

Supporting Information

Bioactive Bis(indole) Alkaloids from a *Spongosorites* sp. Sponge

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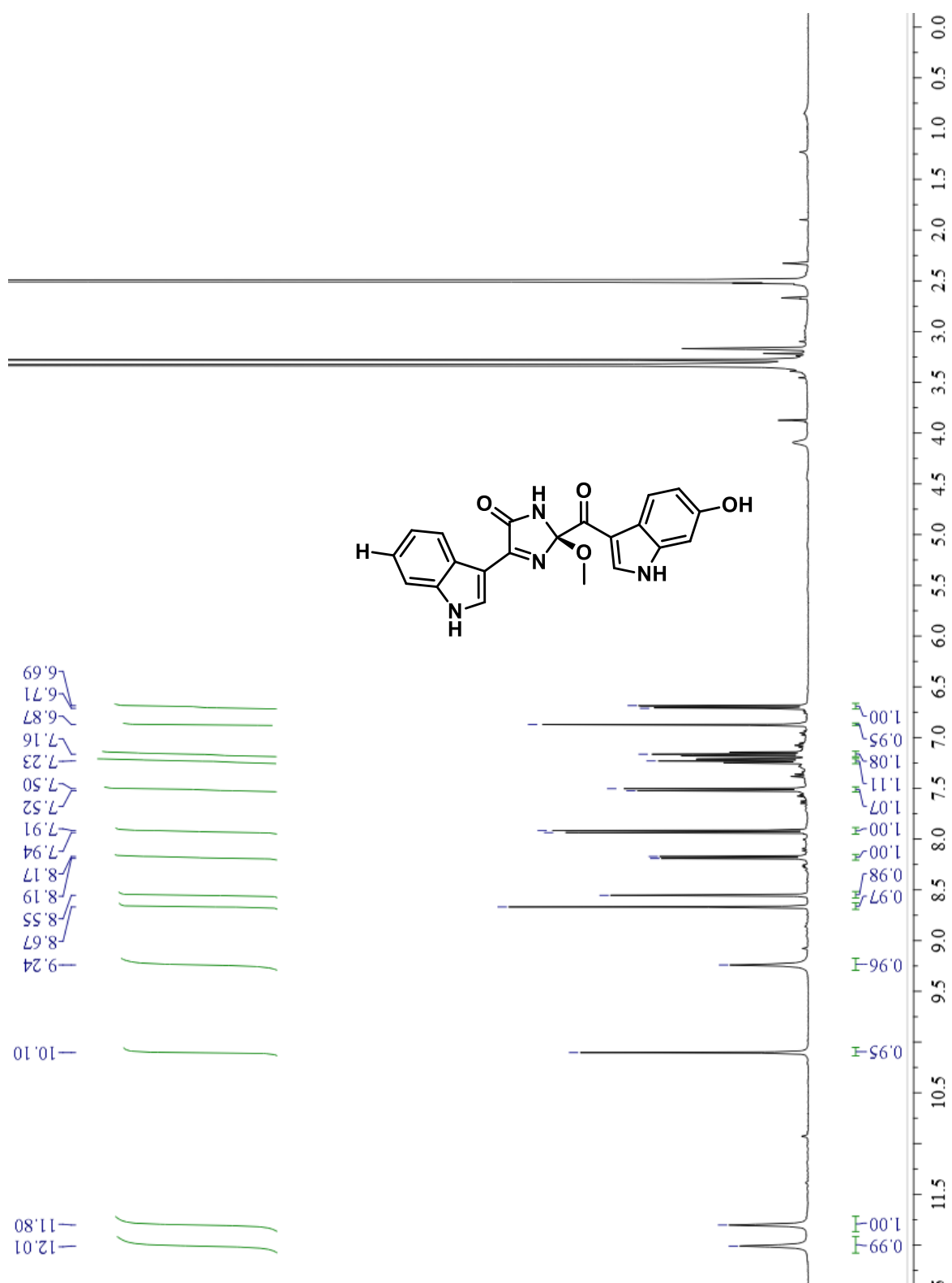


Figure S1. The ^1H NMR (800 MHz, $\text{DMSO-}d_6$) spectrum of **1**.

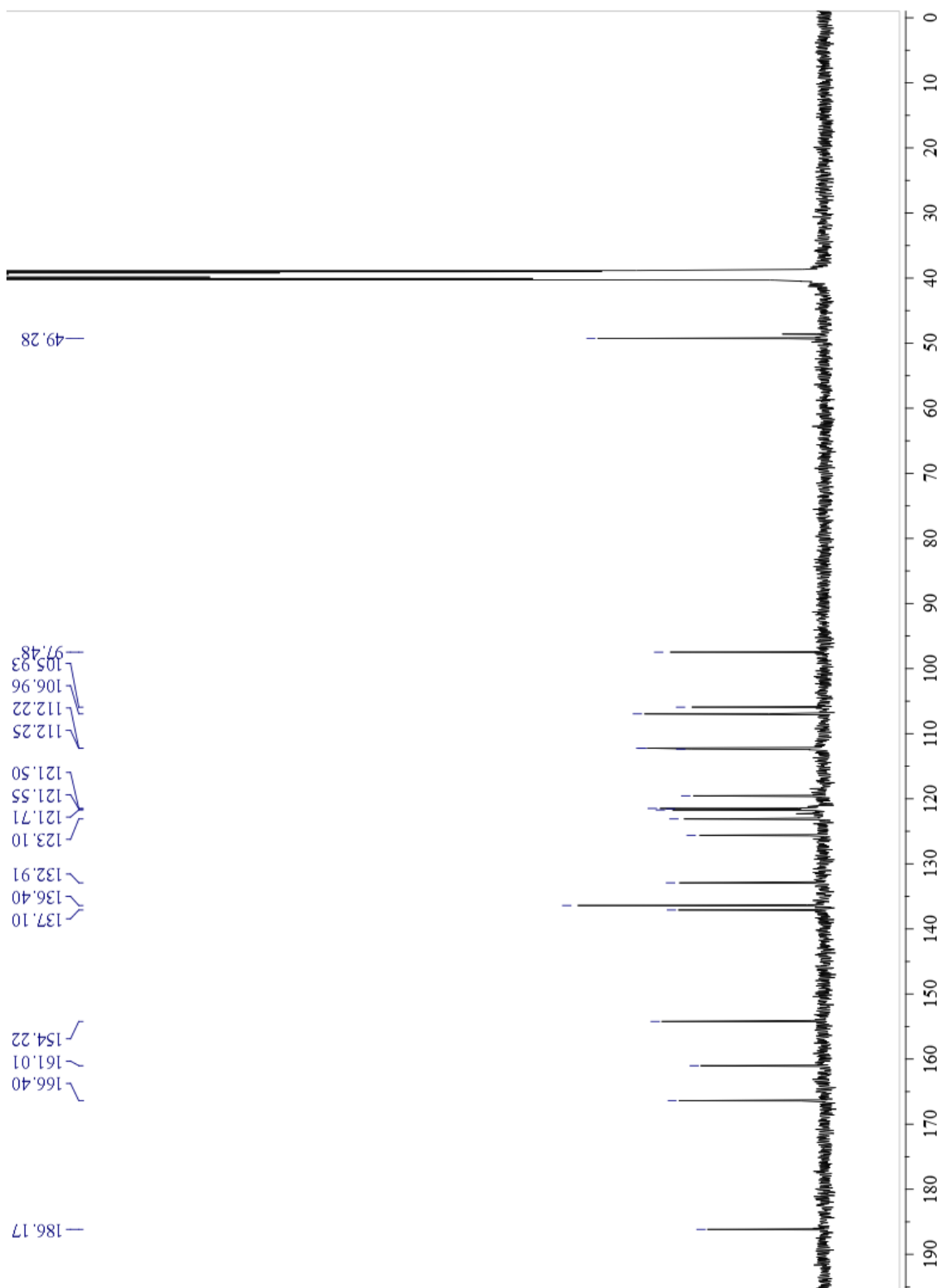


Figure S2. The ^{13}C NMR (200 MHz, $\text{DMSO-}d_6$) spectrum of **1**.

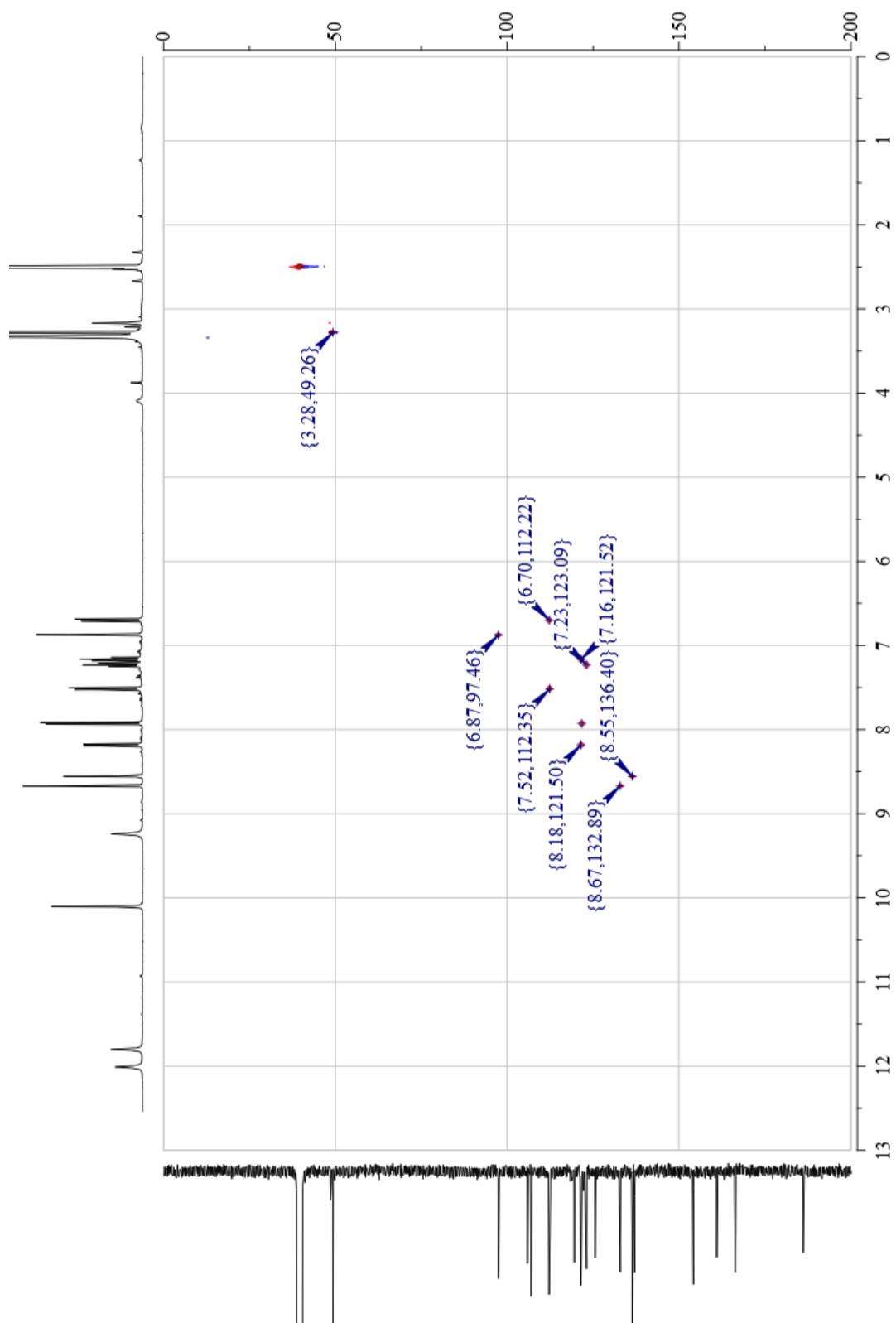


Figure S3. The HSQC (800 MHz, DMSO-*d*₆) spectrum of **1**.

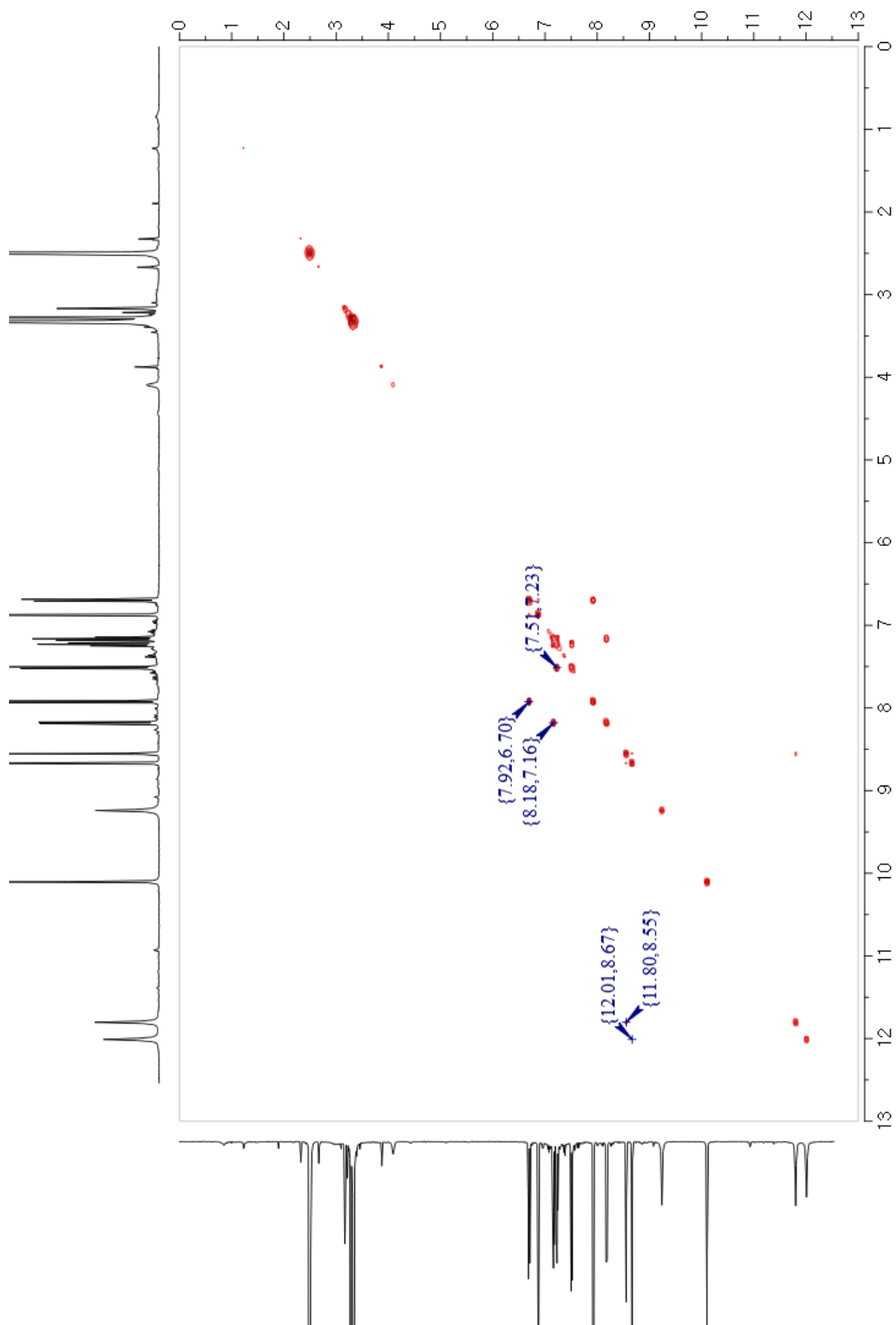


Figure S4. The COSY (800 MHz, DMSO-*d*₆) spectrum of **1**.

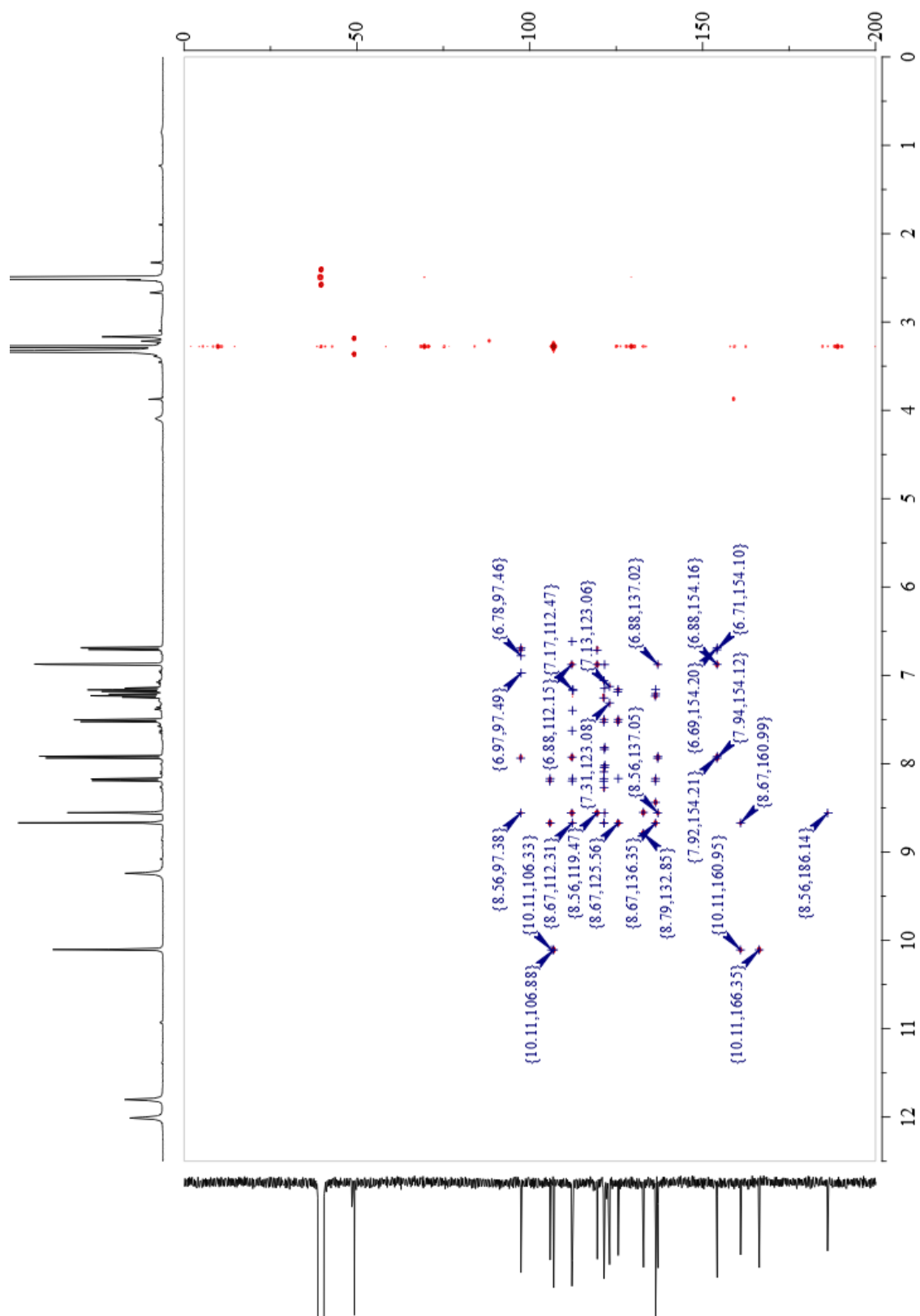


Figure S5. The HMBC (800 MHz, DMSO-*d*₆) spectrum of **1**.

