Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Asperflavipines C−E and Aspermichalasine A: Three Cytochalasan Heterotetramers and an Unusual Cytochalasan Monomer from *Aspergillus micronesiensis*

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Contents of Supporting Information

Table S1 ^{1}H (600 MHz) and ^{13}C (150 MHz) NMR data of **1** and **2** (δ in ppm, DMSO-d_6)

1						**2**					
no.	δ_H (J in Hz)	δ_C	*no.*	δ_H (J in Hz)	$\boldsymbol{\delta_C}$	*no.*	δ_H (J in Hz)	δ_C	*no.*	δ_H (J in Hz)	$\boldsymbol{\delta_C}$
1		174.6	1′		174.0	1		174.6	1′		172.7
3	3.08 m	50.0	3′	2.89 m	51.4	3	3.08 m	49.8	3′	3.12 m	49.3
4	2.35 m	53.5	4′	2.12 m	54.8	4	2.29 m	53.6	4′	2.41 m	53.1
5	2.45 m	35.0	5′	2.47 m	35.8	5	2.45 m	34.9	5′	2.44 m	34.5
6		139.2	6′		138.7	6		139.3	6′		138.6
7	5.23 brs	125.2	7′	5.40 brs	125.8	7	5.24 brs	125.1	7′	5.15 brs	125.6
8	3.06 m	44.1	8′	3.37 m	42.7	8	3.06 m	44.1	8′	2.90 brd (10.8)	43.4
9		68.7	9′		67.4	9		68.7	9′		68.6
10a	1.06 m	50.2	10′a	1.20 m	49.2	10a	1.04 m	50.4	10′a	1.12 m	49.7
10b	1.06 m		10′b	1.07 m		10b	1.04 m		10′b	0.94 m	
11	1.14 d (7.0)	13.1	11′	1.14 d (7.0)	13.6	11	1.14 d (7.0)	13.1	11′	1.14 d (7.0)	13.2
12	1.69 s	19.5	12′	1.72 s	20.0	12	1.69 s	19.5	12′	1.66 s	19.4
13	6.00 d (10.7)	124.7	13′	5.88 d (10.9)	124.2	13	6.03 d (10.7)	124.6	13′	5.84 d (10.8)	123.6
14		135.2	14′		135.4	14		135.2	14′		135.8
15a	2.06 m	34.3	15′a	1.92 m	36.0	15a	2.05 m	34.3	15′a	2.08 m	31.5
15b	1.84 m		15′b	1.81 m		15b	1.84 m		15′b	1.78 m	
16a	1.84 m	28.4	16′a	1.13 m	29.6	16a	1.84 m	28.4	16′a	1.95 m	30.9
16b	1.31 m		16′b	1.13 m		16b	1.32 m		16′b	1.73 m	
17	3.69 m	73.4	17′	3.72 m	69.9	17	3.68 m	73.3	17′	3.79 m	76.5
18	5.21 m	74.8	18′	2.60 dd (11.7, 4.3)	76.2	18	4.48 s	75.9	18′		205.5
19	1.90 m	41.8	19′	2.12 m	53.1	19	1.90 t (5.4)	41.6	19′	3.35 dd (6.4, 5.0)	58.7
20	3.78 d (4.8)	50.2	20′	4.07 d (5.6)	47.2	20	3.79 d (5.4)	50.1	20′	4.63 d (6.4)	46.7
21		214.0	21′		213.6	21		214.6	21′		215.2
22	1.62 m	23.9	22′	1.70 m	24.6	22	1.60 m	23.8	22′	1.57 m	24.0
23	0.83 d (6.5)	23.6	23′	0.97 d (6.5)	23.8	23	0.84 d (6.5)	23.6	23′	0.88 d (6.5)	23.6
24	0.85 d (6.5)	21.3	24′	0.88 d (6.5)	21.9	24	0.85 d (6.5)	21.3	24′	0.85 d (6.5)	21.9
25	1.38 s	15.0	25′	1.38 s	16.0	25	1.39 s	15.0	25′	1.39 s	16.5
1″	4.55 m	75.9	1‴	4.54 m	81.8	1″	5.23 d (5.4)	74.7	1‴	4.59 s	81.9
2″		51.1	2‴		72.0	2″		51.4	2‴		71.8
3″		91.9	3‴		192.8	3″		92.0	3‴		191.8
4″		186.2	4‴		91.2	4″		186.6	4‴		91.1
5″		147.6	5‴		194.1	5″		147.4	5‴		193.9
6″		121.6	6‴		131.7	6″		121.7	6‴		130.9
7″		66.3	7‴		160.7	7″		65.2	7‴		159.0
8″	4.53 s	83.4	8‴	5.09 d (5.0)	80.1	8″	4.50 s	83.1	8‴	5.34 d (5.0)	79.6
9″	1.60 s	16.8	9‴	1.66 s	12.5	9″	1.60 s	16.9	9‴	1.39 s	11.6

Table S2 ^{1}H (800 MHz) and ^{13}C (200 MHz) NMR data of **3** (δ in ppm, CD_3OD).

3					
no.	δ_H (*J* in Hz)	δ_C	*no.*	δ_H (*J* in Hz)	δ_C
1		177.1	1′		176.2
3	3.10 m	52.8	3′	3.17 m	52.8
4	2.47 dd (5.2, 3.5)	56.3.	4′	2.51 dd (5.3, 3.3)	55.5
5	2.61 m	36.9	5′	2.63 m	37.3
6		141.6	6′		141.1
7	5.30 brs	126.7	7′	5.40 brs	126.9
8	3.23 m	45.6	8′	3.25 m	45.9
9		71.3	9′		68.4
10a	1.20 m	51.5	10′a	1.35 m	50.7
10b	1.20 m		10′b	1.35 m	
11	1.23 d (7.2)	14.0	11′	1.28 d (7.3)	14.2
12	1.77 s	20.1	12′	1.79 s	20.1
13	6.14 d (10.9)	126.5	13′	6.05 d (11.1)	125.5
14		138.0	14′		138.4
15a	2.17 dd (13.9, 8.9)	40.0	15′a	2.55 m	33.2
15b	2.10 dd (13.9, 11.0)		15′b	1.99 m	
16a	1.68 m	22.3	16′a	1.33 m	30.8
16b	1.61 m		16′b	1.29 m	
17a	2.23 m	36.8	17′		212.4
17b	1.88 m				
18	5.18 m	73.4	18′	3.04 d (10.9)	78.3
19	2.33 t (5.8)	46.2	19′	2.84 dt (10.9, 5.0)	50.0
20	3.79 d (5.8)	51.8	20′	4.66 d (5.0)	49.0
21		216.7	21′		212.0
22	1.65 m	26.0	22′	1.76 m	26.4
23	0.90 d (6.6)	24.6	23′	1.09 d (6.6)	24.0
24	0.92 d (6.6)	21.3	24′	0.99 d (6.6)	23.5
25	1.52 s	15.4	25′	1.51 s	17.2
1″	5.17 d (5.8)	75.5	1‴	4.86 s	82.54
2″		52.7	2‴		72.9
3″		92.8	3‴		194.4
4″		188.7	4‴		94.4
5″		149.5	5‴		195.6
6″		122.4	6‴		134.1
7″		68.1	7‴		162.0
8″	4.82 s	85.8	8‴	5.37 d (5.0)	82.47
9″	1.66 s	16.9	9‴	1.73 s	12.9

Table S3 ^{1}H (400 MHz) and ^{13}C (100 MHz) NMR data of **4**−**8** (δ in ppm).

4[a]			**5**[a]			**6**[b]		**7**[c]			**8**[a]	
no.	δ_H (J in Hz)	δ_C	*no.*	δ_H (J in Hz)	δ_C	δ_H (J in Hz)	δ_C	*no.*	δ_H (J in Hz)	δ_C	δ_H (J in Hz)	δ_C
1		175.9	1		177.7		176.5	1		174.5		177.3
3	3.41 m	52.0	3	3.25 m	52.3	3.14 m	51.3	3	3.06 m	49.9	3.26 ddd (8.7, 6.1, 2.0)	52.0
4	2.43 m	49.3	4	2.51 dd (6.0, 1.6)	54.5	2.35 dd (5.9, 2.7)	54.9	4	2.40 dd (6.2, 1.9)	51.9	2.65 dd (6.1, 1.8)	53.1
5	2.42 m	37.2	5	2.59 m	36.6	2.62 m	35.5	5	2.45 m	35.0	2.56 m	36.5
6		142.6	6		140.9		139.3	6		139.2		141.1
7	5.79 s	123.5	7	5.41 brs	126.7	5.39 brs	126.2	7	5.33 brs	125.4	5.39 brs	126.7
8	2.26 m	46.2	8	3.29 m	44.6	3.35 m	43.4	8	3.08 m	43.2	3.18 m	44.8
9		67.6	9		69.3		68.3	9		66.9		69.1
10a	1.54 m	49.4	10a	1.19m	50.0	1.20 m	49.2	10a	1.07 m	48.7	1.18 m	49.8
10b	1.43 m		10b	1.13m		1.13 m		10b	1.01 m		1.13 m	
11	1.24 d (6.5)	14.0	11	1.25 d (7.2)	13.8	1.17 d (7.1)	13.6	11	1.16 d (7.0)	13.1	1.26 d (7.2)	13.8
12	1.79 s	20.0	12	1.78 s	19.8	1.73 s	20.0	12	1.70 s	19.6	1.78 d (1.2)	19.8
13	4.59 d	48.6	13	6.03 d (11.1)	125.5	6.12 d (11.0)	125.7	13	6.04 d (10.8)	124.4	6.13 d (10.8)	125.7
14		152.6	14		138.0		137.6	14		135.2		137.8
15a	2.29 m	27.2	15a	2.09 m	38.9	2.54 t (12.6)	33.4	15a	1.99 dd (11.9, 4.8)	39.5	2.12 dd (12.2, 3.8)	41.1
15b	1.82 m		15b	2.09 m		1.94 dd (12.6, 7.5)		15b	1.78 d (12.3)		1.95 m	
16a	2.20 m	40.4	16a	1.56 m	30.2	1.83 m	27.8	16a	1.46 m	19.0	1.61 m	19.9
16b	1.64 m		16b	1.31 m		1.66 m		16b	1.27 m		1.52 m	
17	3.63 m	71.1	17	3.86 m	71.3	3.74 m	71.5	17a	1.69 m	29.1	1.87 m	30.8
18a	2.75 m	36.1	18	3.55 m	80.1	4.51 m	73.3	17b	1.35 m		1.47 m	
18b	2.34 m		19	3.18 d (9.2)	77.9	3.19 d (9.0)	78.4	18	3.40 m	72.3	3.48 m	74.3
19	6.81 ddd (10.6, 7.8, 3.0)	135.1	20a	3.95 d (18.0)	44.3	3.61dd (12.7, 9.0)	41.8	19	3.00 ddd (8.6, 4.1, 3.2)	78.5	3.56 m	69.9
20		143.5	20b	2.00 d (18.0, 4.0)		2.17 d (12.7)		20a	3.82 dd (18.2, 3.2)	43.2	4.00 dd (18.1, 2.8)	46.0
21		202.1	21		212.9		213.6	20b	1.90 dd (18.2, 4.5)		1.96 m	
22	1.67 m	25.5	22	1.60 m	25.8	1.59 m	25.0	21		211.4		212.5
23	0.96 d (6.5)	23.6	23	0.92 d (6.6)	23.8	0.90 d (6.6)	23.7	22	1.57 m	24.0	1.60 m	25.7
24	0.97 d (6.5)	22.7	24	0.91 d (6.6)	22.2	0.90 d (6.6)	21.6	23	0.83 d (6.5)	23.5	0.91 d (6.6)	23.8
25a	5.19 s	115.1	25	1.50 s	16.1	1.52 s	15.6	24	0.83 d (6.5)	21.7	0.91 d (6.6)	22.2
25b	5.08 s		1′a	3.75 dq (9.2, 7.0)	66.6	3.36 s	57.2	25	1.42 s	15.6	1.50 d (0.9)	15.9
			1′b	3.64 m				1′	3.33 s	57.6		
			2′	1.19 t (7.0)	15.7							

[a] in CD_3OD; [b] in $CDCl_3$; [c] in DMSO-d_6.

Table S4. IC_{50} (μM, 48h) values of **1−8** against leukemia cell lines.

Compounds	HL60	A549	Hep3B	SW480
1	16.51	34.72	33.35	26.65
2	9.39	20.14	17.33	23.62
3	5.67	16.29	7.99	12.39
4	>40	>40	>40	>40
5	14.93	39.77	5.60	> 40
6	18.75	>40	>40	24.03
7	13.95	>40	>40	15.56
8	17.50	>40	10.29	17.38
DDP[a]	2.15	7.24	17.58	14.34

[a]DDP was selected as the positive control.

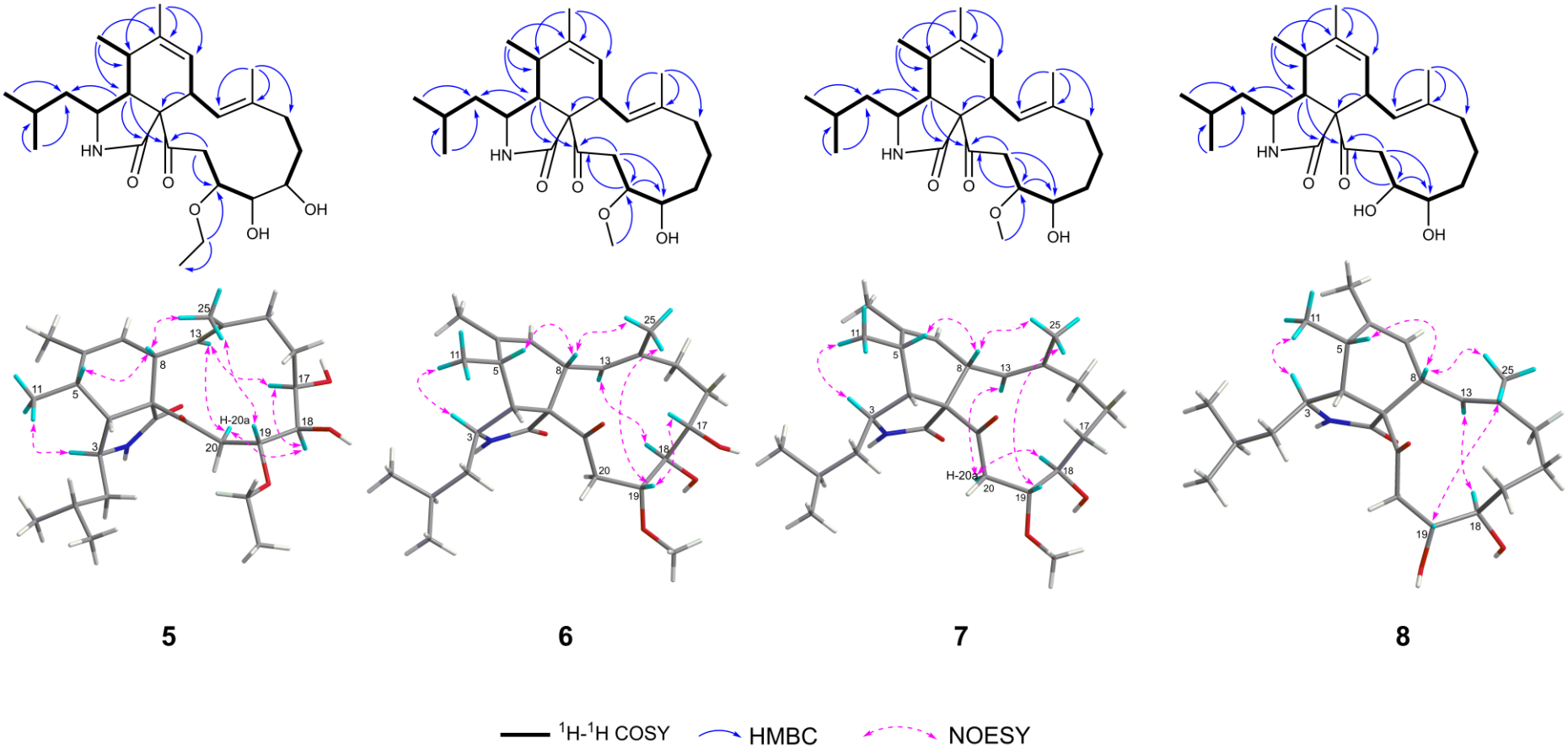

Figure S1. Key ^{1}H–^{1}H COSY, HMBC, and NOESY correlations of **5**–**8**.

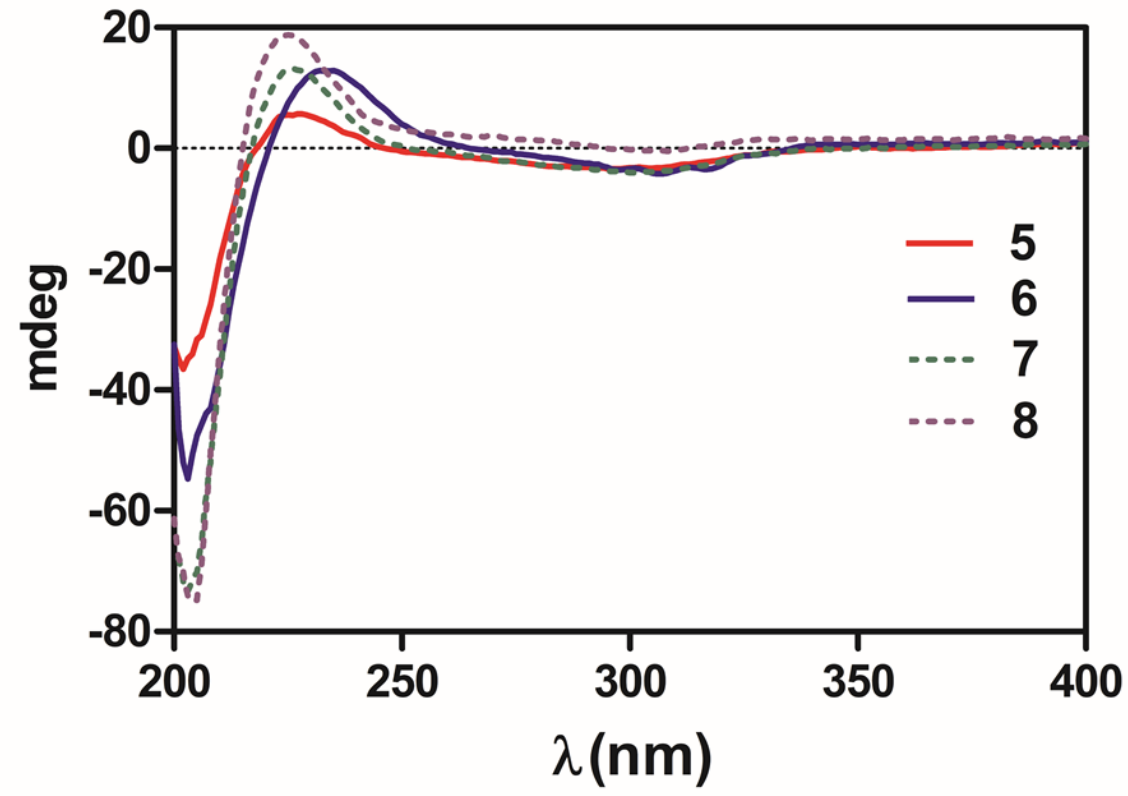

Figure S2. Experimental ECD spectra of **5**−**8.**

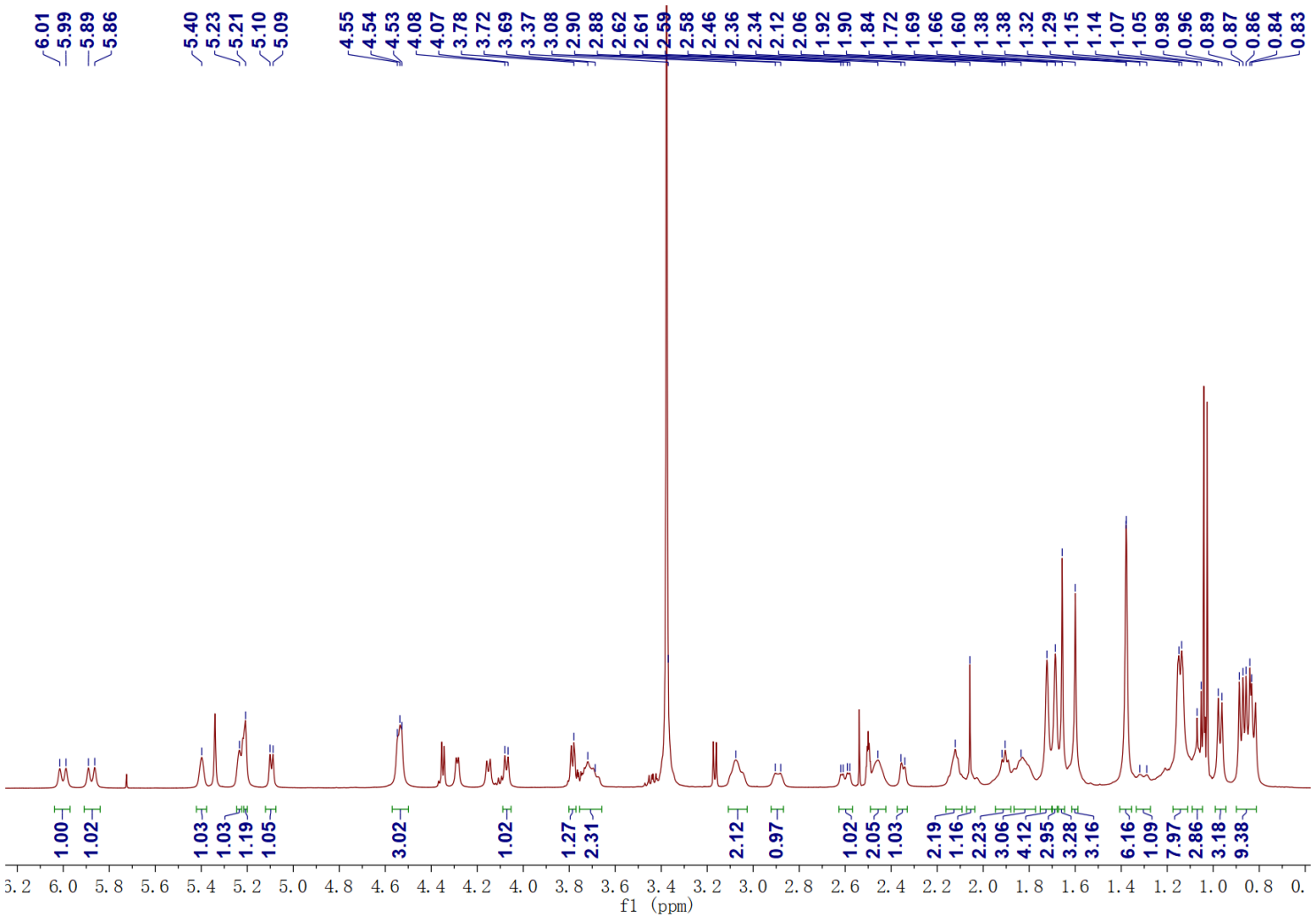

Figure S3. ^{1}H NMR of compound **1** (in DMSO-d_6)

