 66.968°	99.5 %
Data / Restraints / Parameters	8666/1/628
Goodness-of-fit on <i>F</i> ²	10.6387
Final <i>R</i> indexes [<i>I</i> \geq 2 σ (<i>I</i>)]	<i>R</i> ₁ = 0.0362, w <i>R</i> ₂ = 0.0911
Final <i>R</i> indexes [all data]	<i>R</i> ₁ = 0.0439, w <i>R</i> ₂ = 0.1102
Flack X parameter	0.06(9)

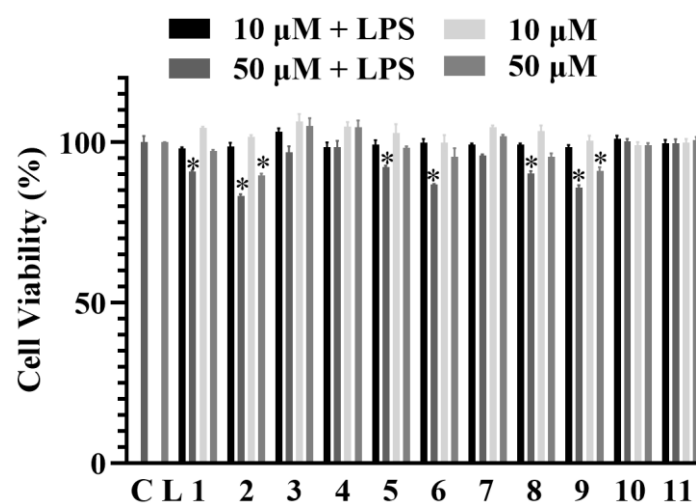


Figure S1. The cell viability of BV-2 cells treated with 1-11

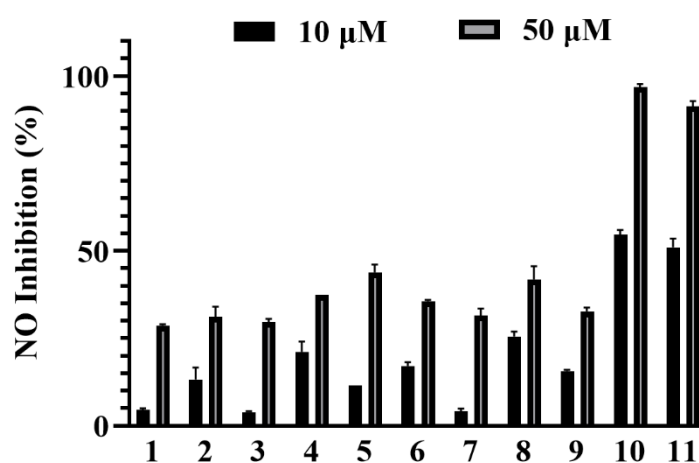


Figure S2. The nitric oxide inhibition of BV-2 cells treated with 1-11

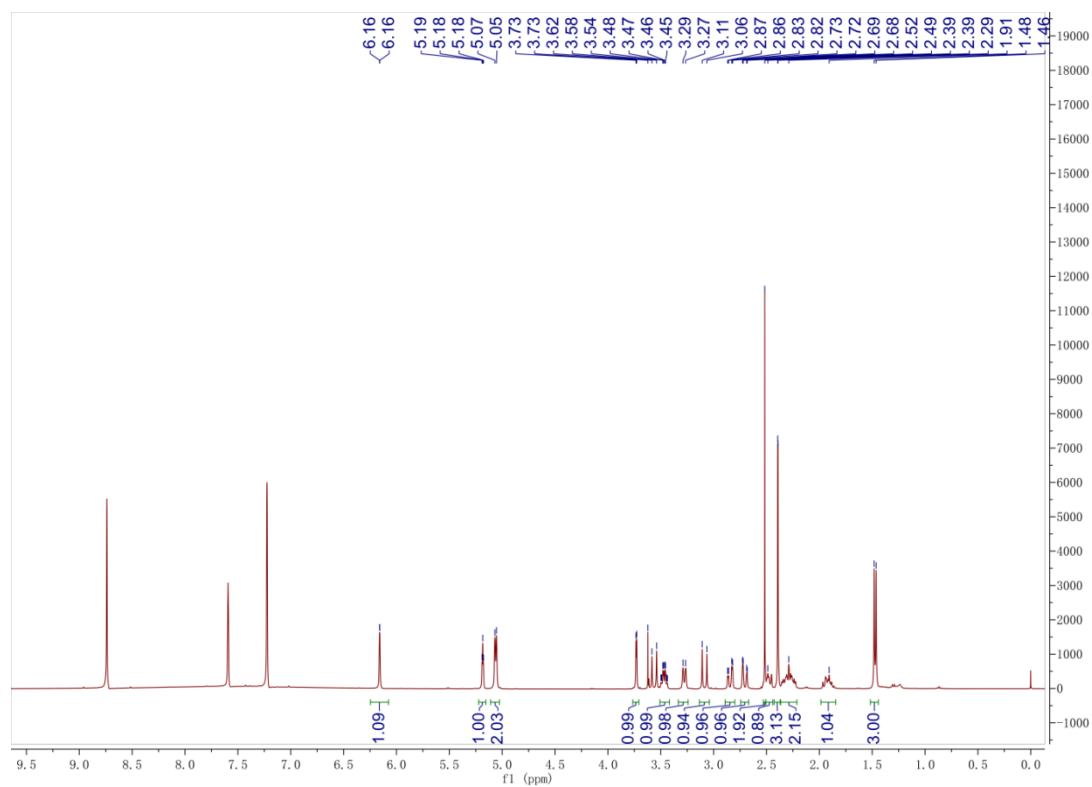


Figure S3. ^1H NMR (400 MHz, Pyridine- d_5) spectrum of **1**

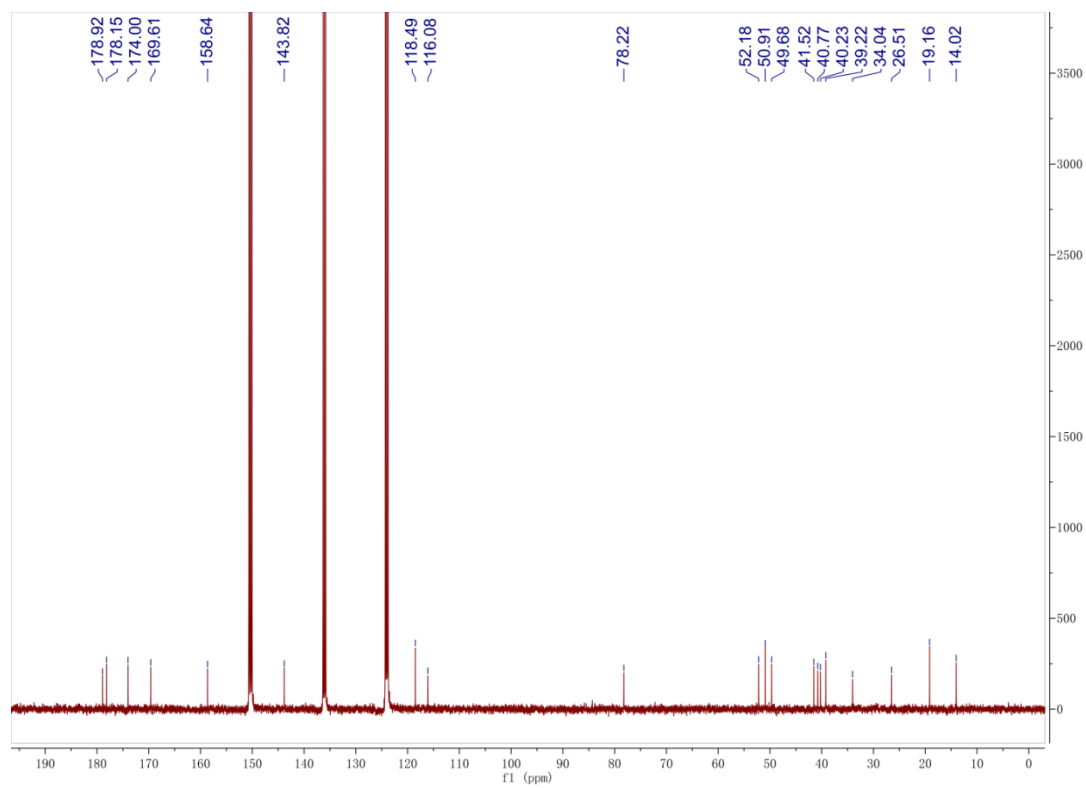