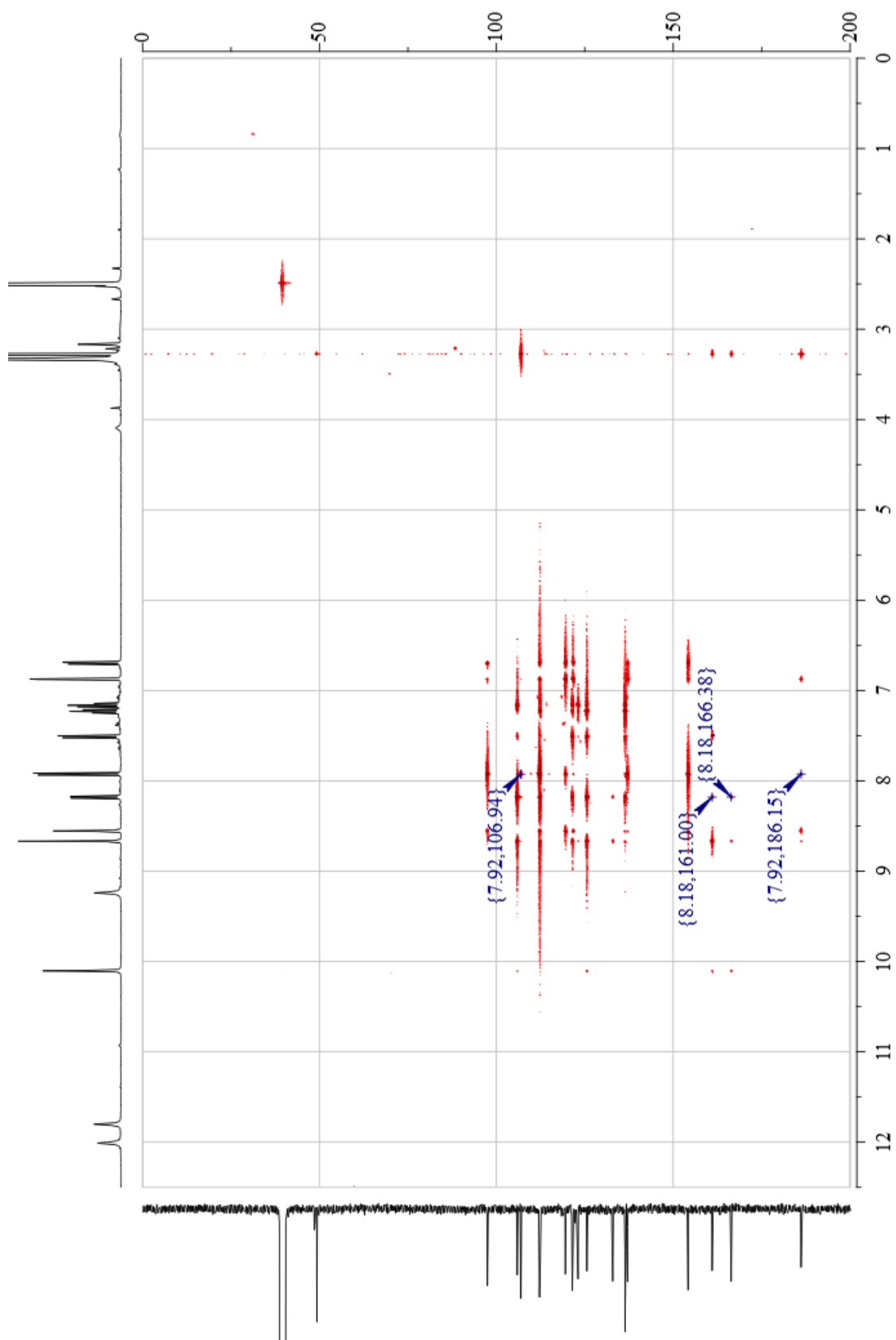


Figure S6. The LRHSQ-MBC at 2 Hz (800 MHz, DMSO-*d*₆) spectrum of **1**.

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
389.1248	5.1	+11.1 / +4.3	24.0	C 30 H 15 N
		-4.0 / -1.6	20.5	C 22 H 13 N 8
		-7.5 / -2.9	20.0	C 24 H 15 N 5 O
		-10.9 / -4.2	19.5	C 26 H 17 N 2 O 2
		+6.3 / +2.5	16.5	C 17 H 13 N 10 O 2
		+18.0 / +7.0	19.5	C 27 H 17 O 3
		+2.9 / +1.1	16.0	C 19 H 15 N 7 O 3
		-0.6 / -0.2	15.5	C 21 H 17 N 4 O 4
		-4.0 / -1.6	15.0	C 23 H 19 N O 5
		-19.1 / -7.4	11.5	C 15 H 17 N 8 O 5
		+13.2 / +5.1	12.0	C 14 H 15 N 9 O 5

[Theoretical Ion Distribution]

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Molecular Formula : C21 H17 N4 O4

(m/z 389.1250, MW 389.3904, U.S. 15.5)

Base Peak : 389.1250, Averaged MW : 389.3889(a), 389.3896(w)

m/z	INT.	
389.1250	100.0000	*****
390.1280	24.9787	*****
391.1306	3.7890	**
392.1331	0.4276	
393.1356	0.0387	
394.1381	0.0029	
395.1405	0.0002	

Figure S7. The HRFABMS data of **1**

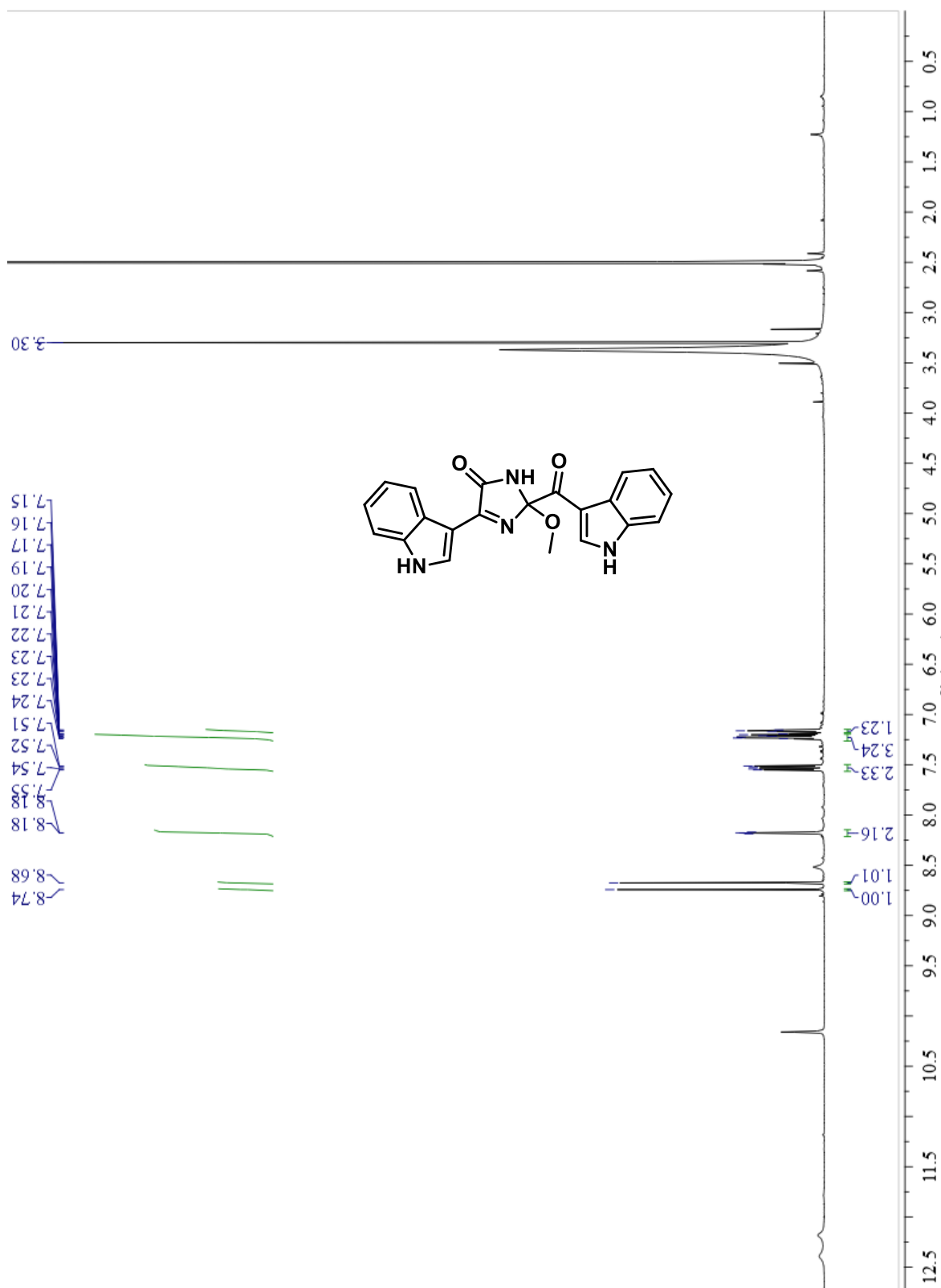


Figure S8. The ^1H NMR (800 MHz, $\text{DMSO-}d_6$) spectrum of **2**

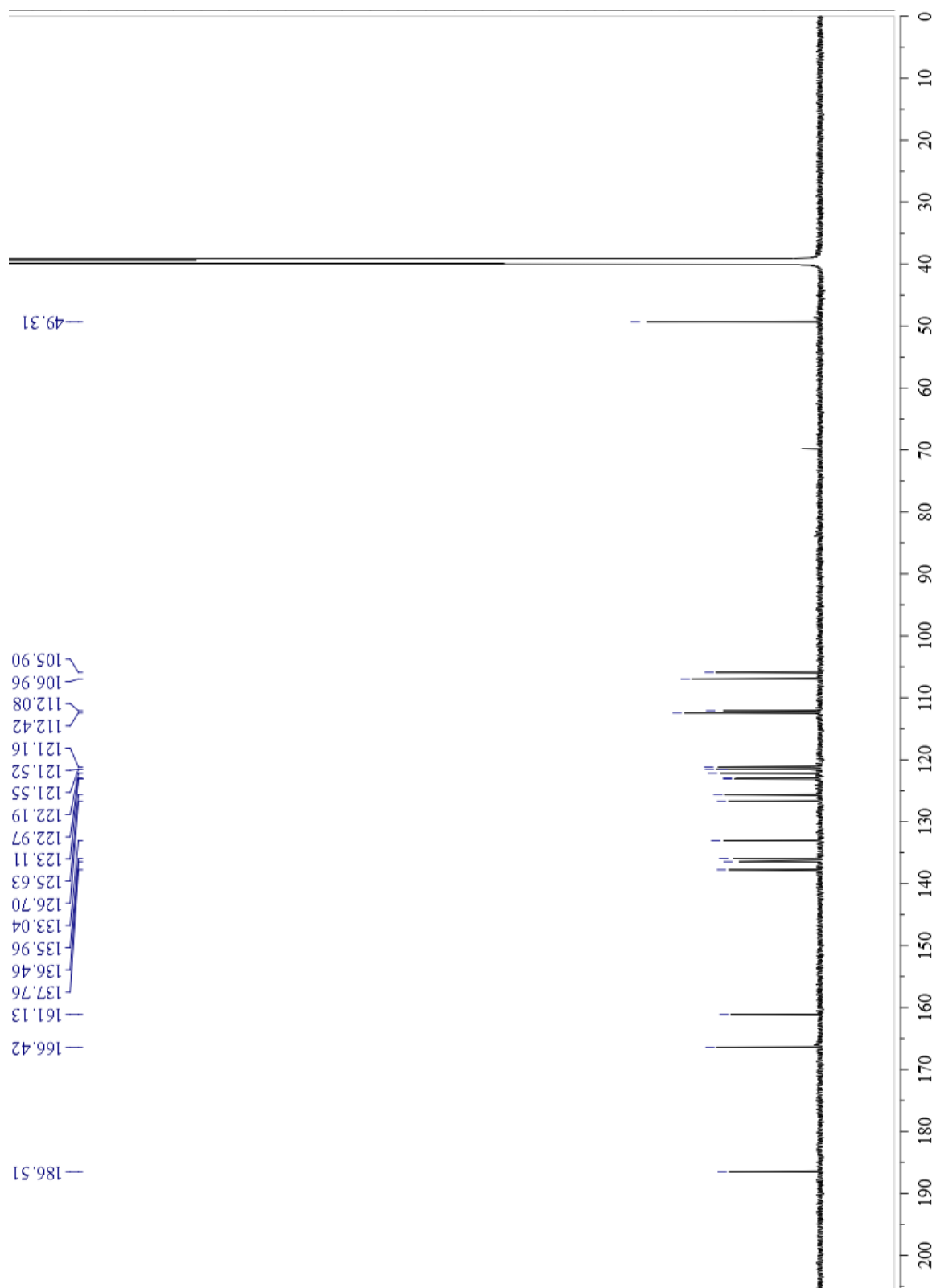


Figure S9. The ^{13}C NMR (200 MHz, $\text{DMSO-}d_6$) spectrum of **2**

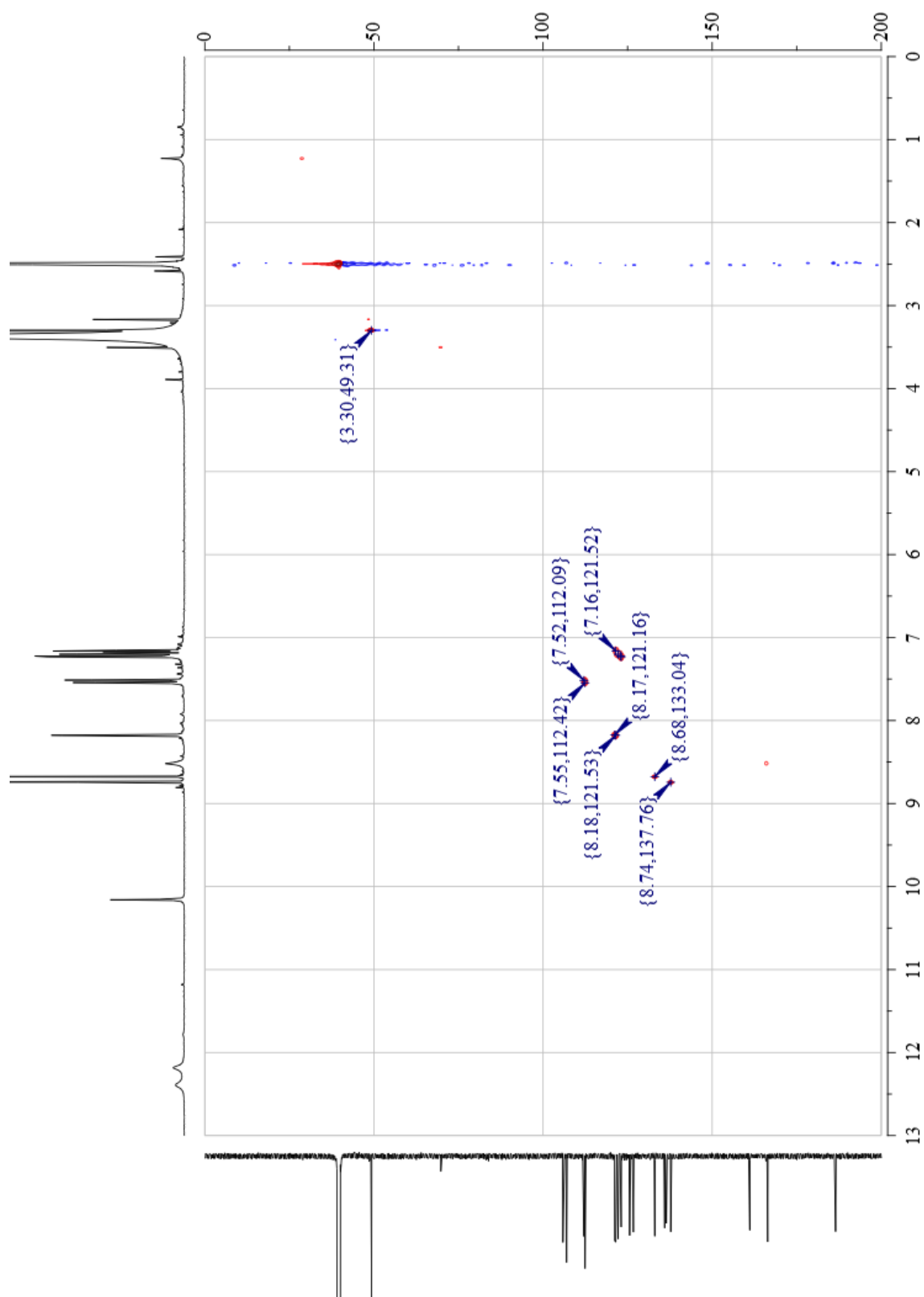


Figure S10. The HSQC spectrum (800 MHz, $\text{DMSO-}d_6$) spectrum of **2**

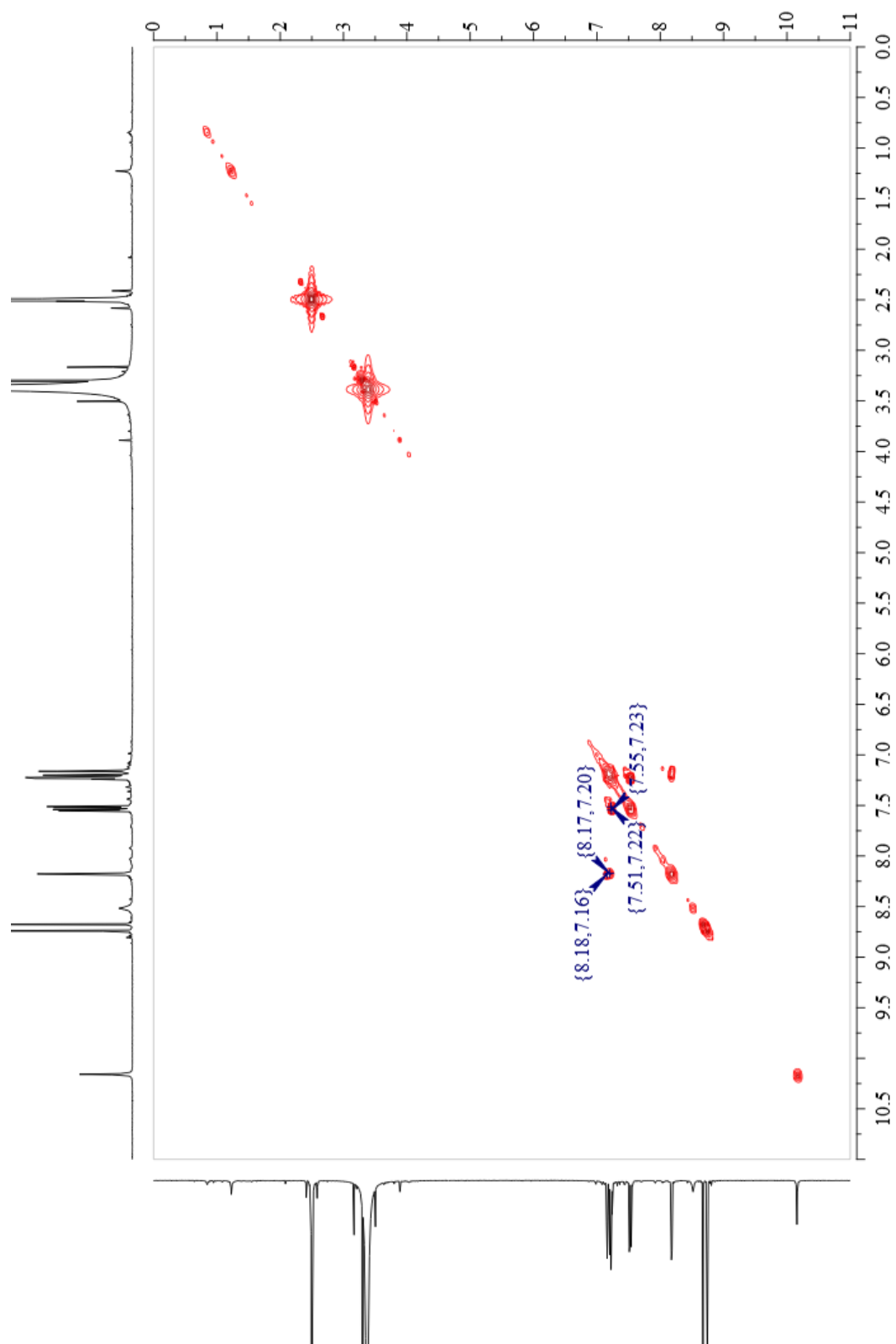


Figure S11. The COSY spectrum (800 MHz, DMSO-*d*₆) spectrum of **2**

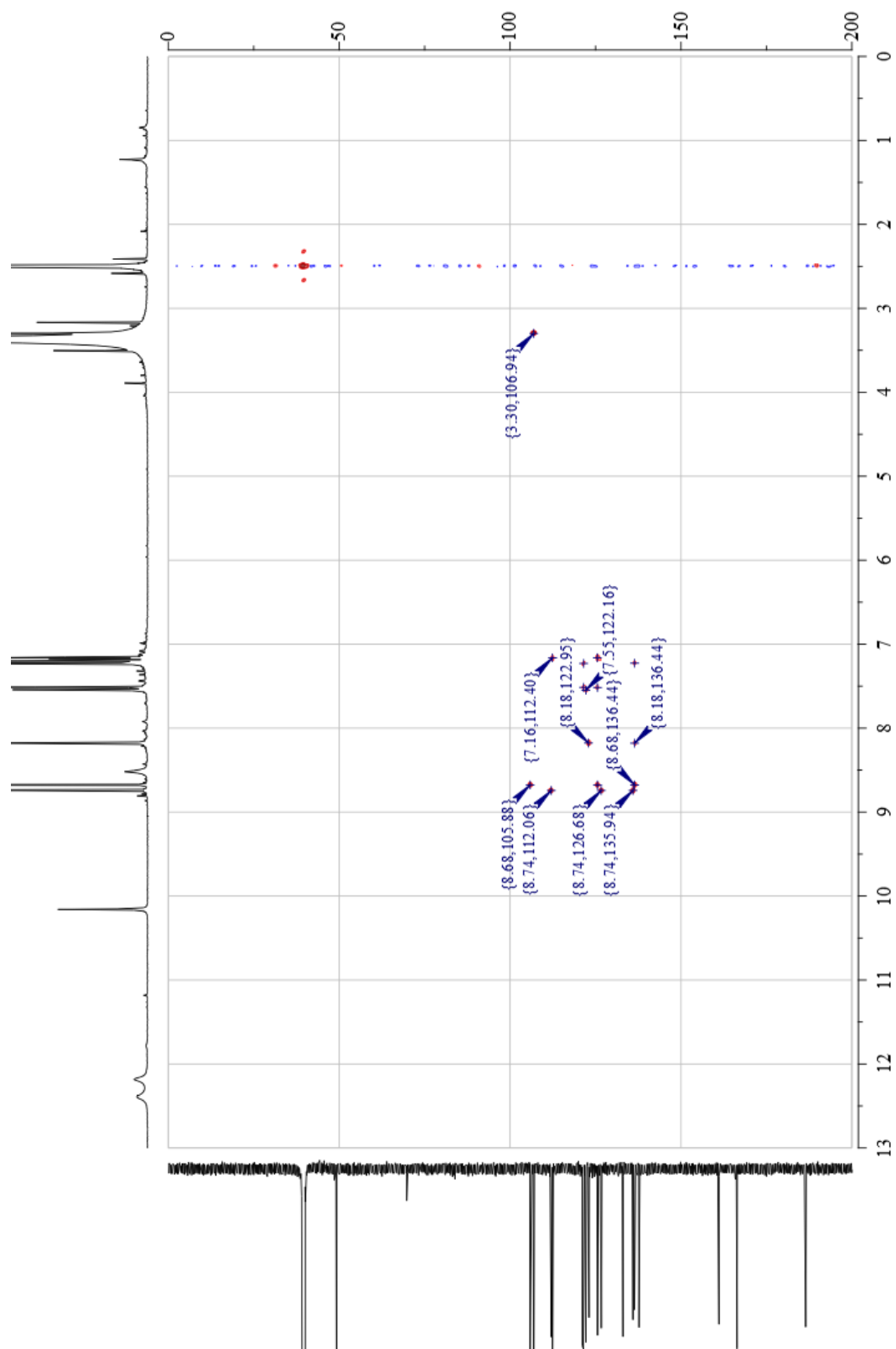


Figure S12. The HMBC spectrum (800 MHz, DMSO-*d*₆) spectrum of **2**

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
373.1303	5.0	-6.4 / -2.4	20.0	C 24 H 15 N 5
		-10.0 / -3.7	19.5	C 26 H 17 N 2 O
		+7.9 / +3.0	16.5	C 17 H 13 N 10 O
		+4.3 / +1.6	16.0	C 19 H 15 N 7 O 2
		+0.7 / +0.3	15.5	C 21 H 17 N 4 O 3
		-2.9 / -1.1	15.0	C 23 H 19 N O 4
		-18.6 / -6.9	11.5	C 15 H 17 N 8 O 4
		+15.1 / +5.6	12.0	C 14 H 15 N 9 O 4
		+11.5 / +4.3	11.5	C 16 H 17 N 6 O 5
		+7.9 / +3.0	11.0	C 18 H 19 N 3 O 6
		-7.8 / -2.9	7.5	C 10 H 17 N 10 O 6
		+4.3 / +1.6	10.5	C 20 H 21 O 7
		-11.4 / -4.3	7.0	C 12 H 19 N 7 O 7
		-15.0 / -5.6	6.5	C 14 H 21 N 4 O 8
		+18.7 / +7.0	7.0	C 13 H 19 N 5 O 8
		-18.6 / -6.9	6.0	C 16 H 23 N O 9
		+15.1 / +5.6	6.5	C 15 H 21 N 2 O 9
		-0.6 / -0.2	3.0	C 7 H 19 N 9 O 9
		-4.2 / -1.6	2.5	C 9 H 21 N 6 O 10