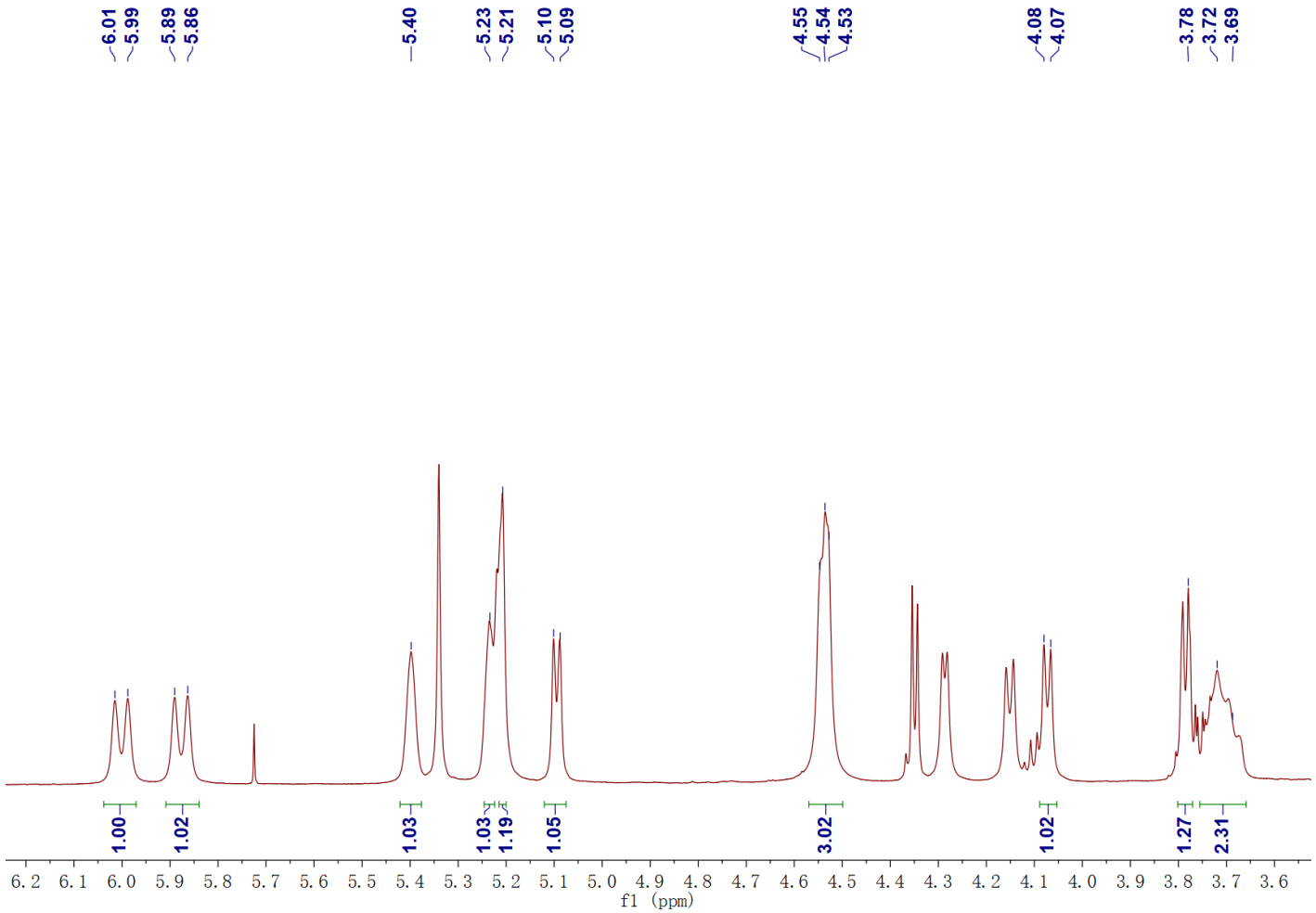

Figure S4. Enlarged ^{1}H NMR spectrum (6.0 ~ 3.6 ppm) of compound **1**

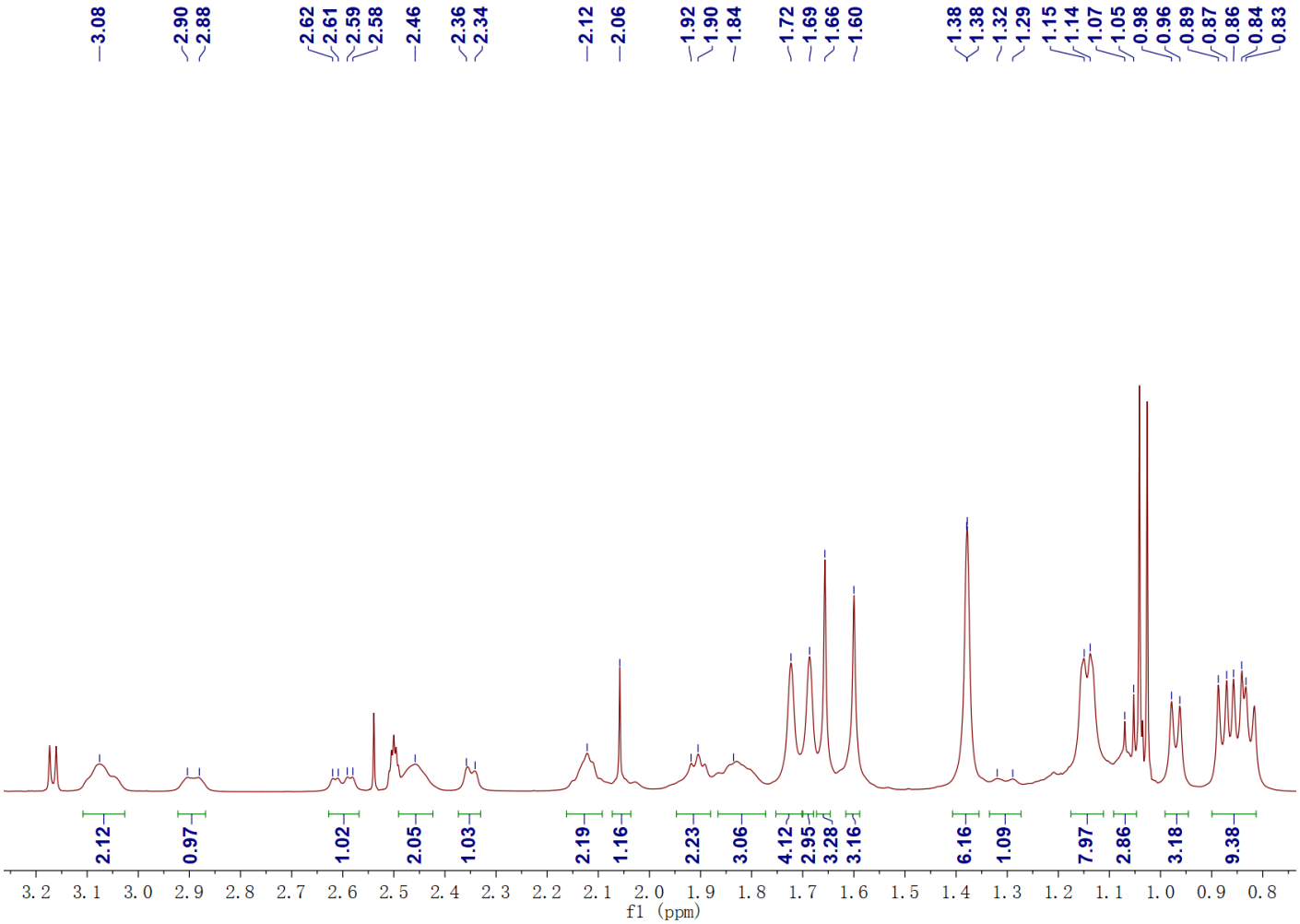

Figure S5. Enlarged ^{1}H NMR spectrum (3.2 ~ 0.8 ppm) of compound **1**

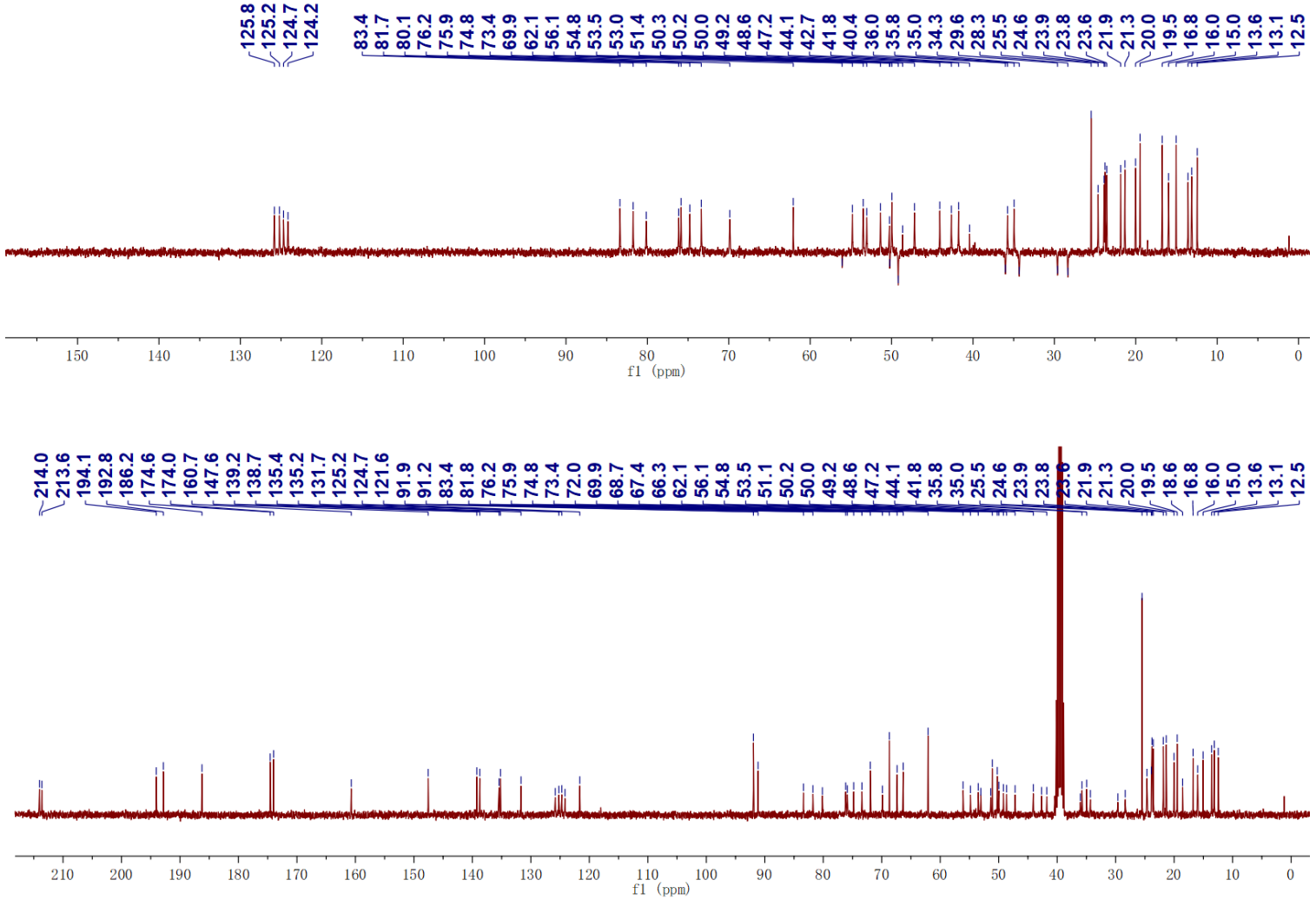

Figure S6. ^{13}C NMR of compound **1** (in DMSO-d_6)

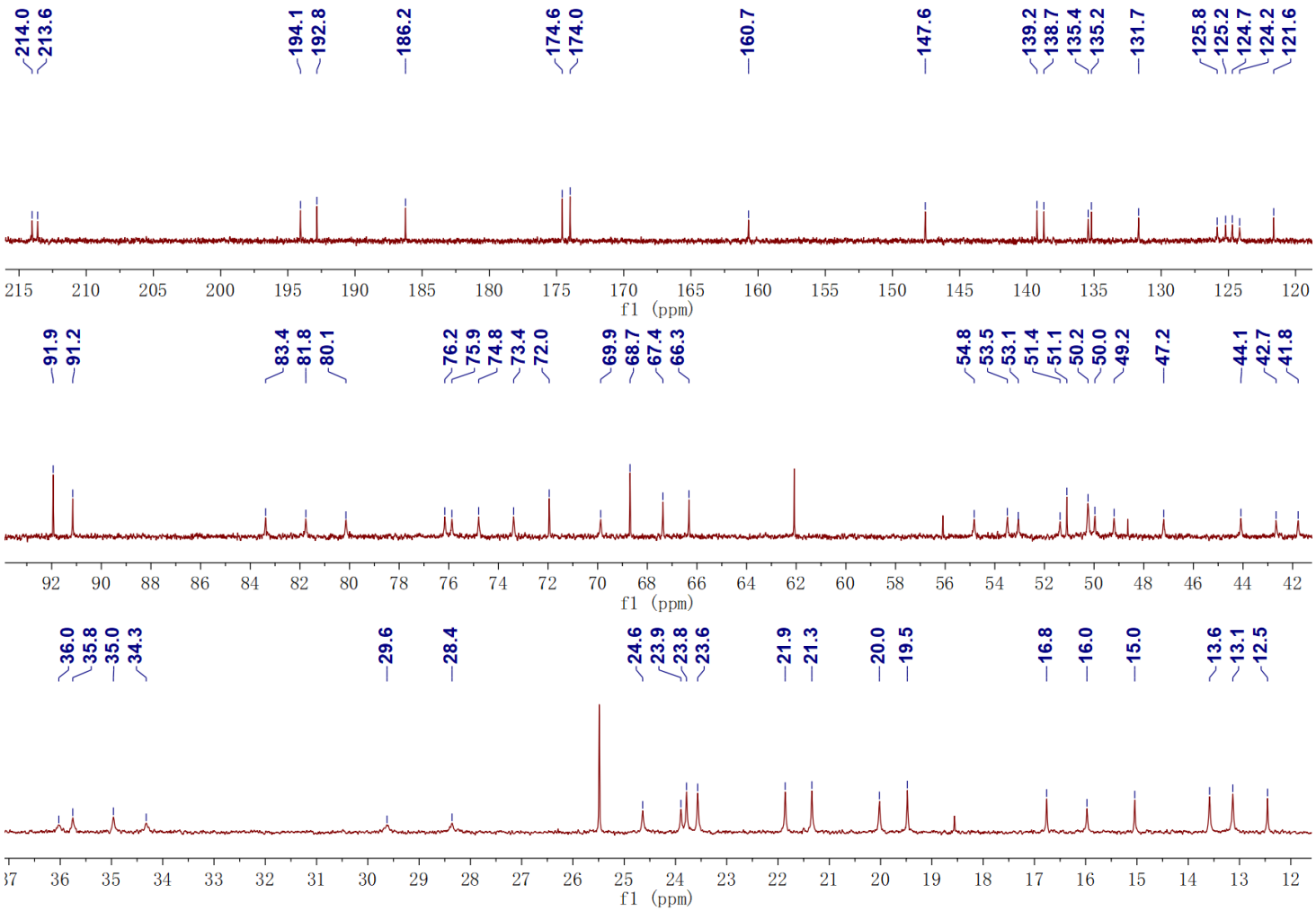

Figure S7. Enlarged ^{13}C NMR spectrum of compound **1**

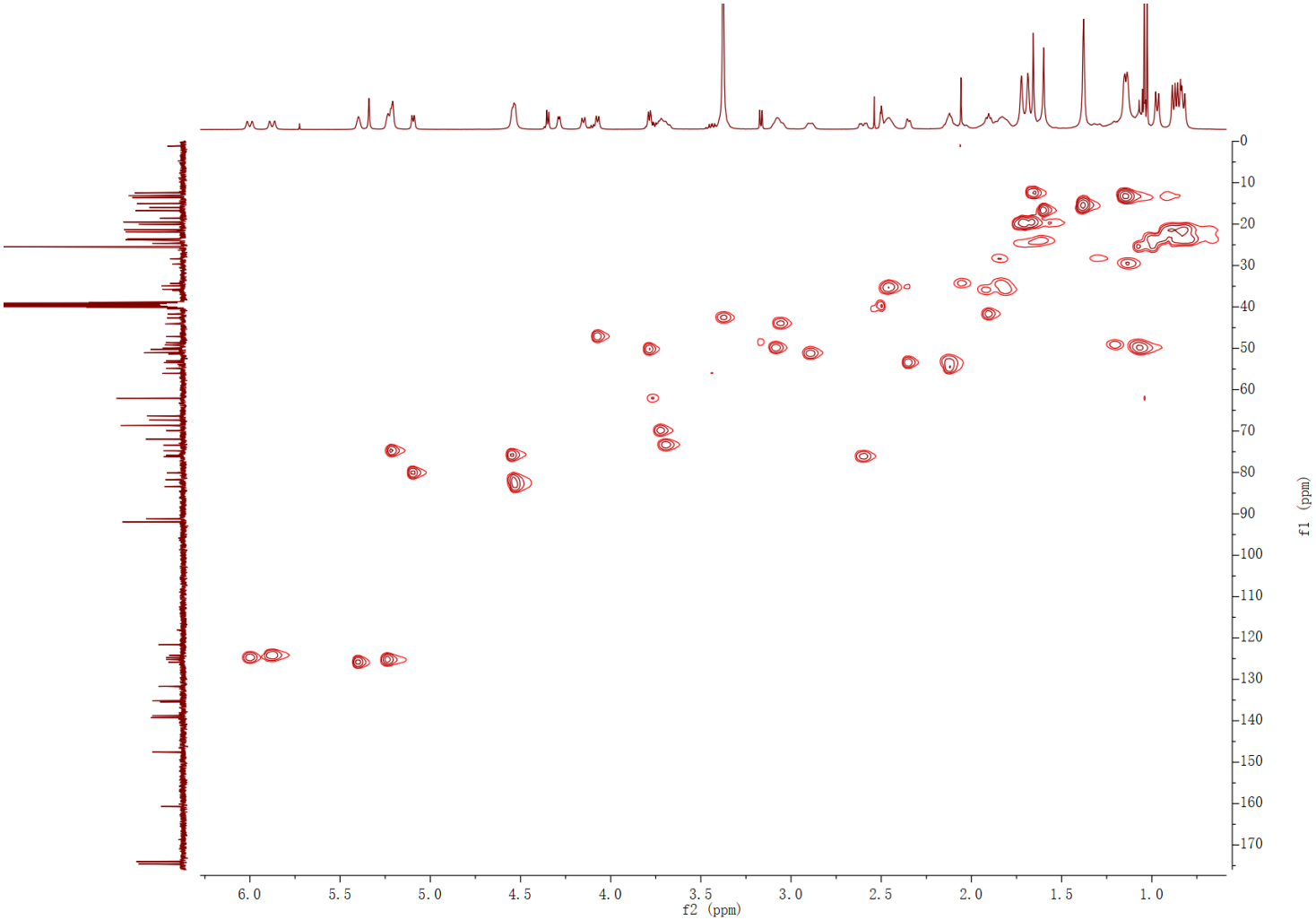

Figure S8. HSQC of compound **1** (in DMSO-d_6)