Figure S4. ^{13}C NMR (100 MHz, Pyridine- d_5) spectrum of **1**

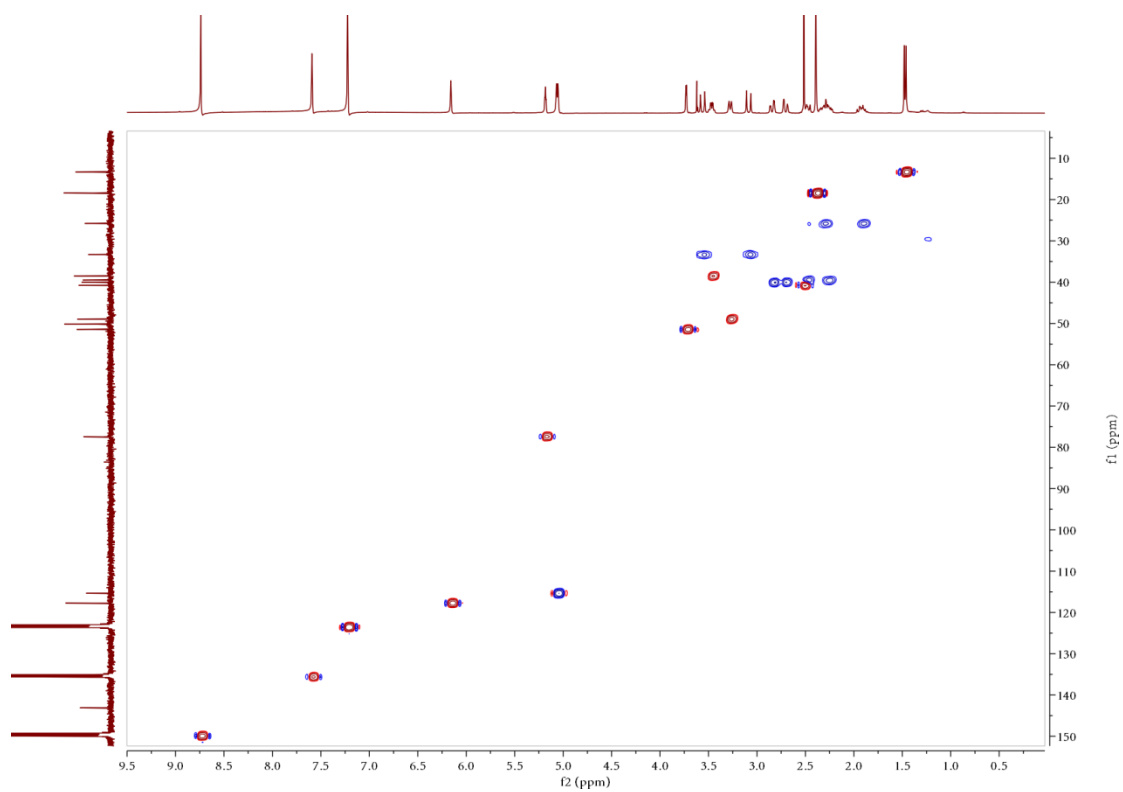


Figure S5. HMQC (Pyridine- d_5) spectrum of **1**

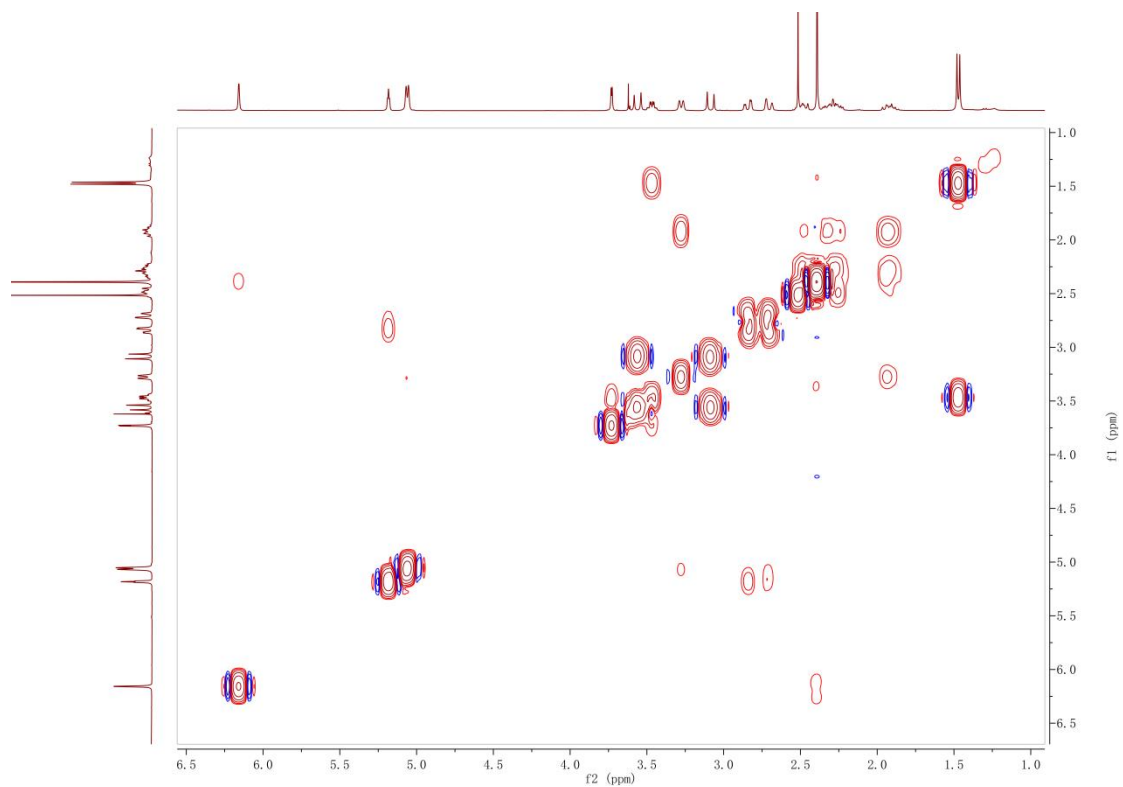


Figure S6. ^1H - ^1H COSY (Pyridine- d_5) spectrum of **1**

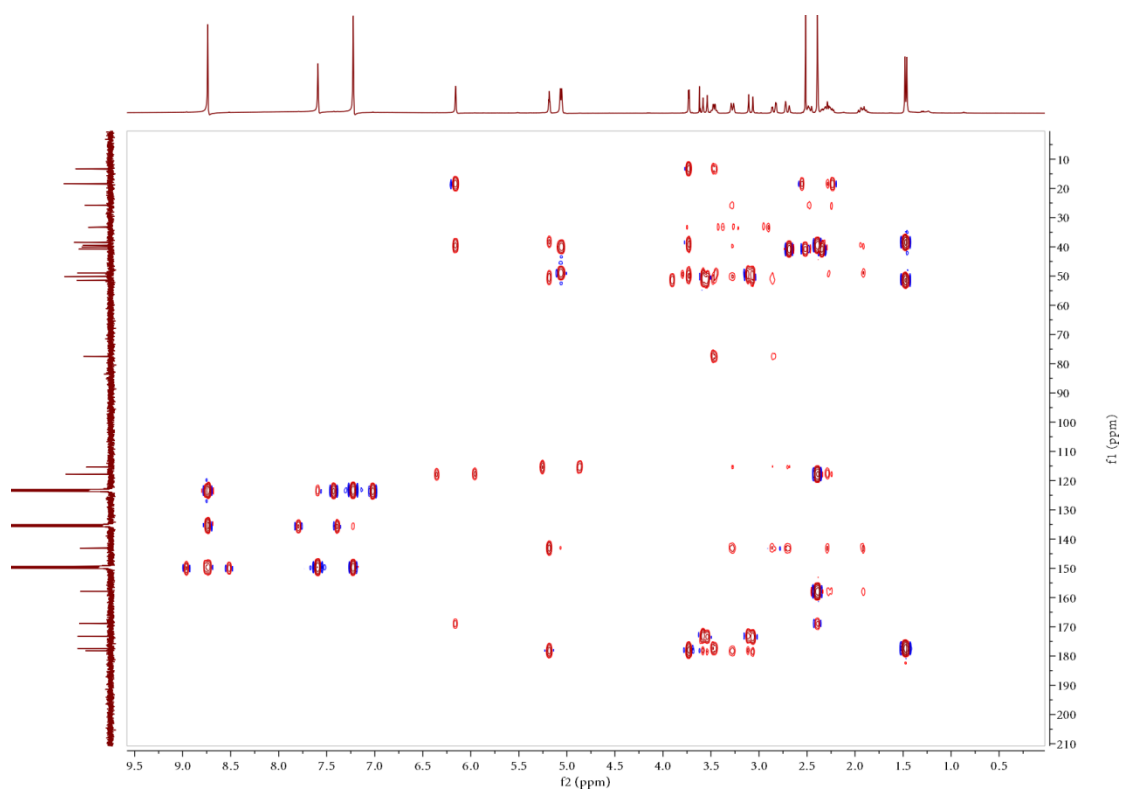


Figure S7. HMBC (Pyridine- d_5) spectrum of **1**

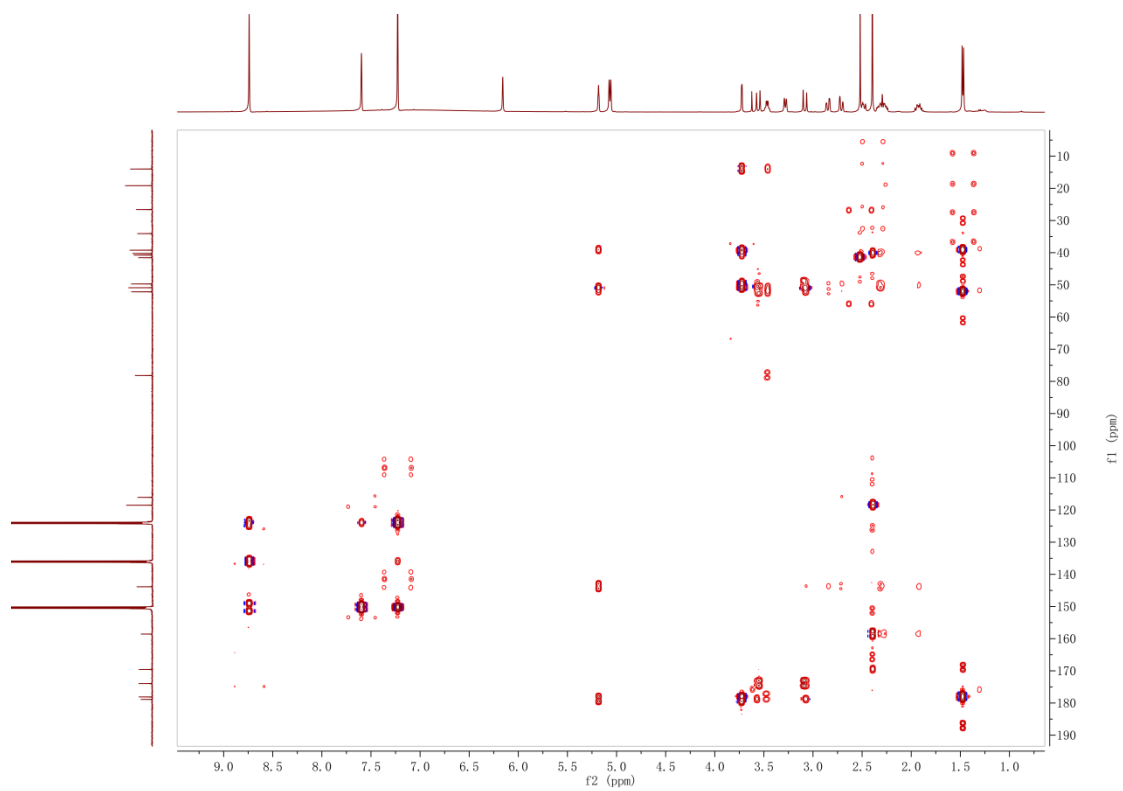


Figure S8. J-HMBC (Pyridine- d_5) spectrum of **1**

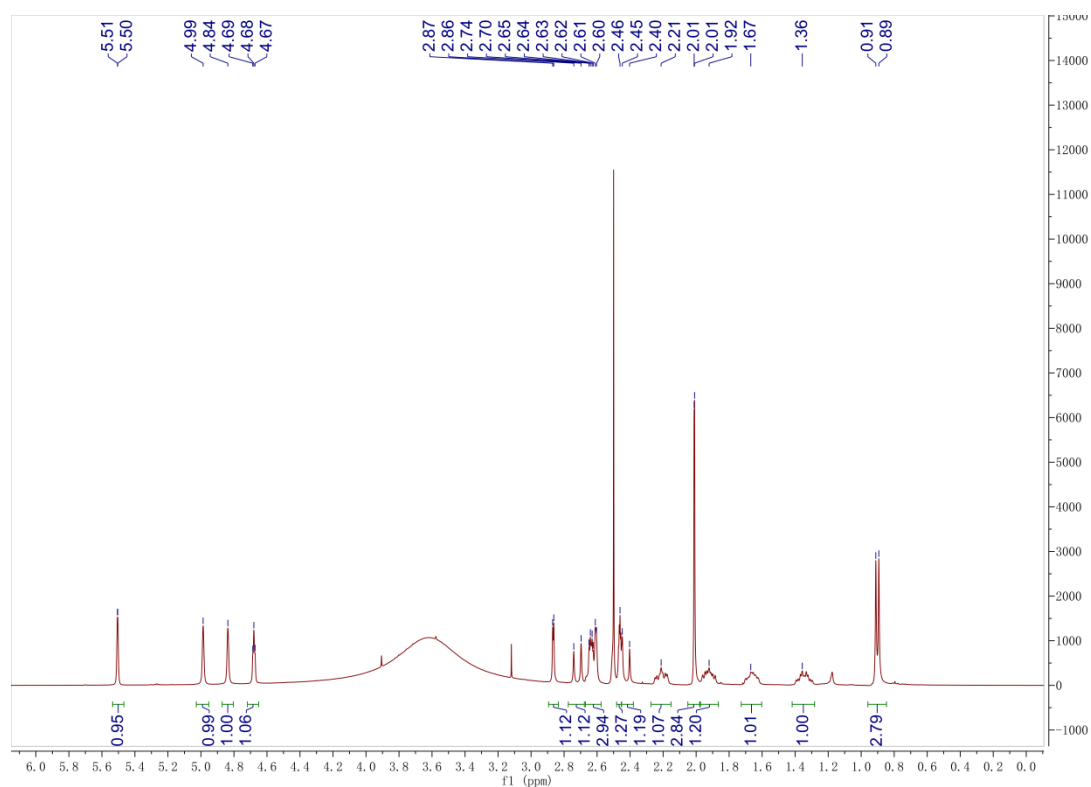


Figure S9. ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of **1**

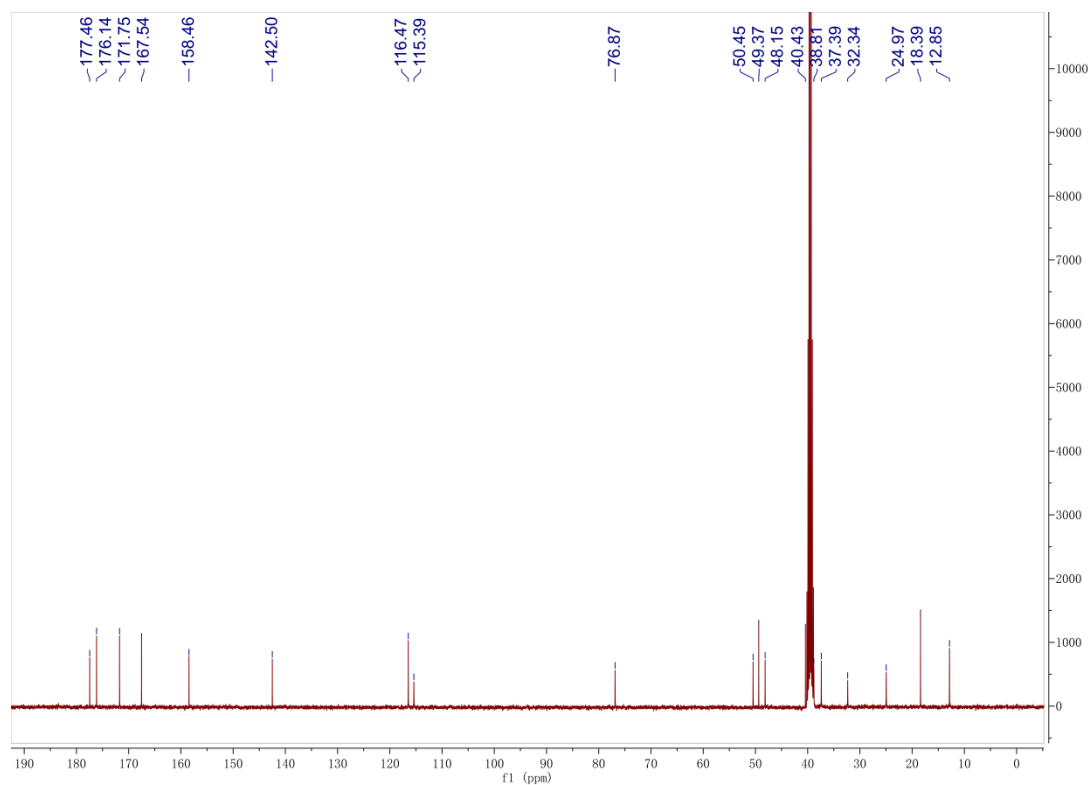


Figure S10. ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of **1**