[Theoretical Ion Distribution]

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Molecular Formula : C21 H17 N4 O3

(m/z 373.1301, MW 373.3910, U.S. 15.5)

Base Peak : 373.1301, Averaged MW : 373.3896(a), 373.3903(w)

m/z	INT.	
373.1301	100.0000	*****
374.1331	24.9406	*****
375.1357	3.5790	**
376.1383	0.3762	
377.1408	0.0314	
378.1433	0.0022	
379.1459	0.0001	

Figure S13. The HRFABMS data of 2

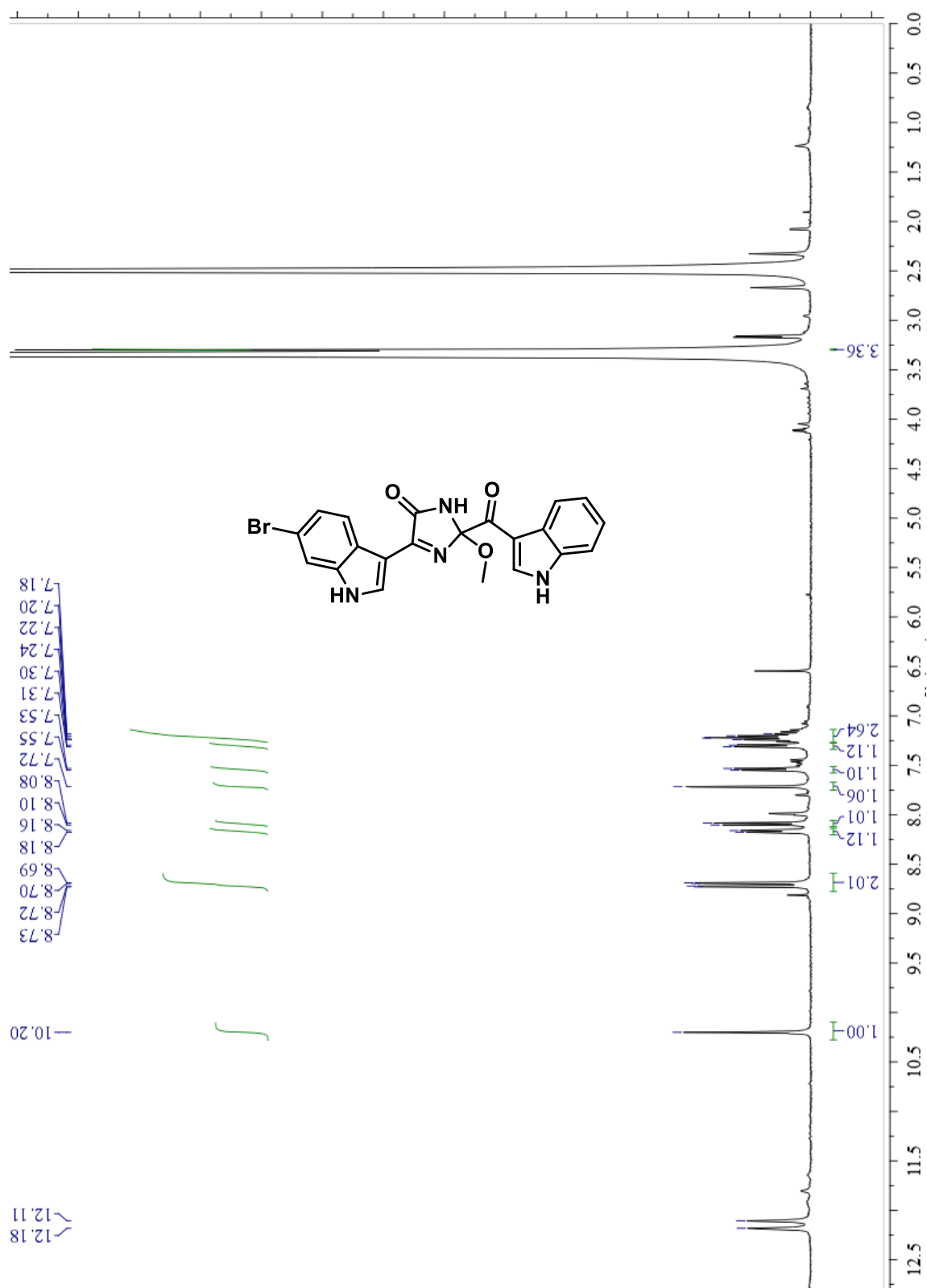


Figure S14. The ¹H NMR (800 MHz, DMSO-*d*₆) spectrum of **3**

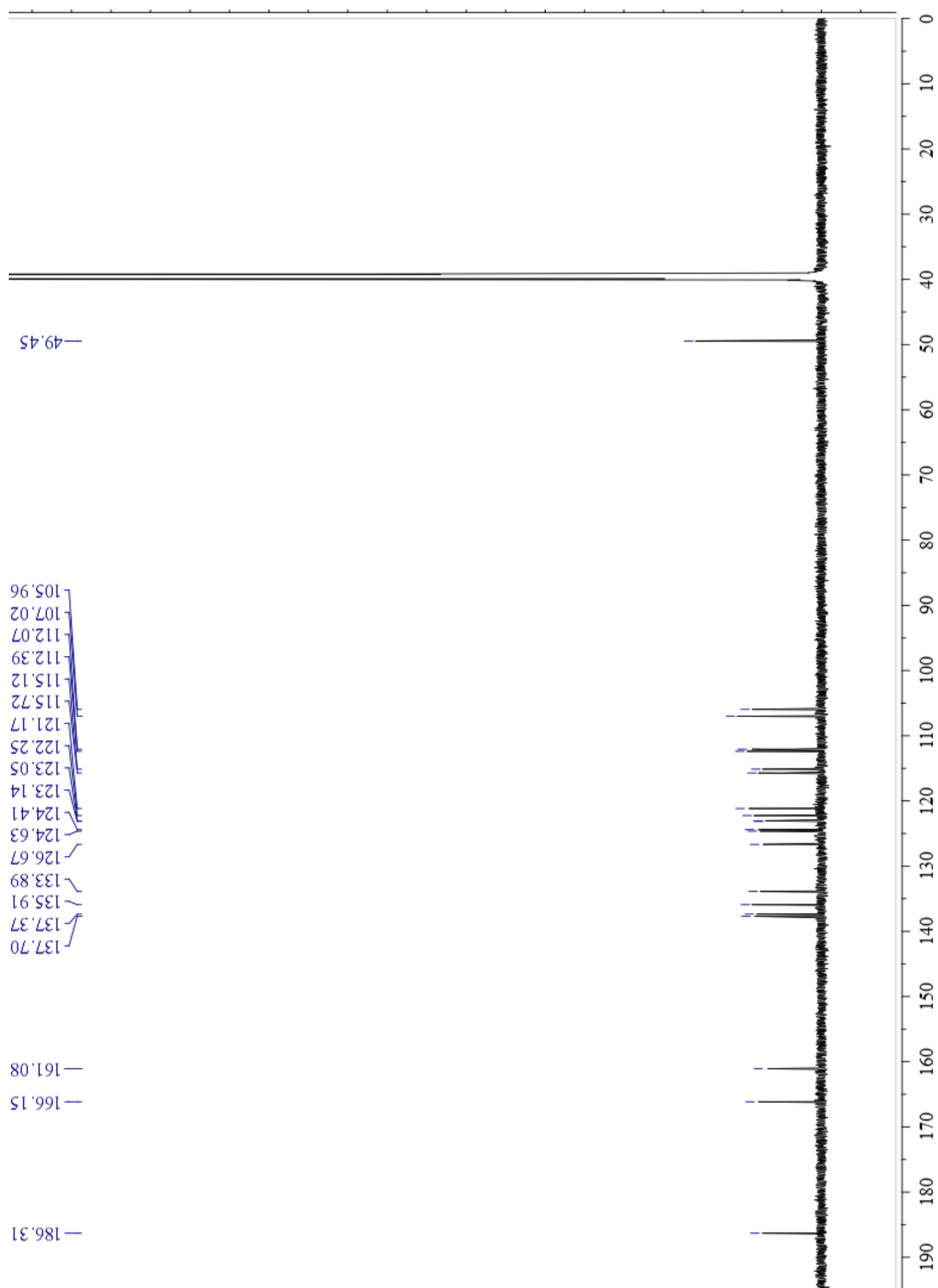


Figure S15. The ^{13}C NMR (200 MHz, $\text{DMSO-}d_6$) spectrum of **3**

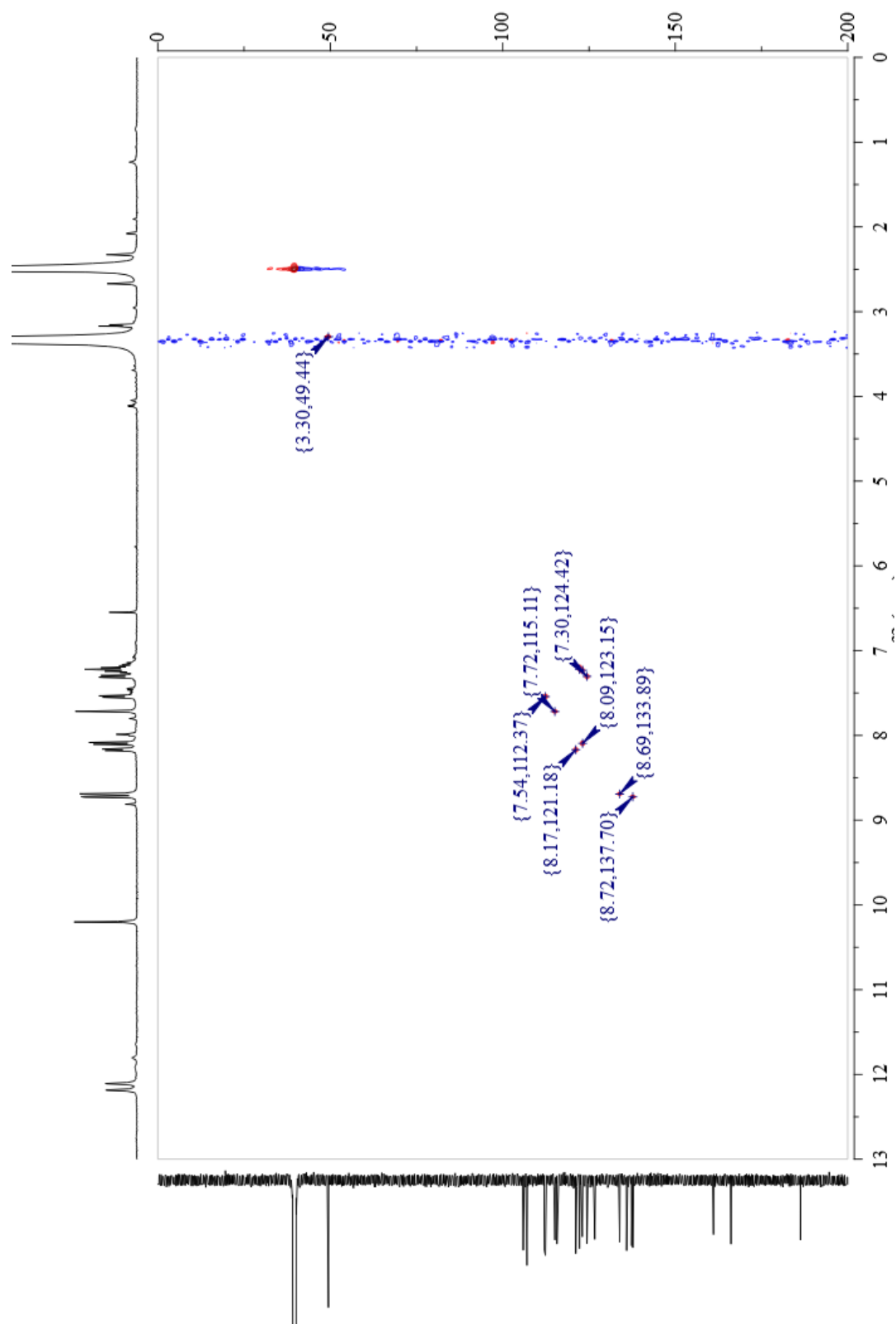


Figure S16. The HSQC (800 MHz, DMSO-*d*₆) spectrum of **3**

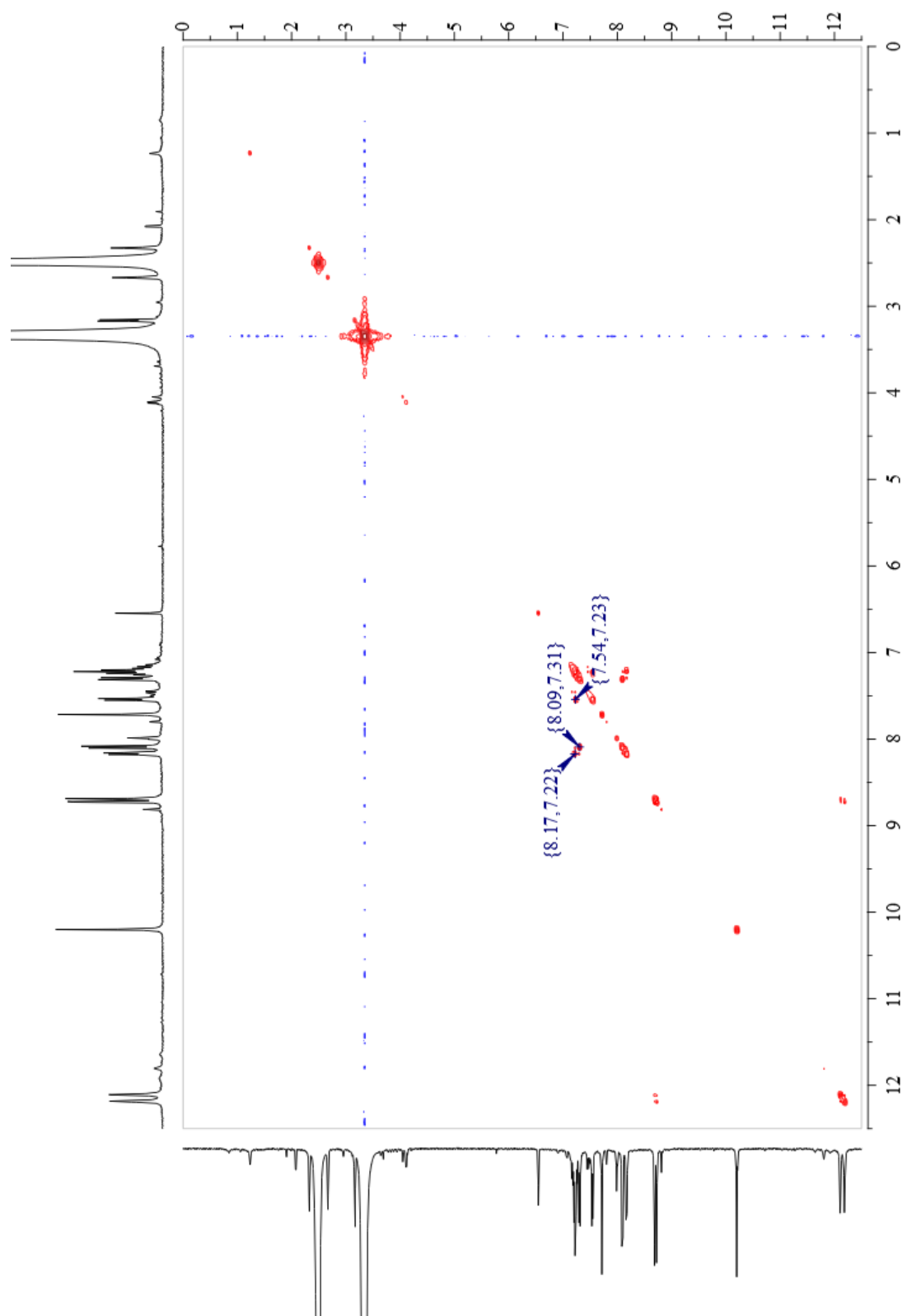


Figure S17. The COSY (800 MHz, DMSO-*d*₆) spectrum of **3**

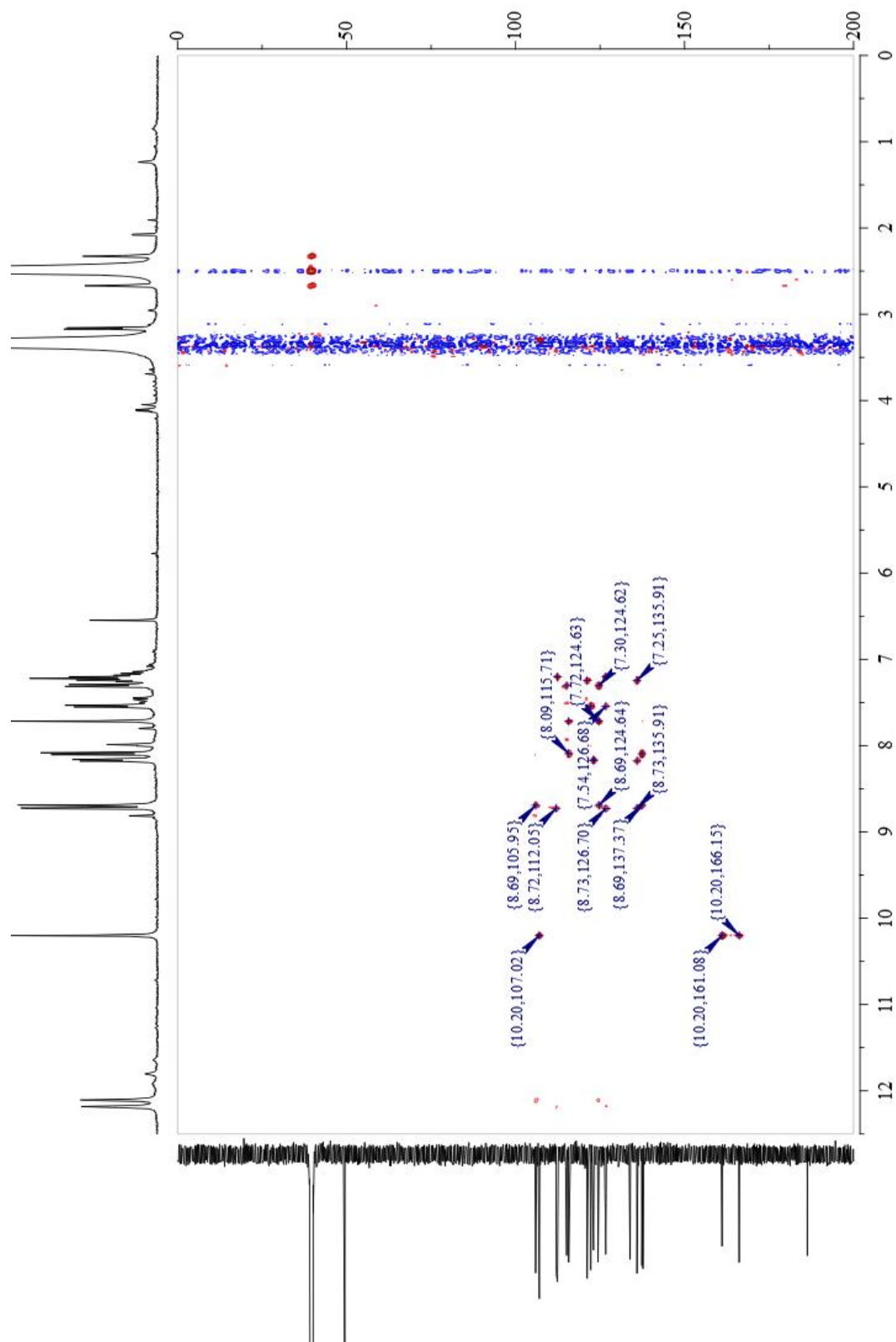


Figure S18. The HMBC (800 MHz, DMSO-*d*₆) spectrum of **3**

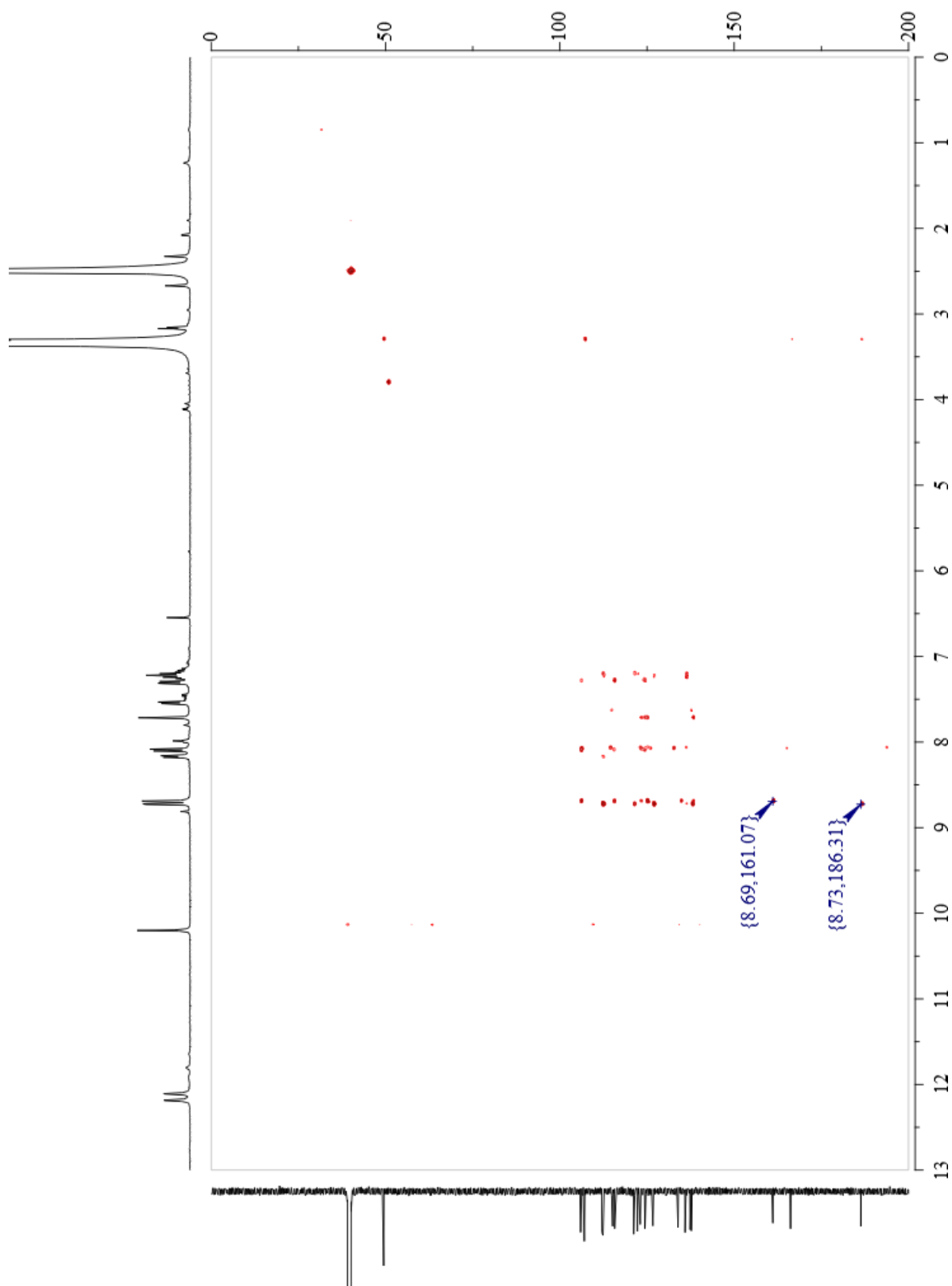


Figure S19. The dHMBC at 2Hz (800 MHz, DMSO-*d*₆) spectrum of **3**

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
1	451.0413	4.07	-10.2 / -4.6	8.5 C22 H27 79Br 81Br
2			+17.7 / +8.0	9.0 C21 H25 79Br 81Br N
3			-20.9 / -9.4	20.0 C26 H16 81Br N3
4			-4.3 / -2.0	20.0 C24 H14 79Br N5
5			+4.0 / +1.8	20.0 C27 H16 81Br N O
6			-7.3 / -3.3	19.5 C26 H16 79Br N2 O
7			+20.6 / +9.3	20.0 C25 H14 79Br N3 O
8			+1.7 / +0.8	5.0 C15 H25 79Br 81Br N5 O
9			+17.6 / +7.9	19.5 C27 H16 79Br O2
10			-1.3 / -0.6	4.5 C17 H27 79Br 81Br N2 O2
11			-11.9 / -5.4	16.0 C21 H16 81Br N5 O2
12			-14.9 / -6.7	15.5 C23 H18 81Br N2 O3
13			+13.0 / +5.8	16.0 C22 H16 81Br N3 O3
14			+1.6 / +0.7	15.5 C21 H16 79Br N4 O3
15			+10.0 / +4.5	15.5 C24 H18 81Br O4
16			-1.4 / -0.6	15.0 C23 H18 79Br N O4
17			-20.2 / -9.1	0.0 C13 H29 79Br 81Br N3 O4
18			+7.6 / +3.4	0.5 C12 H27 79Br 81Br N4 O4
19			+4.7 / +2.1	0.0 C14 H29 79Br 81Br N O5
20			-6.0 / -2.7	11.5 C18 H18 81Br N4 O5
21			-17.4 / -7.8	11.0 C17 H18 79Br N5 O5
22			+21.9 / +9.9	12.0 C17 H16 81Br N5 O5

[Theoretical Ion Distribution]

Molecular Formula : C21 H16 Br N4 O3

(m/z 451.0406, MW 452.2870, U.S. 15.5)

Base Peak : 453.0388, Averaged MW : 452.2853(a), 452.2881(w)

m/z	INT.
451.0406	99.1507*****
452.0436	24.7288*****
453.0388	100.0000*****
454.0416	24.4286*****
455.0443	3.4831**
456.0468	0.3650
457.0493	0.0304
458.0518	0.0021
459.0543	0.0001