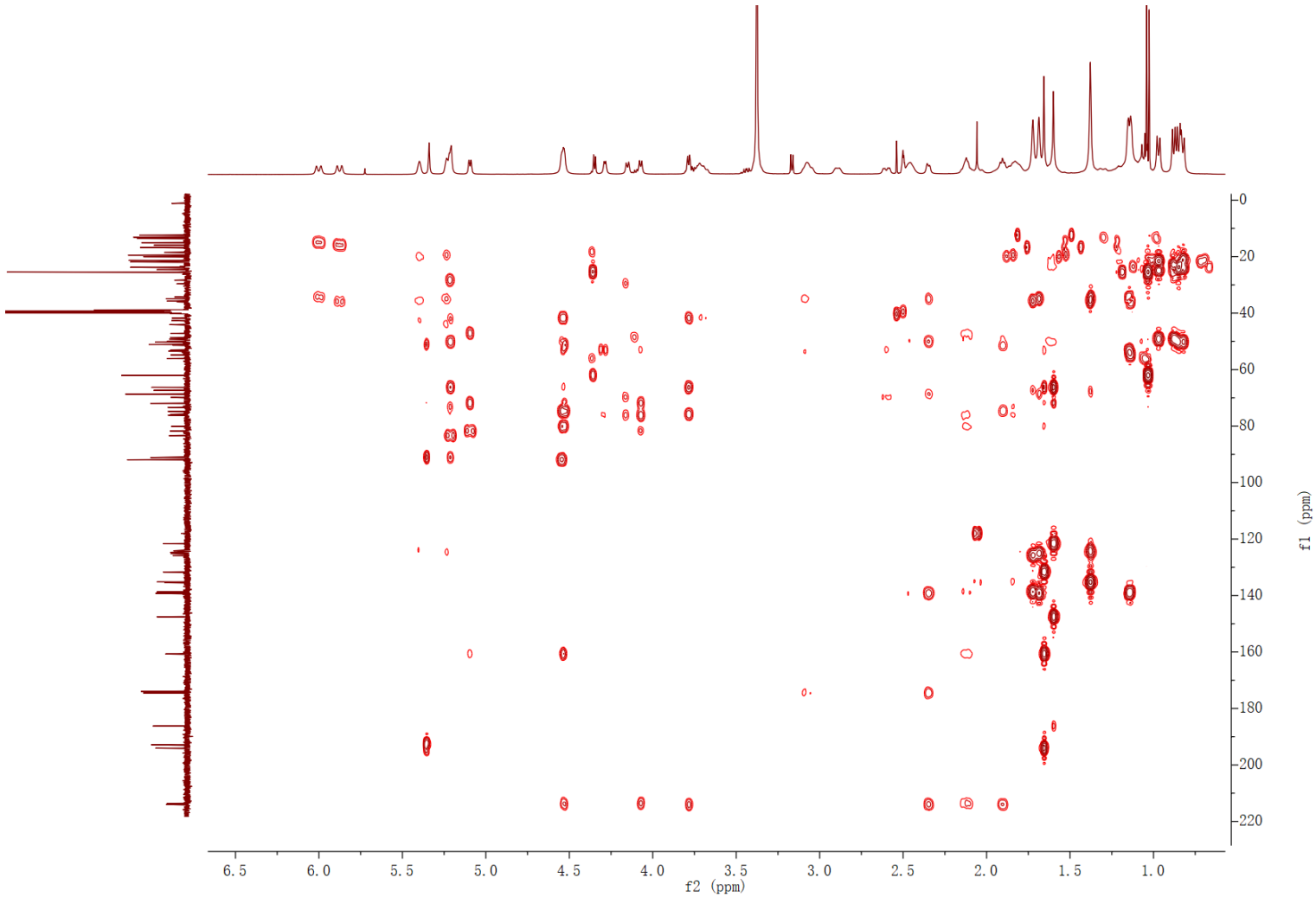

Figure S9. HMBC of compound **1** (in DMSO-d_6)

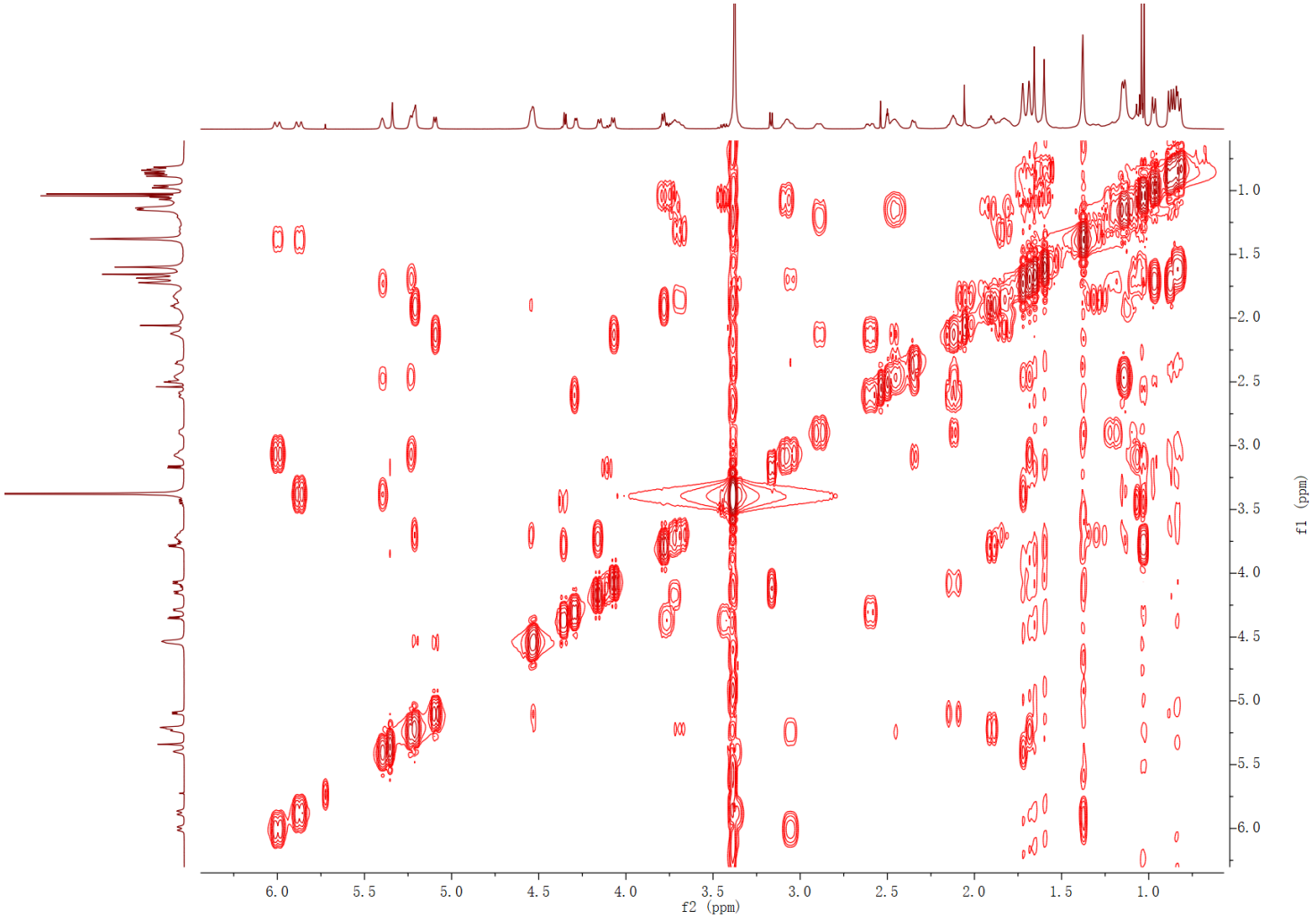

Figure S10. ^{1}H–^{1}H COSY of compound **1** (in DMSO-d_6)

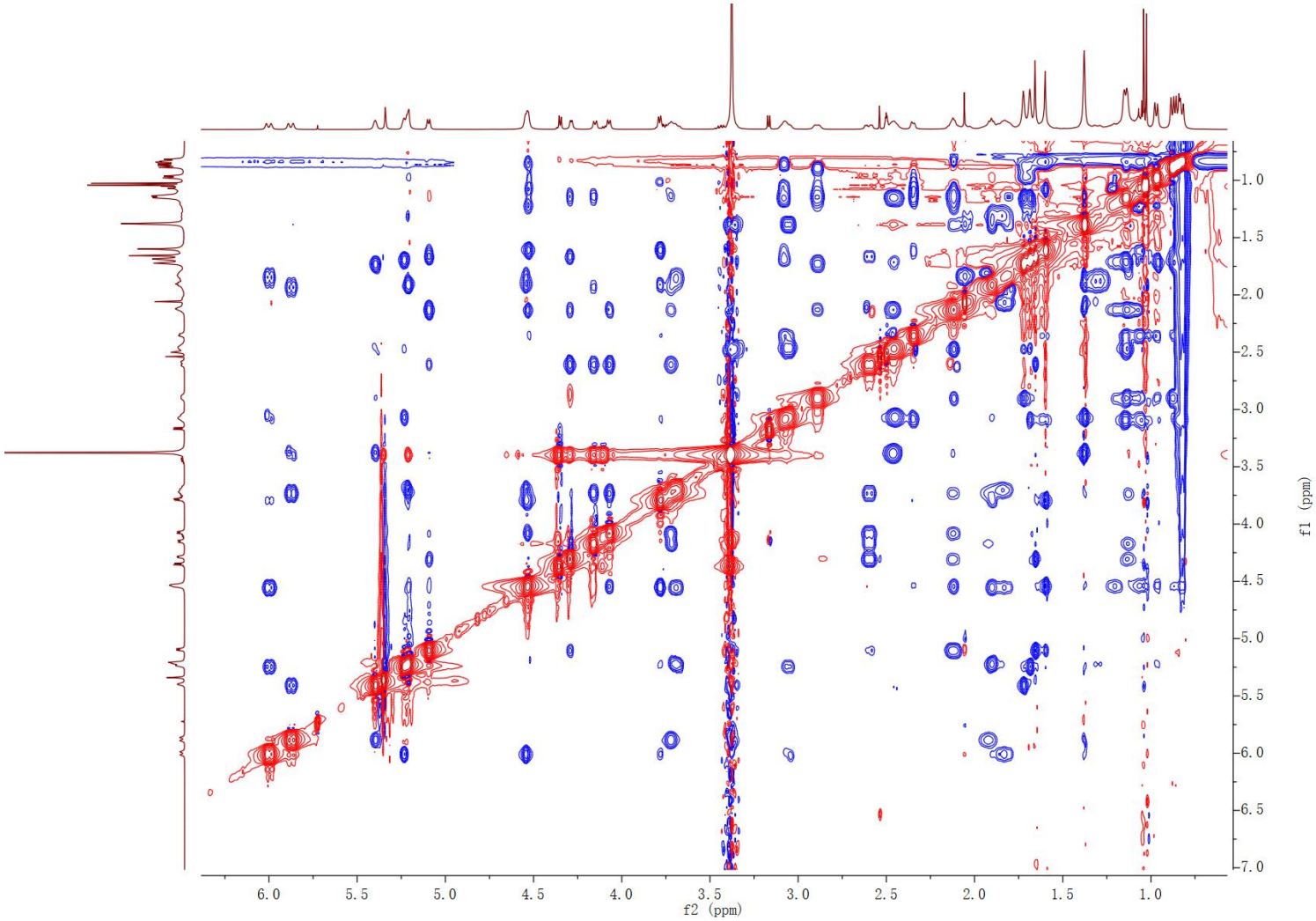

Figure S11. ROESY of compound**1** (in DMSO-d_6)