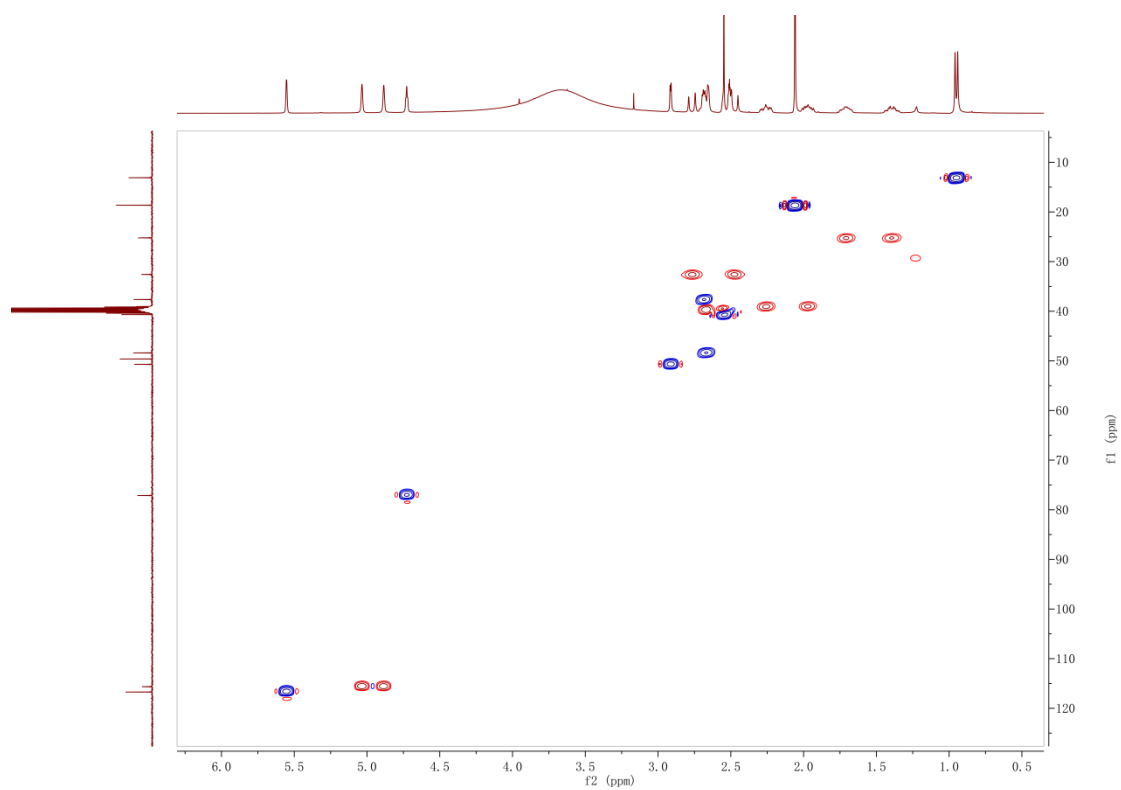


Figure S11. HMQC (DMSO-*d*₆) spectrum of **1**

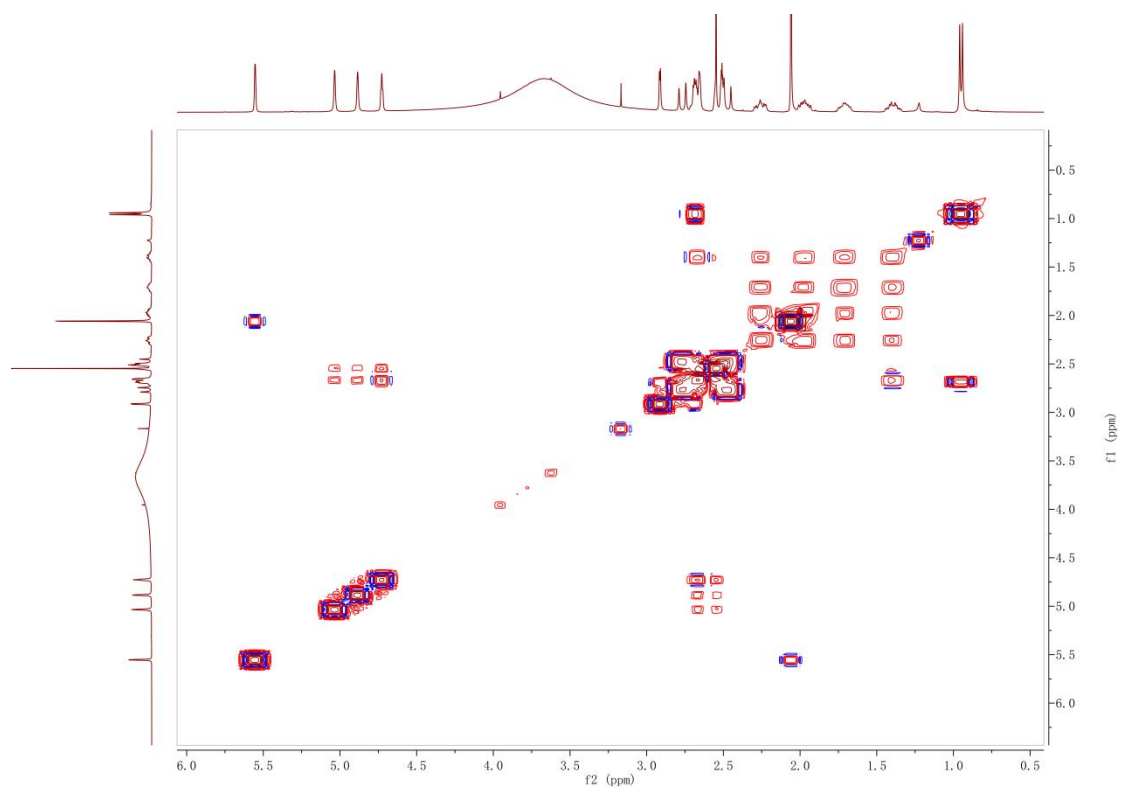


Figure S12. ¹H-¹H COSY (DMSO-*d*₆) spectrum of **1**

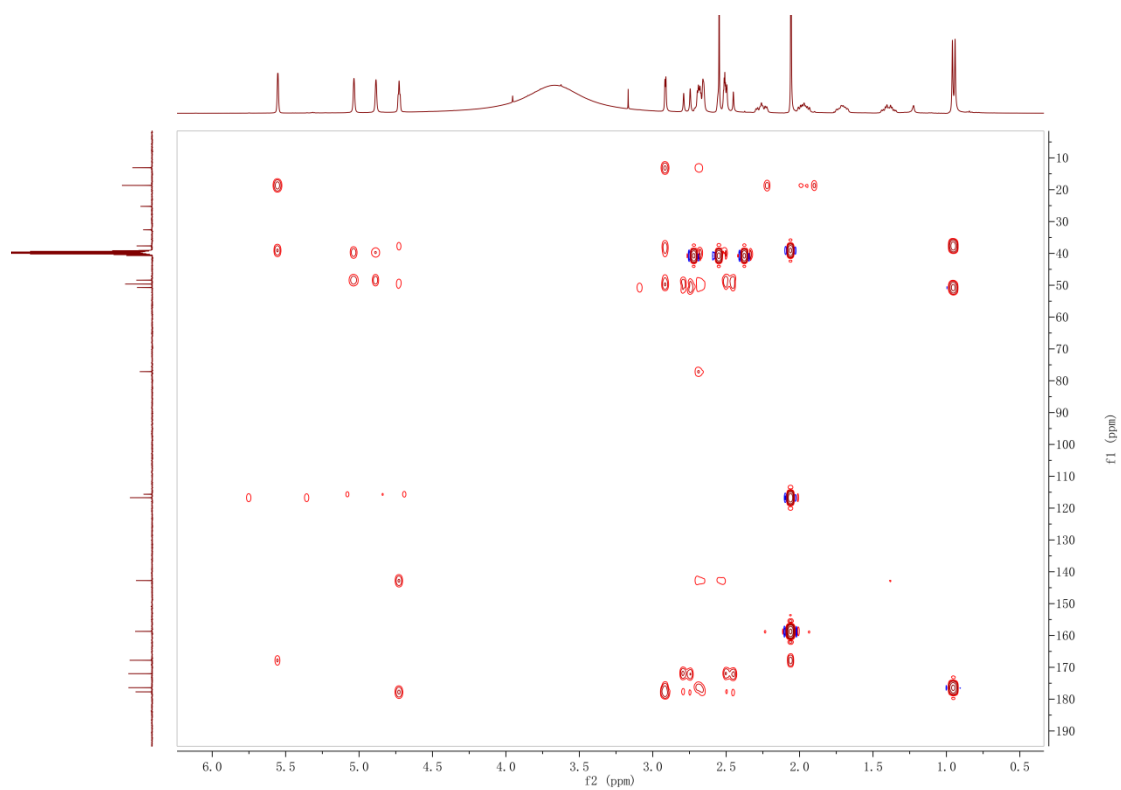


Figure S13. HMBC (DMSO- d_6) spectrum of **1**

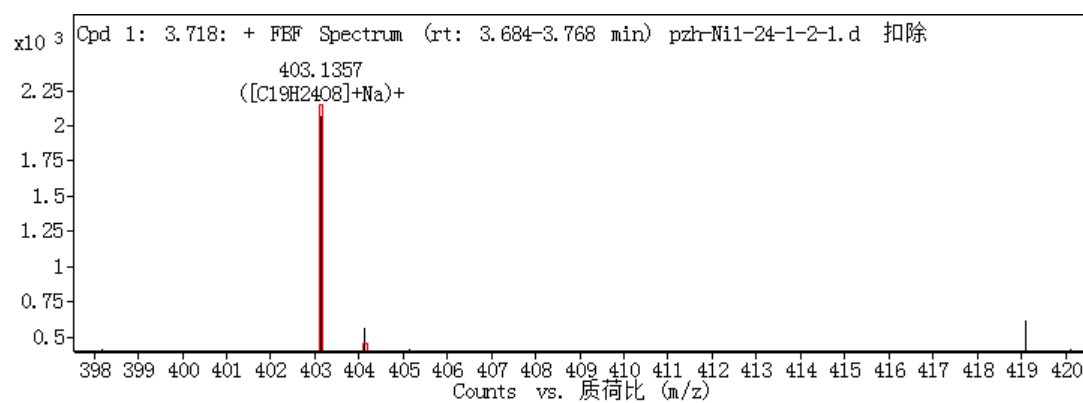


Figure S14. HRESIMS spectrum of **1**

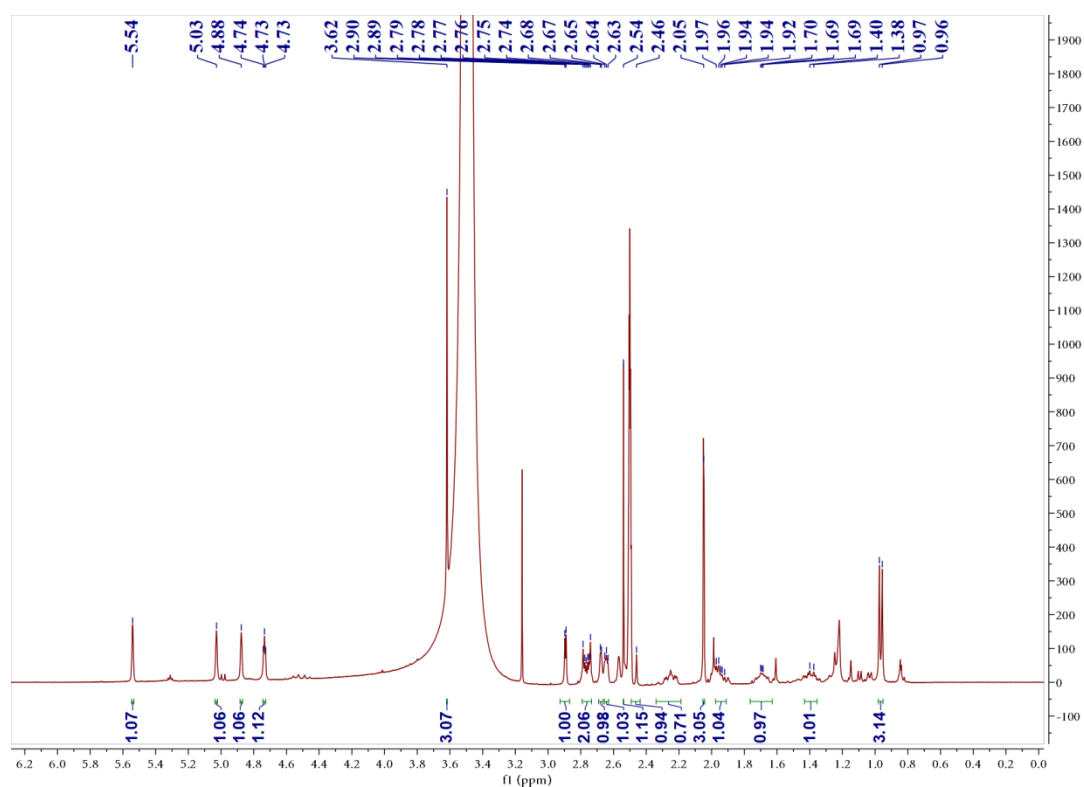


Figure S15. ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of 2

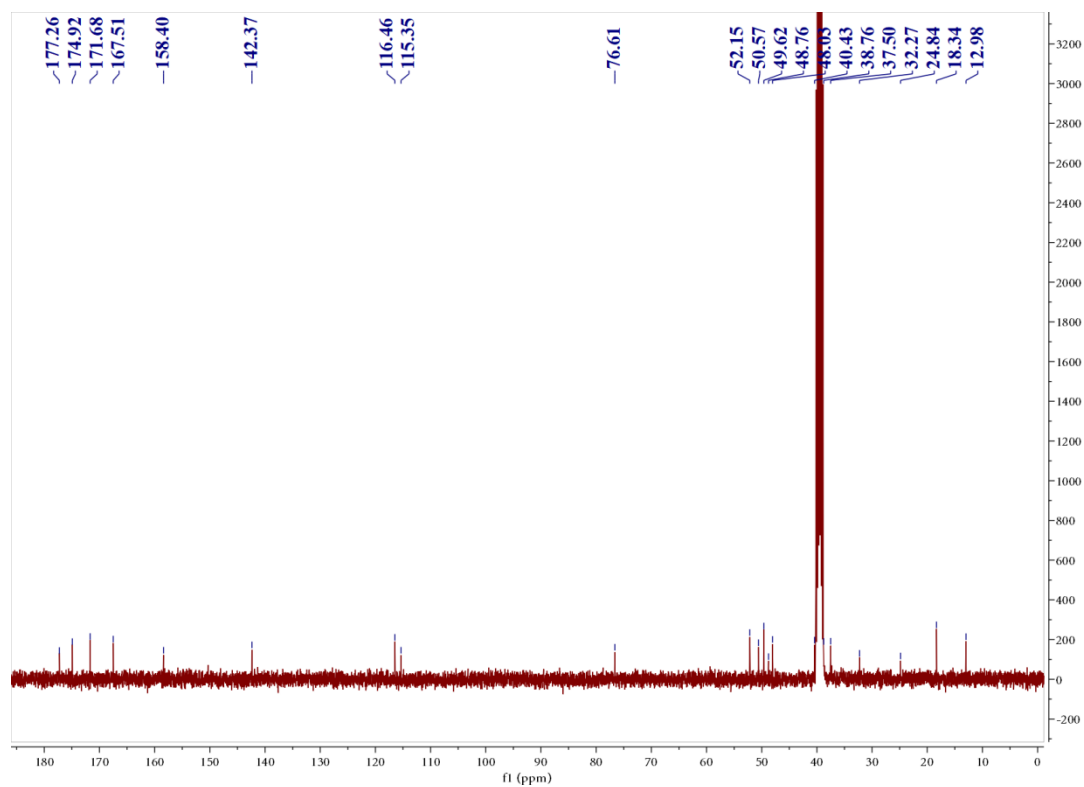


Figure S16. ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of 2

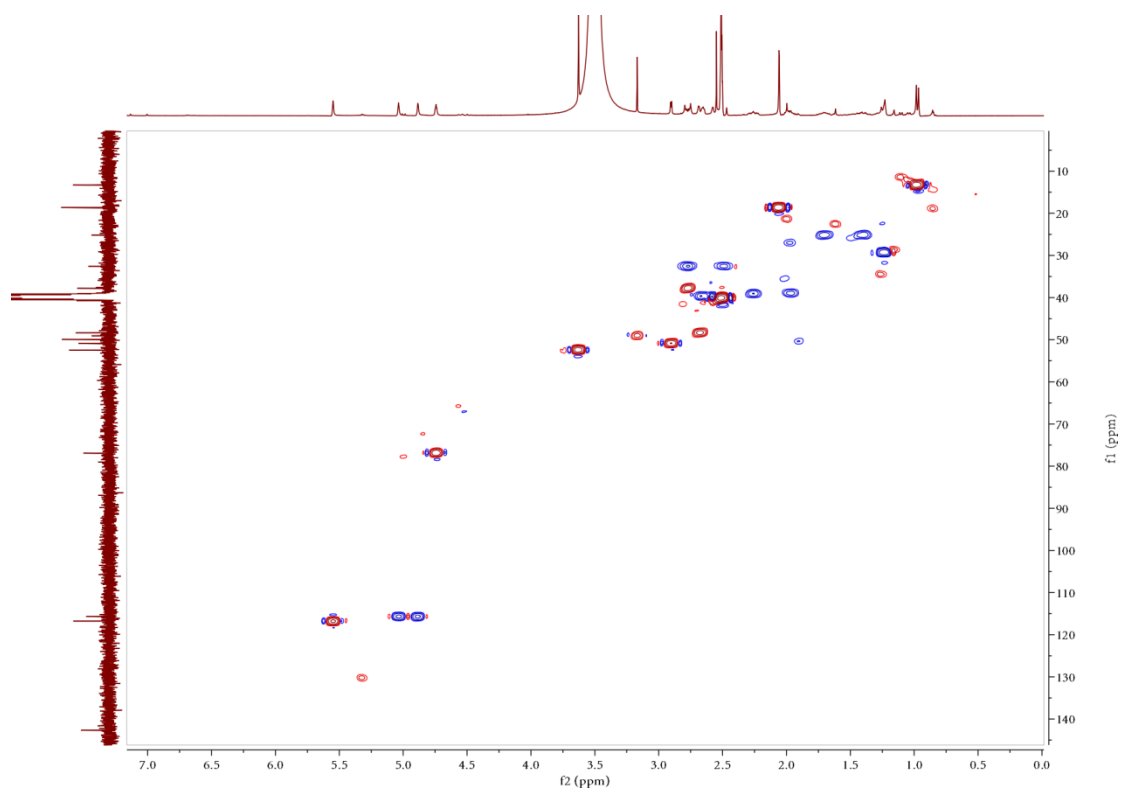