Figure S20. The HRFABMS data of **3**

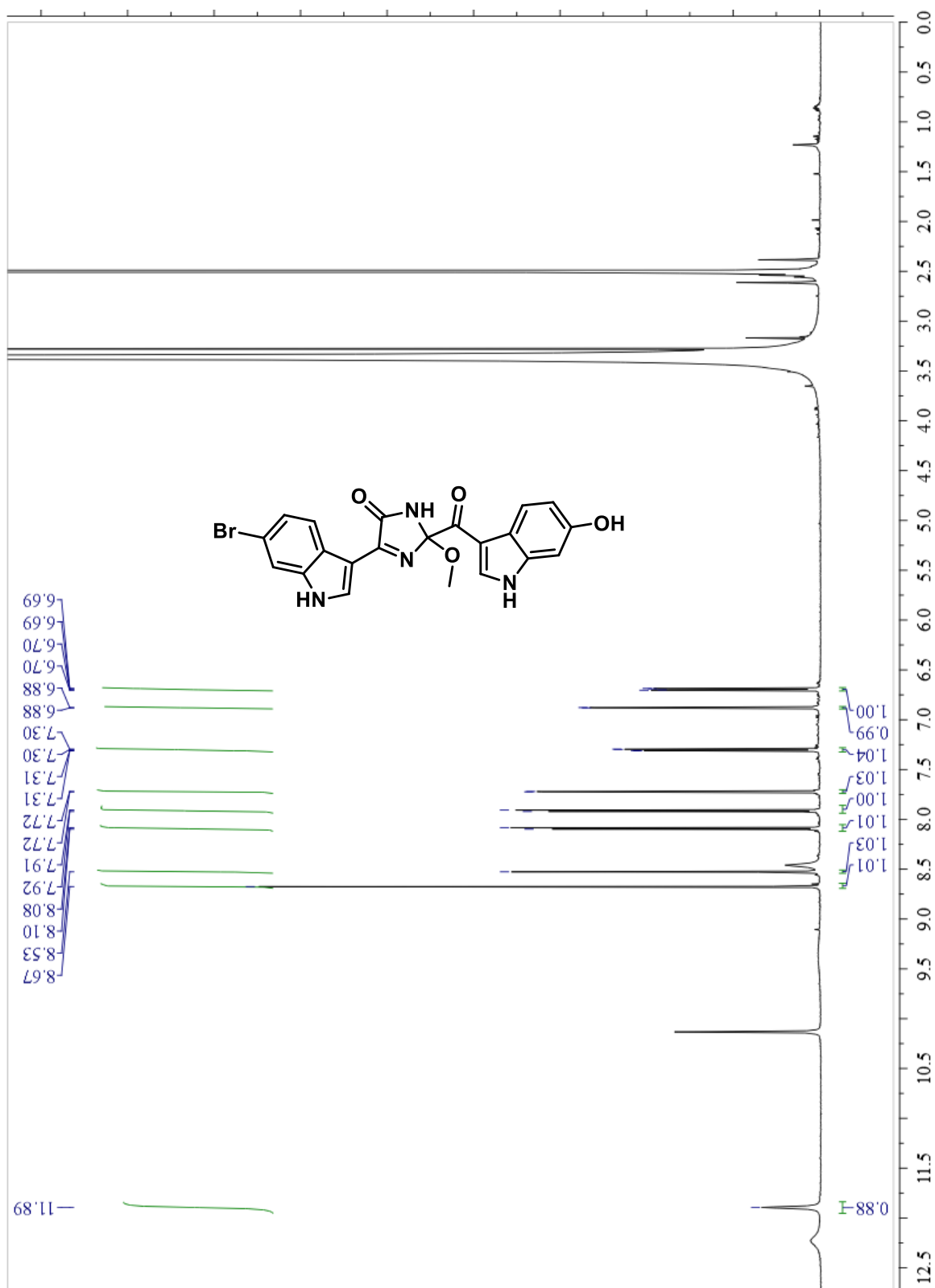


Figure S21. The ¹H NMR (800 MHz, DMSO-*d*₆) spectrum of **4**

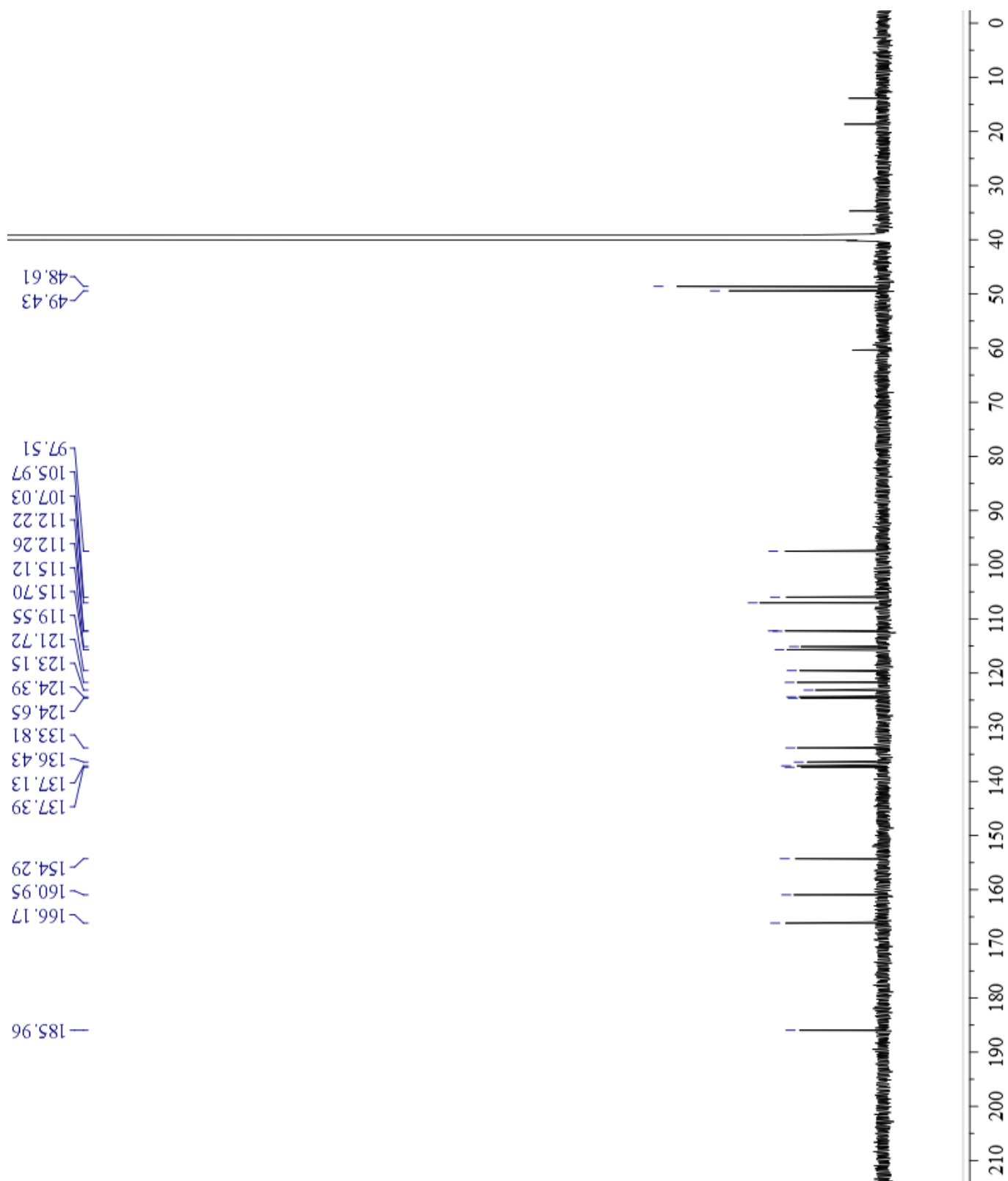


Figure S22. The ^{13}C NMR (200 MHz, $\text{DMSO-}d_6$) spectrum of **4**

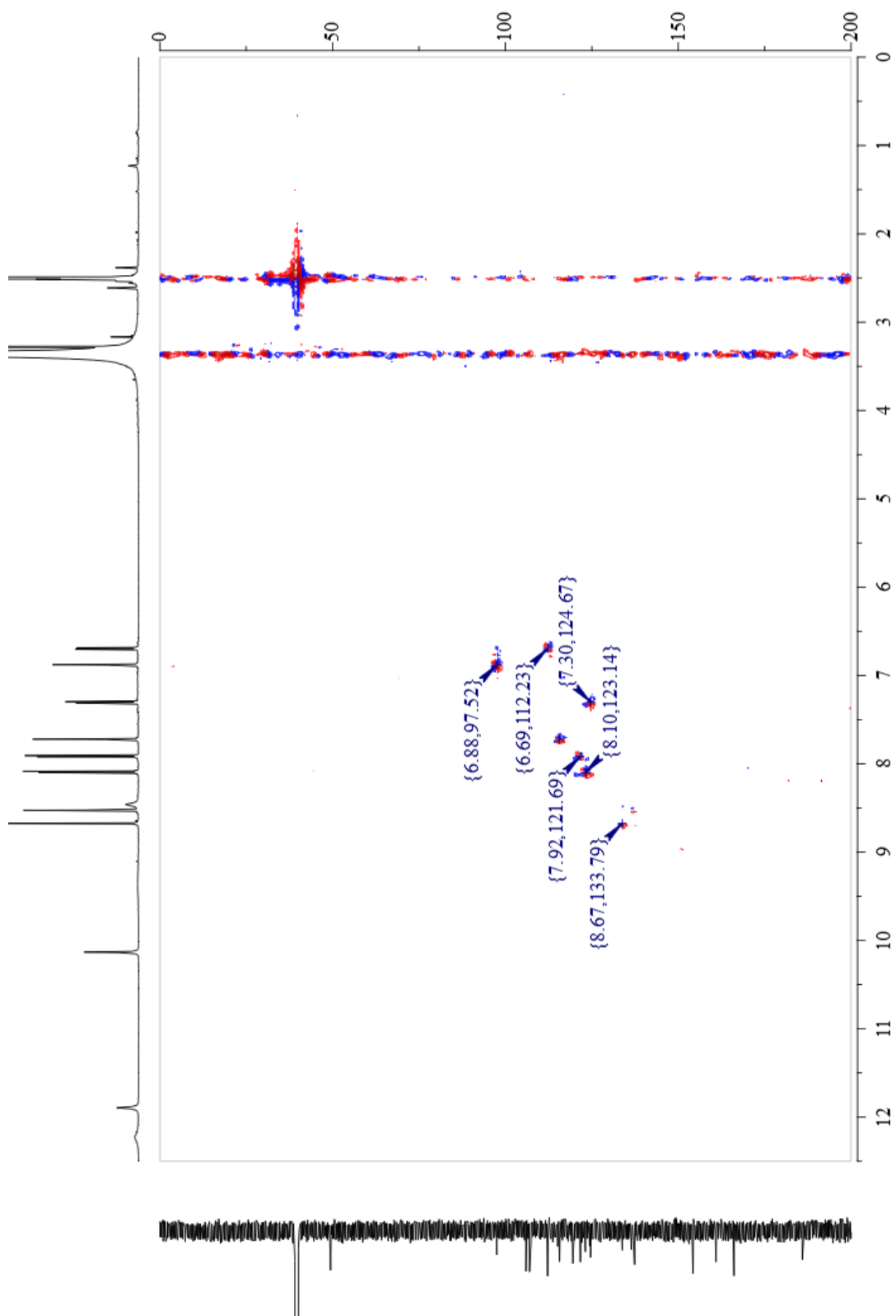


Figure S23. The HSQC (800 MHz, DMSO-*d*₆) spectrum of **4**

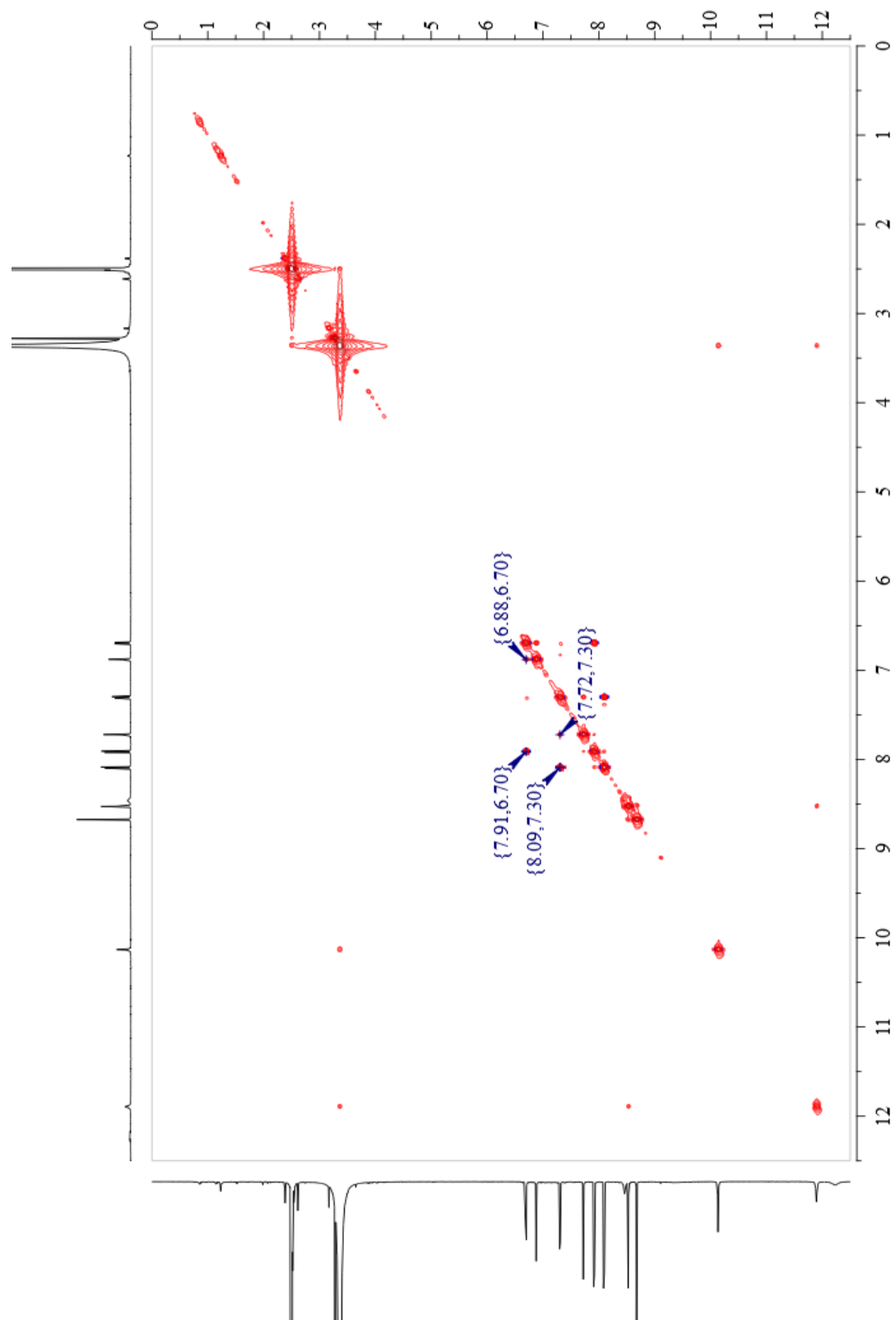


Figure S24. The COSY (800 MHz, DMSO-*d*6) spectrum of **4**

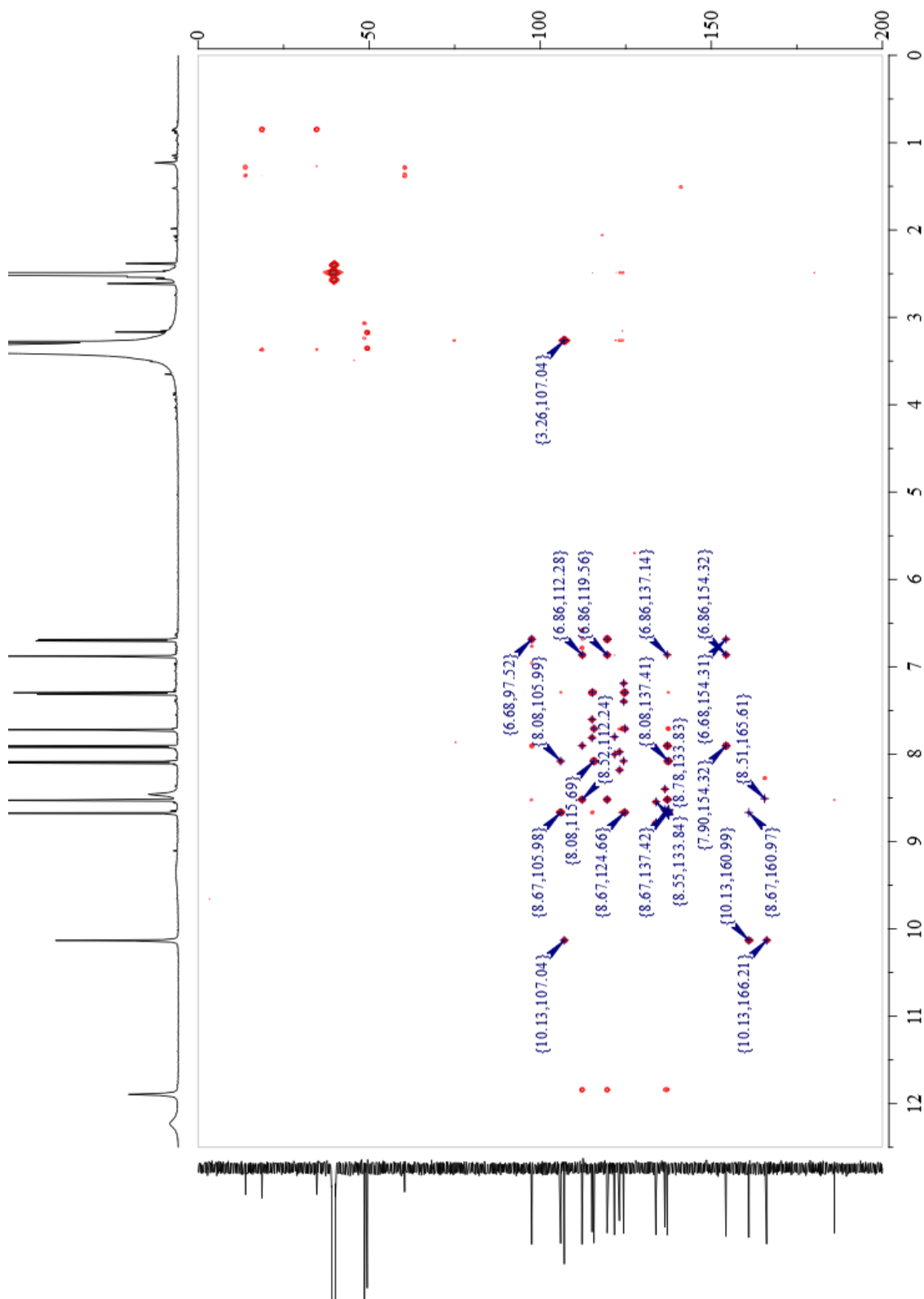


Figure S25. The HMBC (800 MHz, DMSO-*d*₆) spectrum of **4**

Observed m/z Int%		467.0351 2.2							
Err [ppm / mmu]	U.S.	Composition							
-18.0 / -8.4	23.5	C 31	H 16 79Br	-9.5 / +4.4	4.0	C 17	H 27 79Br 2 N O 4		
+19.9 / +9.3	24.5	C 31	H 14 81Br	-16.7 / -7.8	15.5	C 23	H 18 81Br N 2 O 4		
+8.9 / +4.2	24.0	C 30	H 14 79Br N	+10.2 / +4.8	16.0	C 22	H 16 81Br N 3 O 4		
+1.7 / +0.8	9.5	C 21	H 25 81Br 2 N 2	-0.8 / -0.4	15.5	C 21	H 16 79Br N 4 O 4		
-9.3 / -4.3	9.0	C 20	H 25 79Br 81Br N 3	-8.0 / -3.8	1.0	C 12	H 27 81Br 2 N 5 O 4		
-1.4 / -0.6	35.5	C 34	H 3 N 4	-19.0 / -8.9	0.5	C 11	H 27 79Br 81Br N 6 O 4		
+17.6 / +8.2	9.5	C 19	H 23 79Br 81Br N 4	+18.9 / +8.8	1.5	C 11	H 25 81Br 2 N 6 O 4		
+6.7 / +3.1	9.0	C 18	H 23 79Br 2 N 5	-11.1 / -5.2	27.0	C 25	H 5 N 7 O 4		
-19.6 / -9.2	20.5	C 24	H 14 81Br N 6	+7.9 / +3.7	1.0	C 10	H 25 79Br 81Br N 7 O 4		
+7.3 / +3.4	21.0	C 23	H 12 81Br N 7	+15.8 / +7.4	27.5	C 24	H 3 N 8 O 4		
-3.6 / -1.7	20.5	C 22	H 12 79Br N 8	-3.0 / -1.4	0.5	C 9	H 25 79Br 2 N 8 O 4		
-10.9 / -5.1	6.0	C 13	H 23 81Br 2 N 9	-2.4 / -1.1	12.5	C 14	H 14 81Br N 10 O 4		
+16.0 / +7.5	6.5	C 12	H 21 81Br 2 N 10	+7.3 / +3.4	15.5	C 24	H 18 81Br O 5		
-12.2 / -5.7	8.5	C 22	H 27 79Br 81Br O	-3.7 / -1.7	15.0	C 23	H 18 79Br N O 5		
-4.3 / -2.0	35.0	C 36	H 5 N O	-10.9 / -5.1	0.5	C 14	H 29 81Br 2 N 2 O 5		
+14.7 / +6.9	9.0	C 21	H 25 79Br 81Br N O	+16.0 / +7.5	1.0	C 13	H 27 81Br 2 N 3 O 5		
+3.8 / +1.8	8.5	C 20	H 25 79Br 2 N 2 O	-14.0 / -6.5	26.5	C 27	H 7 N 4 O 5		
+4.4 / +2.1	20.5	C 25	H 14 81Br N 4 O	+5.0 / +2.4	0.5	C 12	H 27 79Br 81Br N 4 O 5		
-6.5 / -3.0	20.0	C 24	H 14 79Br N 5 O	+13.0 / +6.1	27.0	C 26	H 5 N 5 O 5		
-13.8 / -6.4	5.5	C 15	H 25 81Br 2 N 6 O	-5.9 / -2.8	0.0	C 11	H 27 79Br 2 N 5 O 5		
+13.1 / +6.1	6.0	C 14	H 23 81Br 2 N 7 O	-5.3 / -2.5	12.0	C 16	H 16 81Br N 7 O 5		
-16.8 / -7.9	31.5	C 28	H 3 N 8 O	-16.2 / -7.6	11.5	C 15	H 16 79Br N 8 O 5		
+2.2 / +1.0	5.5	C 13	H 23 79Br 81Br N 8 O	+10.7 / +5.0	12.0	C 14	H 14 79Br N 9 O 5		
+10.1 / +4.7	32.0	C 27	H N 9 O	+13.1 / +6.1	0.5	C 15	H 29 81Br 2 O 6		
-8.8 / -4.1	5.0	C 12	H 23 79Br 2 N 9 O	-16.8 / -7.9	26.0	C 29	H 9 N O 6		
+18.1 / +8.5	5.5	C 11	H 21 79Br 2 N 10 O	+2.2 / +1.0	0.0	C 14	H 29 79Br 81Br N O 6		
+1.6 / +0.7	20.0	C 27	H 16 81Br N O 2	+10.1 / +4.7	26.5	C 28	H 7 N 2 O 6		
-9.4 / -4.4	19.5	C 26	H 16 79Br N 2 O 2	-8.8 / -4.1	-0.5	C 13	H 29 79Br 2 N 2 O 6		