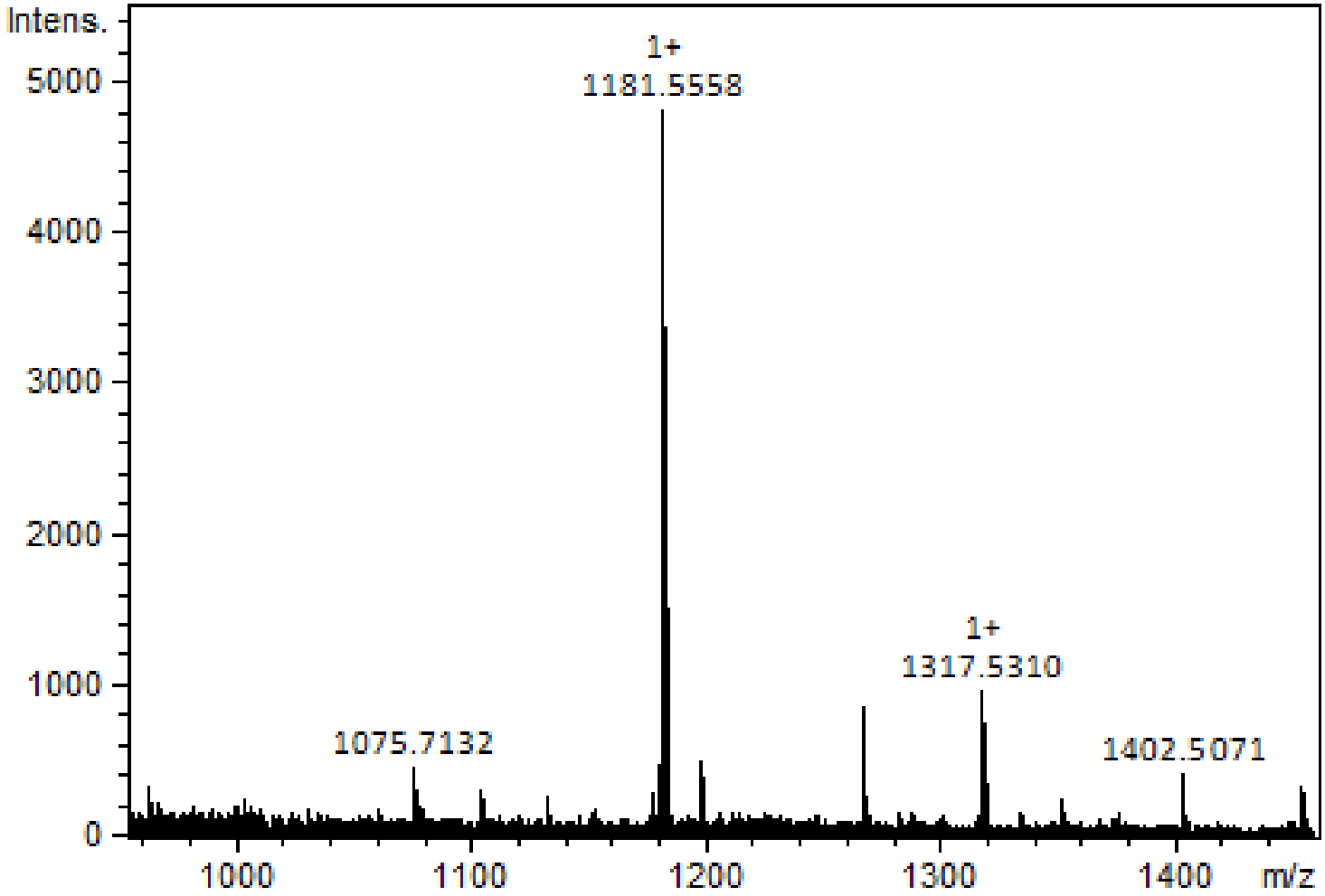

Figure S12. HRESIMS of compound **1**

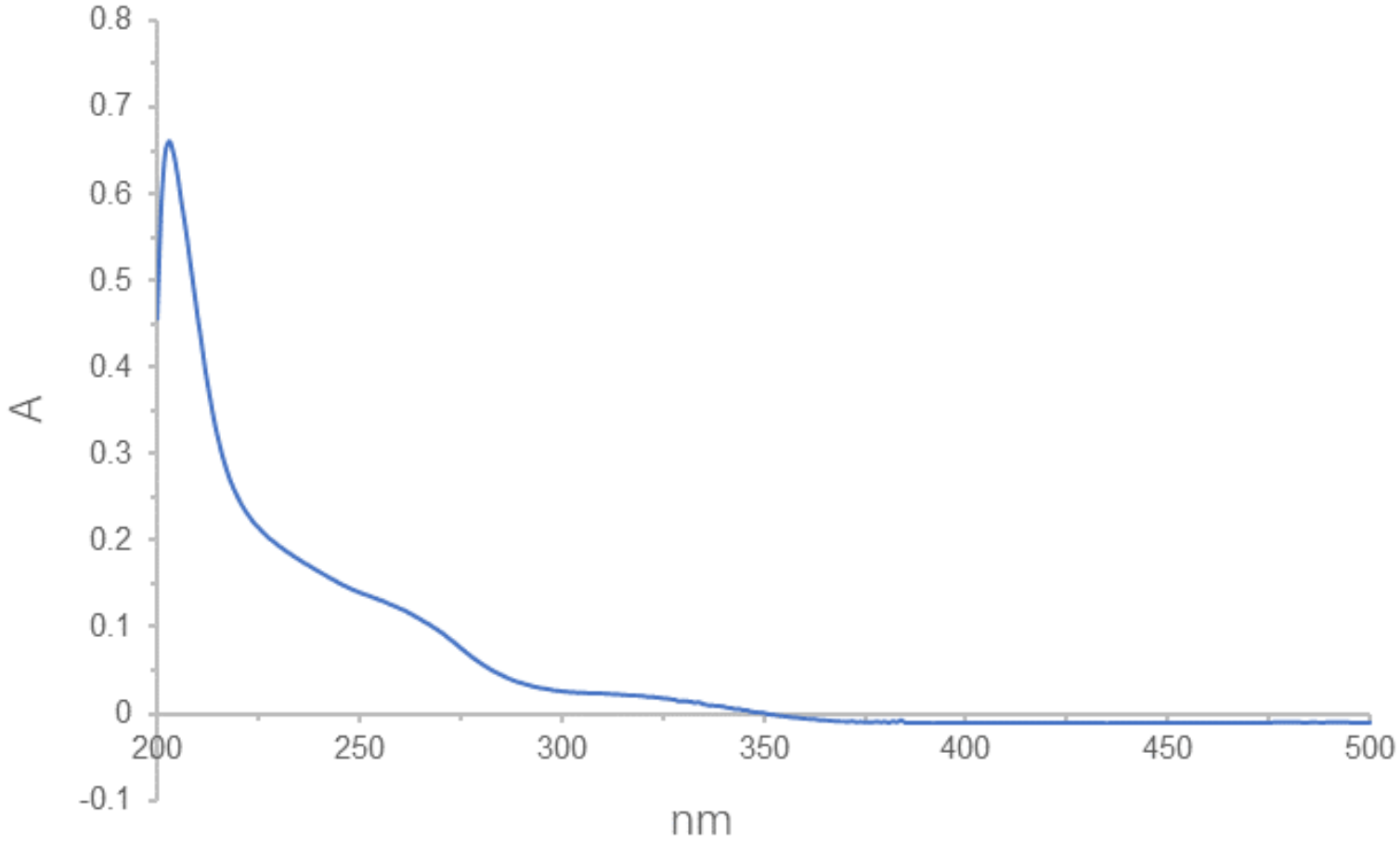

Figure S13. UV of compound **1**

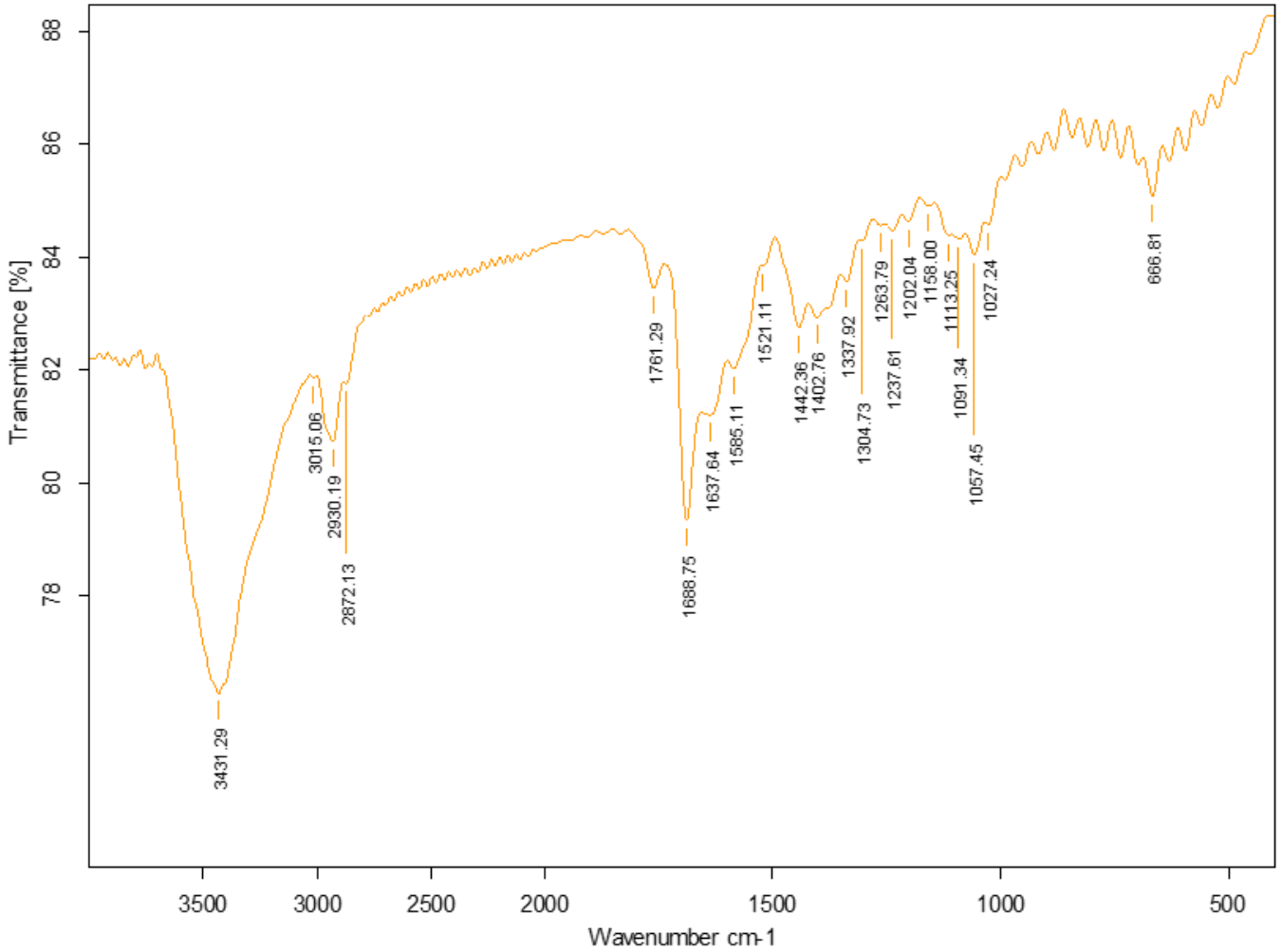

Figure S14. IR of compound **1**

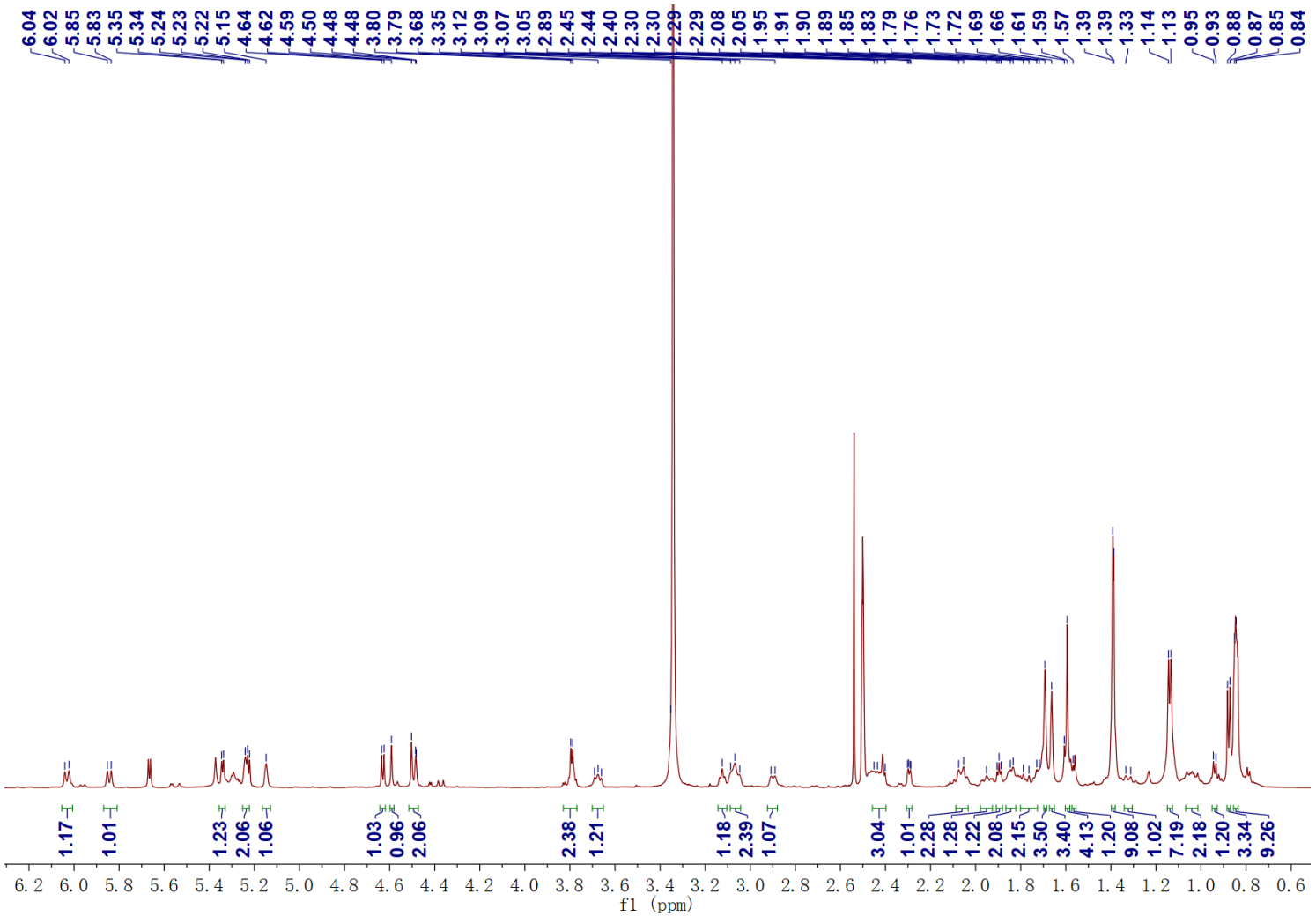

Figure S15. ^{1}H NMR of compound **2** (in DMSO-d_6)

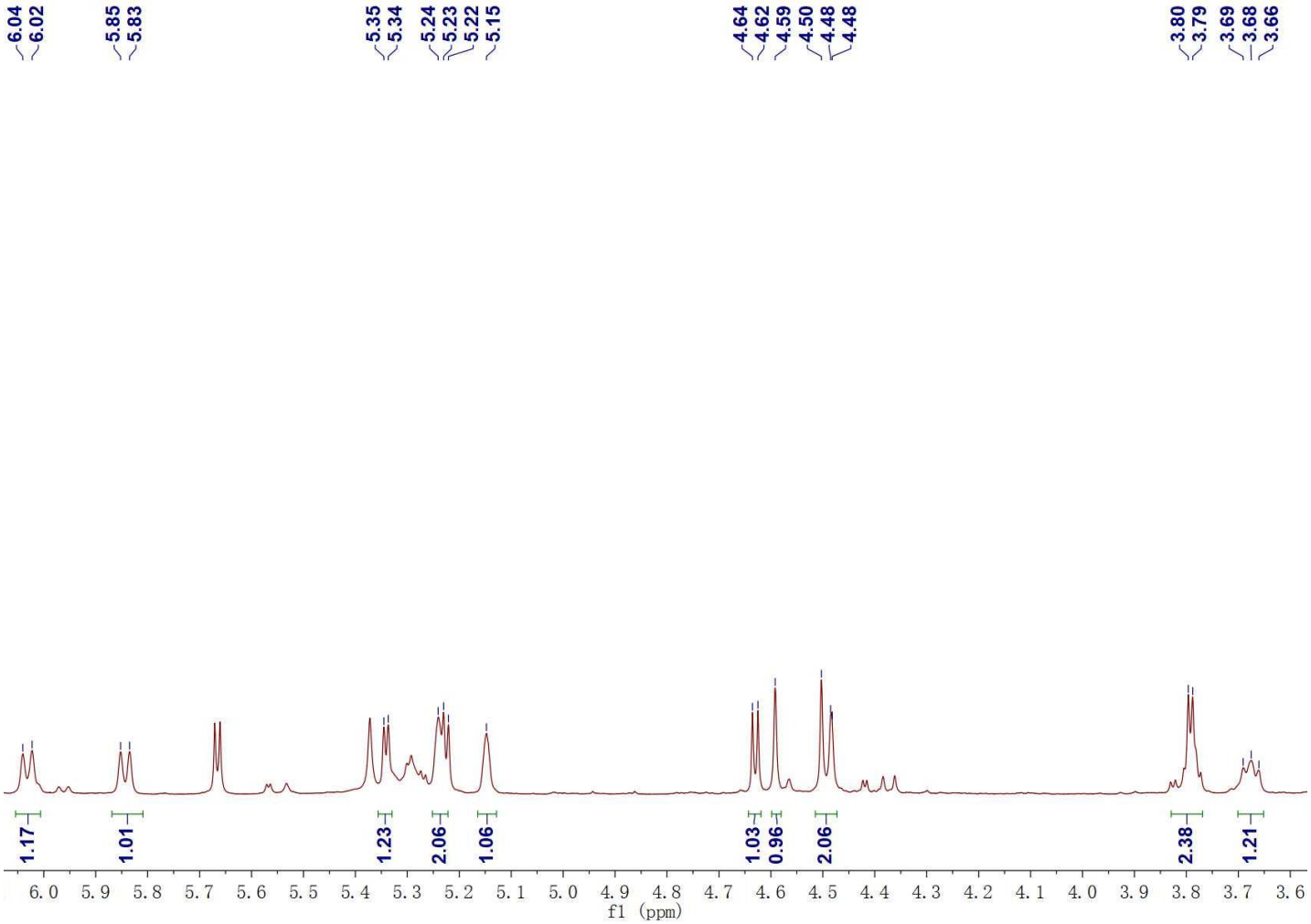

Figure S16. Enlarged ^{1}H NMR spectrum (6.1 ~ 3.6 ppm) of compound **2**

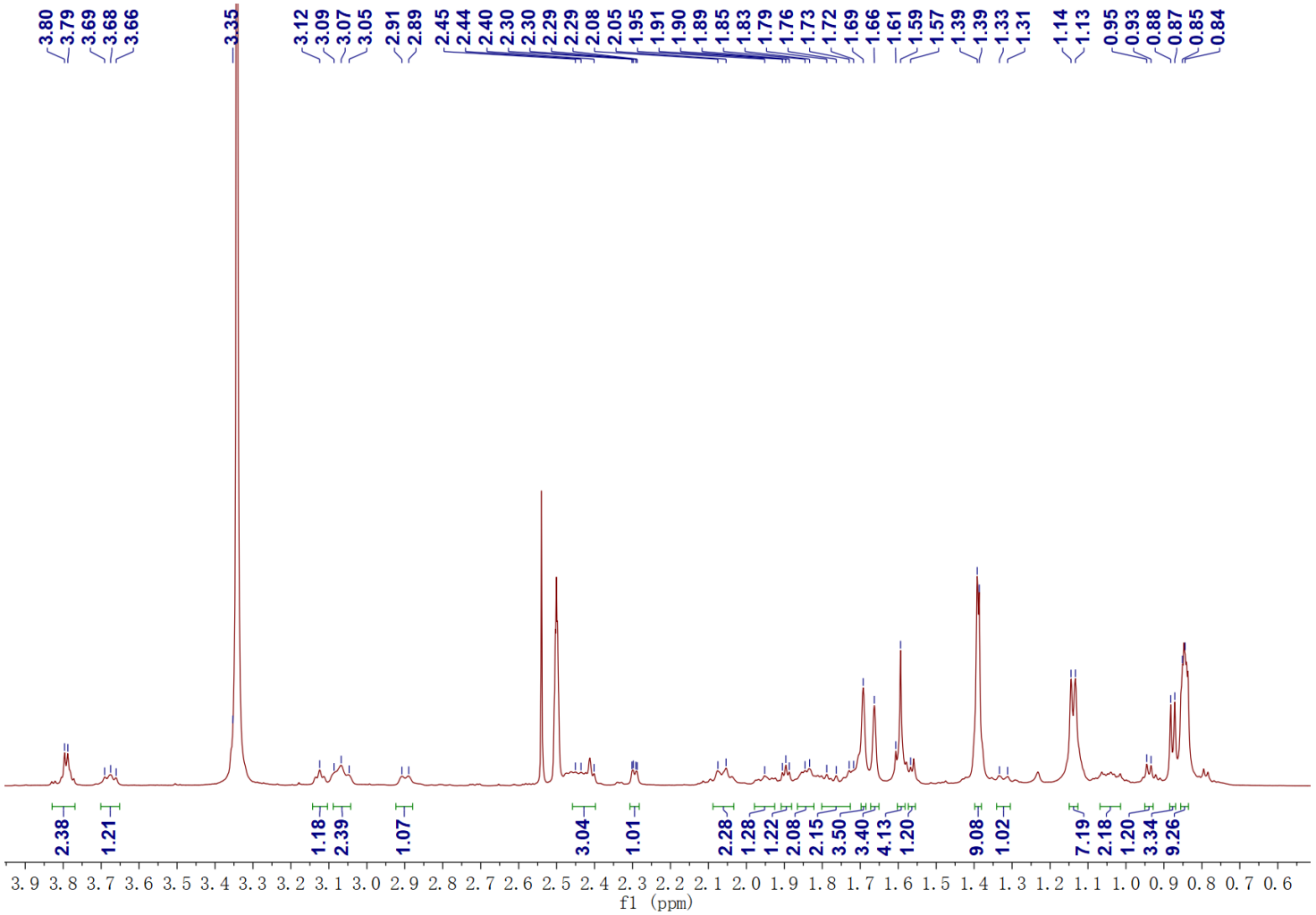

Figure S17. Enlarged ^{1}H NMR spectrum (3.9 ~ 0.7 ppm) of compound **2**

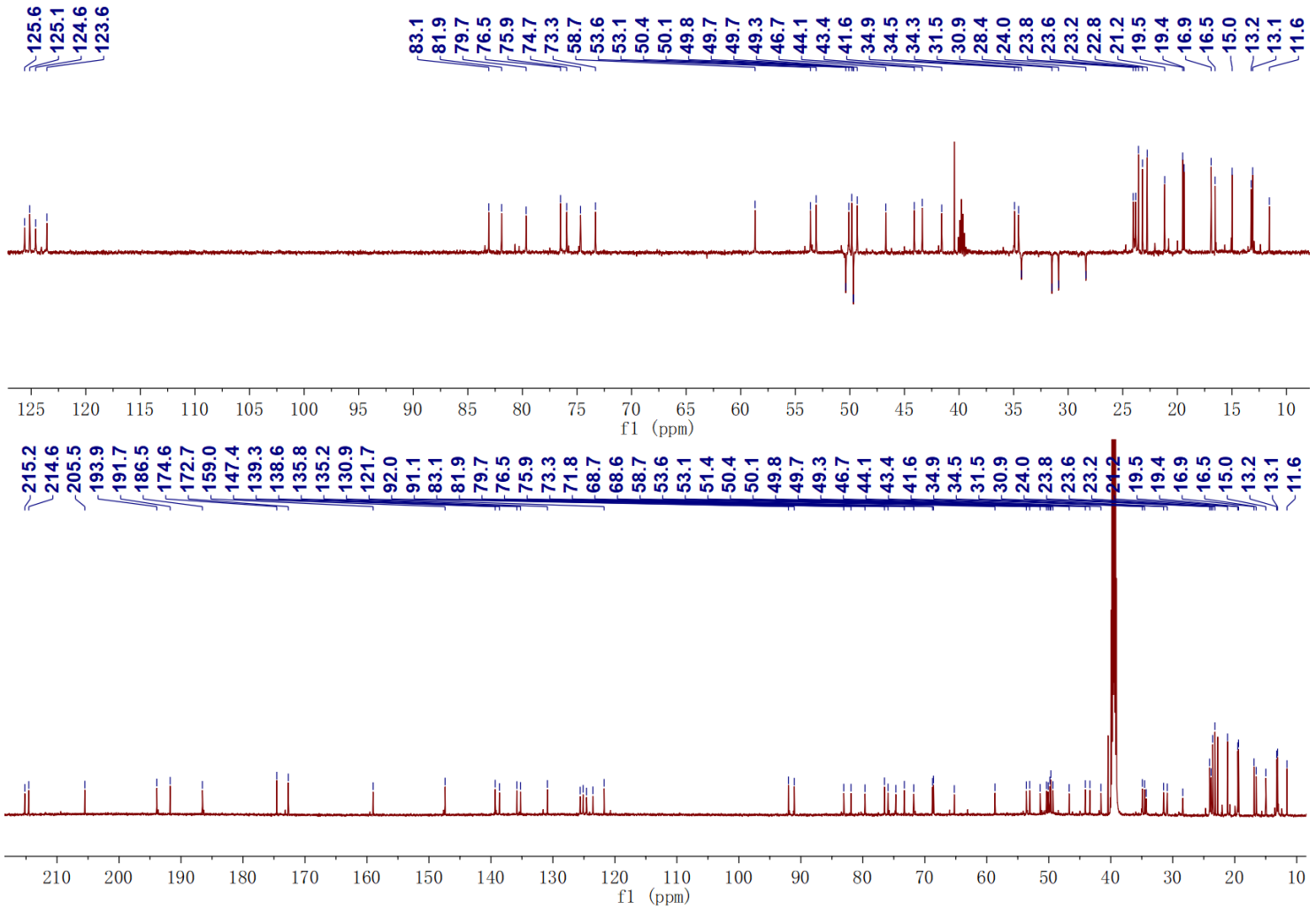

Figure S18. ^{13}C NMR NMR of compound **2** (in DMSO-d_6)

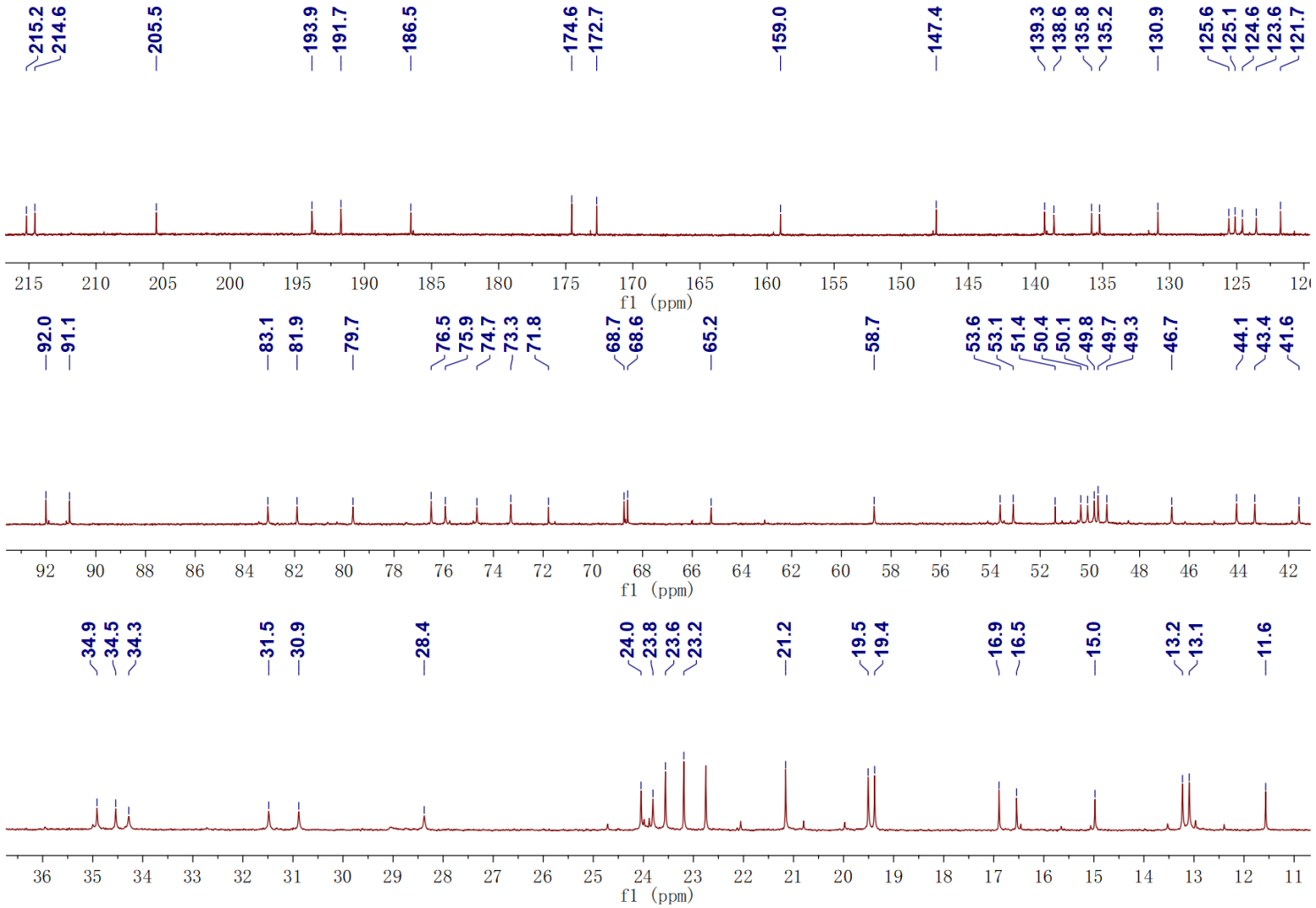

Figure S19. Enlarged ^{13}C NMR spectrum of compound **2**

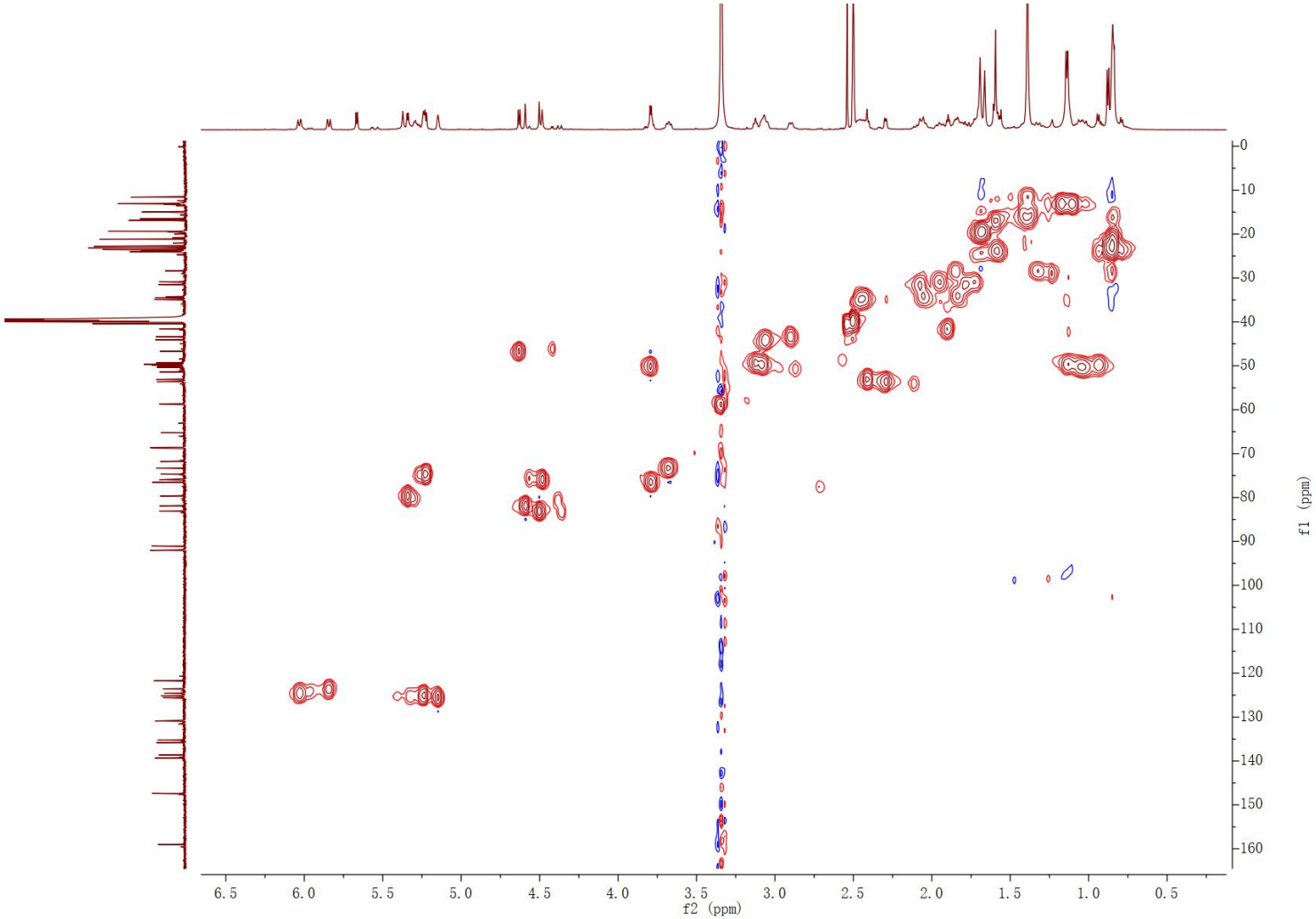

Figure S20. HSQC of compound **2** (in DMSO-d_6)