Figure S17. HMQC (DMSO- d_6) spectrum of **2**

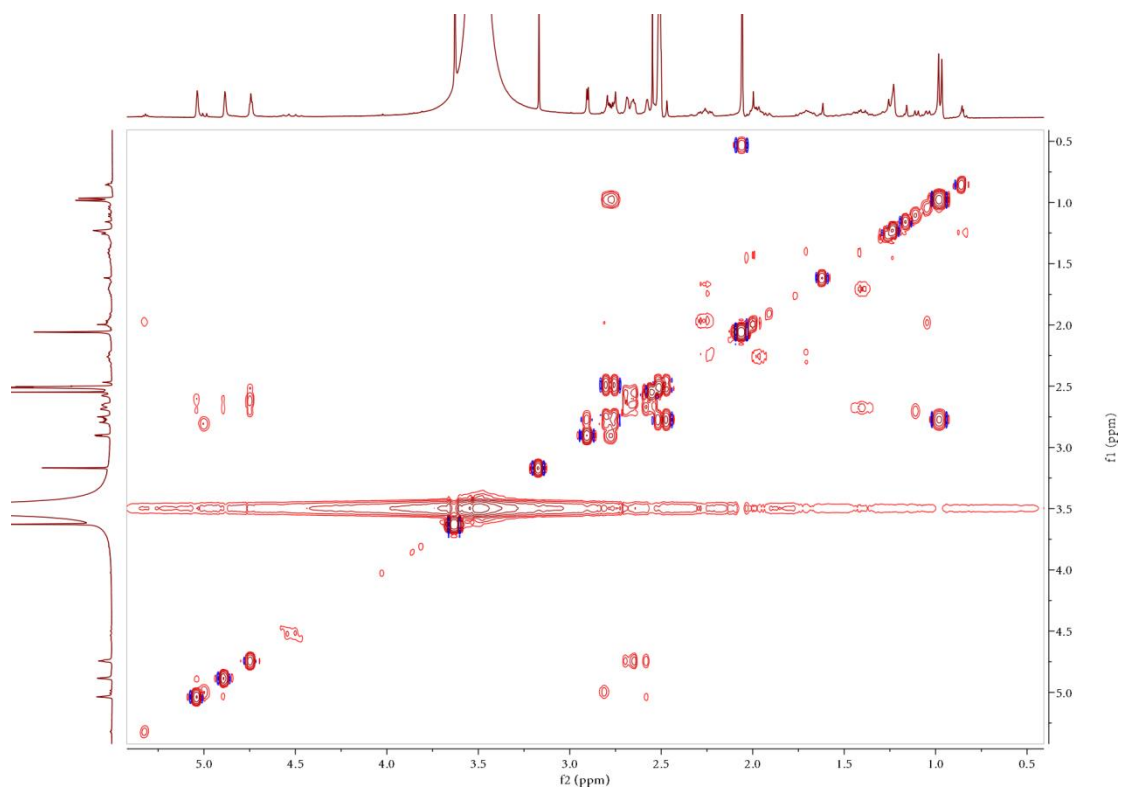


Figure S18. ^1H - ^1H COSY (DMSO- d_6) spectrum of **2**

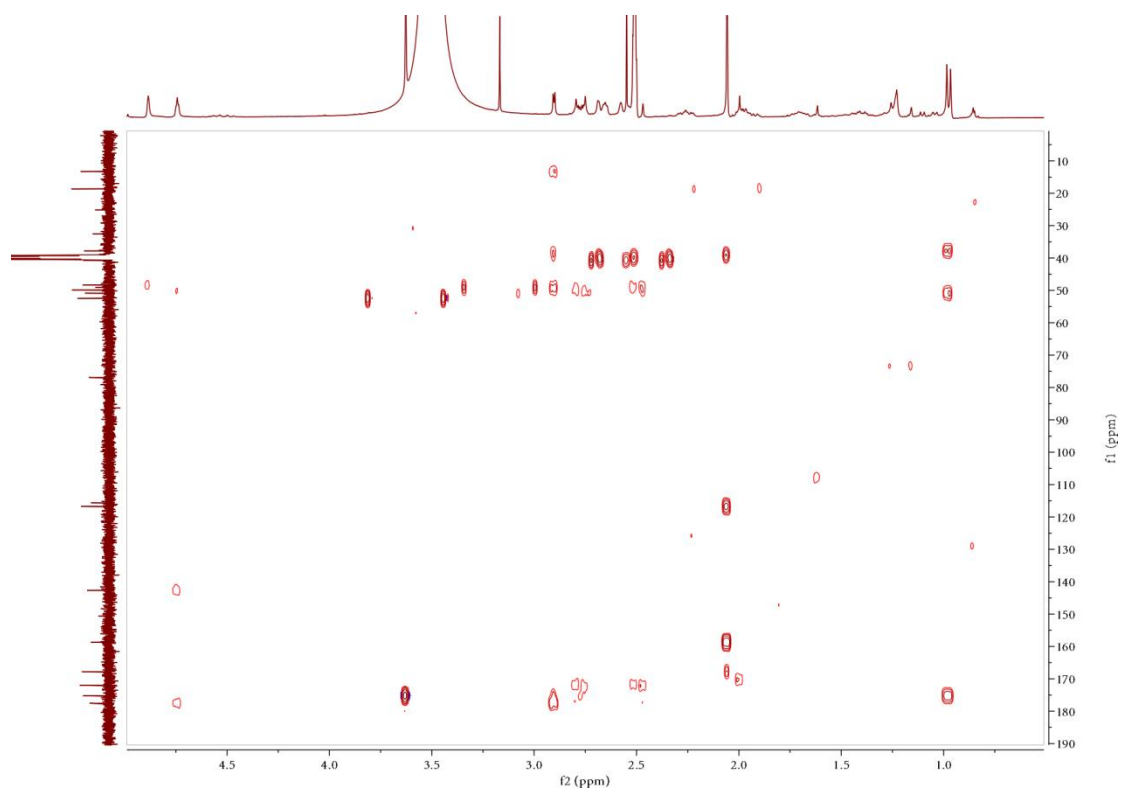


Figure S19. HMBC (DMSO- d_6) spectrum of **2**

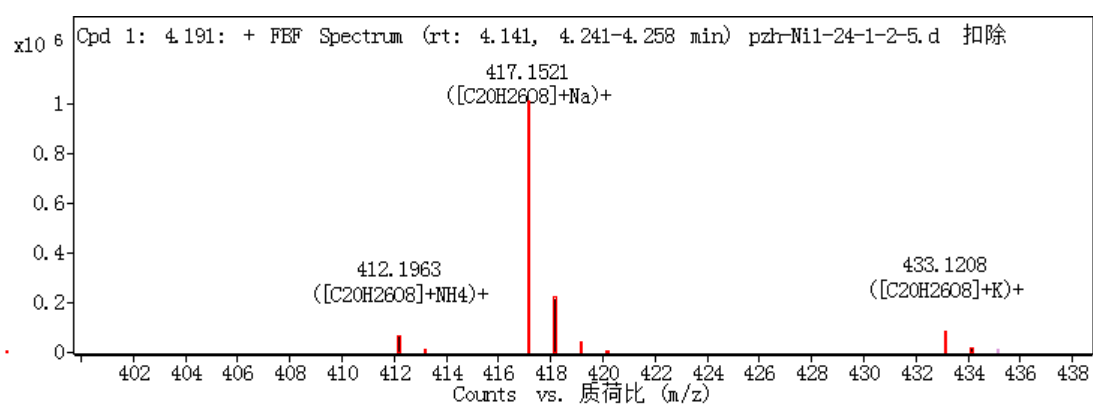


Figure S20. HRESIMS spectrum of **2**

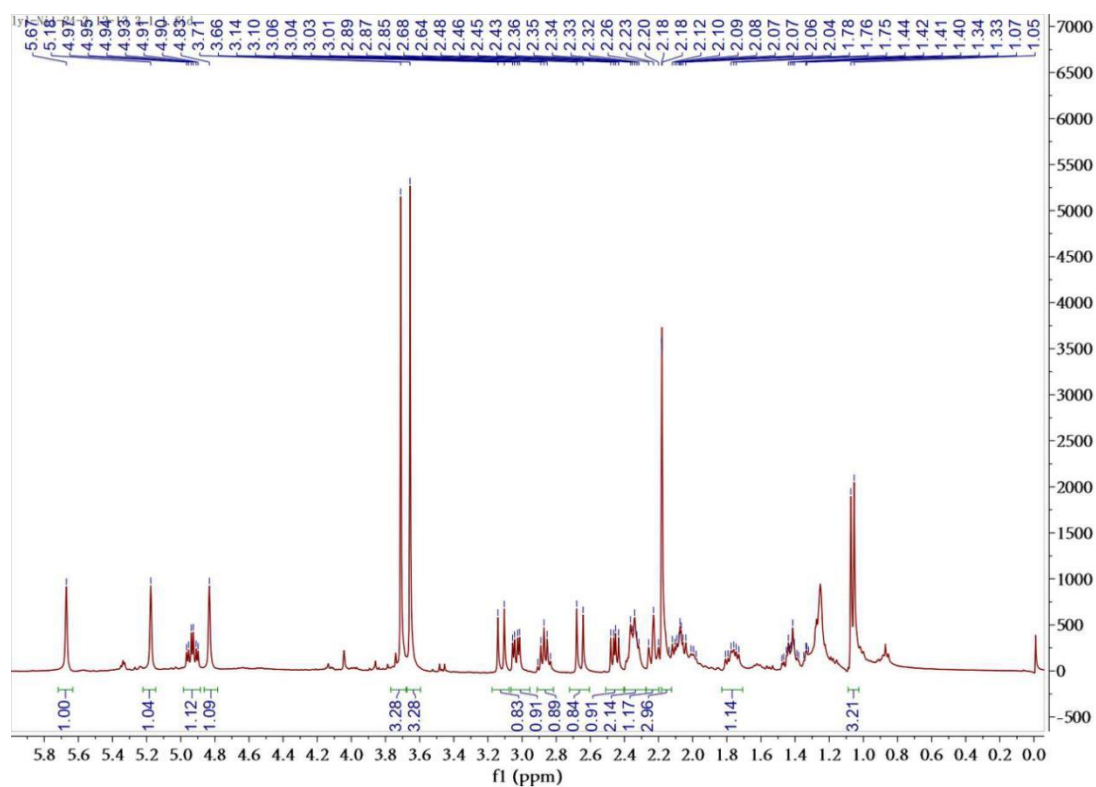


Figure S21. ¹H NMR (400 MHz, CDCl₃) spectrum of **3**

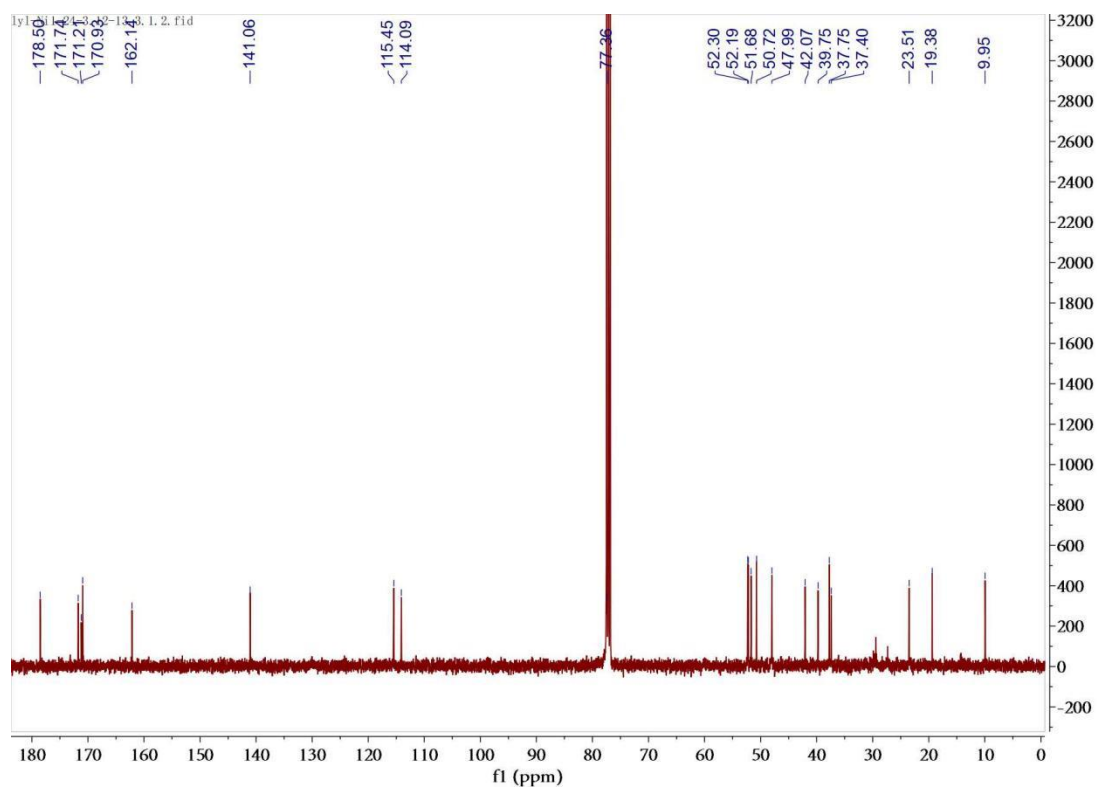


Figure S22. ¹³C NMR (100 MHz, CDCl₃) spectrum of **3**

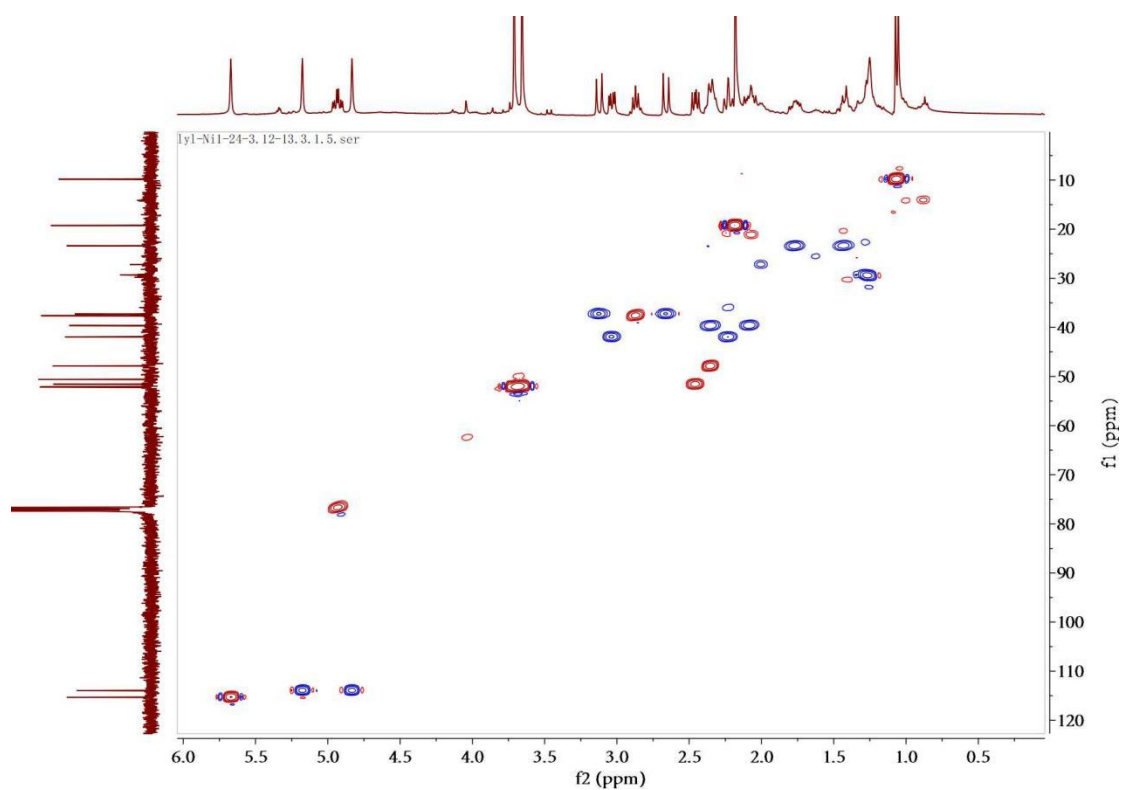


Figure S23. HMQC (CDCl₃) spectrum of **3**

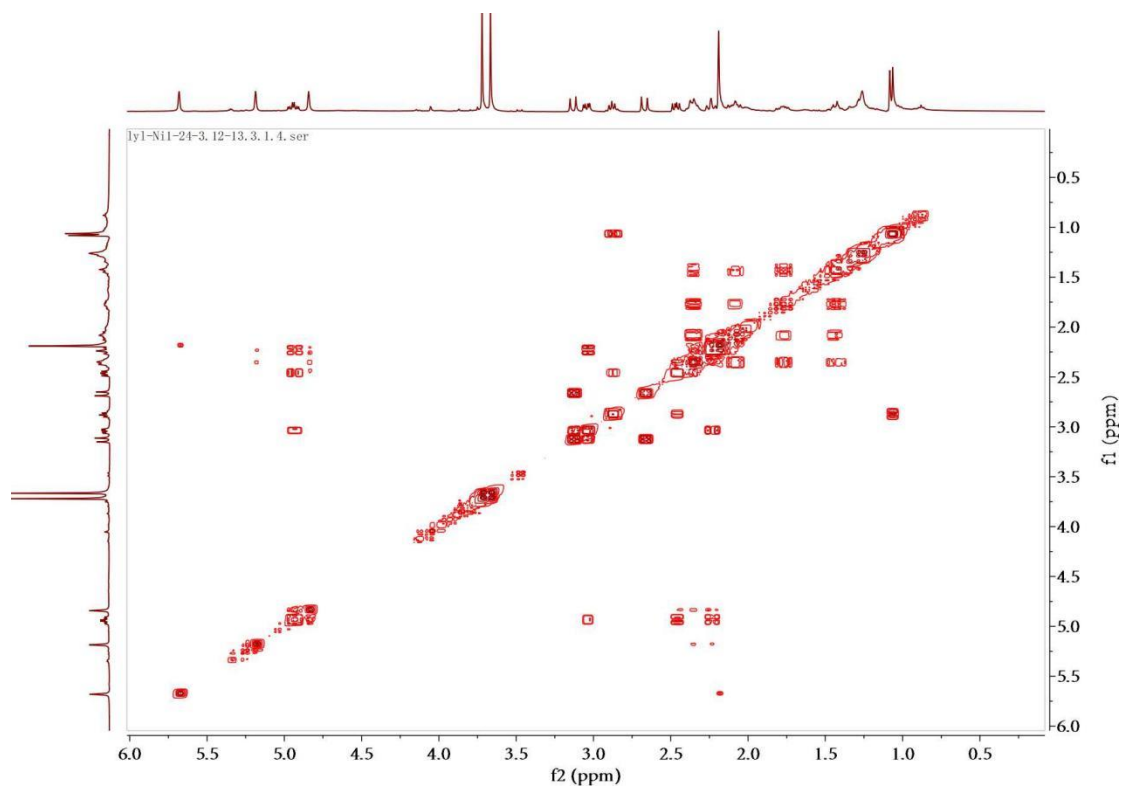