+17.5 / +8.2	20.0	C 25	H 14 79Br N 3 O 2	+18.1 / +8.5	0.0	C 12	H 27 79Br 2 N 3 O 6		
-16.7 / -7.8	5.0	C 17	H 27 81Br 2 N 3 O 2	-8.1 / -3.8	11.5	C 18	H 18 81Br N 4 O 6		
+10.3 / +4.8	5.5	C 16	H 25 81Br 2 N 4 O 2	-19.1 / -8.9	11.0	C 17	H 18 79Br N 5 O 6		
-19.7 / -9.2	31.0	C 30	H 5 N 5 O 2	+18.8 / +8.8	12.0	C 17	H 16 81Br N 5 O 6		
-0.7 / -0.3	5.0	C 15	H 25 79Br 81Br N 5 O 2	+7.8 / +3.7	11.5	C 16	H 16 79Br N 6 O 6		
+7.2 / +3.4	31.5	C 29	H 3 N 6 O 2	-2.5 / -1.2	23.0	C 20	H 5 N 9 O 6		
-11.7 / -5.4	4.5	C 14	H 25 79Br 2 N 6 O 2	+15.3 / +7.1	-0.5	C 14	H 29 79Br 2 O 7		
+15.3 / +7.1	5.0	C 13	H 23 79Br 2 N 7 O 2	-11.0 / -5.1	11.0	C 20	H 20 81Br N O 7		
-11.0 / -5.1	16.5	C 19	H 14 81Br N 8 O 2	+15.9 / +7.4	11.5	C 19	H 18 81Br N 2 O 7		
+15.9 / +7.4	17.0	C 18	H 12 81Br N 9 O 2	+5.0 / +2.3	11.0	C 18	H 18 79Br N 3 O 7		
+5.0 / +2.3	16.5	C 17	H 12 79Br N 10 O 2	-5.3 / -2.5	22.5	C 22	H 7 N 6 O 7		
+14.7 / +6.8	19.5	C 27	H 16 79Br O 3	+3.4 / +1.6	8.0	C 11	H 16 81Br N 9 O 7		
-19.5 / -9.1	4.5	C 19	H 29 81Br 2 O 3	-7.6 / -3.6	7.5	C 10	H 16 79Br N 10 O 7		
+7.4 / +3.5	5.0	C 18	H 27 81Br 2 N O 3	+2.1 / +1.0	10.5	C 20	H 20 79Br O 8		
-3.6 / -1.7	4.5	C 17	H 27 79Br 81Br N 2 O 3	-8.2 / -3.8	22.0	C 24	H 9 N 3 O 8		
+4.4 / +2.0	31.0	C 31	H 5 N 3 O 3	+18.7 / +8.7	22.5	C 23	H 7 N 4 O 8		
-14.5 / -6.8	4.0	C 16	H 27 79Br 2 N 3 O 3	+0.5 / +0.2	7.5	C 13	H 18 81Br N 6 O 8		
+12.4 / +5.8	4.5	C 15	H 25 79Br 2 N 4 O 3	-10.5 / -4.9	7.0	C 12	H 18 79Br N 7 O 8		
-13.9 / -6.5	16.0	C 21	H 16 81Br N 5 O 3	+16.4 / +7.7	7.5	C 11	H 16 79Br N 8 O 8		
+13.1 / +6.1	16.5	C 20	H 14 81Br N 6 O 3	-11.1 / -5.2	21.5	C 26	H 11 O 9		
+2.1 / +1.0	16.0	C 19	H 14 79Br N 7 O 3	+15.8 / +7.4	22.0	C 25	H 9 N O 9		
-5.2 / -2.4	1.5	C 10	H 25 81Br 2 N 8 O 3	-2.4 / -1.1	7.0	C 15	H 20 81Br N 3 O 9		
-16.1 / -7.5	1.0	C 9	H 25 79Br 81Br N 9 O 3	-13.4 / -6.2	6.5	C 14	H 20 79Br N 4 O 9		
-8.2 / -3.8	27.5	C 23	H 3 N 10 O 3	+13.6 / +6.3	7.0	C 13	H 18 79Br N 5 O 9		
+10.8 / +5.0	1.5	C 8	H 23 79Br 81Br N 10 O 3	+3.3 / +1.5	18.5	C 17	H 7 N 8 O 9		
+1.5 / +0.7	30.5	C 33	H 7 O 4	-15.0 / -7.0	3.5	C 7	H 18 81Br N 10 O 9		
-17.4 / -8.1	3.5	C 18	H 29 79Br 2 O 4	-5.3 / -2.5	6.5	C 17	H 22 81Br N O 10		
				-16.2 / -7.6	6.0	C 16	H 22 79Br N O 10		
				+10.7 / +5.0	6.5	C 15	H 20 79Br N 2 O 10		
				+0.4 / +0.2	18.0	C 19	H 9 N 5 O 10		
				-17.8 / -8.3	3.0	C 9	H 20 81Br N 7 O 10		
				+9.1 / +4.2	3.5	C 8	H 18 81Br N 8 O 10		
				-1.9 / -0.9	3.0	C 7	H 18 79Br N 9 O 10		

[Theoretical Ion Distribution]

Molecular Formula : C21 H16 Br N4 O4

(m/z 467.0355, MW 468.2864, U.S. 15.5)

Base Peak : 469.0337, Averaged MW : 468.2846(a), 468.2873(w)

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m/z	INT.	
467.0355	98.9447	*****
468.0385	24.7151	*****
469.0337	100.0000	*****
470.0366	24.4653	*****
471.0391	3.6852	**
472.0416	0.4145	
473.0441	0.0374	
474.0465	0.0028	
475.0490	0.0002	