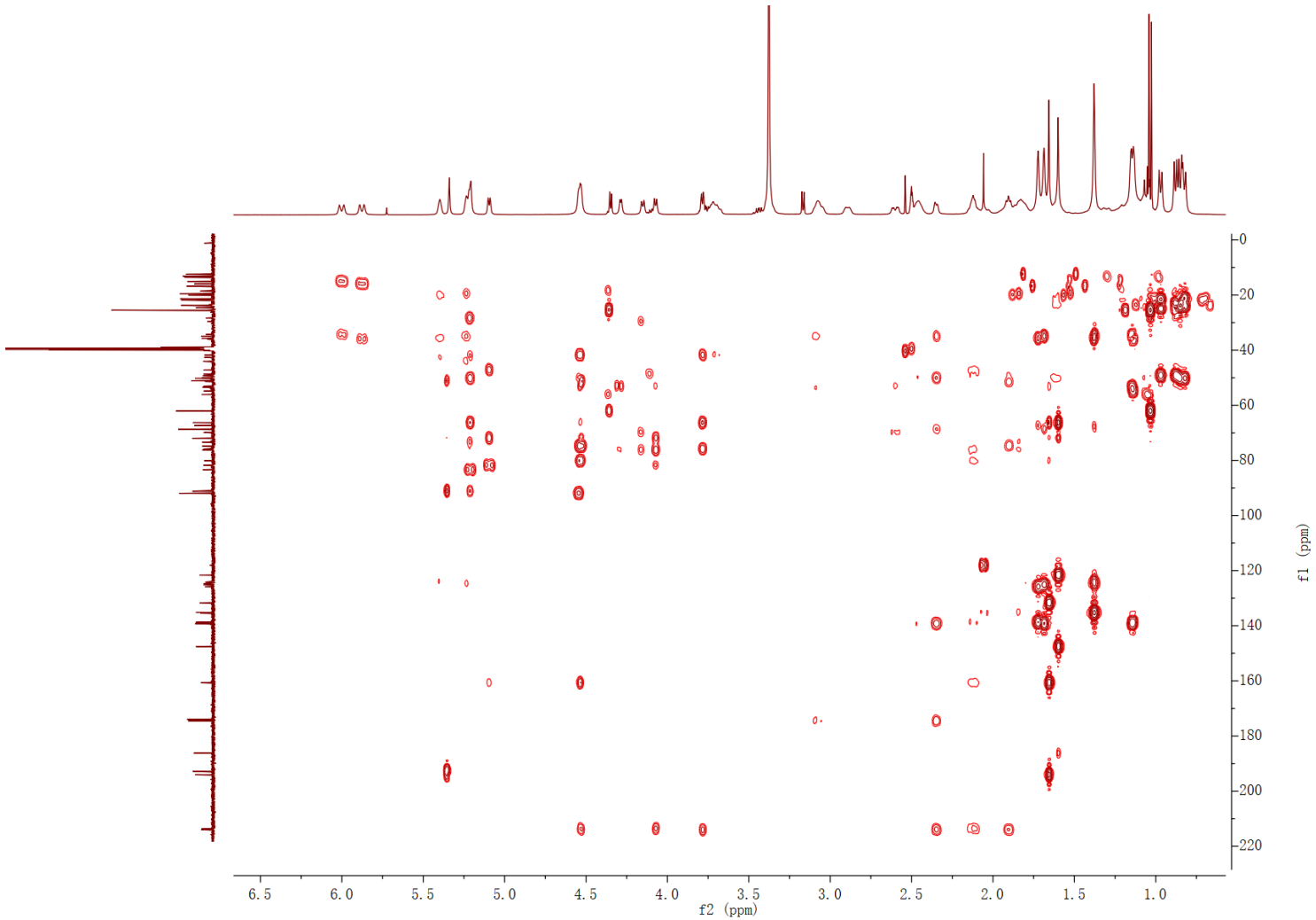

Figure S21. HMBC of compound **2** (in DMSO-d_6)

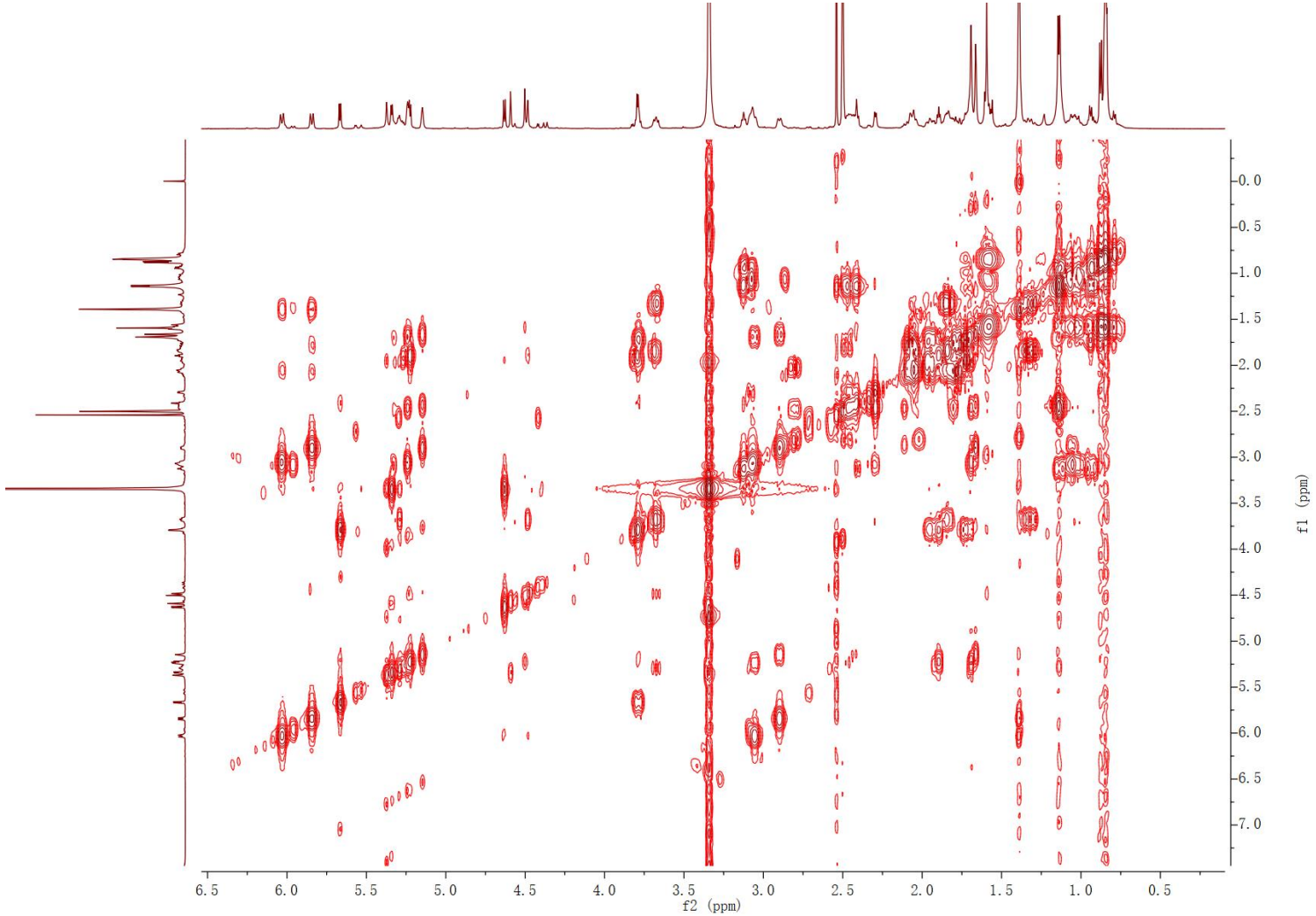

Figure S22. ^{1}H–^{1}H COSY of compound **2** (in DMSO-d_6)

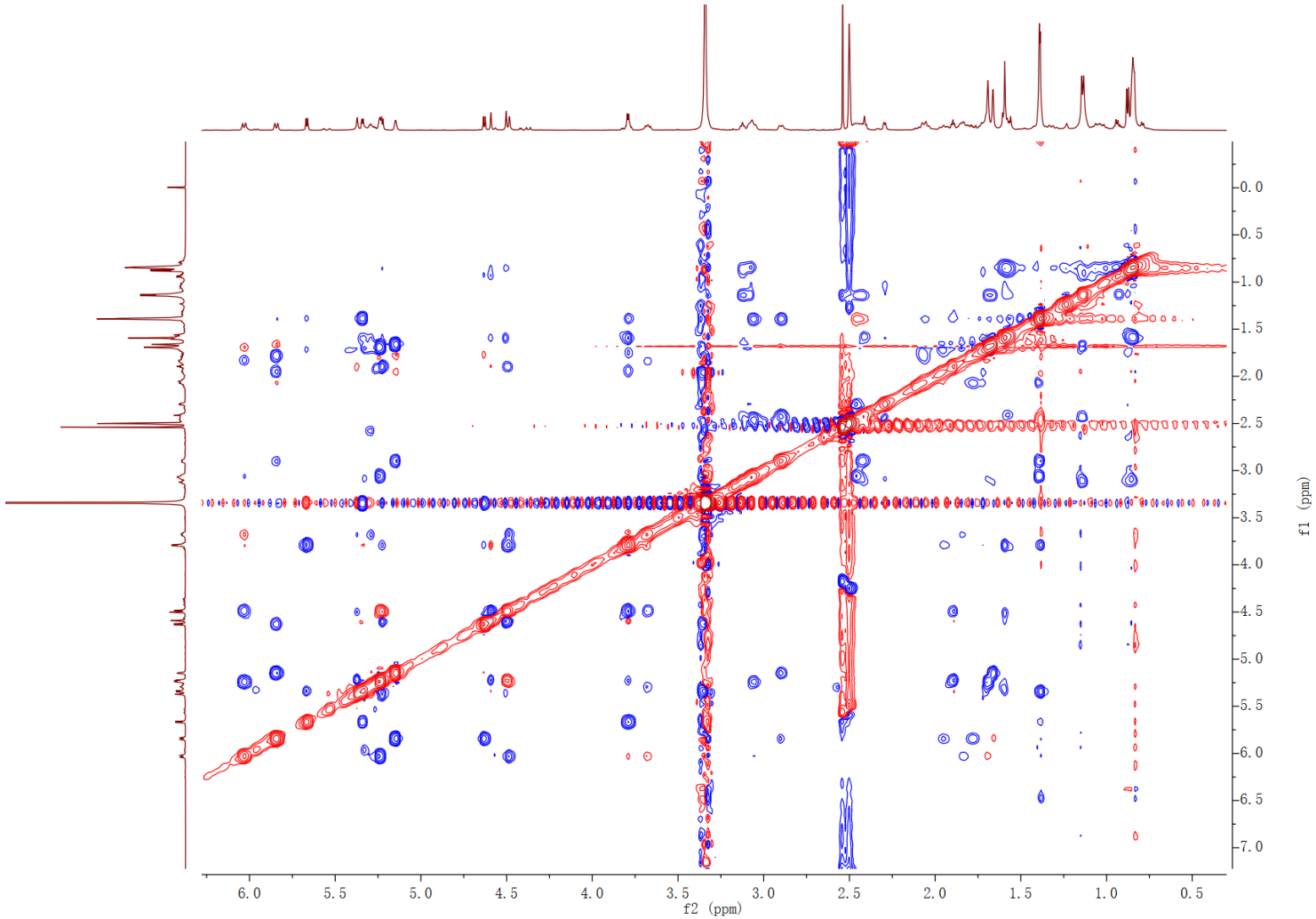

Figure S23. ROESY of compound **2** (in DMSO-d_6)