Figure S24. ¹H-¹H COSY (CDCl₃) spectrum of **3**

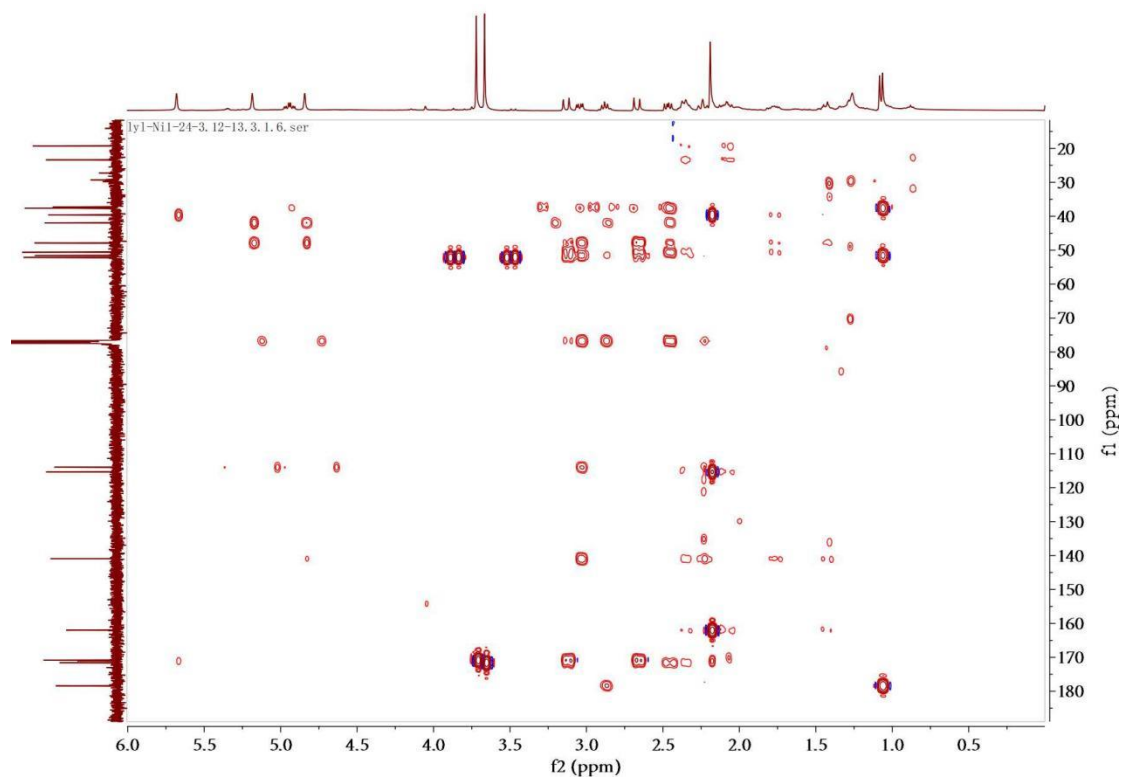


Figure S25. HMBC (CDCl₃) spectrum of **3**

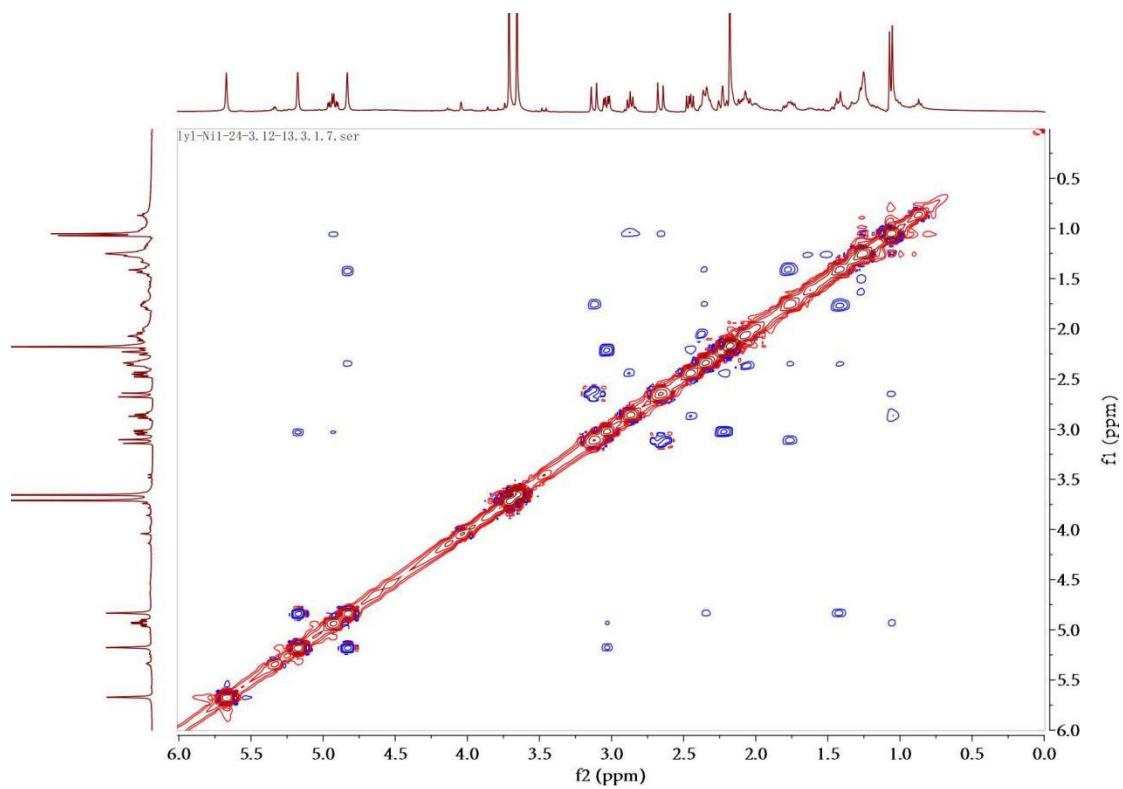


Figure S26. NOESY (CDCl₃) spectrum of **3**

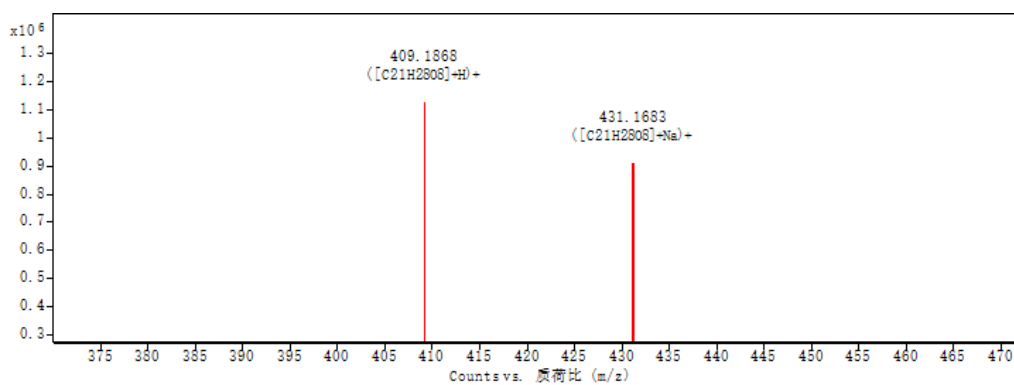


Figure S27. HRESIMS spectrum of **3**

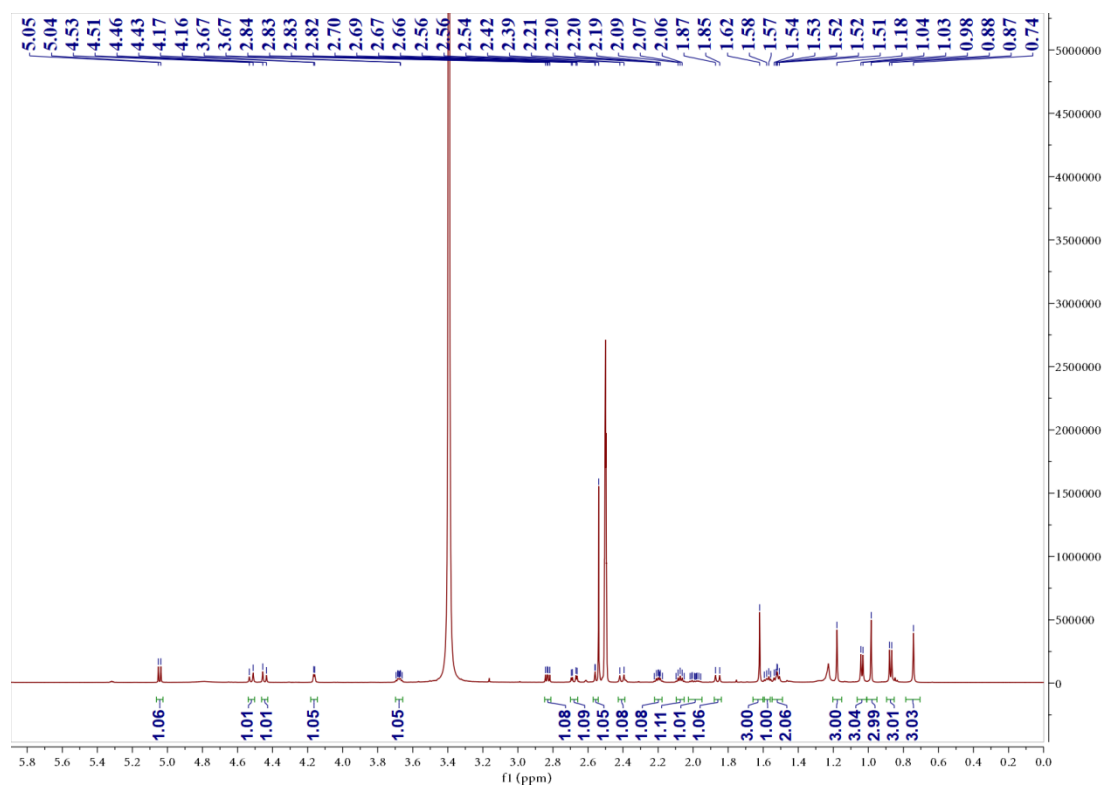


Figure S28. ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **6**

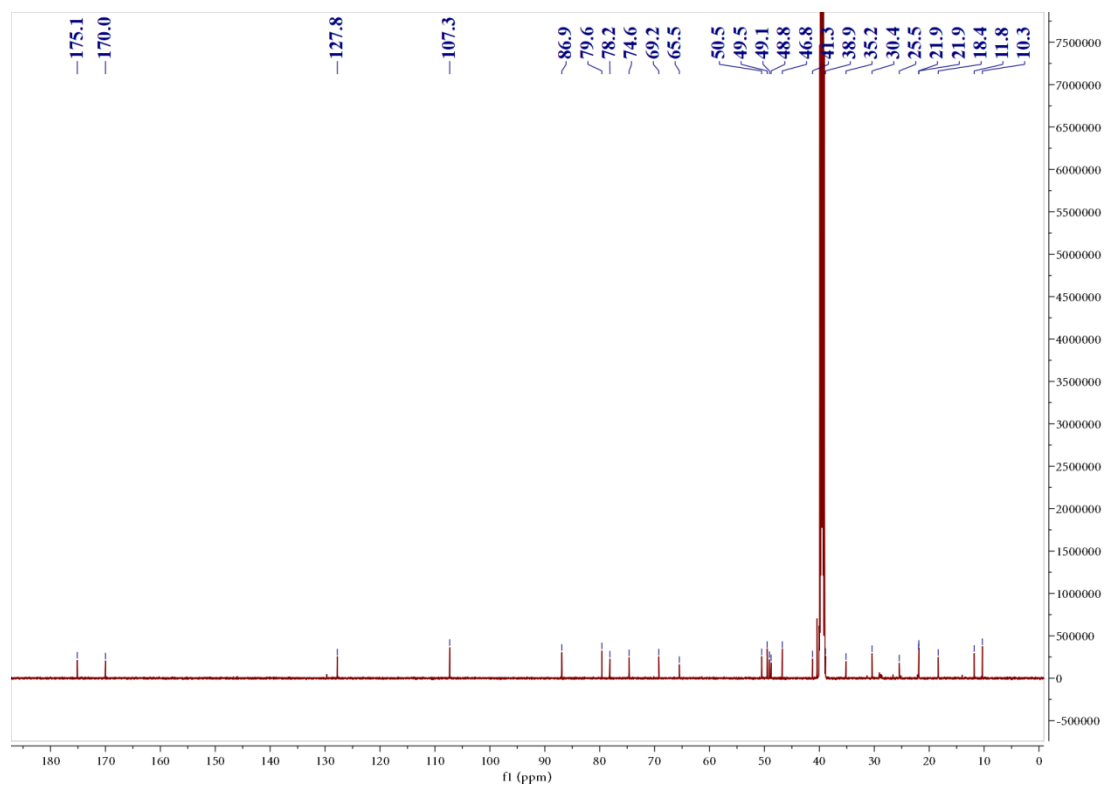


Figure S29. ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of **6**

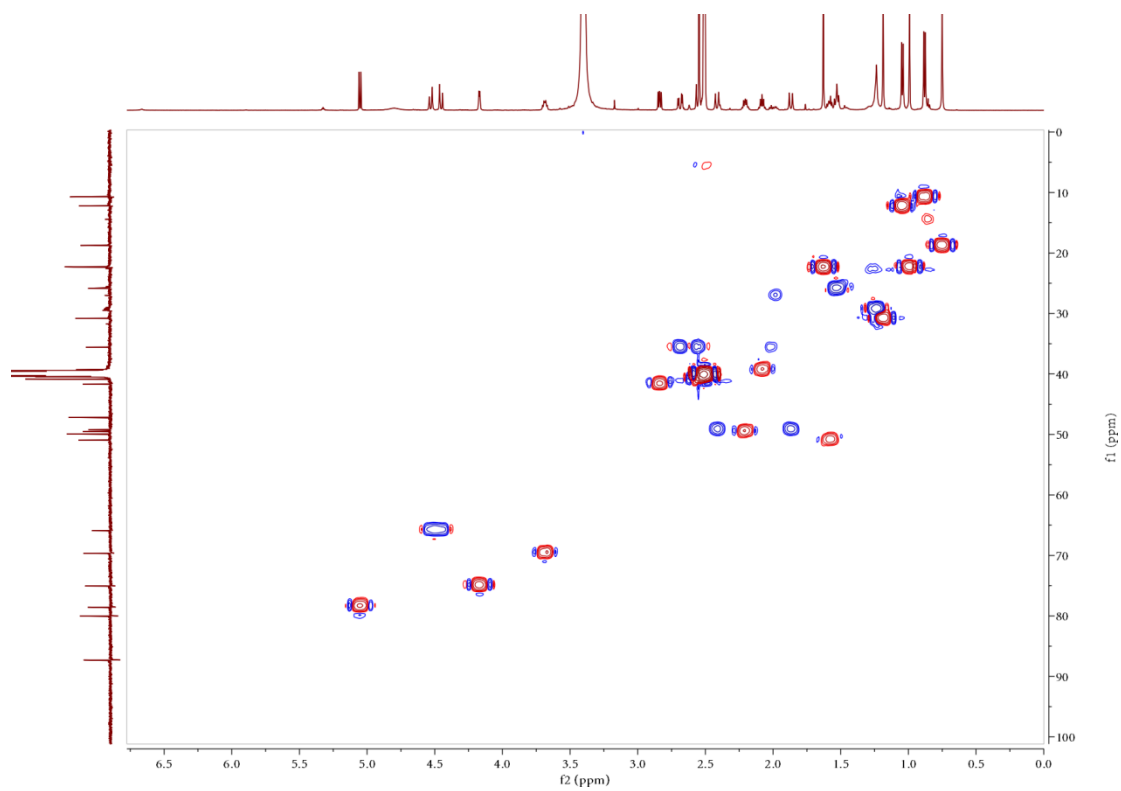


Figure S30. HMQC ($\text{DMSO-}d_6$) spectrum of **6**

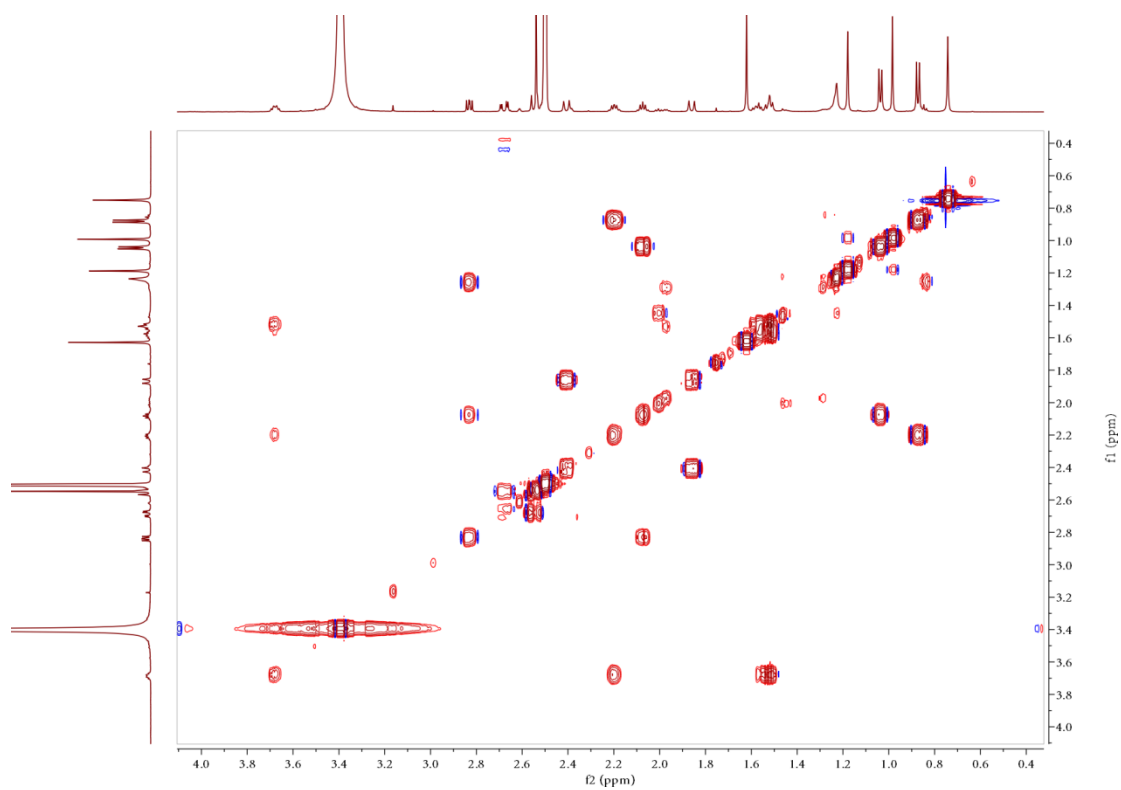