Figure S26. The HRFABMS data of 4

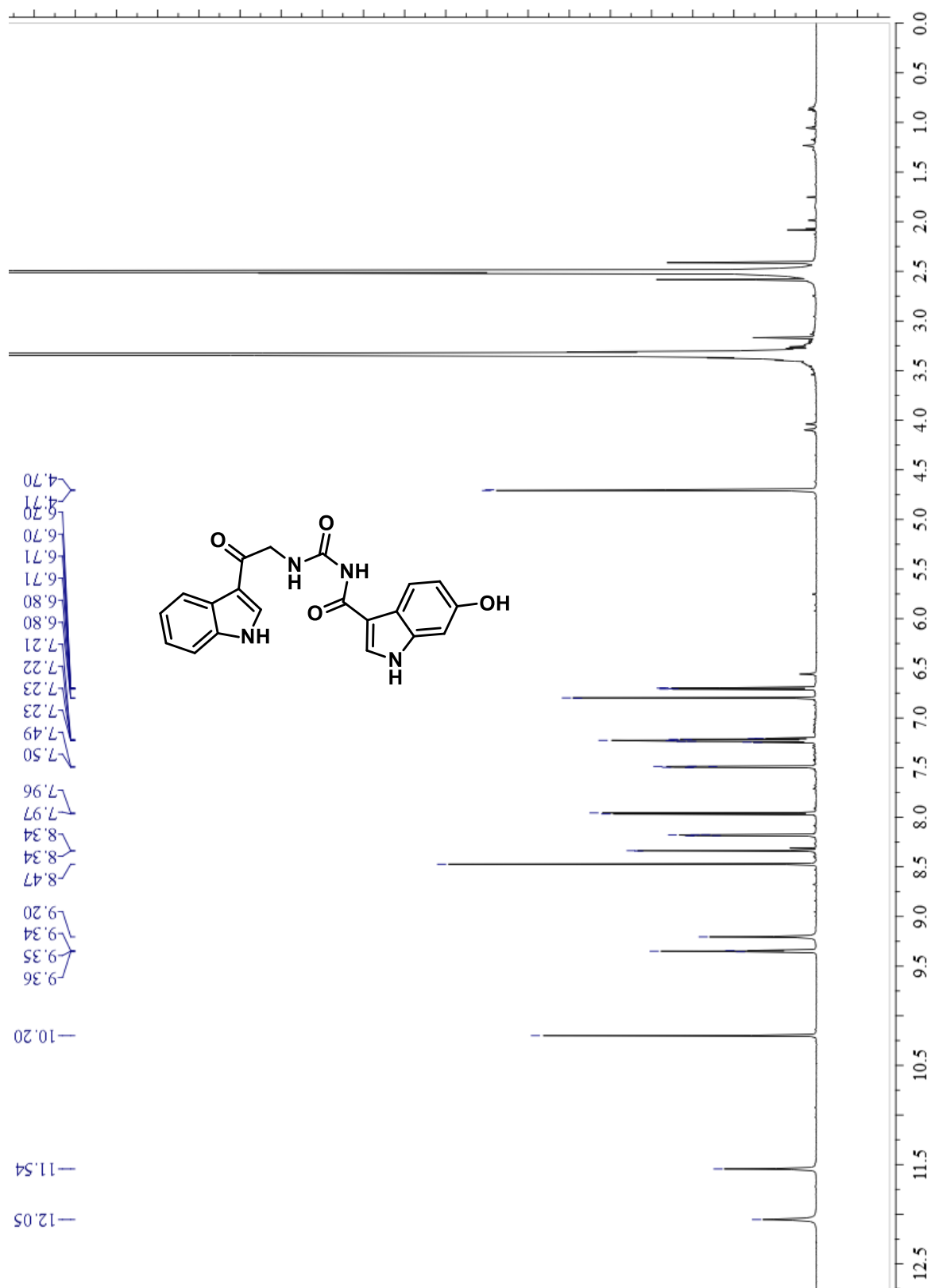


Figure S27. The ^1H NMR (800 MHz, $\text{DMSO-}d_6$) spectrum of **5**

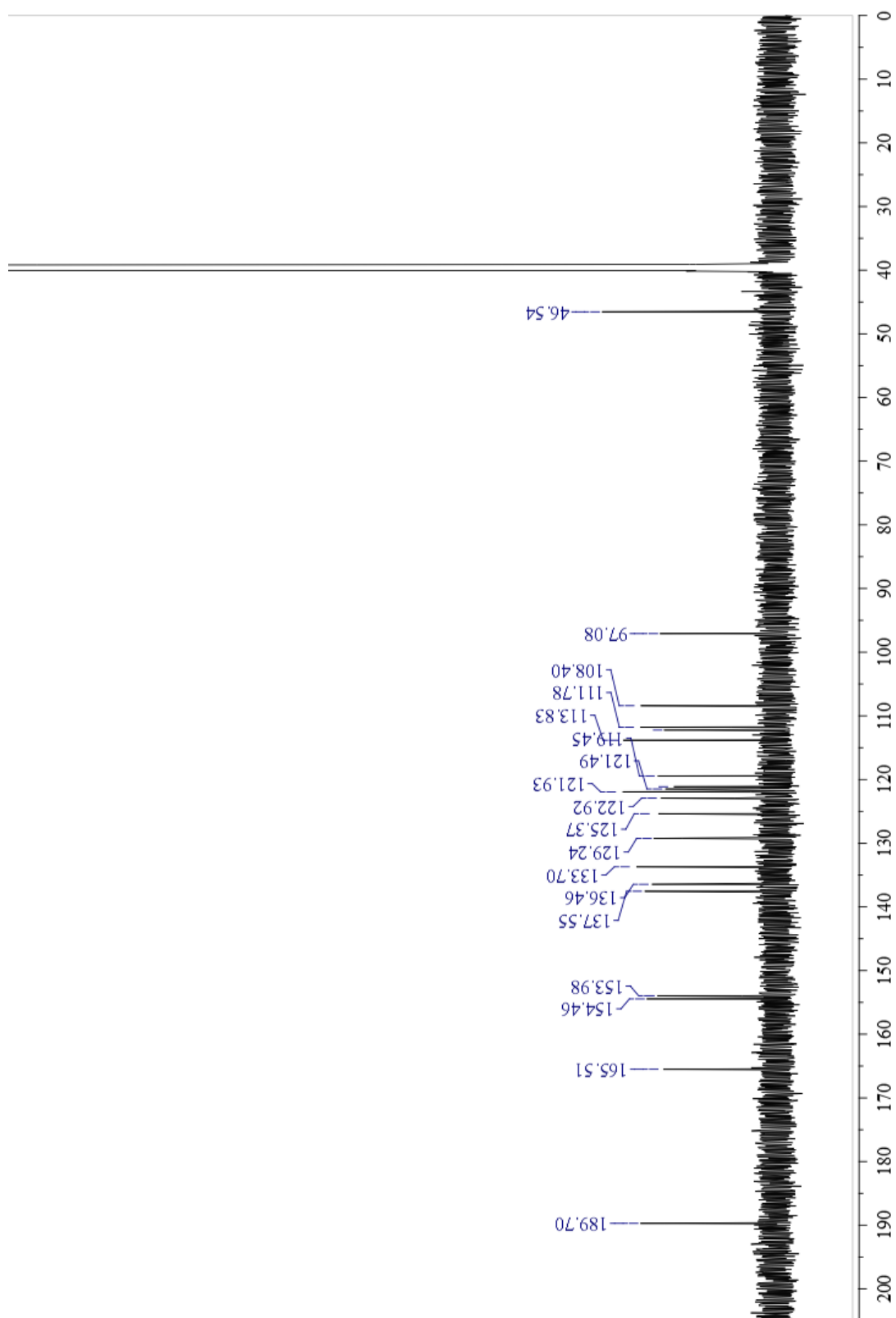


Figure S28. The ^{13}C NMR (200 MHz, $\text{DMSO-}d_6$) spectrum of **5**

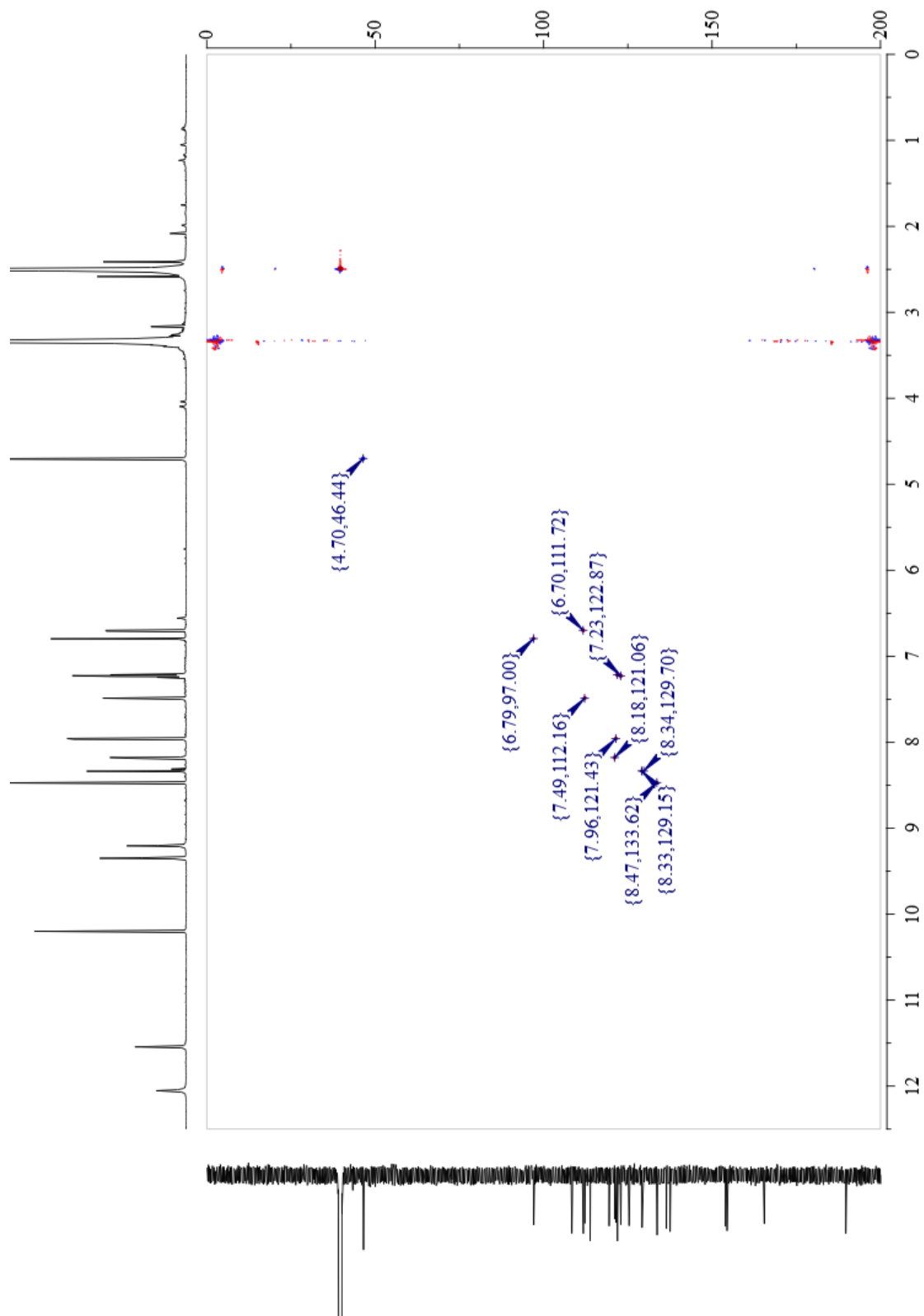


Figure S29. The HSQC (800 MHz, DMSO-*d*₆) spectrum of **5**

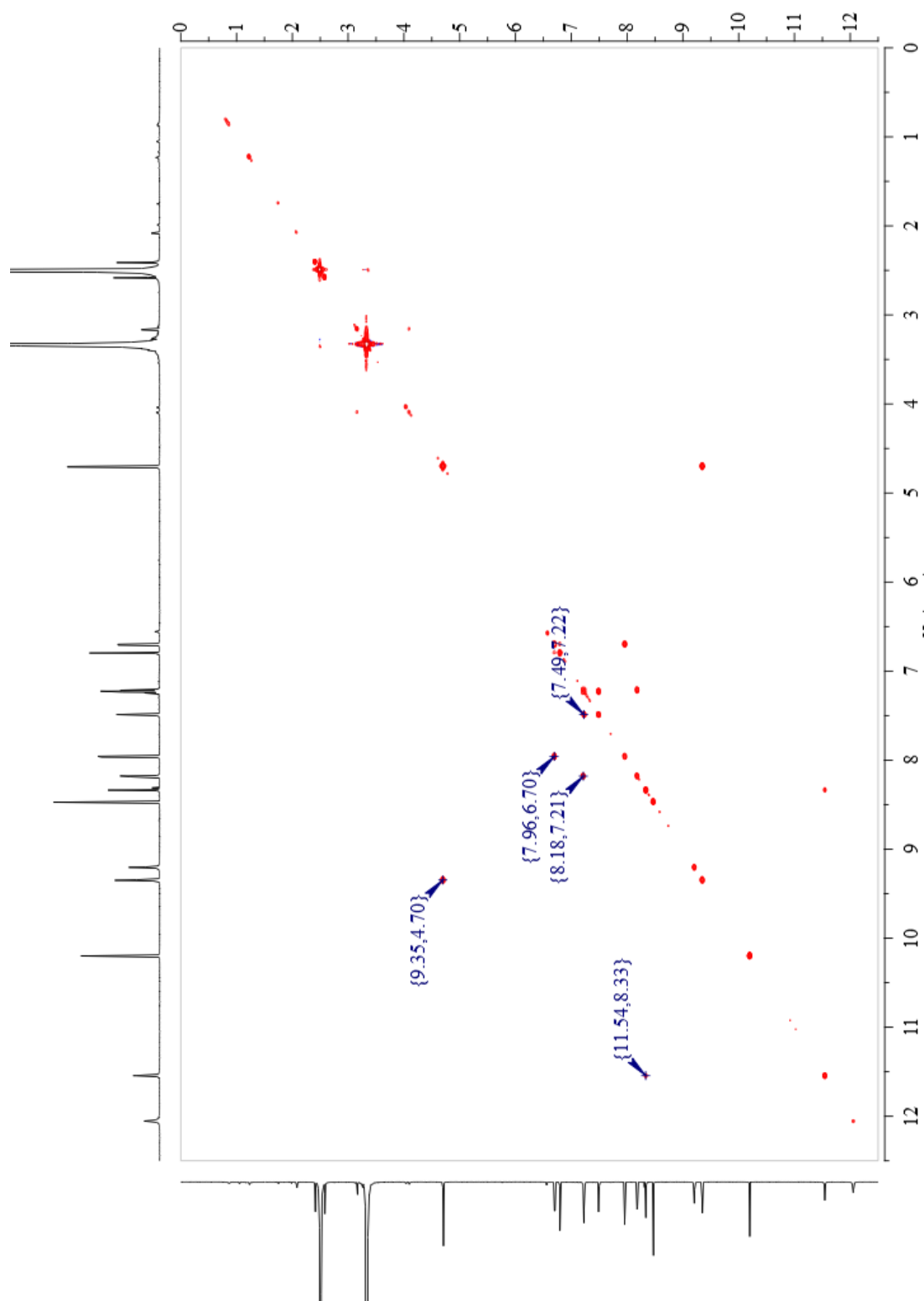


Figure S30. The COSY (800 MHz, DMSO-*d*₆) spectrum of **5**

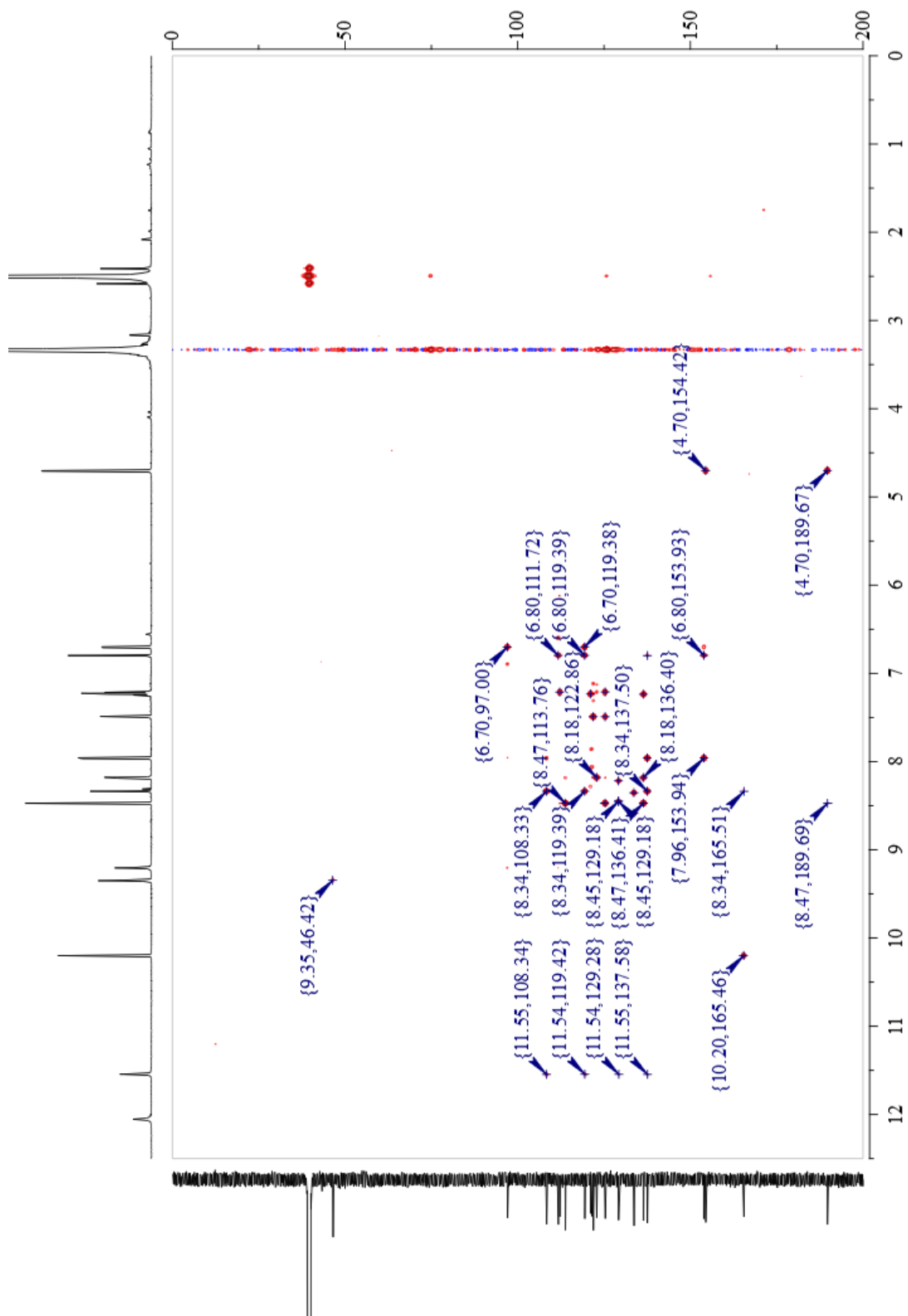


Figure S31. The HMBC (800 MHz, DMSO-*d*₆) spectrum of **5**

Observed m/z	Int%	Err [ppm / mmu]	U.S.	Composition
377.1249	14.3	+11.8 / +4.5	23.0	C 29 H 15 N
		-3.7 / -1.4	19.5	C 21 H 13 N 8
		-7.3 / -2.8	19.0	C 23 H 15 N 5 O
		-10.9 / -4.1	18.5	C 25 H 17 N 2 O 2
		+6.9 / +2.6	15.5	C 16 H 13 N 10 O 2
		+18.9 / +7.1	18.5	C 26 H 17 O 3
		+3.4 / +1.3	15.0	C 18 H 15 N 7 O 3
		-0.2 / -0.1	14.5	C 20 H 17 N 4 O 4
		-3.8 / -1.4	14.0	C 22 H 19 N O 5
		-19.3 / -7.3	10.5	C 14 H 17 N 8 O 5
		+14.0 / +5.3	11.0	C 13 H 15 N 9 O 5
		+10.5 / +4.0	10.5	C 15 H 17 N 6 O 6
		+6.9 / +2.6	10.0	C 17 H 19 N 3 O 7
		-8.6 / -3.3	6.5	C 9 H 17 N 10 O 7
		+3.4 / +1.3	9.5	C 19 H 21 O 8
		-12.2 / -4.6	6.0	C 11 H 19 N 7 O 8
		-15.8 / -5.9	5.5	C 13 H 21 N 4 O 9
		+17.6 / +6.6	6.0	C 12 H 19 N 5 O 9
		-19.3 / -7.3	5.0	C 15 H 23 N O 10
		+14.0 / +5.3	5.5	C 14 H 21 N 2 O 10
		-1.5 / -0.6	2.0	C 6 H 19 N 9 O 10

[Theoretical Ion Distribution]

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Molecular Formula : C20 H17 N4 O4

(m/z 377.1250, MW 377.3794, U.S. 14.5)

Base Peak : 377.1250, Averaged MW : 377.3779(a), 377.3786(w)

m/z	INT.	
377.1250	100.0000	*****
378.1280	23.8664	*****
379.1305	3.5235	**
380.1330	0.3884	
381.1355	0.0344	
382.1379	0.0025	
383.1404	0.0002	