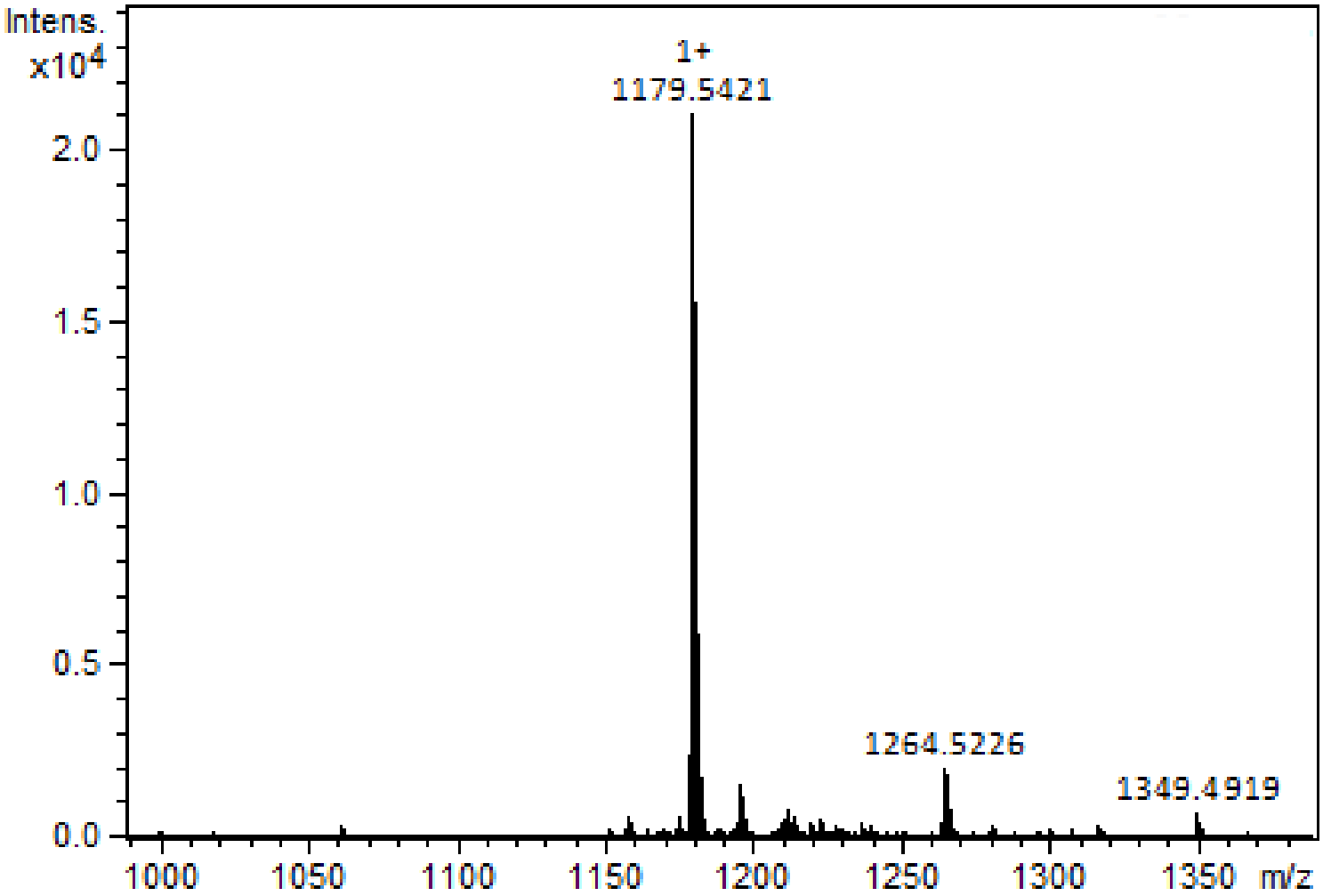

Figure S24. HRESIMS of compound **2**

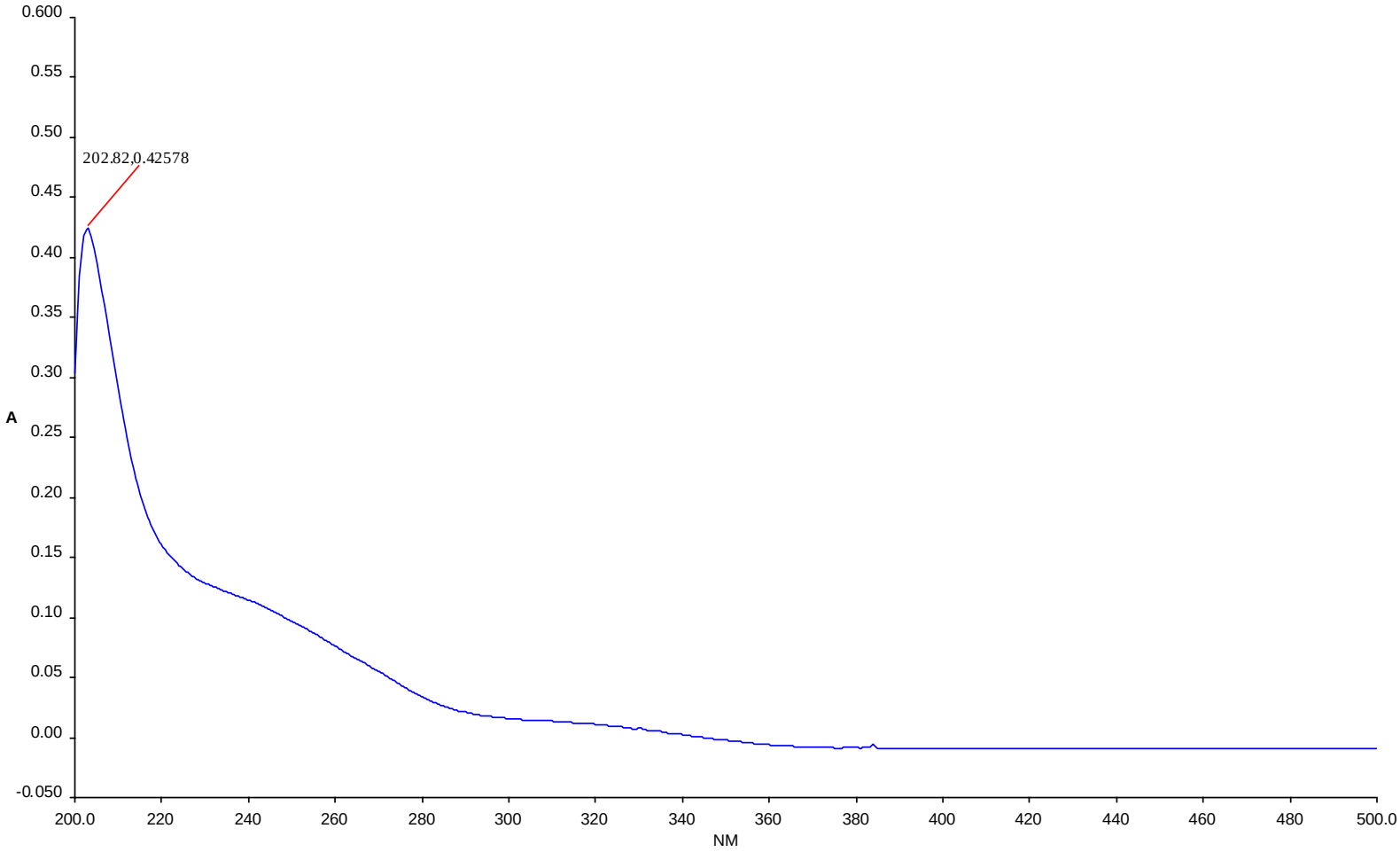

Figure S25. UV of compound **2**

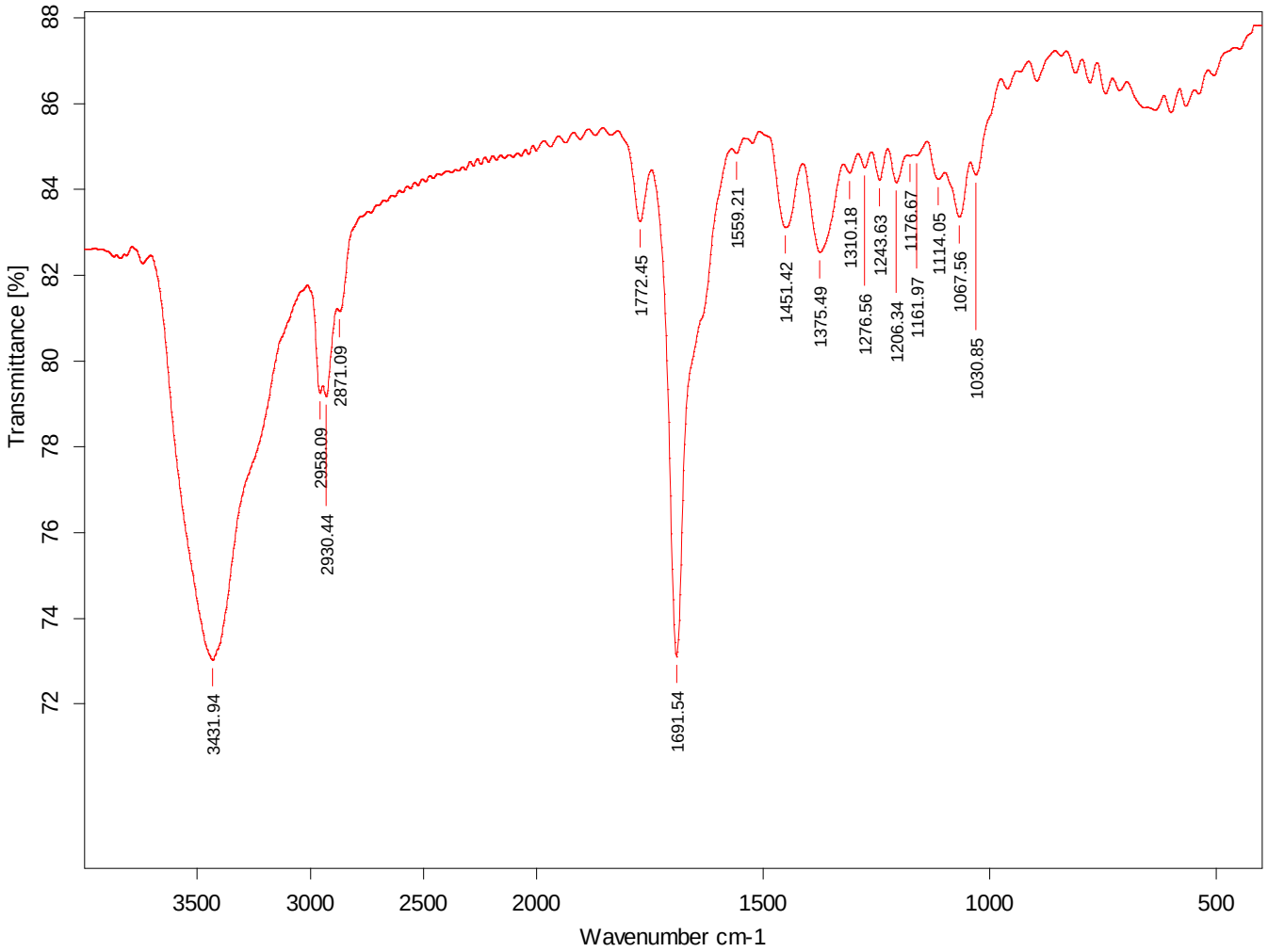

Figure S26. IR of compound **2**

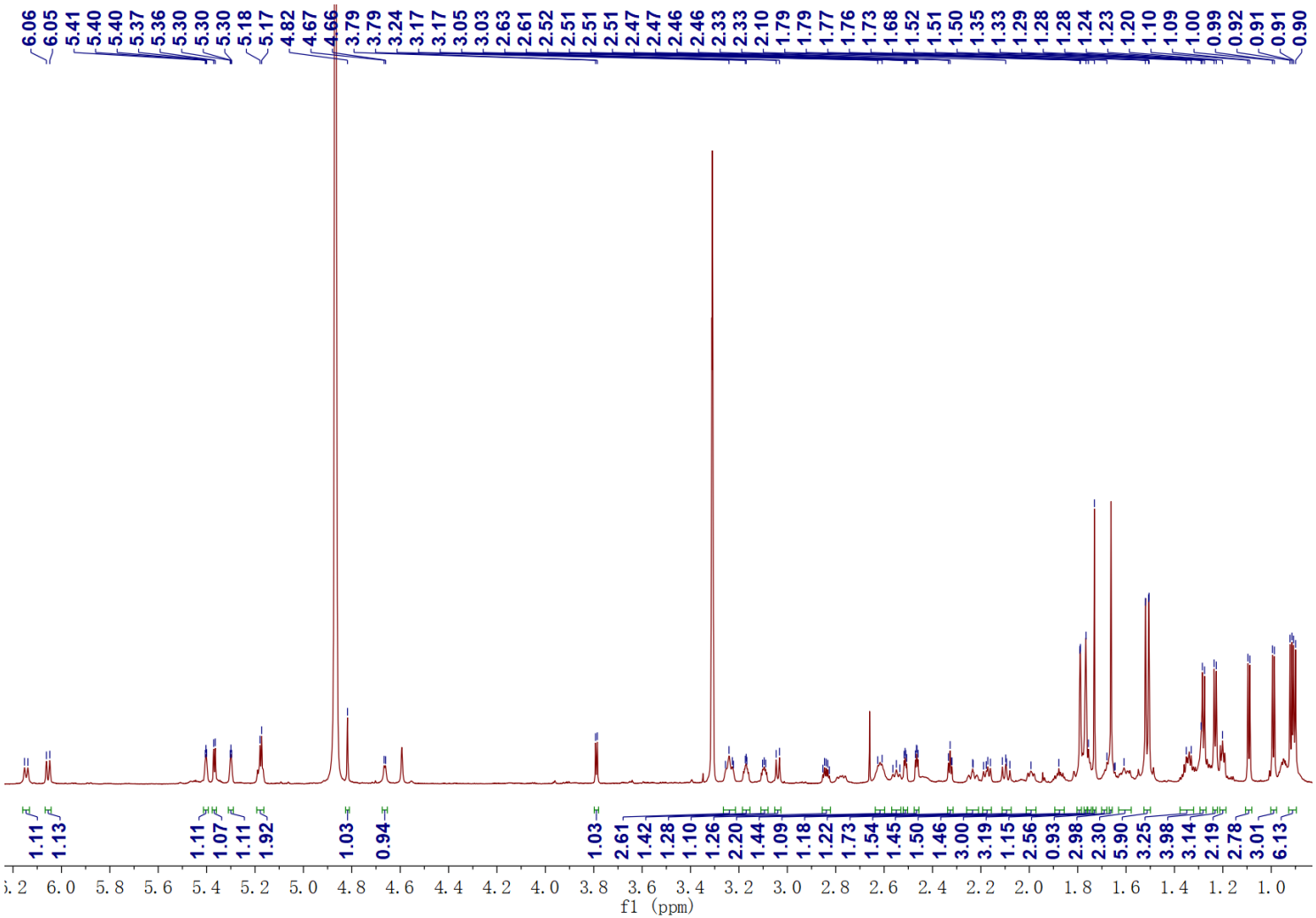

Figure S27. ^{1}H NMR of compound **3** (in CD_3OD)

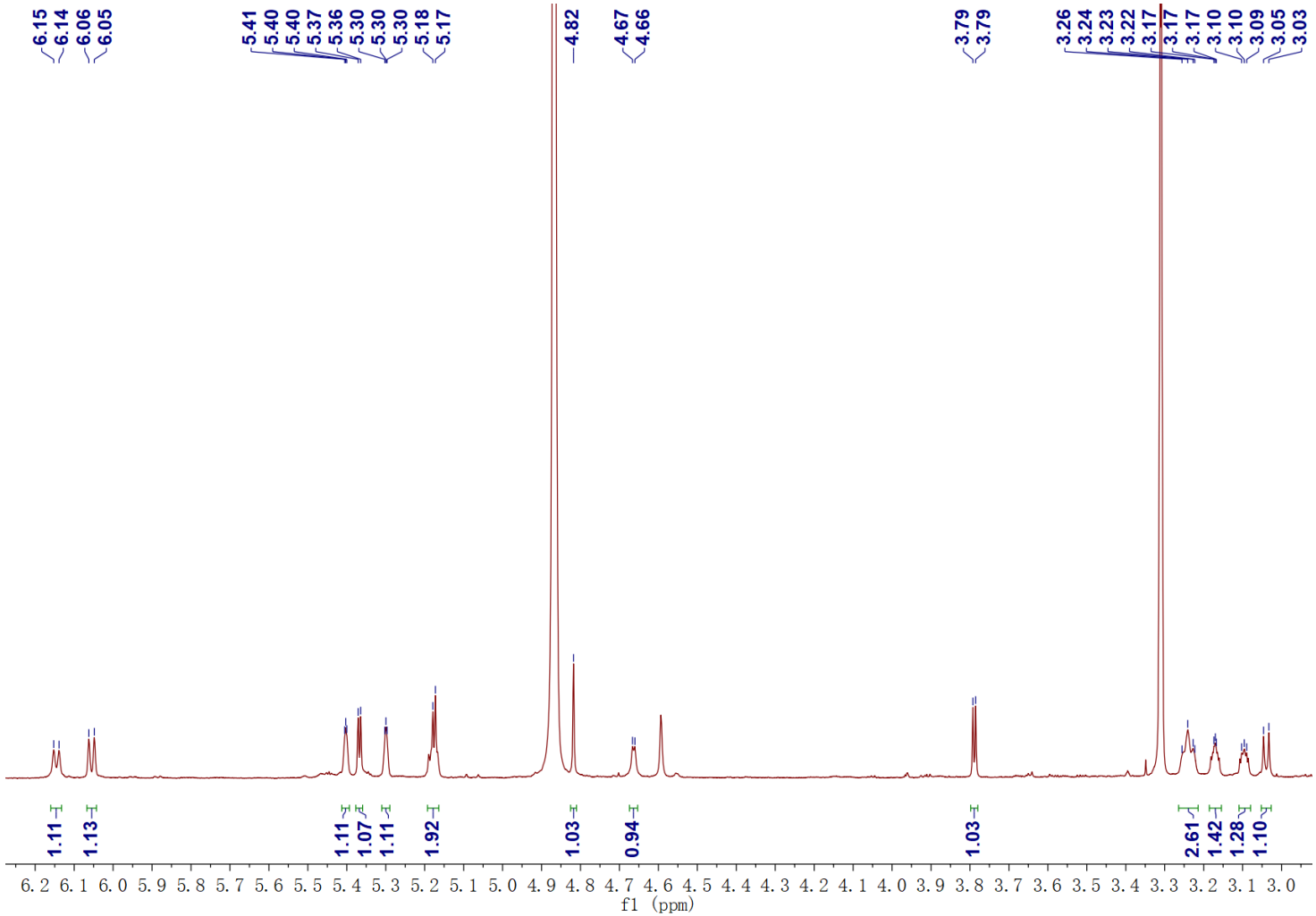

Figure S28. Enlarged ^{1}H NMR spectrum (6.2 ~ 3.0 ppm) of compound **3**

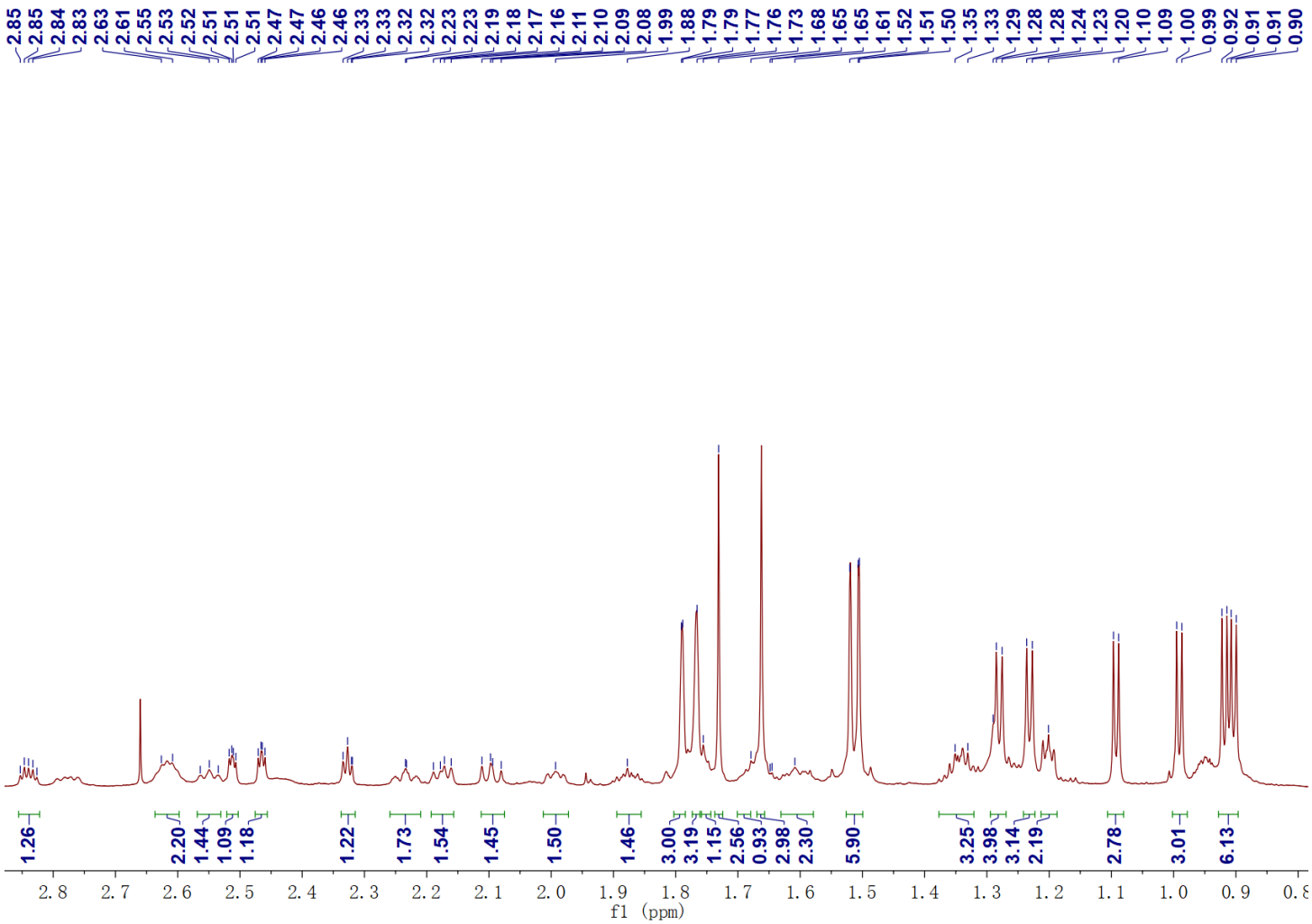

Figure S29. Enlarged ^{1}H NMR spectrum (3.0 ~ 0.8 ppm) of compound **3**

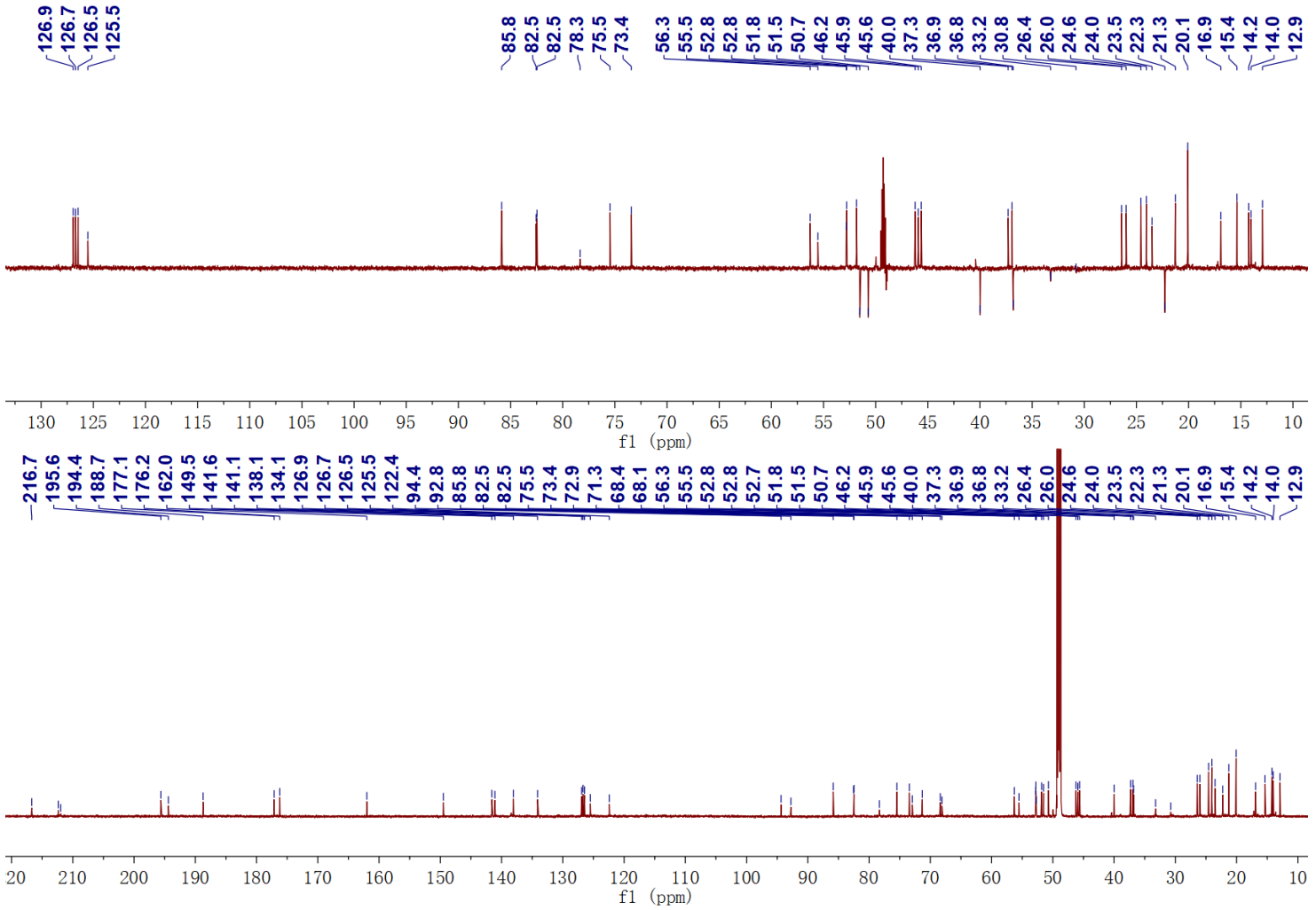

Figure S30. ^{13}C NMR of compound **3** (in CD_3OD)