Figure S31. ^1H - ^1H COSY (DMSO- d_6) spectrum of **6**

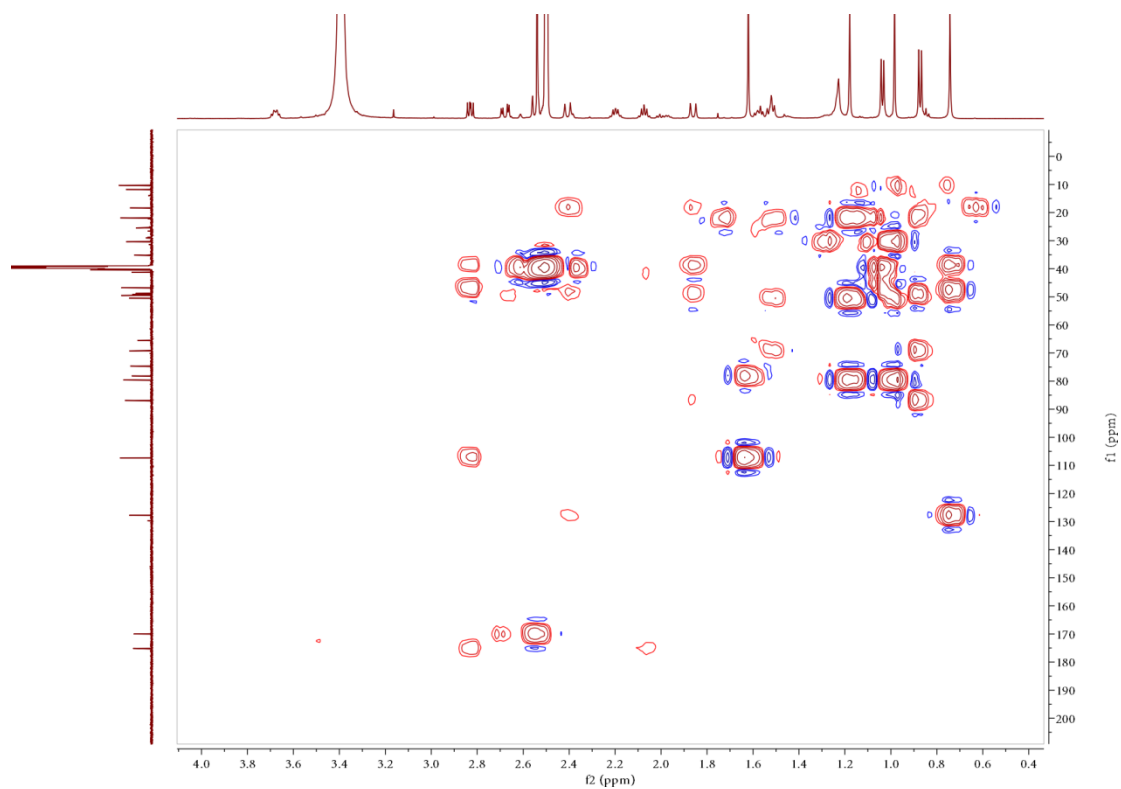


Figure S32. HMBC (DMSO- d_6) spectrum of **6**

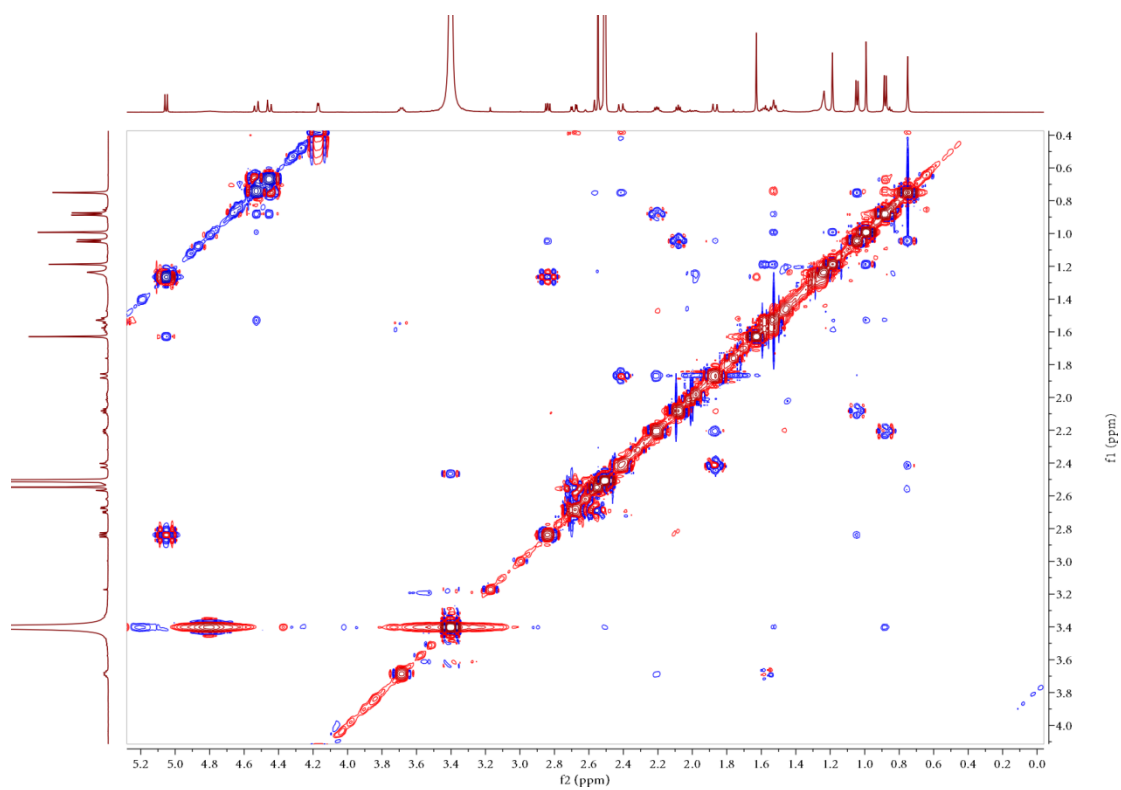


Figure S33. NOESY (DMSO- d_6) spectrum of **6**

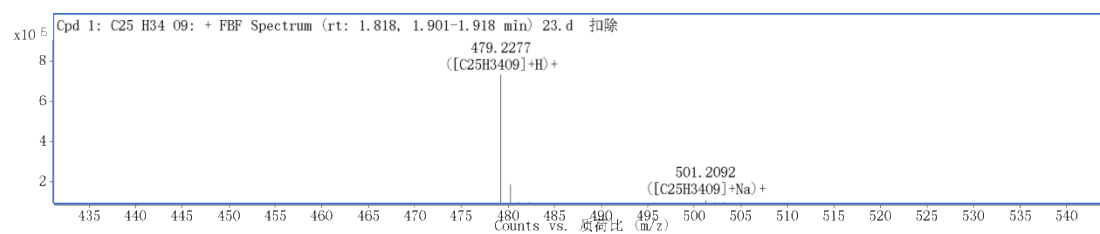


Figure S34. HRESIMS spectrum of **6**

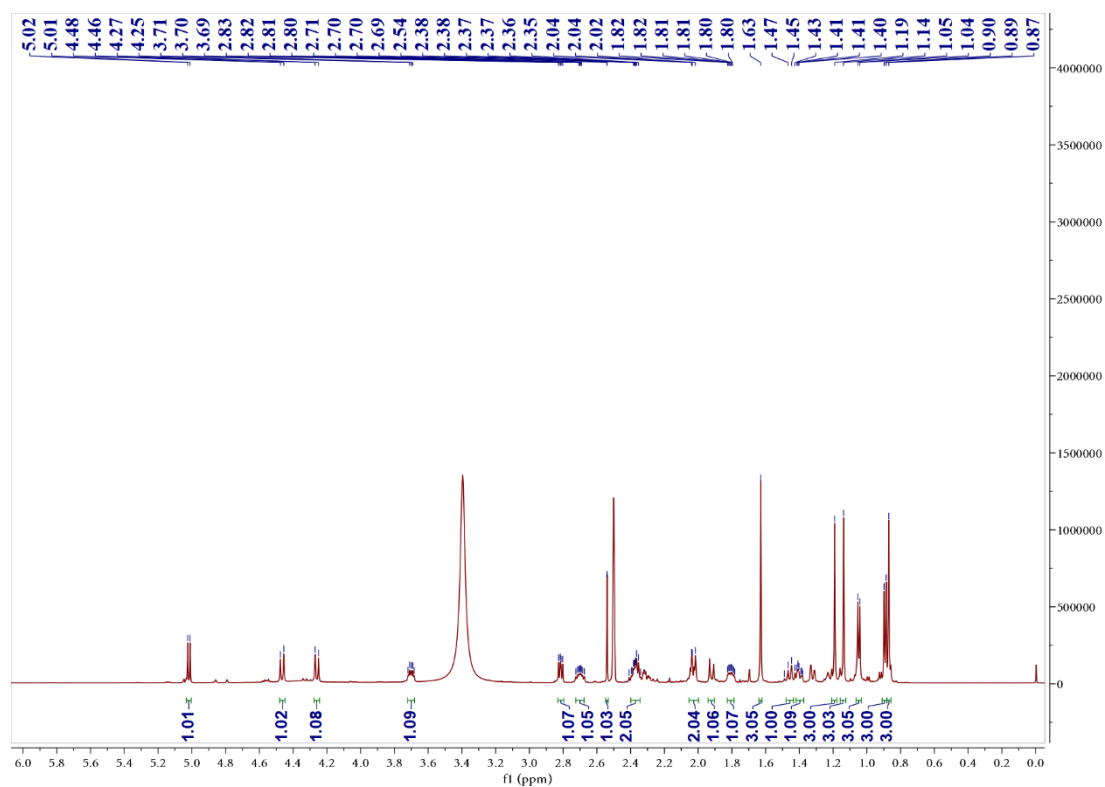


Figure S35. ^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of **7**

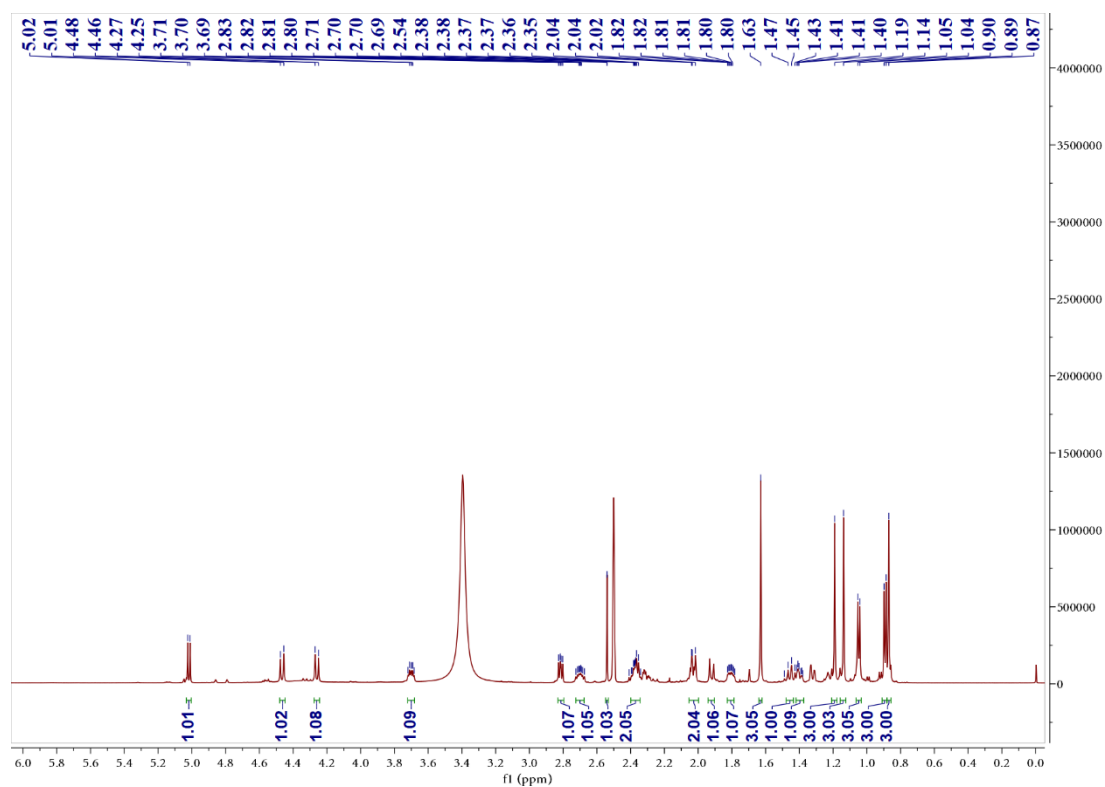


Figure S36. ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of **7**

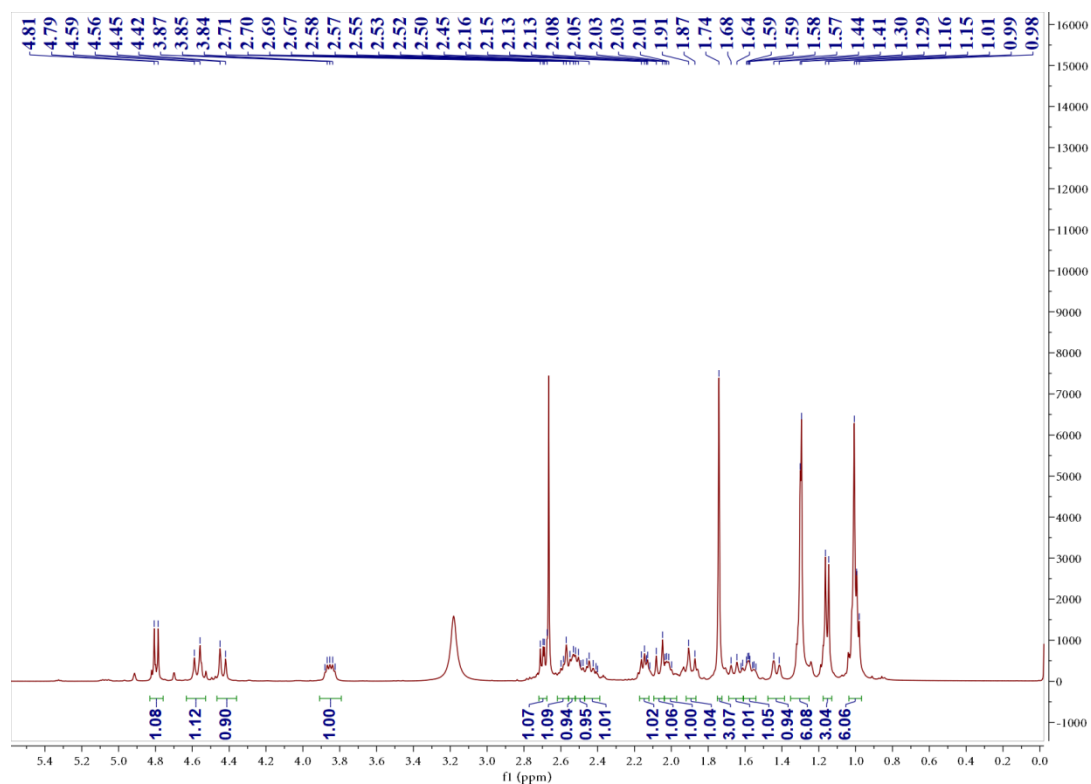


Figure S37. ¹H NMR (400 MHz, CDCl₃) spectrum of 7