Figure S32. The HRFABMS data of **5**

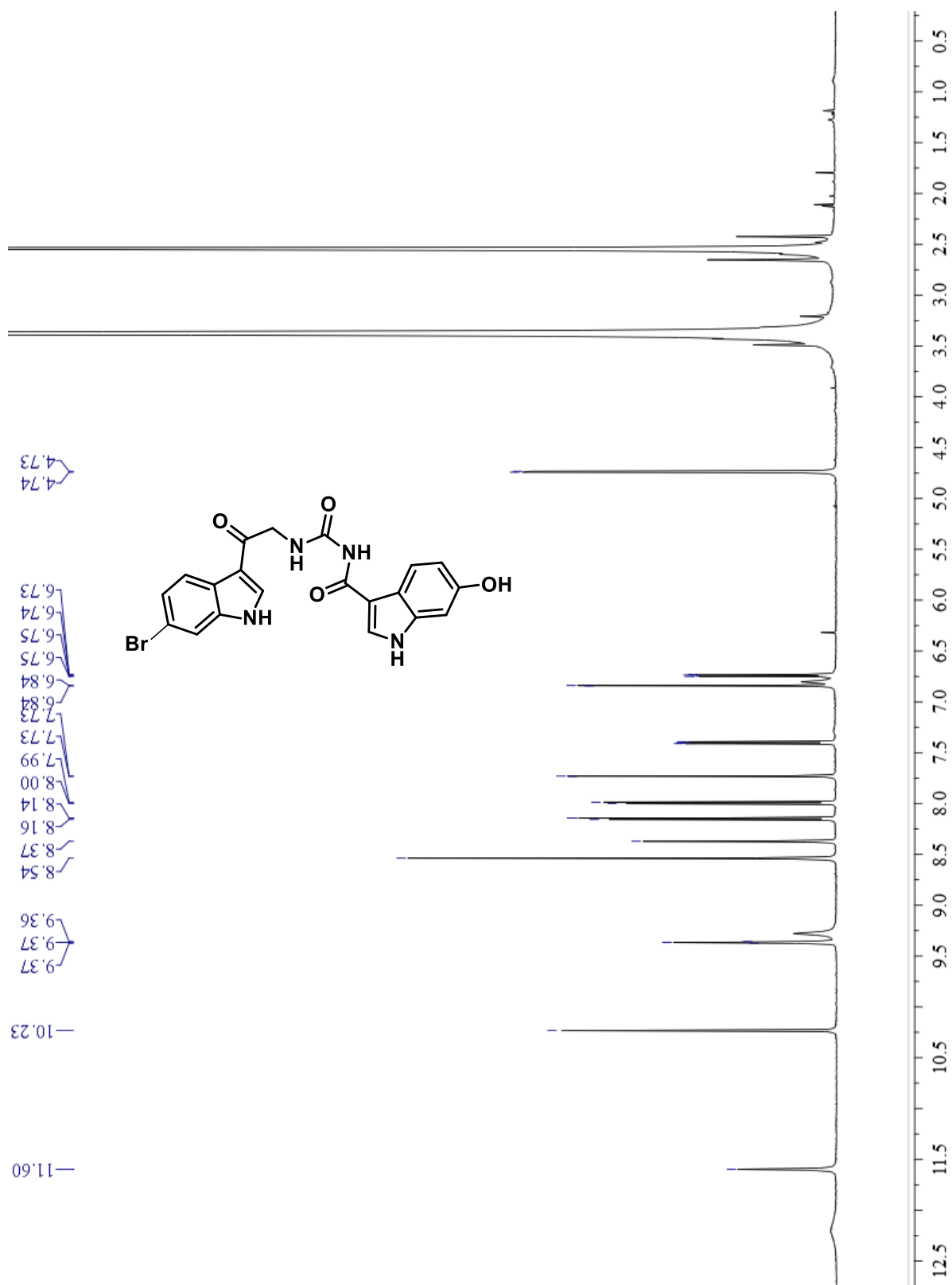


Figure S33. The ^1H NMR (800 MHz, $\text{DMSO-}d_6$) spectrum of **6**

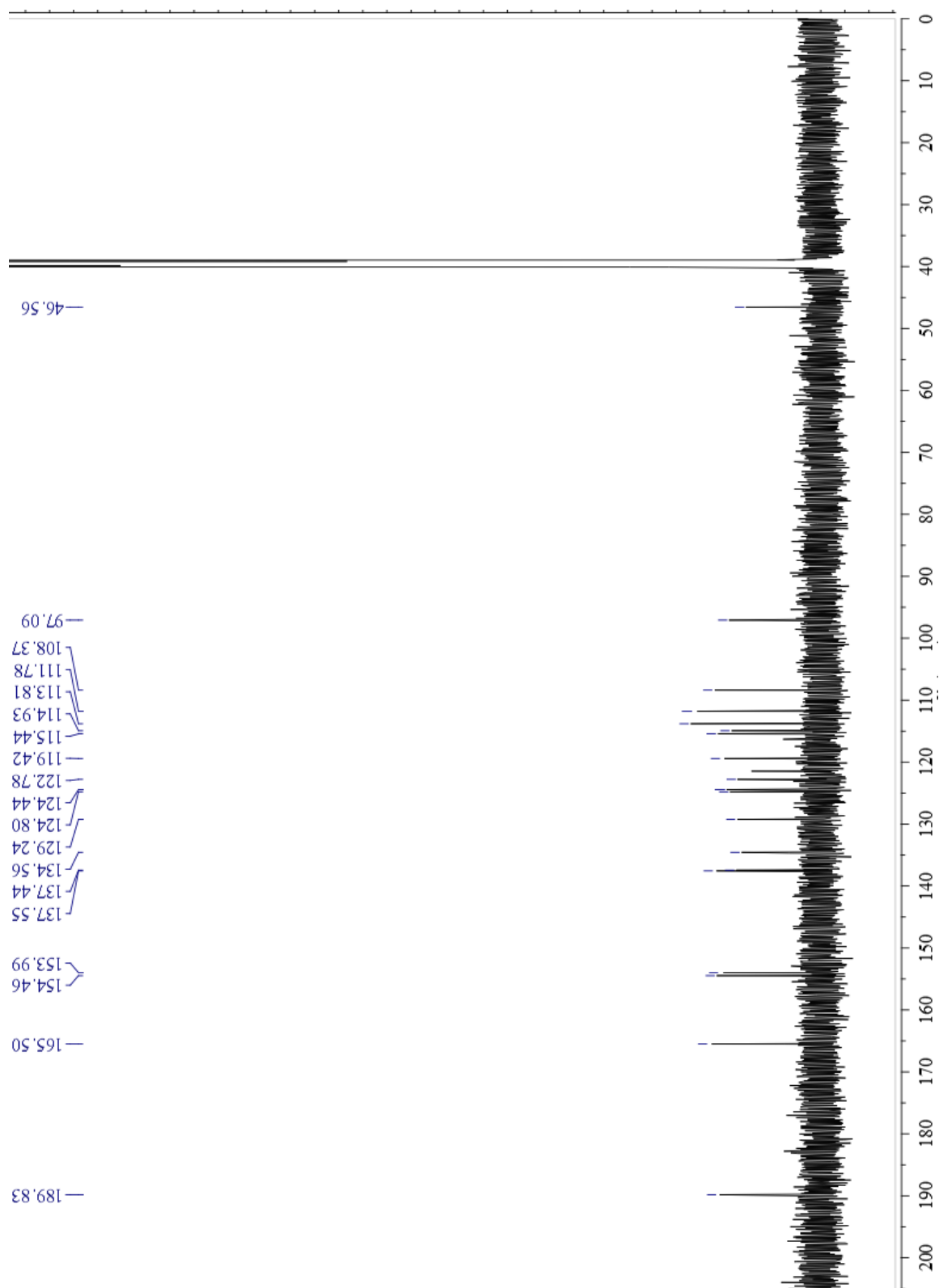


Figure S34. The ^{13}C NMR (200 MHz, $\text{DMSO-}d_6$) spectrum of **6**

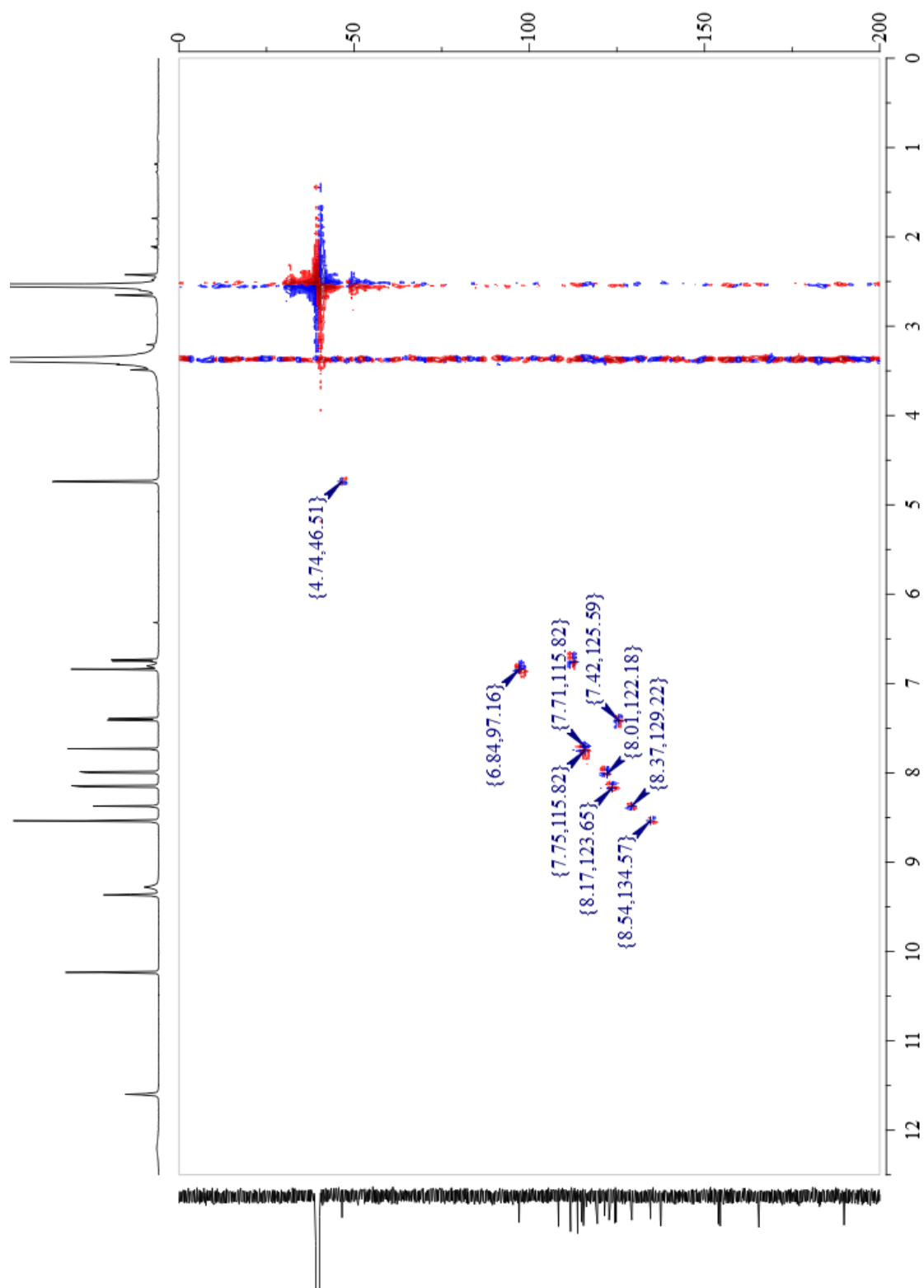


Figure S35. The HSQC (800 MHz, DMSO-*d*₆) spectrum of **6**

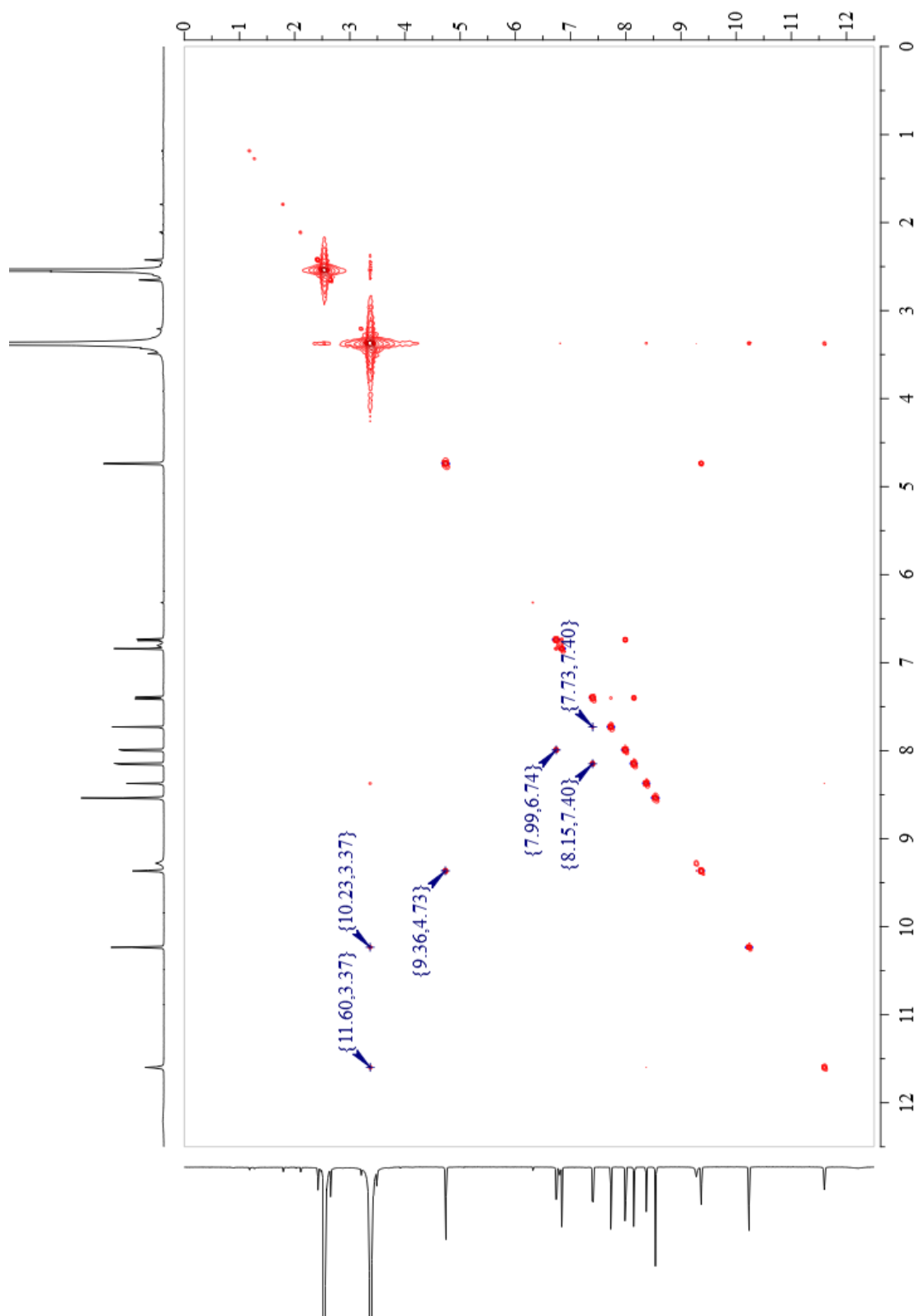


Figure S36. The COSY (800 MHz, DMSO-*d*₆) spectrum of **6**

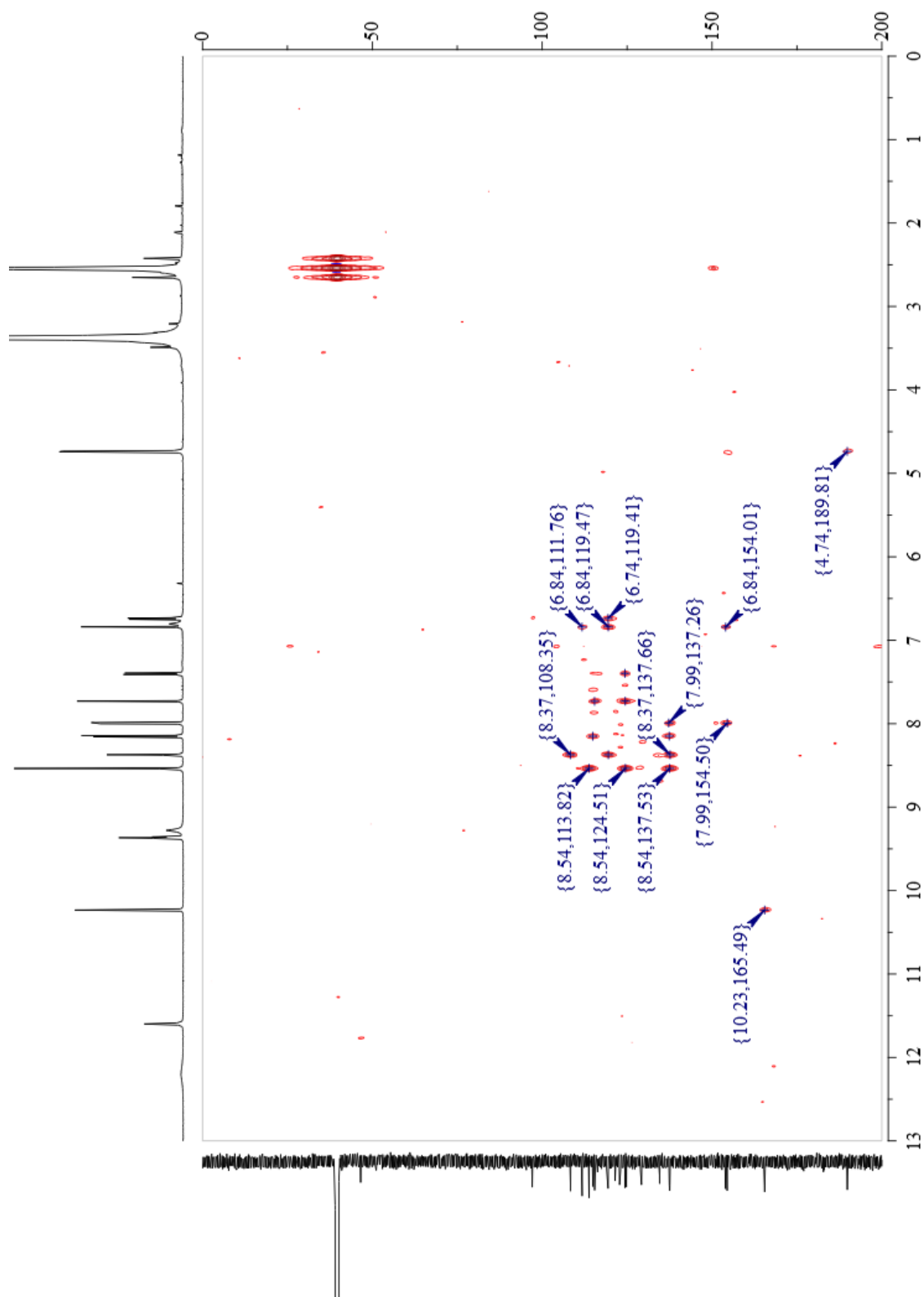


Figure S37. The HMBC (800 MHz, DMSO-*d*₆) spectrum of **6**

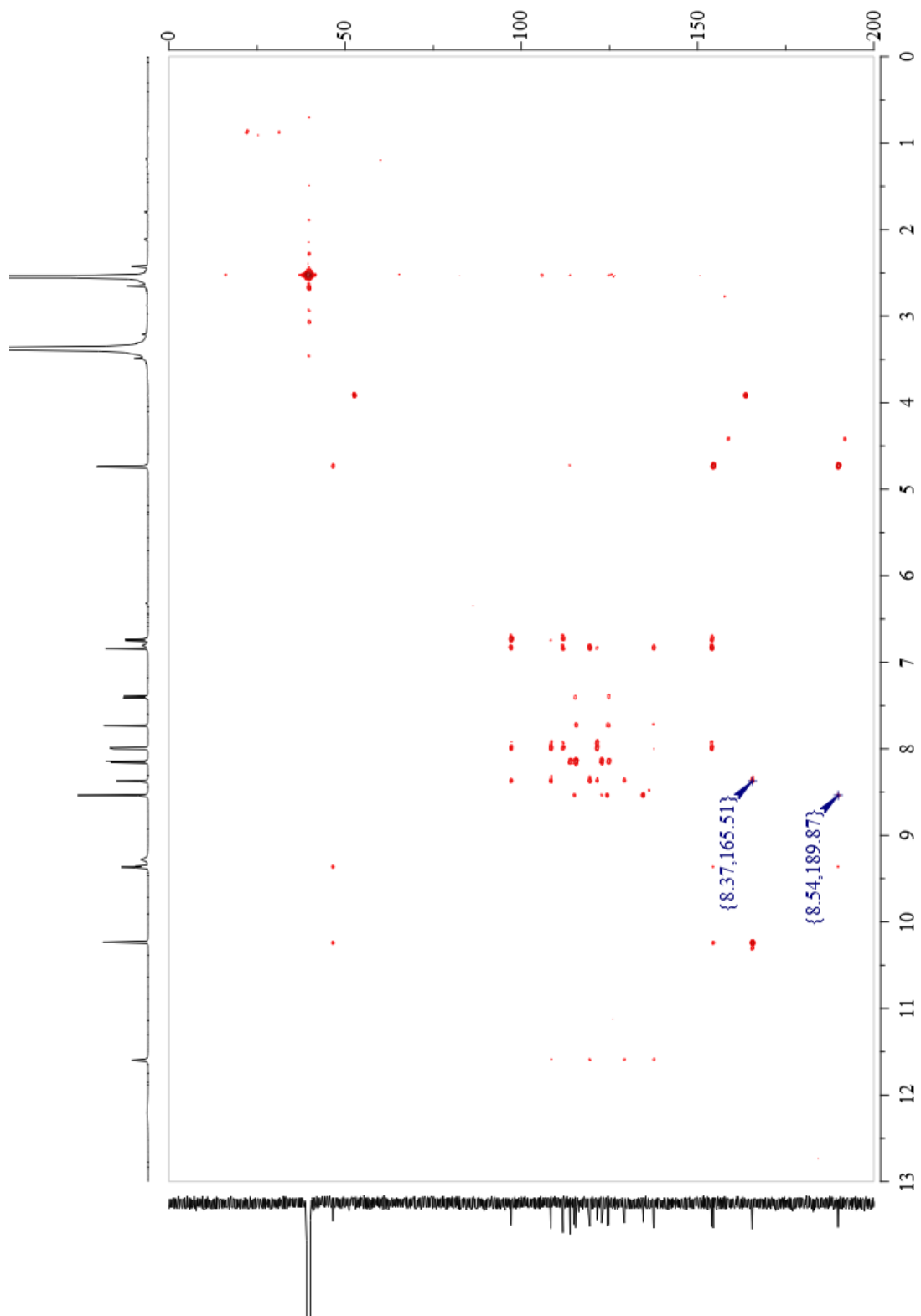


Figure S38. The dHMQC at 4Hz (800 MHz, DMSO-*d*₆) spectrum of **6**

Observed m/z Int%
455.0356 0.6

Err [ppm / mmu]	U.S. Composition				
-17.5 / -8.0	22.5 C 30 H 16 79Br				
+10.1 / +4.6	23.0 C 29 H 14 79Br N				
+2.6 / +1.2	8.5 C 20 H 25 81Br 2 N 2				
-8.6 / -3.9	8.0 C 19 H 25 79Br 81Br N 3				
-0.5 / -0.2	34.5 C 33 H 3 N 4				
-19.9 / -9.0	7.5 C 18 H 25 79Br 2 N 4				
+19.0 / +8.7	8.5 C 18 H 23 79Br 81Br N 4				
+7.8 / +3.5	8.0 C 17 H 23 79Br 2 N 5				
-19.2 / -8.7	19.5 C 23 H 14 81Br N 6				
+8.4 / +3.8	20.0 C 22 H 12 81Br N 7				
-2.8 / -1.3	19.5 C 21 H 12 79Br N 8				
-10.3 / -4.7	5.0 C 12 H 23 81Br 2 N 9				
+17.4 / +7.9	5.5 C 11 H 21 81Br 2 N 10				
-11.6 / -5.3	7.5 C 21 H 27 79Br 81Br O				
-3.4 / -1.6	34.0 C 35 H 5 N O				
+16.1 / +7.3	8.0 C 20 H 25 79Br 81Br N O				
+4.8 / +2.2	7.5 C 19 H 25 79Br 2 N 2 O				
+5.5 / +2.5	19.5 C 24 H 14 81Br N 4 O				
-5.8 / -2.6	19.0 C 23 H 14 79Br N 5 O				
-13.2 / -6.0	4.5 C 14 H 25 81Br 2 N 6 O				
+14.4 / +6.6	5.0 C 13 H 23 81Br 2 N 7 O				
-16.3 / -7.4	30.5 C 27 H 3 N 8 O				
+3.2 / +1.4	4.5 C 12 H 23 79Br 81Br N 8 O				
+11.3 / +5.1	31.0 C 26 H N 9 O				
-8.1 / -3.7	4.0 C 11 H 23 79Br 2 N 9 O				
+19.6 / +8.9	4.5 C 10 H 21 79Br 2 N 10 O				
+2.5 / +1.2	19.0 C 26 H 16 81Br N O 2				
-8.7 / -4.0	18.5 C 25 H 16 79Br N 2 O 2				
+18.9 / +8.6	19.0 C 24 H 14 79Br N 3 O 2				
-16.2 / -7.4	4.0 C 16 H 27 81Br 2 N 3 O 2				
+11.5 / +5.2	4.5 C 15 H 25 81Br 2 N 4 O 2				
-19.3 / -8.8	30.0 C 29 H 5 N 5 O 2				
+0.2 / +0.1	4.0 C 14 H 25 79Br 81Br N 5 O 2				
+8.4 / +3.8	30.5 C 28 H 3 N 6 O 2				
-11.0 / -5.0	3.5 C 13 H 25 79Br 2 N 6 O 2				
+16.6 / +7.6	4.0 C 12 H 23 79Br 2 N 7 O 2				
-10.3 / -4.7	15.5 C 18 H 14 81Br N 8 O 2				
+17.3 / +7.9	16.0 C 17 H 12 81Br N 9 O 2				
+6.0 / +2.7	15.5 C 16 H 12 79Br N 10 O 2				
+16.0 / +7.3	18.5 C 26 H 16 79Br O 3				
-19.1 / -8.7	3.5 C 18 H 29 81Br 2 O 3				
+8.5 / +3.9	4.0 C 17 H 27 81Br 2 N O 3				
-2.7 / -1.2	3.5 C 16 H 27 79Br 81Br N 2 O 3				
+5.4 / +2.5	30.0 C 30 H 5 N 3 O 3				
-14.0 / -6.4	3.0 C 15 H 27 79Br 2 N 3 O 3				
+13.7 / +6.2	3.5 C 14 H 25 79Br 2 N 4 O 3				
-13.3 / -6.1	15.0 C 20 H 16 81Br N 5 O 3				
+14.3 / +6.5	15.5 C 19 H 14 81Br N 6 O 3				
+3.1 / +1.4	15.0 C 18 H 14 79Br N 7 O 3				
-4.4 / -2.0	0.5 C 9 H 25 81Br 2 N 8 O 3				
-15.6 / -7.1	0.0 C 8 H 25 79Br 81Br N 9 O 3				
-7.5 / -3.4	26.5 C 22 H 3 N 10 O 3				
+12.0 / +5.5	0.5 C 7 H 23 79Br 81Br N 10 O 3				
+2.5 / +1.1	29.5 C 32 H 7 O 4				
-16.9 / -7.7	2.5 C 17 H 29 79Br 2 O 4				
+10.7 / +4.9	3.0 C 16 H 27 79Br 2 N O 4				
-16.2 / -7.4	14.5 C 22 H 18 81Br N 2 O 4				
+11.4 / +5.2	15.0 C 21 H 16 81Br N 3 O 4				
+0.1 / +0.1	14.5 C 20 H 16 79Br N 4 O 4				
-7.3 / -3.3	0.0 C 11 H 27 81Br 2 N 5 O 4				
-18.6 / -8.5	-0.5 C 10 H 27 79Br 81Br N 6 O 4				
-10.4 / -4.7	26.0 C 24 H 5 N 7 O 4				
+9.1 / +4.1	0.0 C 9 H 25 79Br 81Br N 7 O 4				
+17.2 / +7.8	26.5 C 23 H 3 N 8 O 4				
-2.2 / -1.0	-0.5 C 8 H 25 79Br 2 N 8 O 4				
-1.5 / -0.7	11.5 C 13 H 14 81Br N 10 O 4				
+8.4 / +3.8	14.5 C 23 H 18 81Br O 5				
-2.8 / -1.3	14.0 C 22 H 18 79Br N O 5				
-10.3 / -4.7	-0.5 C 13 H 29 81Br 2 N 2 O 5				
+17.4 / +7.9	0.0 C 12 H 27 81Br 2 N 3 O 5				
-13.4 / -6.1	25.5 C 26 H 7 N 4 O 5				
+6.1 / +2.8	-0.5 C 11 H 27 79Br 81Br N 4 O 5				
+14.3 / +6.5	26.0 C 25 H 5 N 5 O 5				
-4.5 / -2.0	11.0 C 15 H 16 81Br N 7 O 5				
-15.7 / -7.1	10.5 C 14 H 16 79Br N 8 O 5				
+11.9 / +5.4	11.0 C 13 H 14 79Br N 9 O 5				
+14.4 / +6.6	-0.5 C 14 H 29 81Br 2 O 6				
-16.3 / -7.4	25.0 C 28 H 9 N O 6				
+11.3 / +5.1	25.5 C 27 H 7 N 2 O 6				
-7.4 / -3.4	10.5 C 17 H 18 81Br N 4 O 6				
-18.7 / -8.5	10.0 C 16 H 18 79Br N 5 O 6				
+9.0 / +4.1	10.5 C 15 H 16 79Br N 6 O 6				
-1.6 / -0.7	22.0 C 19 H 5 N 9 O 6				
-10.4 / -4.7	10.0 C 19 H 20 81Br N O 7				
+17.3 / +7.9	10.5 C 18 H 18 81Br N 2 O 7				
+6.0 / +2.7	10.0 C 17 H 18 79Br N 3 O 7				
-4.5 / -2.1	21.5 C 21 H 7 N 6 O 7				