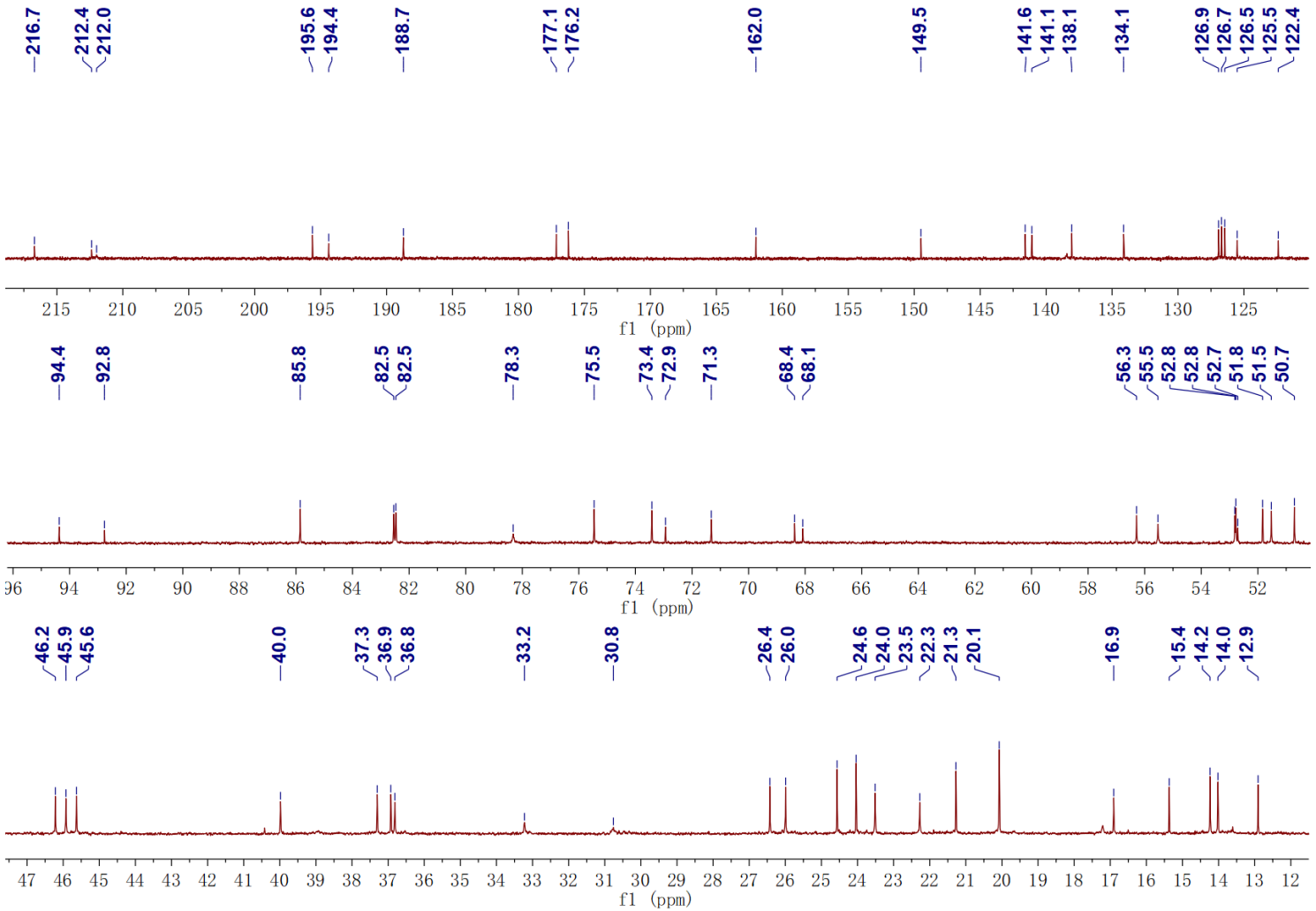

Figure S31. Enlarged ^{13}C NMR spectrum of compound **3**

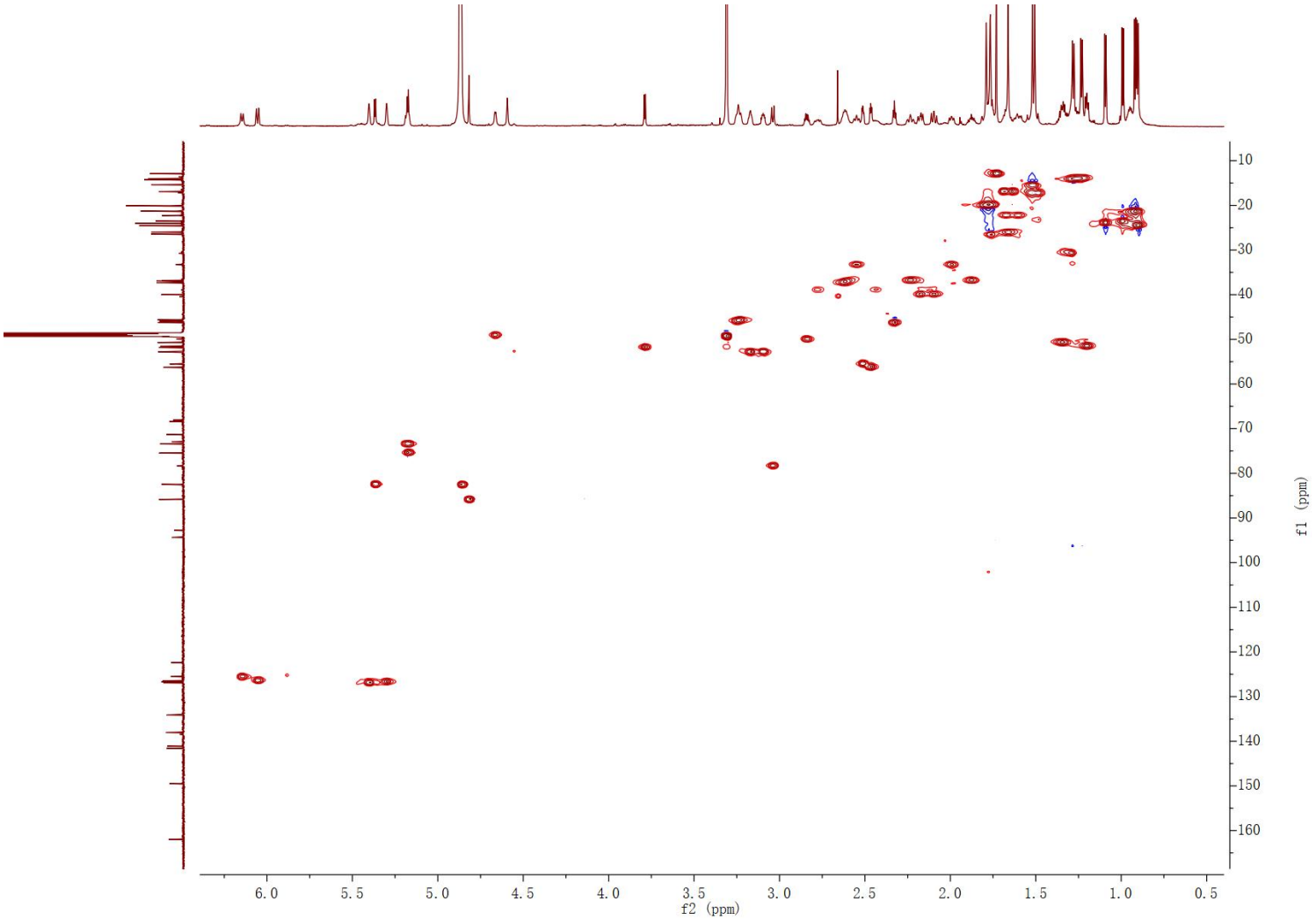

Figure S32. HSQC of compound **3** (in CD_3OD)

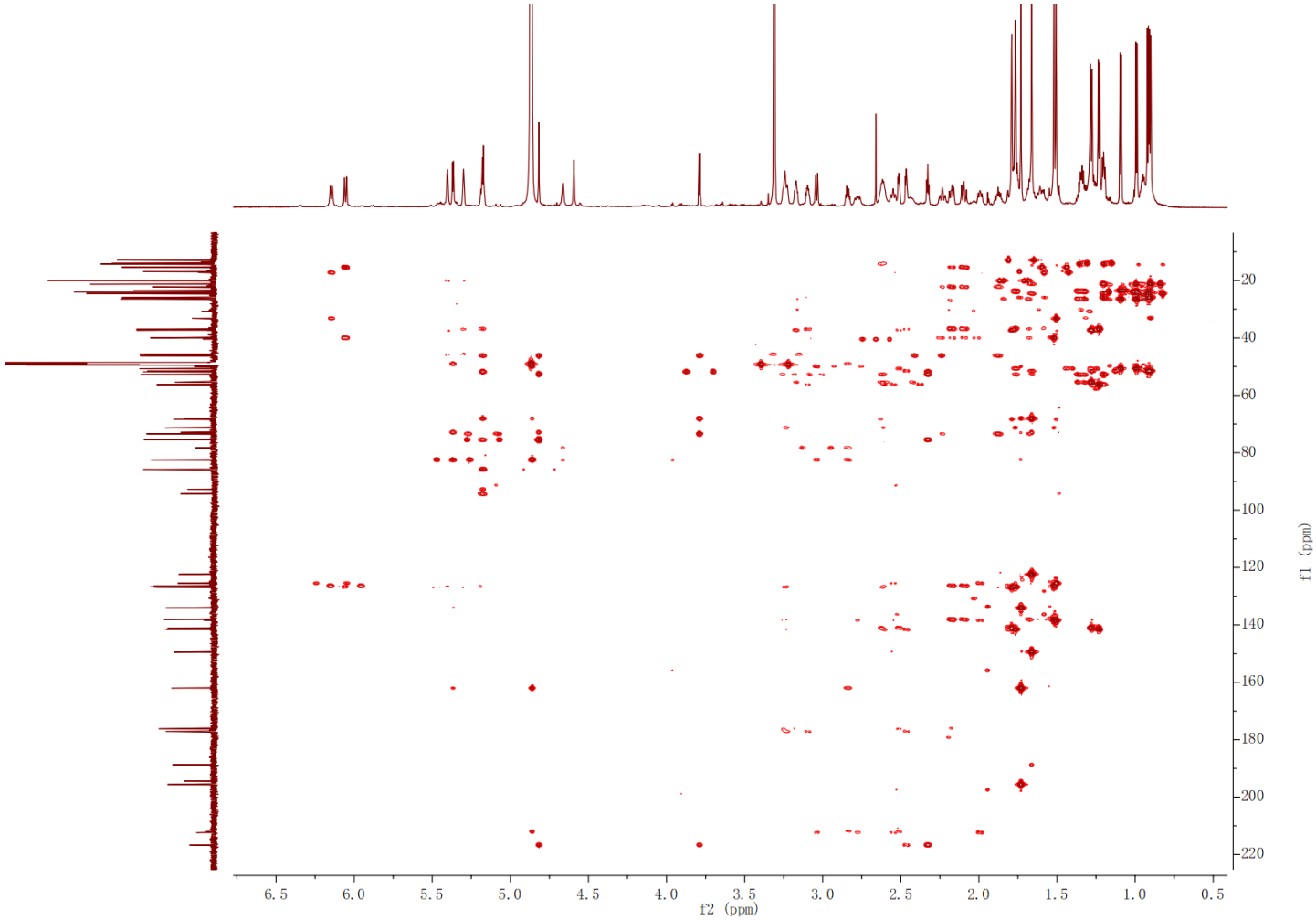

Figure S33. HMBC of compound **3** (in CD_3OD)

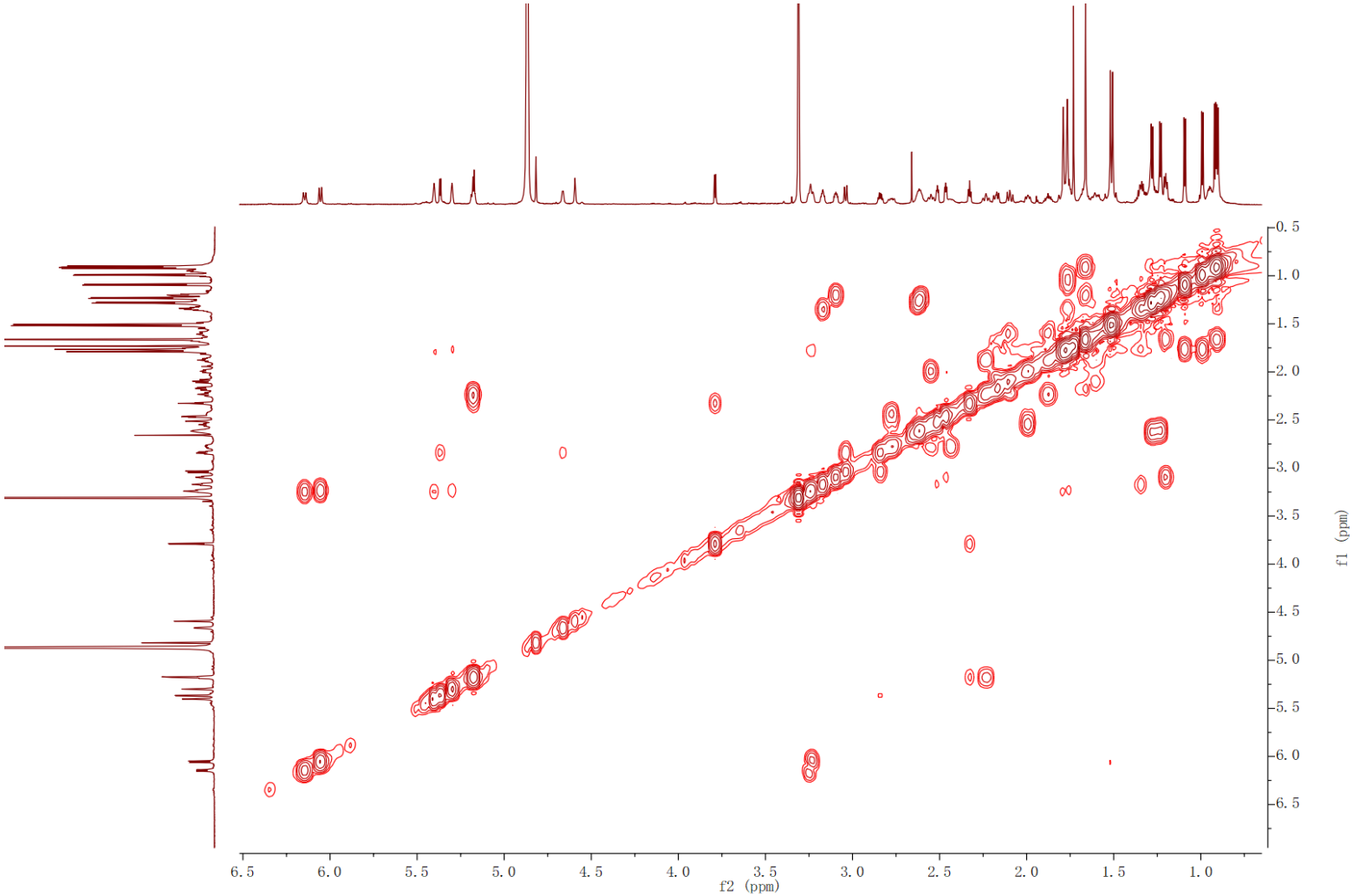

Figure S34. ^{1}H–^{1}H COSY of compound **3** (in CD_3OD)

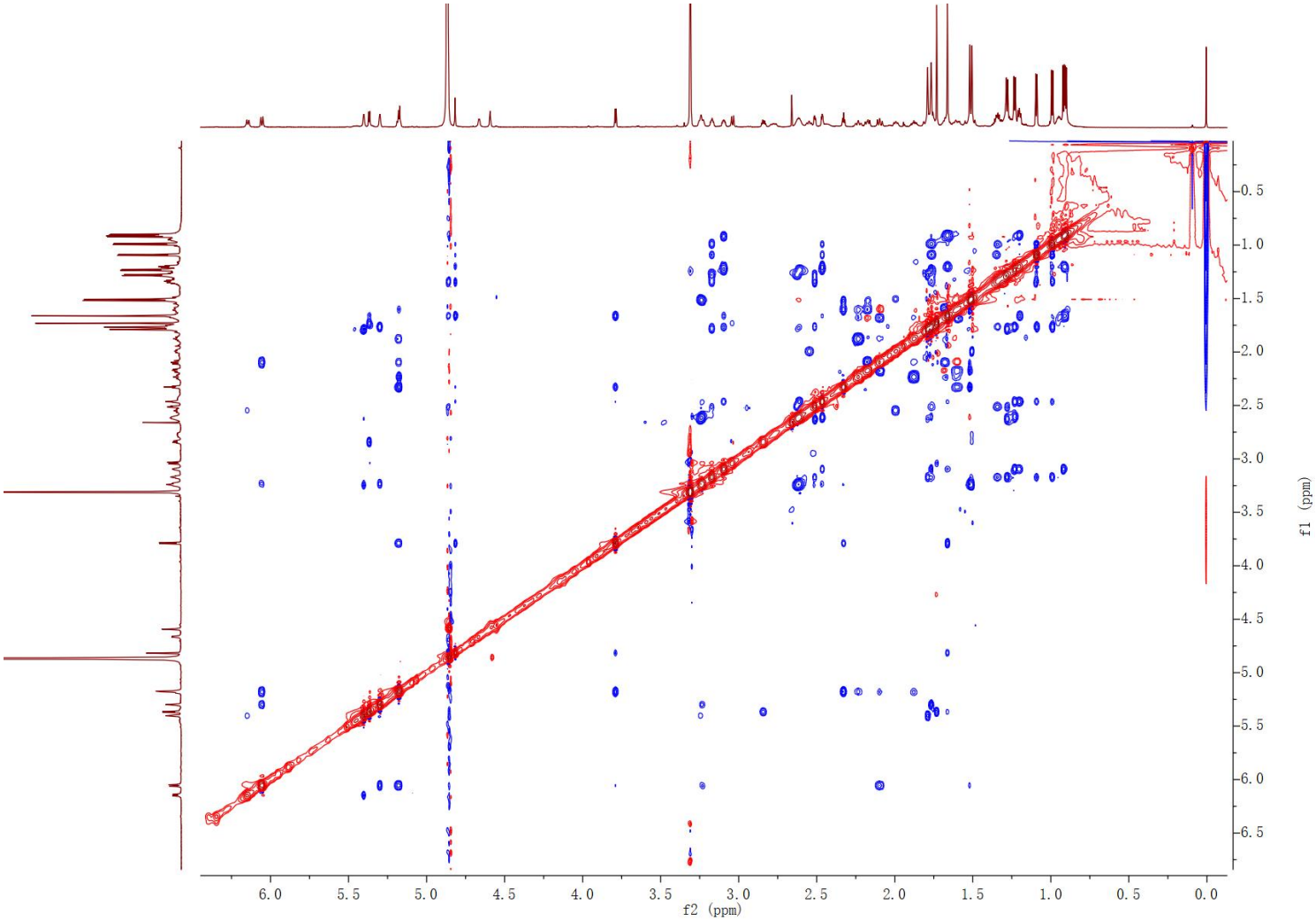

Figure S35. ROESY of compound **3** (in CD_3OD)