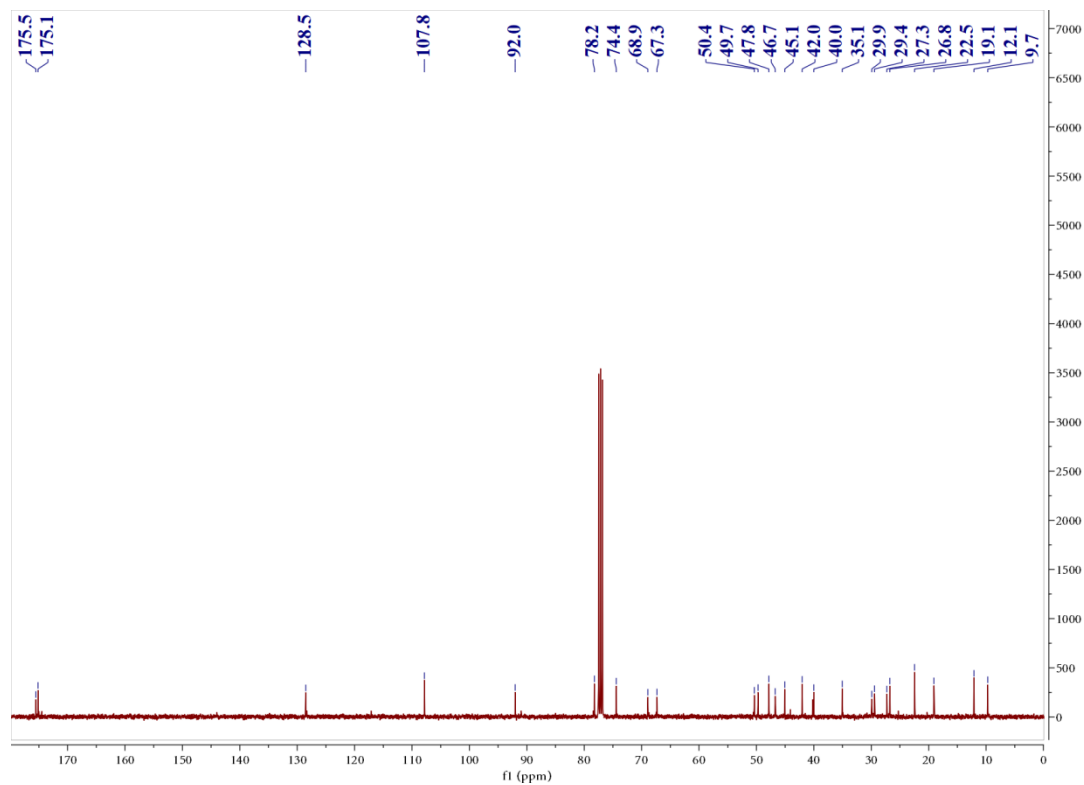


Figure S38. ¹³C NMR (100 MHz, CDCl₃) spectrum of 7

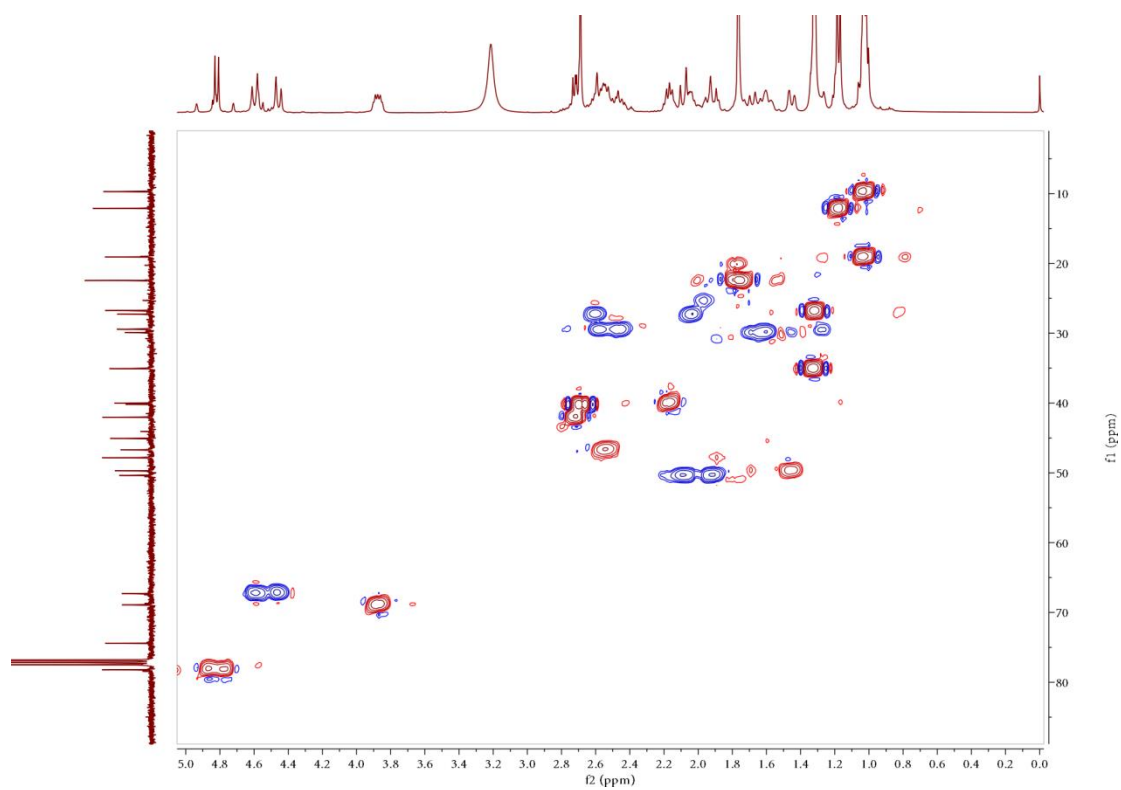


Figure S39. HMQC (CDCl₃) spectrum of **7**

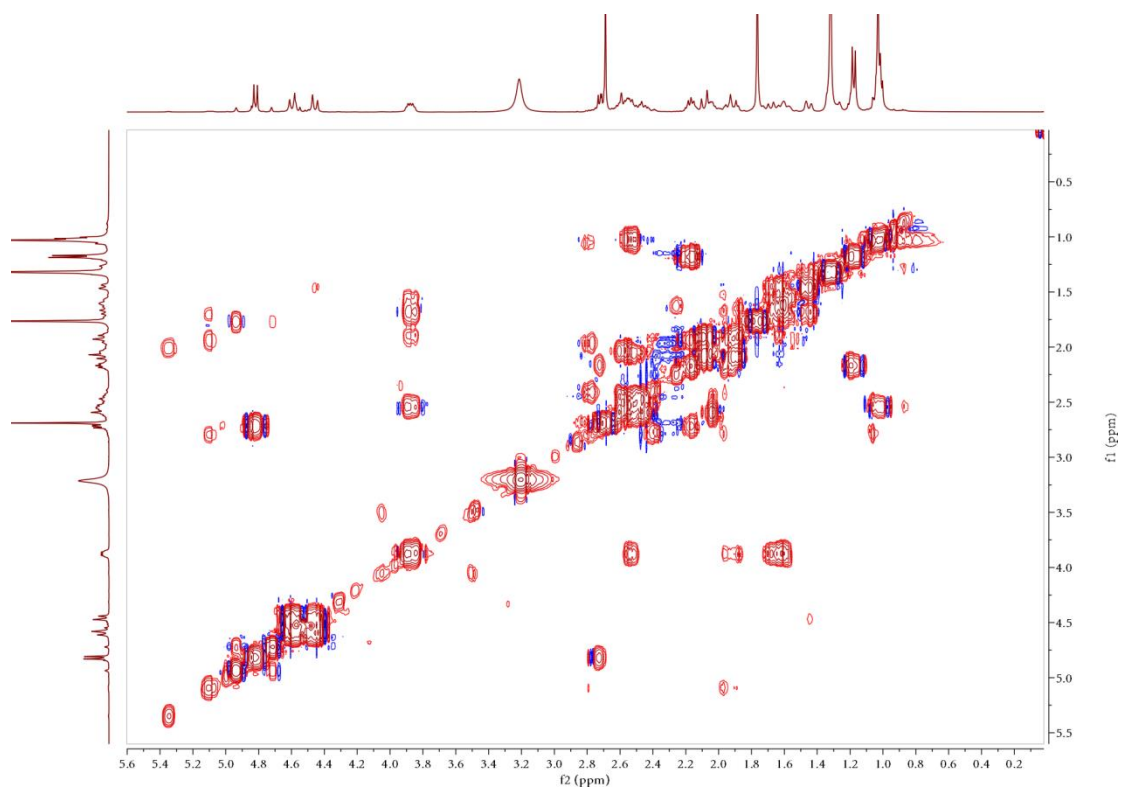


Figure S40. ¹H-¹H COSY (CDCl₃) spectrum of **7**

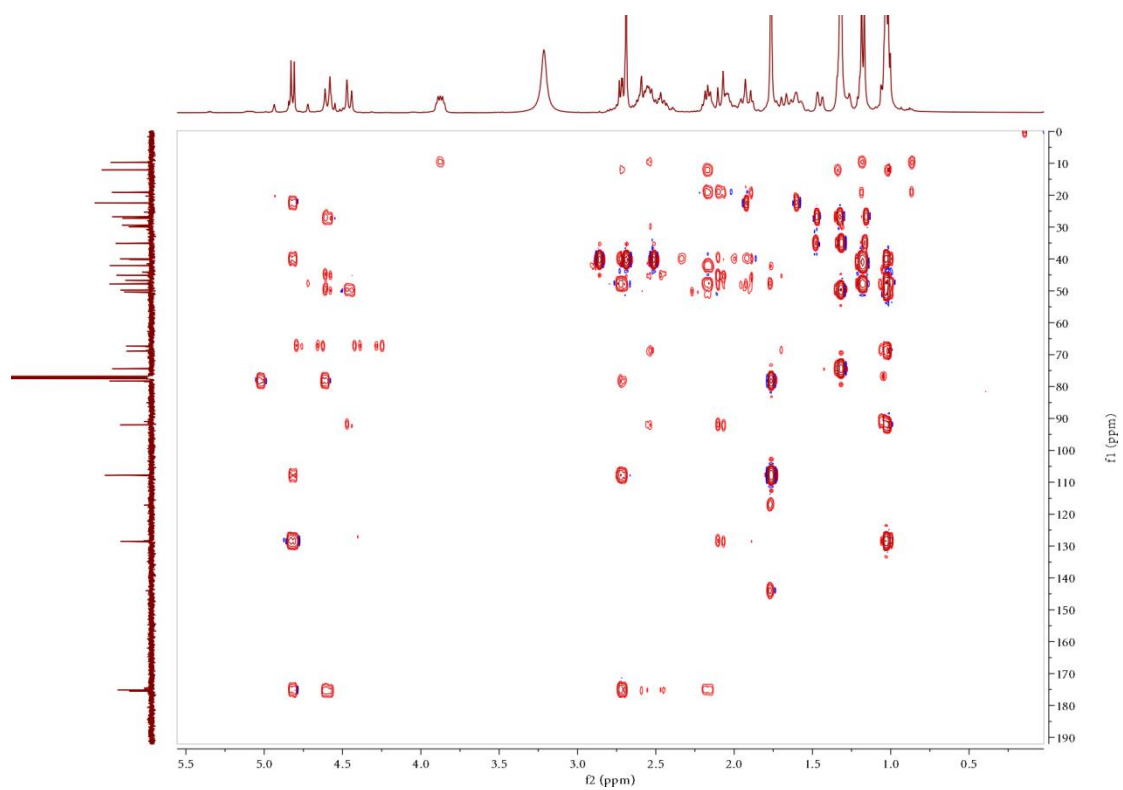


Figure S41. HMBC (CDCl₃) spectrum of **7**

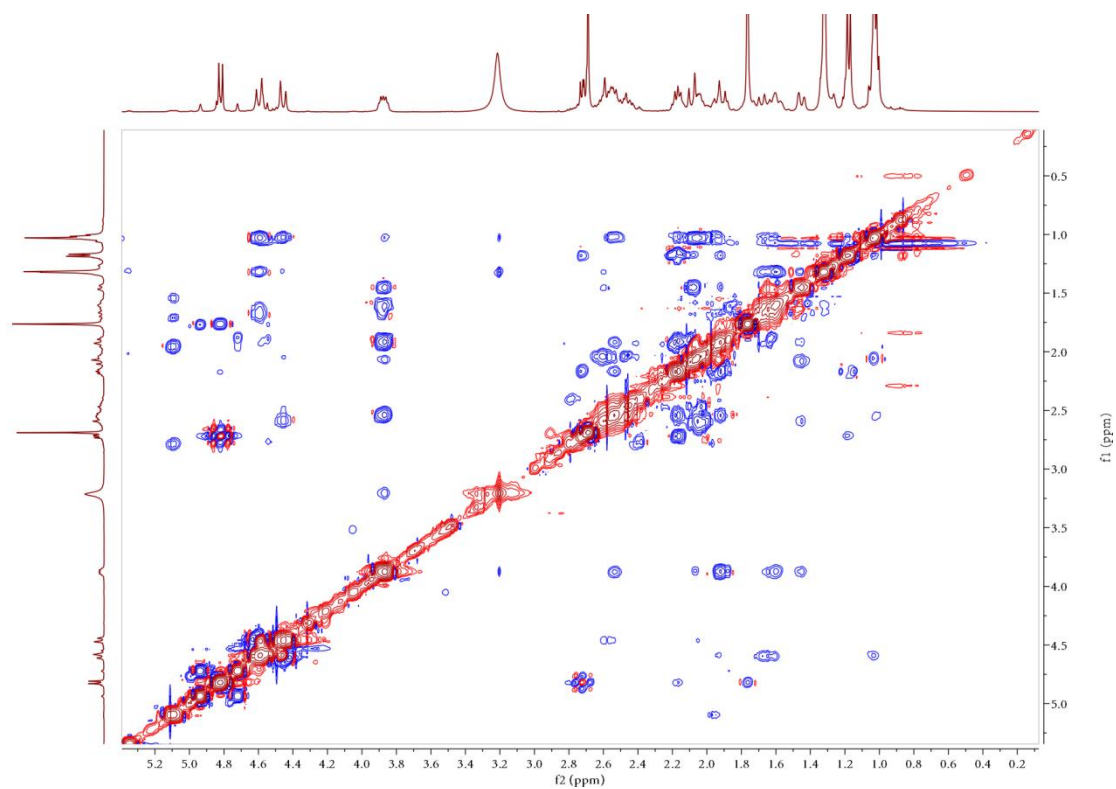


Figure S42. NOESY (CDCl₃) spectrum of **7**

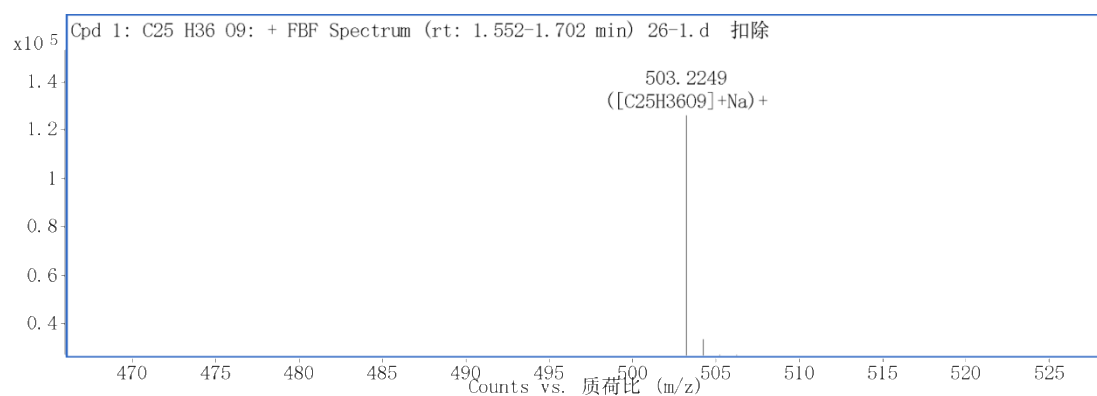


Figure S43. HRESIMS spectrum of **7**

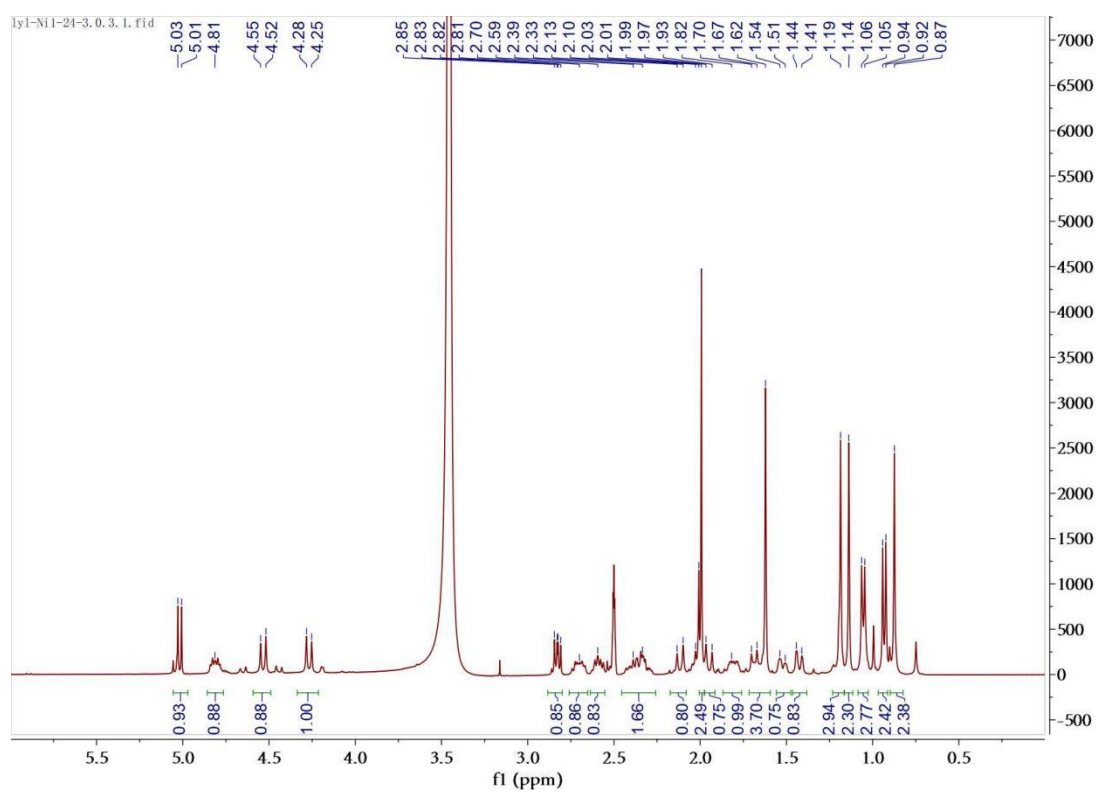


Figure S44. ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of **8**

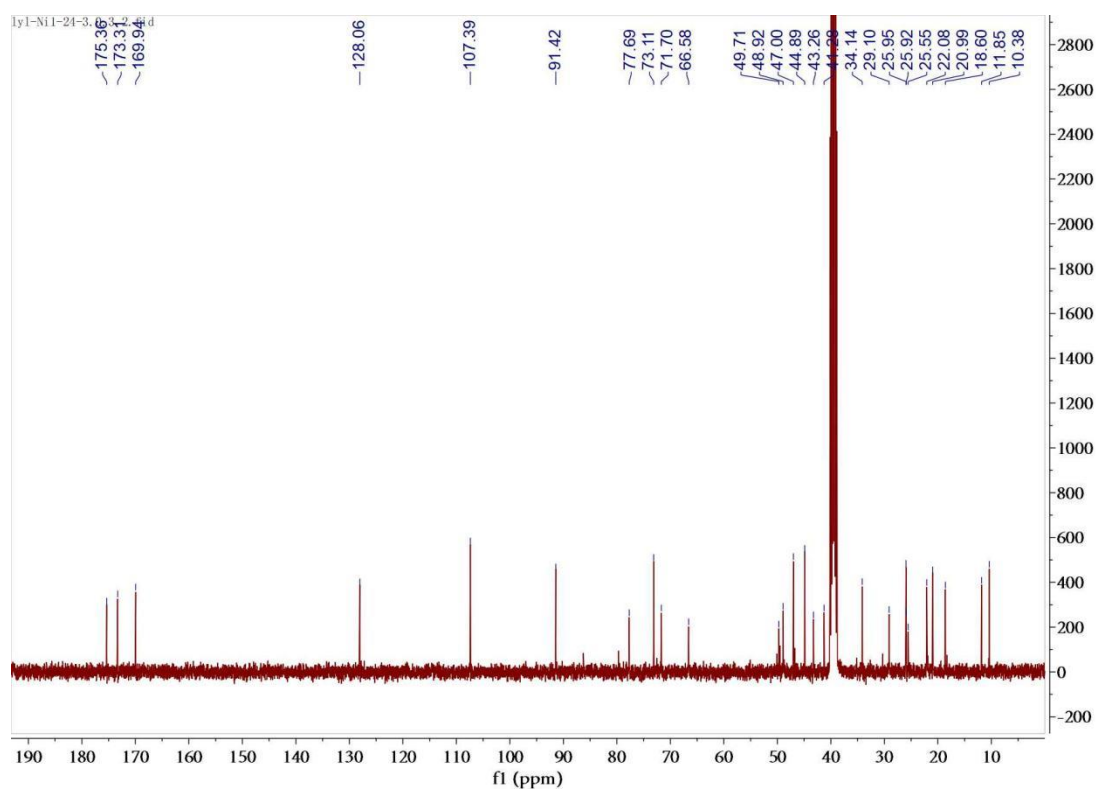