+4.4 / +2.0	7.0 C 10 H 16 81Br N 9 O 7				
-6.9 / -3.1	6.5 C 9 H 16 79Br N 10 O 7				
+3.1 / +1.4	9.5 C 19 H 20 79Br O 8				
-7.5 / -3.4	21.0 C 23 H 9 N 3 O 8				
+1.4 / +0.7	6.5 C 12 H 18 81Br N 6 O 8				
-9.8 / -4.5	6.0 C 11 H 18 79Br N 7 O 8				
+17.8 / +8.1	6.5 C 10 H 16 79Br N 8 O 8				
-10.4 / -4.8	20.5 C 25 H 11 O 9				
+17.2 / +7.8	21.0 C 24 H 9 N O 9				
-1.5 / -0.7	6.0 C 14 H 20 81Br N 3 O 9				
-12.8 / -5.8	5.5 C 13 H 20 79Br N 4 O 9				
+14.9 / +6.8	6.0 C 12 H 18 79Br N 5 O 9				
+4.3 / +2.0	17.5 C 16 H 7 N 8 O 9				
-14.4 / -6.6	2.5 C 6 H 18 81Br N 10 O 9				
-4.5 / -2.0	5.5 C 16 H 22 81Br O 10				
-15.7 / -7.2	5.0 C 15 H 22 79Br N O 10				
+11.9 / +5.4	5.5 C 14 H 20 79Br N 2 O 10				
+1.3 / +0.6	17.0 C 18 H 9 N 5 O 10				
-17.4 / -7.9	2.0 C 8 H 20 81Br N 7 O 10				
+10.3 / +4.7	2.5 C 7 H 18 81Br N 8 O 10				
-1.0 / -0.4	2.0 C 6 H 18 79Br N 9 O 10				

[Theoretical Ion Distribution]
Molecular Formula : C20 H17 N4 O4

Page: 1

(m/z 377.1250, MW 377.3794, U.S. 14.5)
Base Peak : 377.1250, Averaged MW : 377.3779(a), 377.3786(w)

m/z	INT.	
377.1250	100.0000	*****
378.1280	23.8664	*****
379.1305	3.5235	**
380.1330	0.3884	
381.1355	0.0344	
382.1379	0.0025	
383.1404	0.0002	

Figure S39. The HRFABMS data of 6

Parameters for calculating specific rotations

Functional: B3-LYP

Basis set: def-SVP

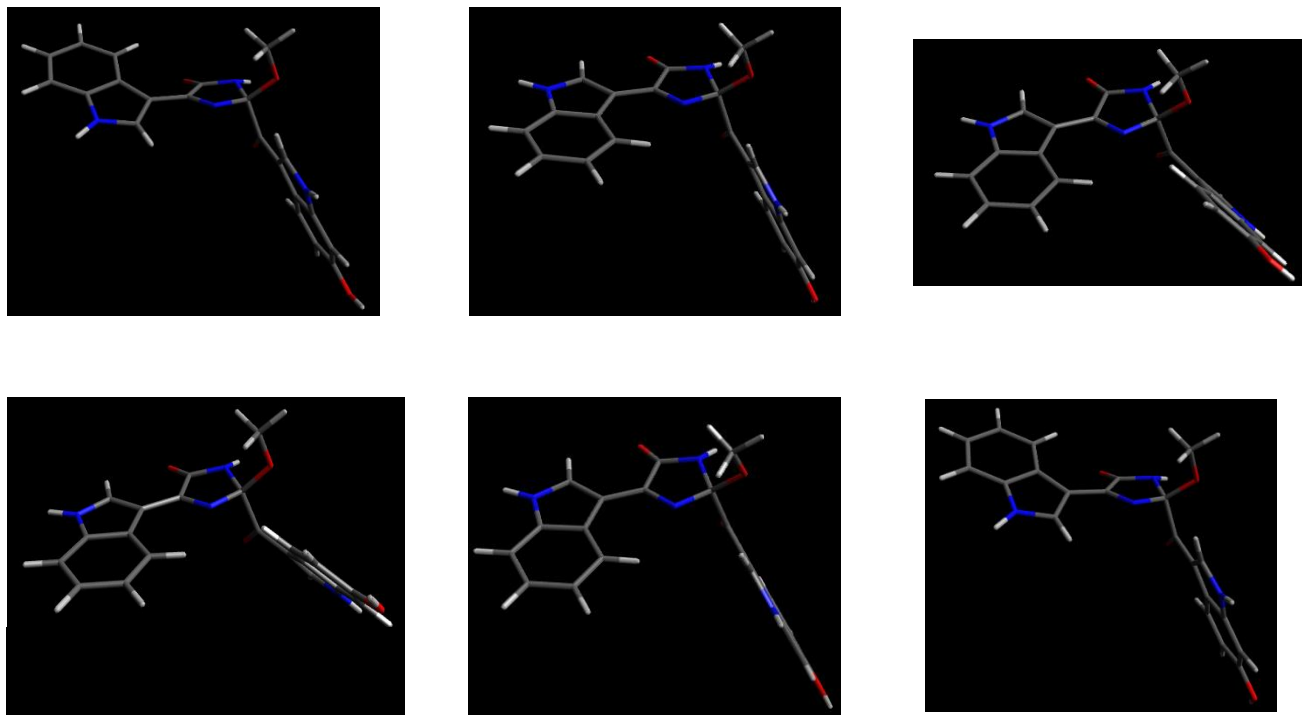
Gridsize: m3

Frequency: 0.7735713524617996E-01

Frequency / eV: 2.104995653760073

Frequency / nm: 589.0000000000000

Frequency / cm⁻¹: 16977.92869016530



Major conformers (> 2% population) under the relative energy of 10 kJ/mol in calculated Boltzmann distribution.

Compound 1	1/3*trace (dipole polarizability)	1/3*trace (rotatory dispersion)	Specific rotation [α] in deg*[dm(g/cc)] ⁽⁻¹⁾
26.305 %	297.9	4.4	+ 440.4
23.069 %	298.6	5.5	+ 545.0
11.573 %	292.6	-9.4	-932.6
9.939 %	292.6	-10.4	-1033.8
5.847 %	306.8	-0.9	-90.9
5.141 %	292.6	-10.4	-1033.8

Figure S40. Calculated optical rotations of major conformers of **1**.

Parameters for calculating specific rotations

Functional: B3-LYP

Basis set: def-SVP

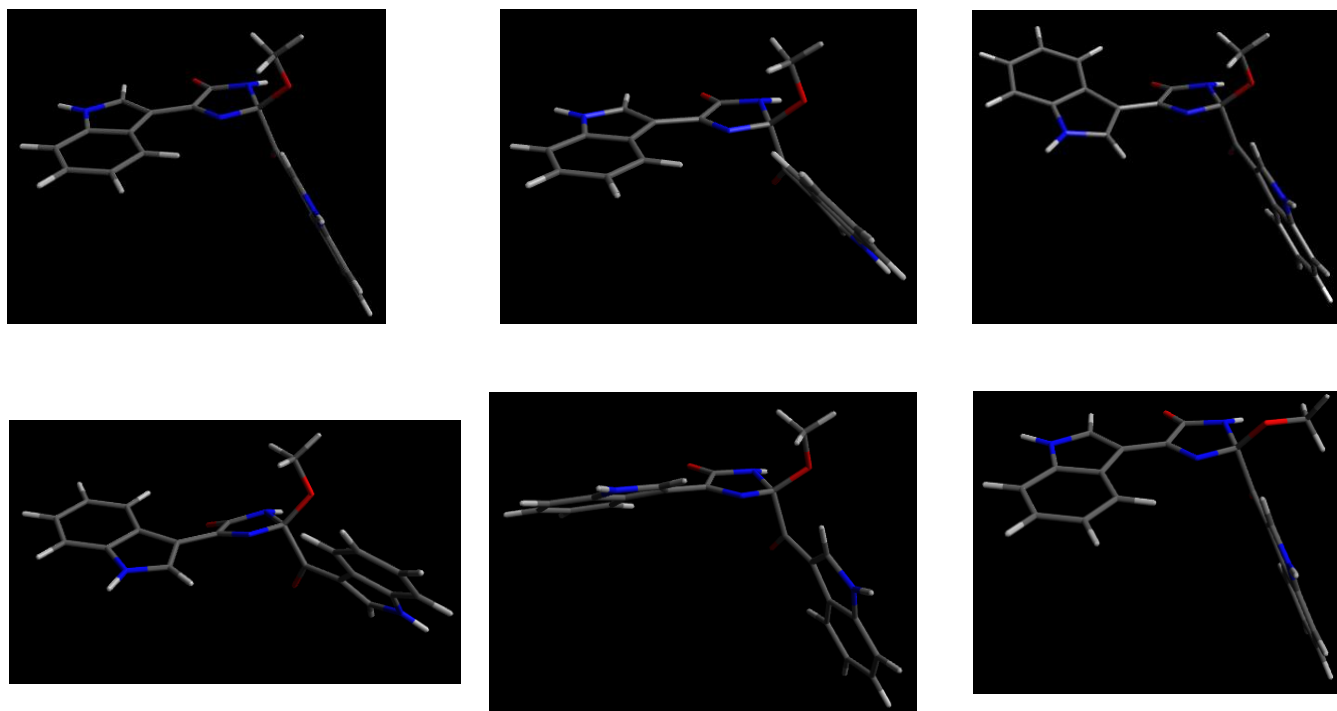
Gridsize: m3

Frequency: 0.7735713524617996E-01

Frequency / eV: 2.104995653760073

Frequency / nm: 589.0000000000000

Frequency / cm⁻¹: 16977.92869016530



Major conformers (> 2% population) under the relative energy of 10 kJ/mol in calculated Boltzmann distribution.

Compound 2	1/3*trace (dipole polarizability)	1/3*trace (rotatory dispersion)	Specific rotation [α] in deg*[dm(g/cc)] ⁽⁻¹⁾
40.086 %	290.7	4.3	+ 446.6
23.392 %	285.9	-8.6	-893.2
10.293 %	299.5	-0.5	-53.7
4.800 %	295.4	-10.5	-1086.9
3.492 %	299.5	-0.5	-47.9
3.260 %	292.0	5.4	+ 560.4

Figure S41. Calculated optical rotations of major conformers of **2**.

Parameters for calculating specific rotations

Functional: B3-LYP

Basis set: def-SVP

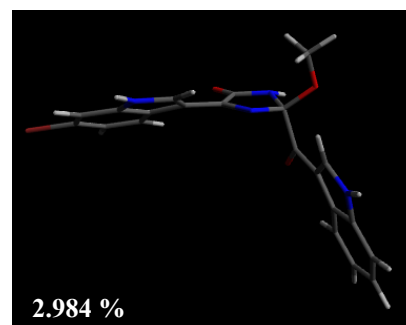
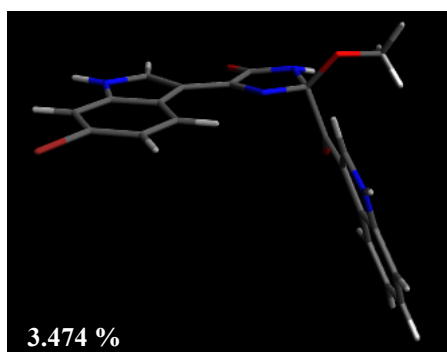
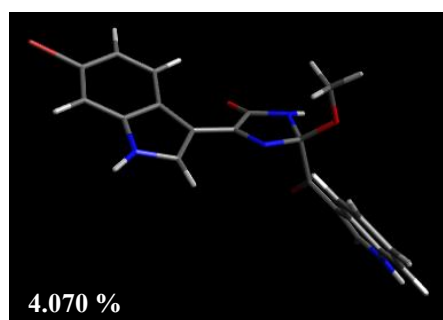
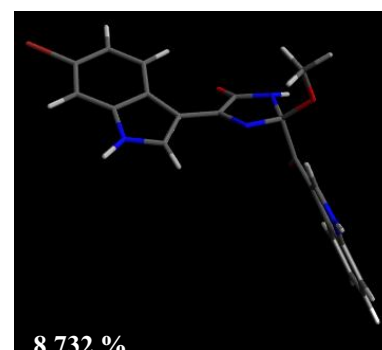
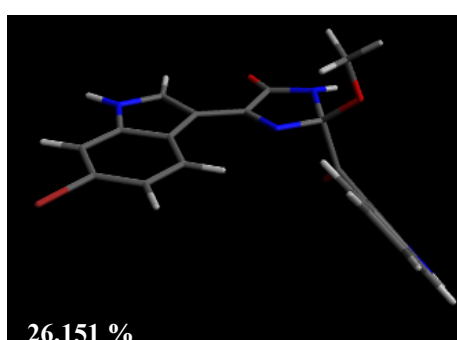
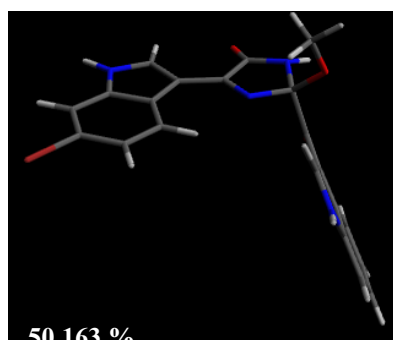
Gridsize: m3

Frequency: 0.7735713524617996E-01

Frequency / eV: 2.104995653760073

Frequency / nm: 589.0000000000000

Frequency / cm⁻¹: 16977.92869016530



Major conformers (> 2% population) under the relative energy of 10 kJ/mol in calculated Boltzmann distribution.

Compound 3	1/3*trace (dipole polarizability)	1/3*trace (rotatory dispersion)	Specific rotation [α] in deg*[dm(g/cc)] ⁽⁻¹⁾
50.163 %	314.1	7.5	+ 646.6
26.151 %	308.5	-8.1	- 691.4
8.732 %	324.4	0.3	+ 33.0
4.070 %	322.6	-13.7	- 1176.2
3.474 %	315.1	8.6	+ 738.7
2.984 %	324.5	1.1	+ 93.5

Figure S42. Calculated optical rotations of major conformers of **3**.

Parameters for calculating specific rotations

Functional: B3-LYP

Basis set: def-SVP

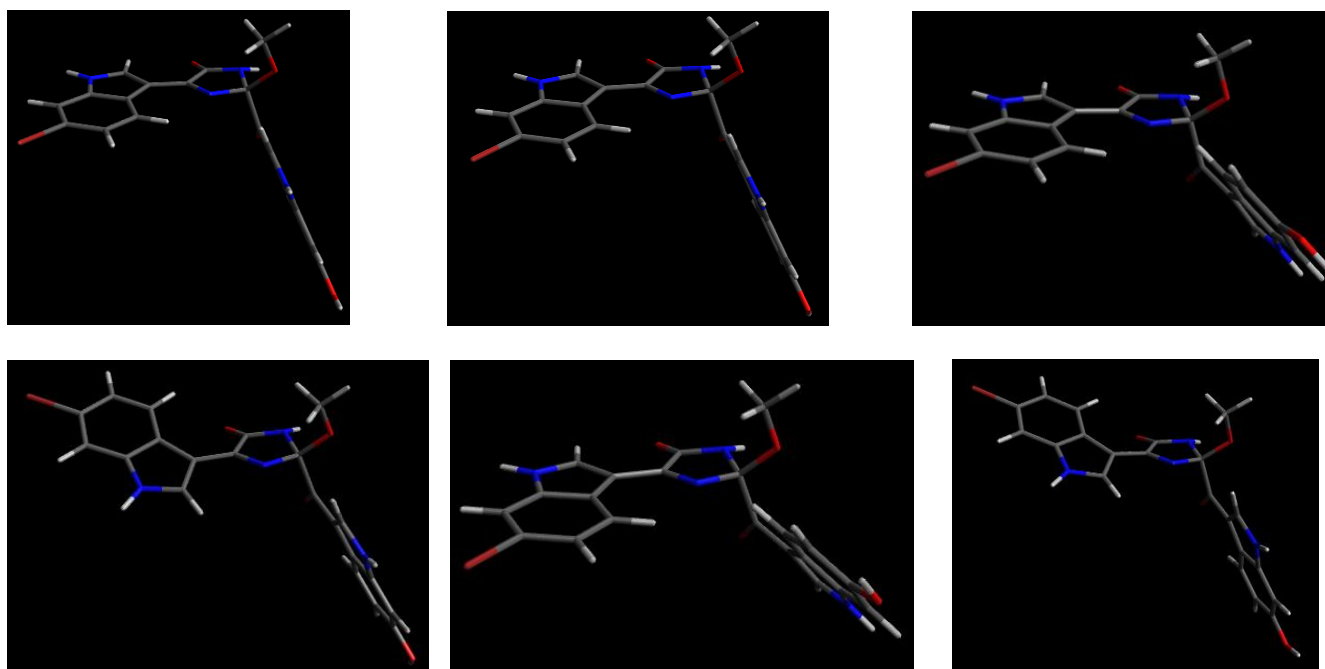
Gridsize: m3

Frequency: 0.7735713524617996E-01

Frequency / eV: 2.104995653760073

Frequency / nm: 589.0000000000000

Frequency / cm⁻¹: 16977.92869016530



Major conformers (> 2% population) under the relative energy of 10 kJ/mol in calculated Boltzmann distribution.

Compound 4	1/3*trace (dipole polarizability)	1/3*trace (rotatory dispersion)	Specific rotation [α] in deg*[dm(g/cc)] ⁽⁻¹⁾
27.577 %	321.9	3.5	- 287.2
24.151 %	322.8	3.9	+ 327.2
12.285 %	318.2	-12.8	- 1064.0
10.592 %	318.3	-13.3	- 1103.5
4.826 %	333.0	-4.6	-344.3
4.222 %	333.9	-4.0	-330.6

Figure S43. Calculated optical rotations of major conformers of **4**.