Figure S45. ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of **8**

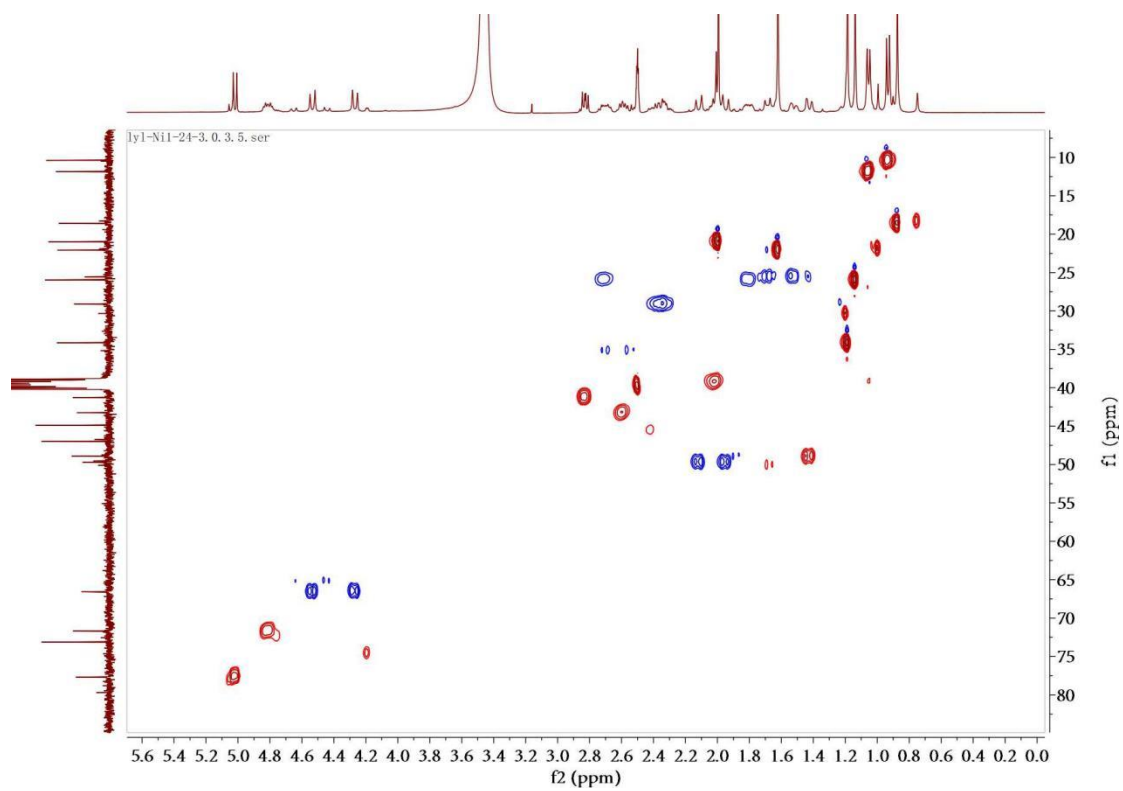


Figure S46. HMQC (DMSO-*d*₆) spectrum of **8**

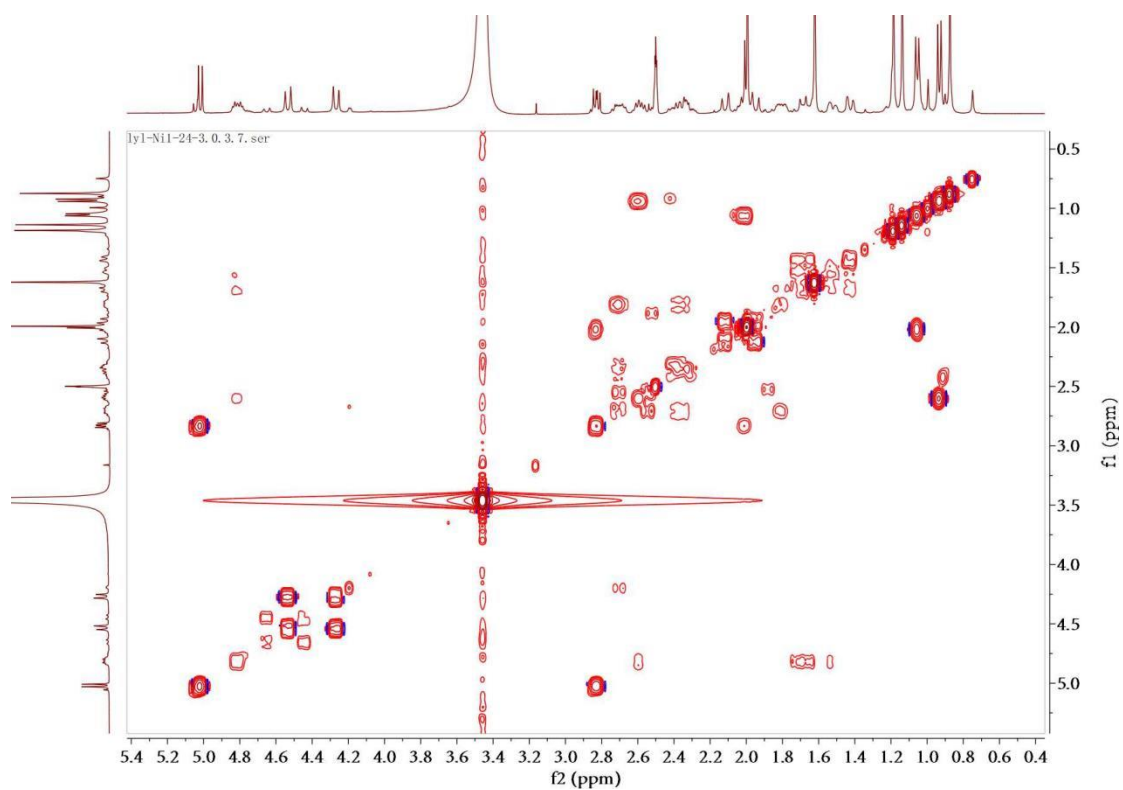


Figure S47. ^1H - ^1H COSY (DMSO- d_6) spectrum of **8**

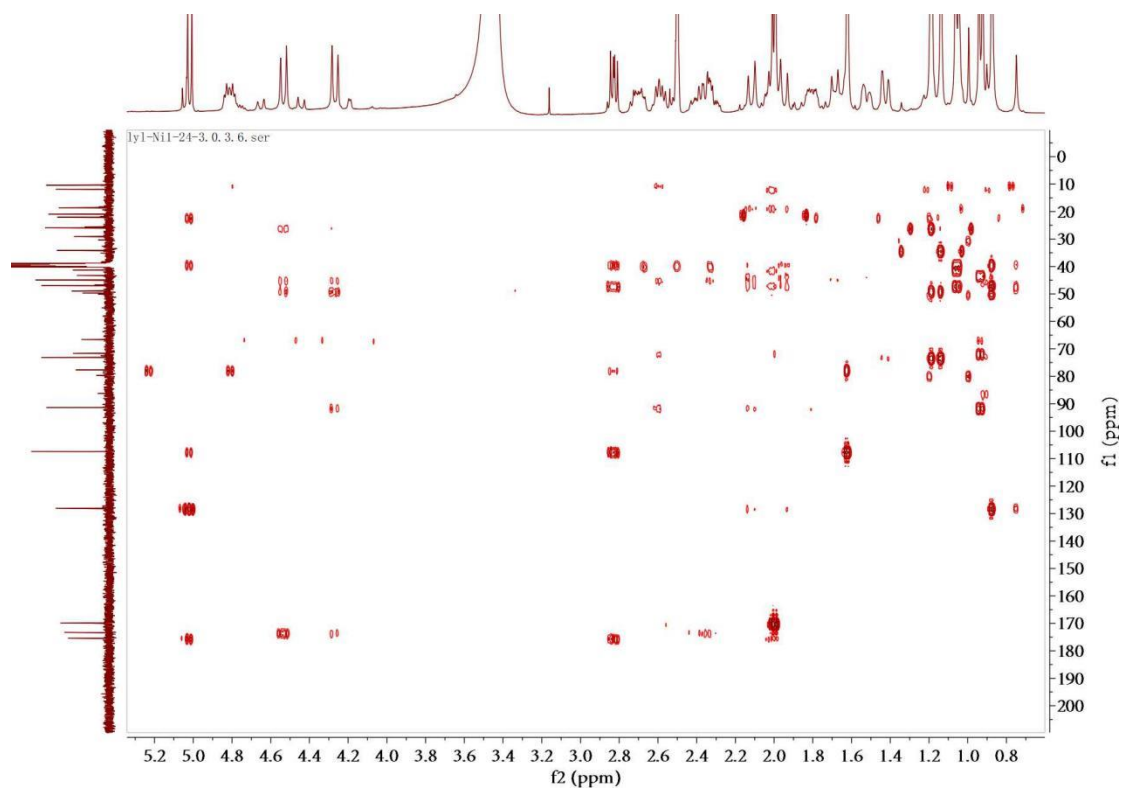


Figure S48. HMBC (DMSO- d_6) spectrum of **8**

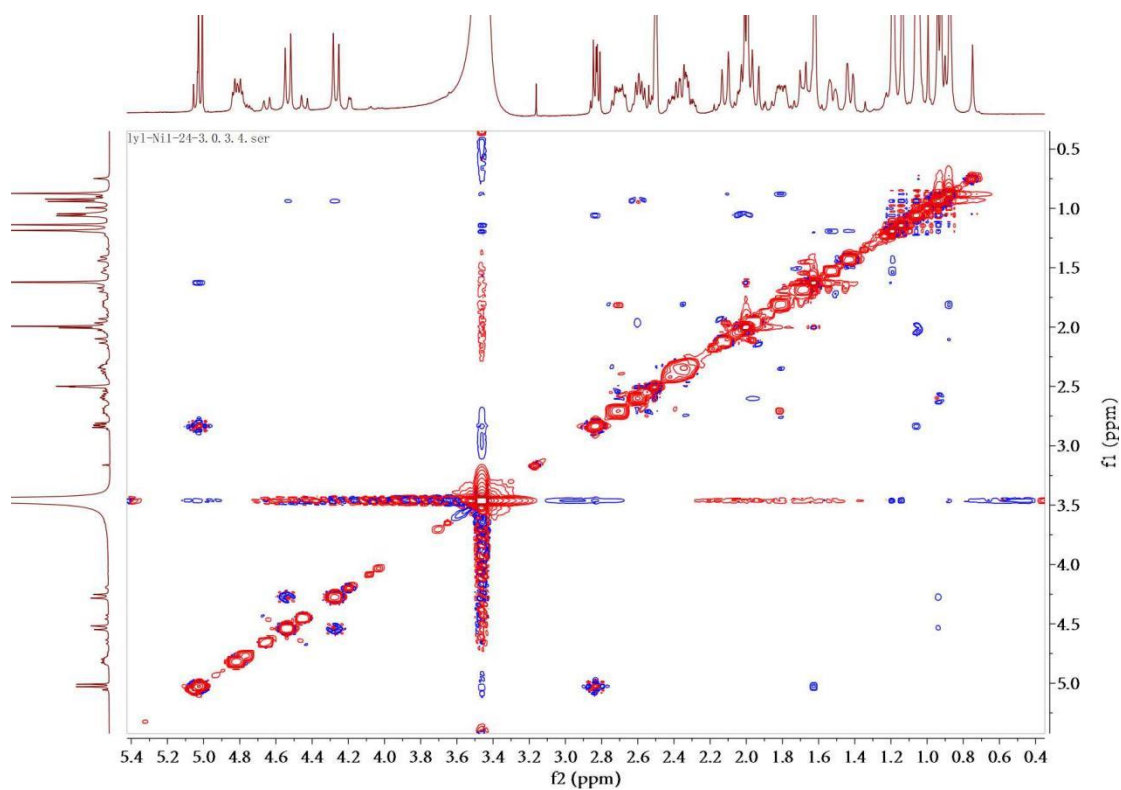


Figure S49. NOESY (DMSO- d_6) spectrum of **8**

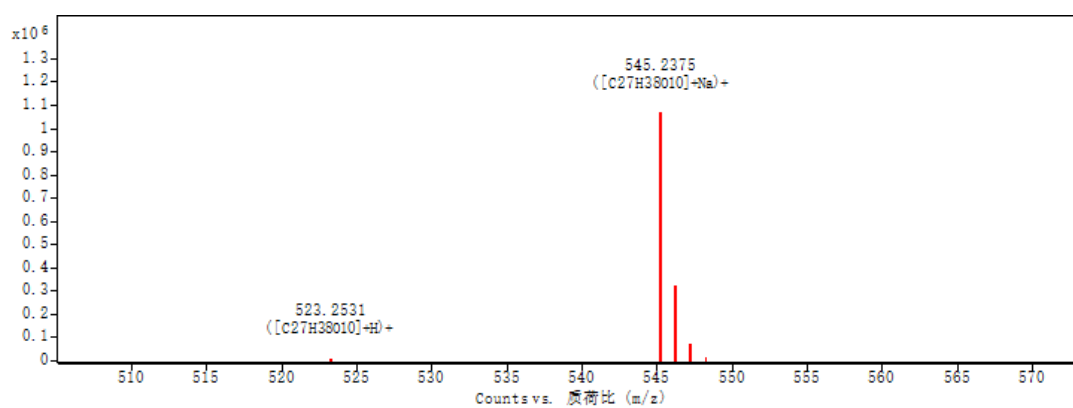


Figure S50. HRESIMS spectrum of **8**

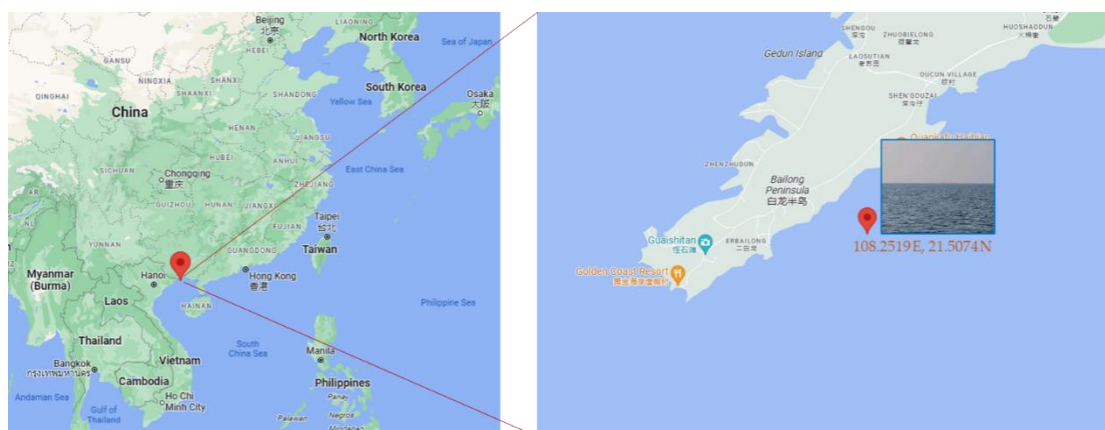


Figure S51. Map of location sites of sea sediment sample used in this study