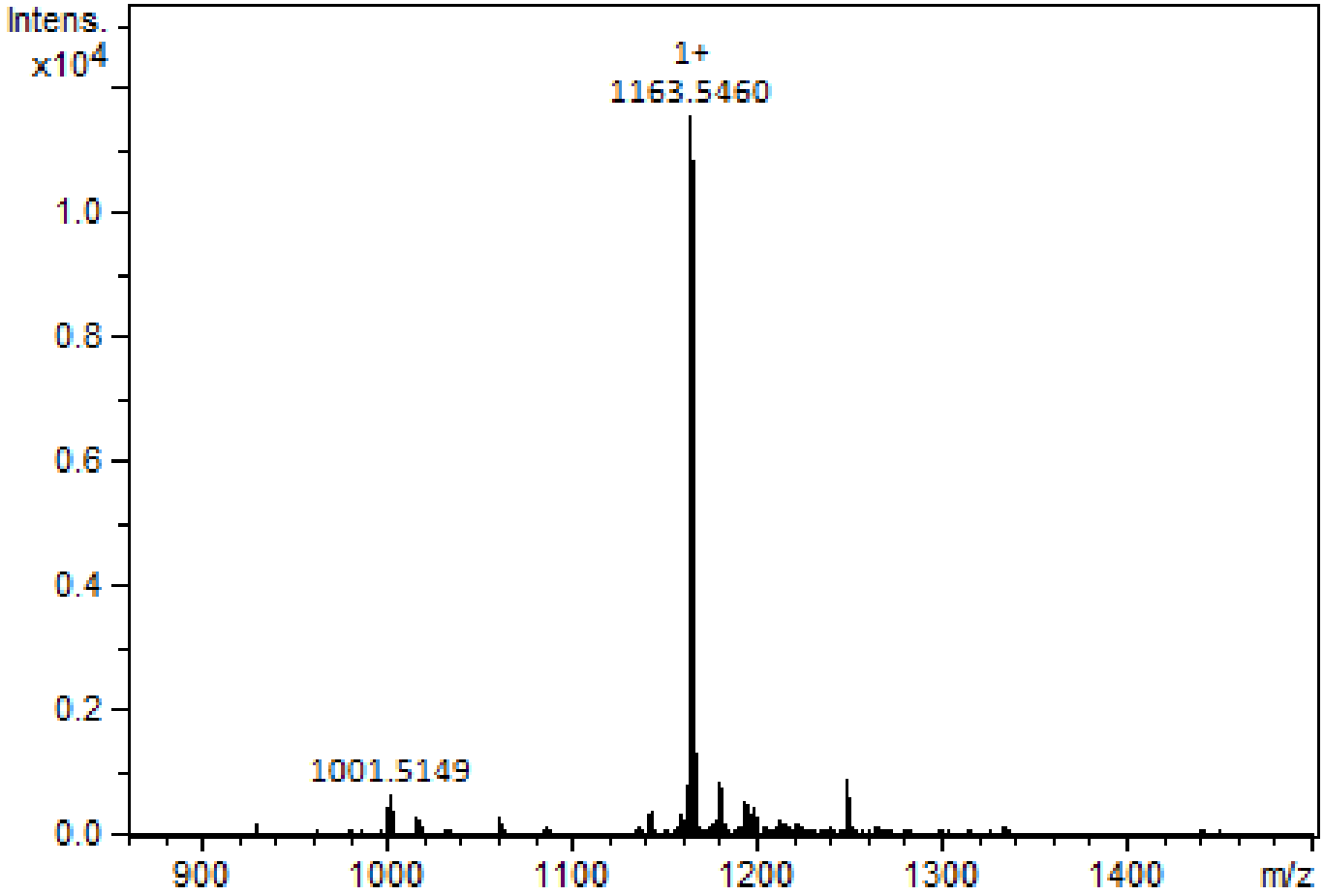

Figure S36. HRESIMS of compound **3**

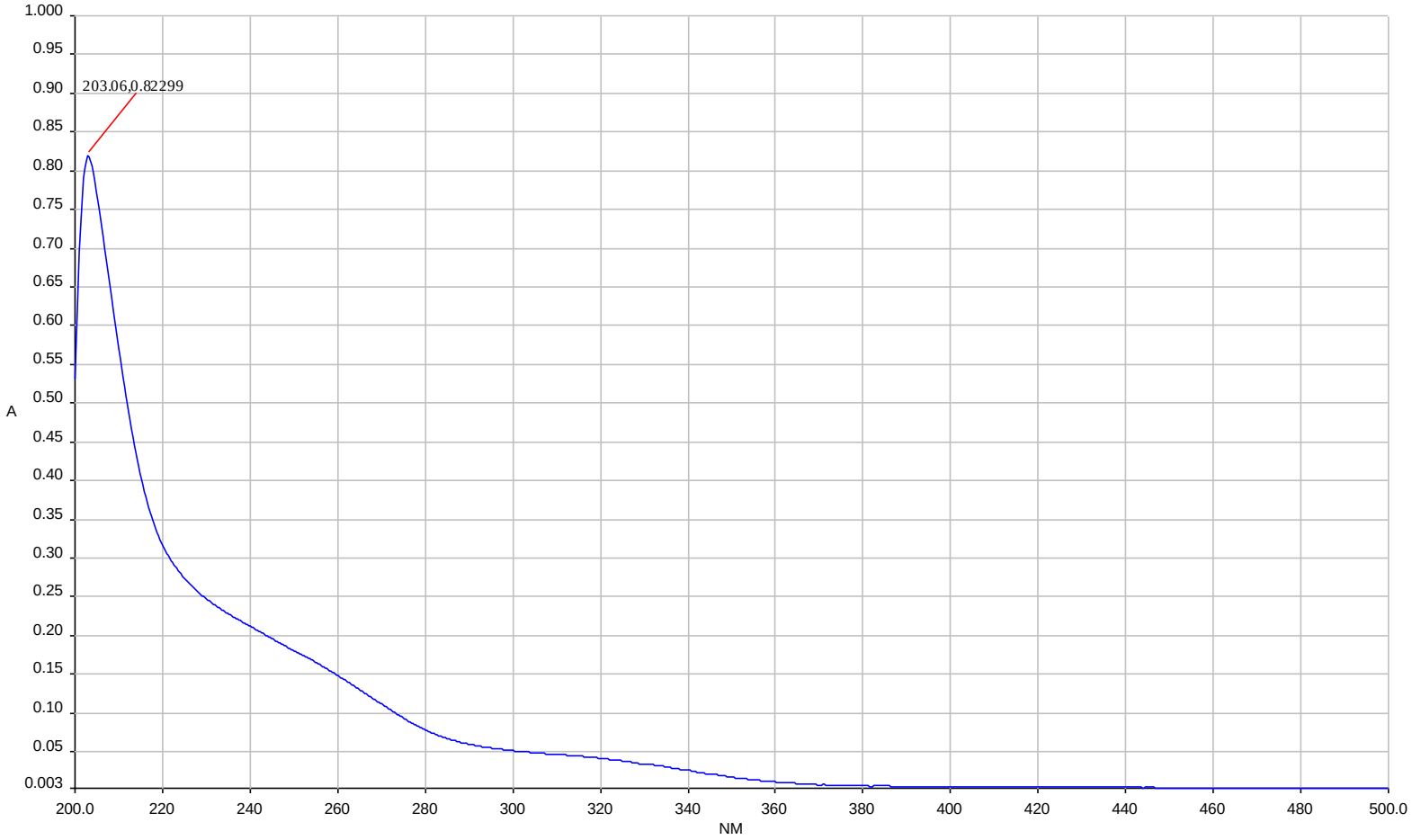

Figure S37. UV of compound **3**

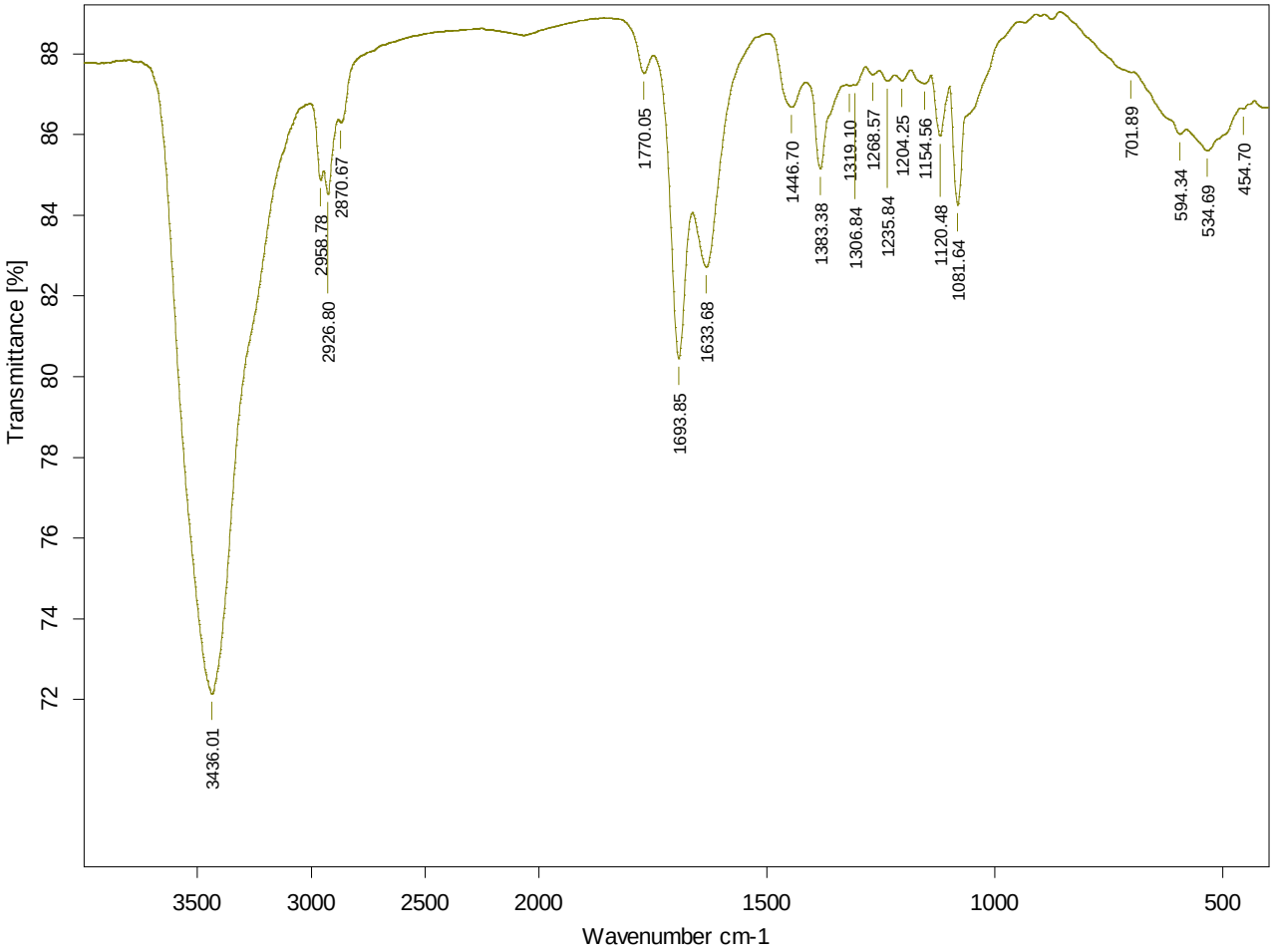

Figure S38. IR of compound **3**

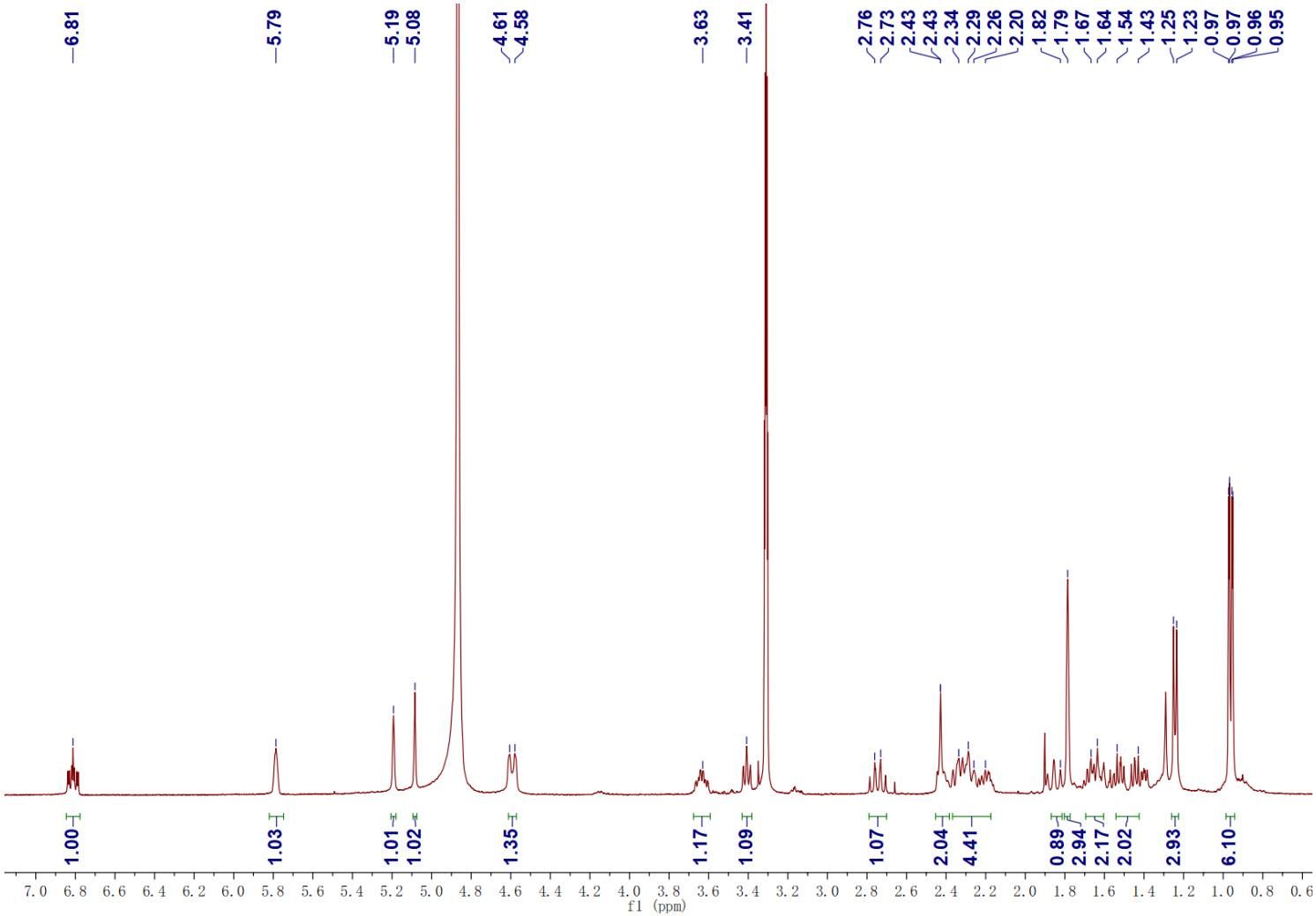

Figure S39. ^{1}H NMR of compound **4** (in CD_3OD)

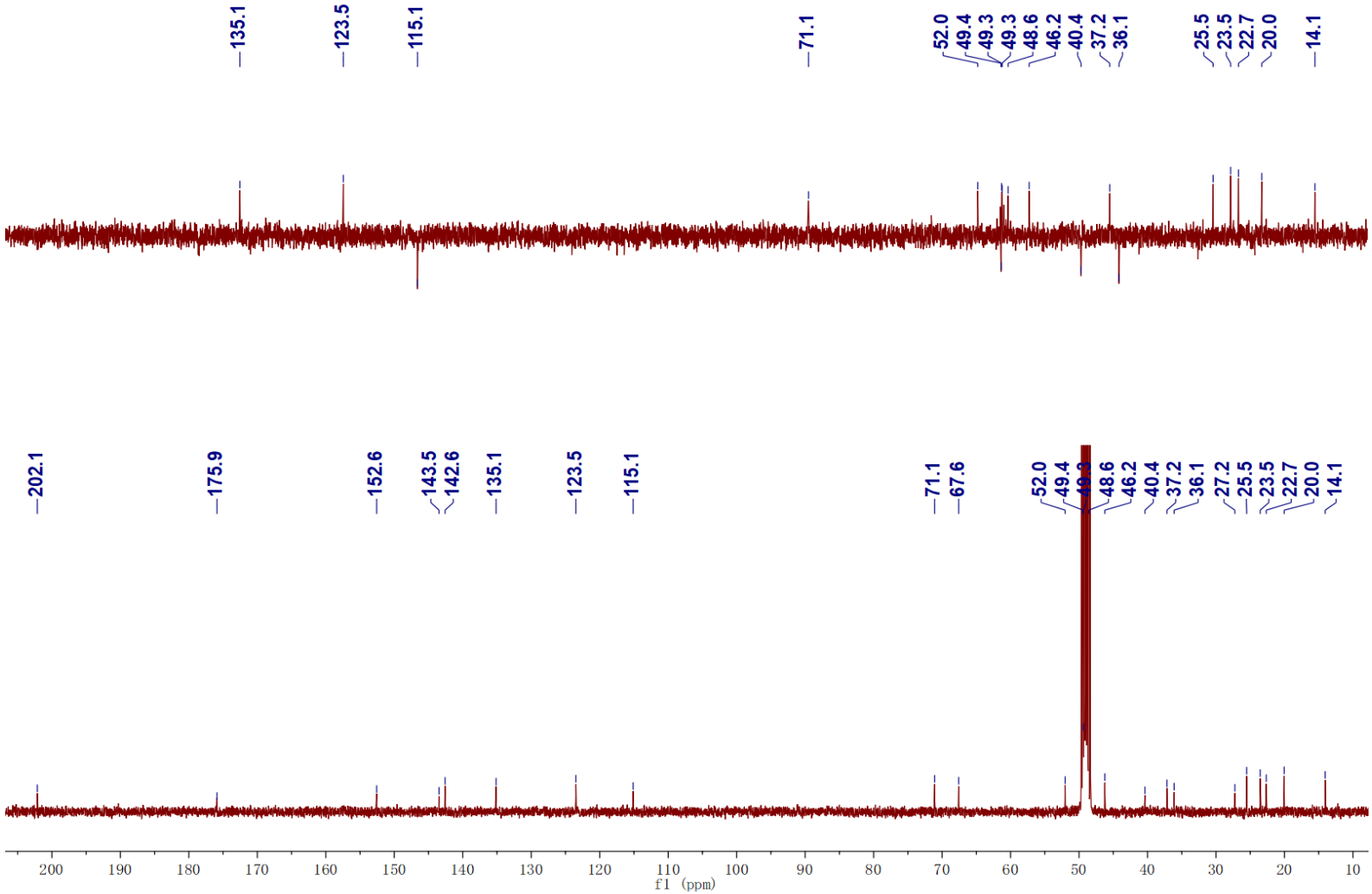

Figure S40. ^{13}C NMR of compound **4** (in CD_3OD)

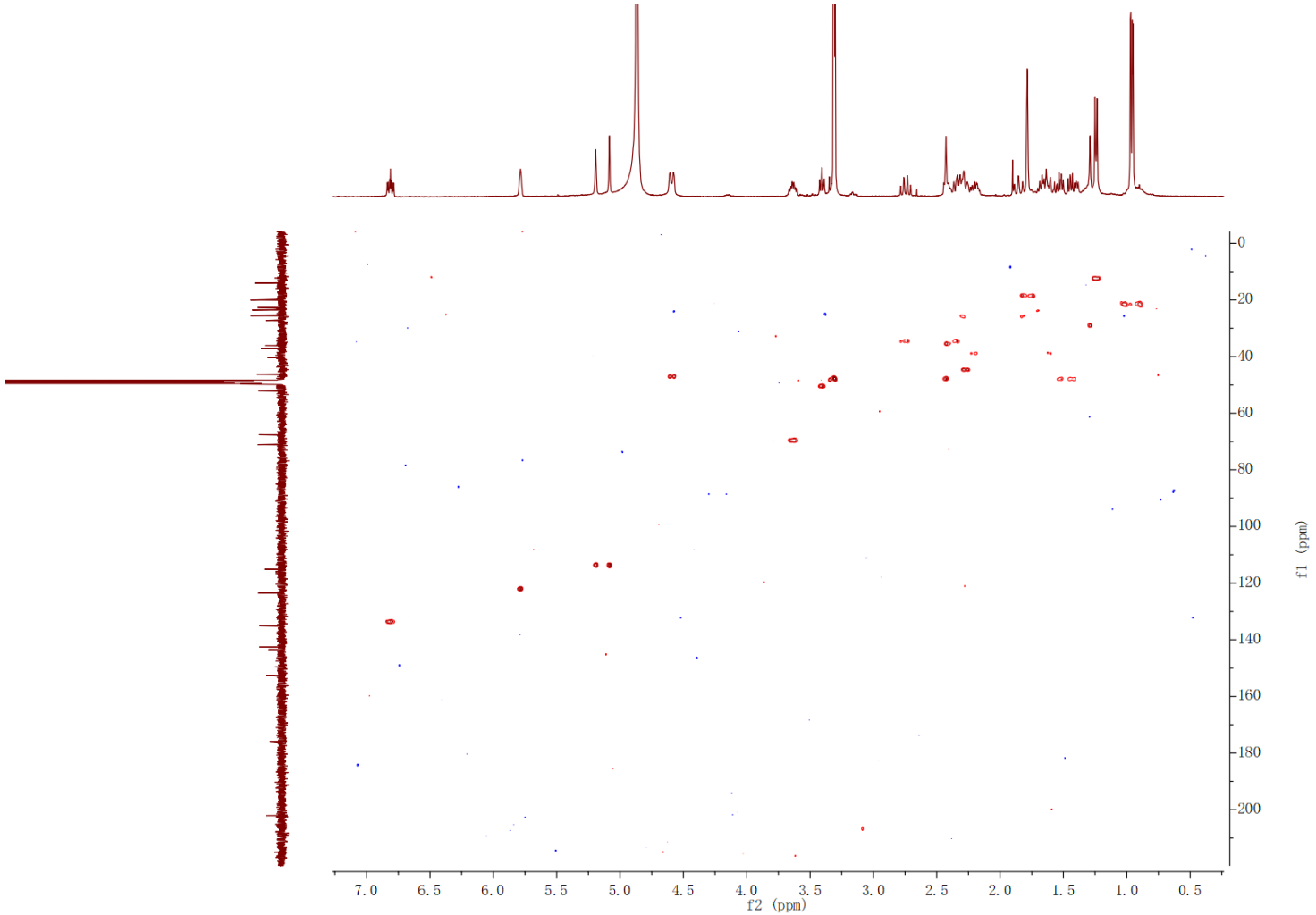

Figure S41. HSQC of compound **4** (in CD_3OD)

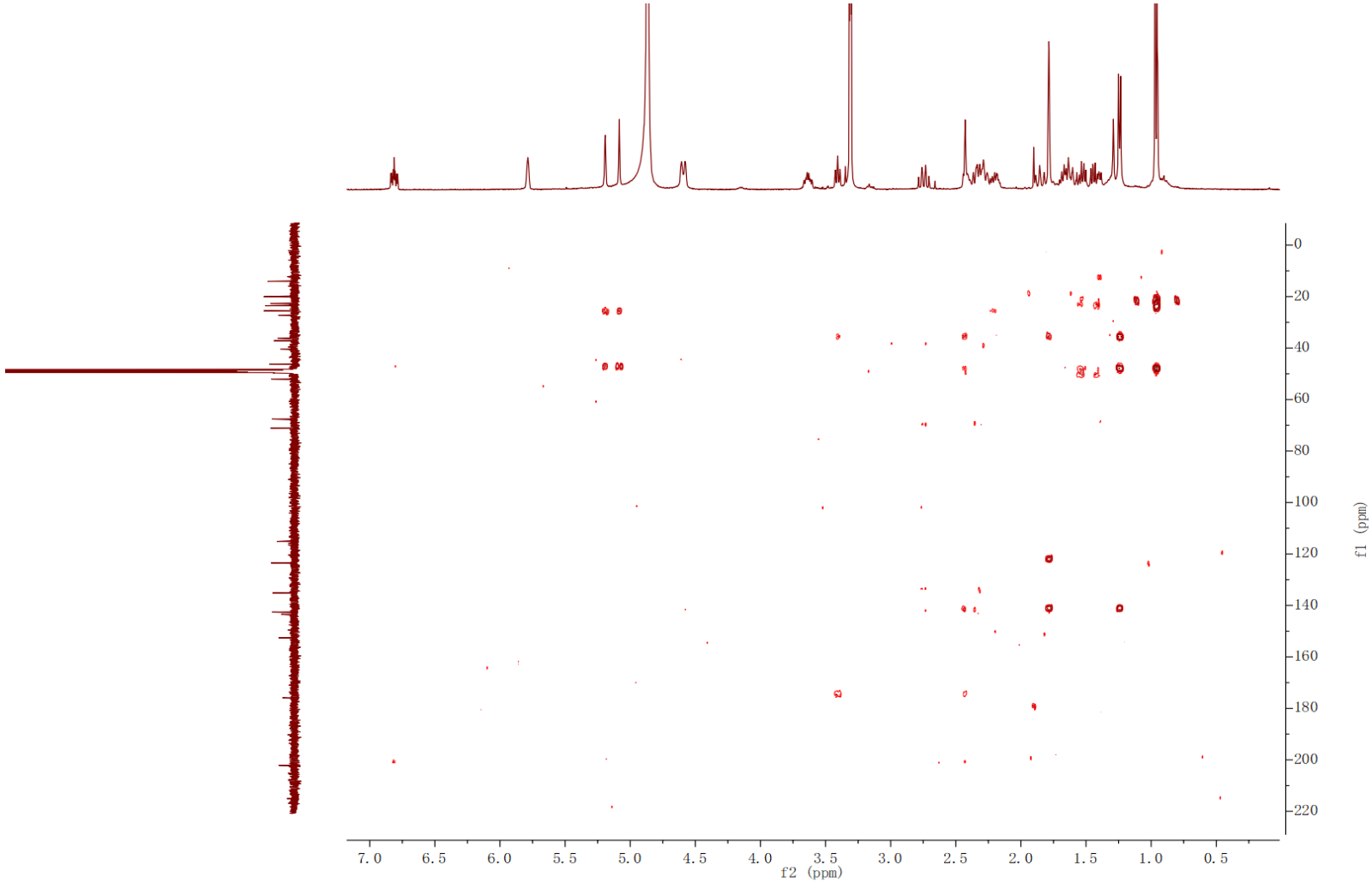

Figure S42. HMBC of compound **4** (in CD_3OD)

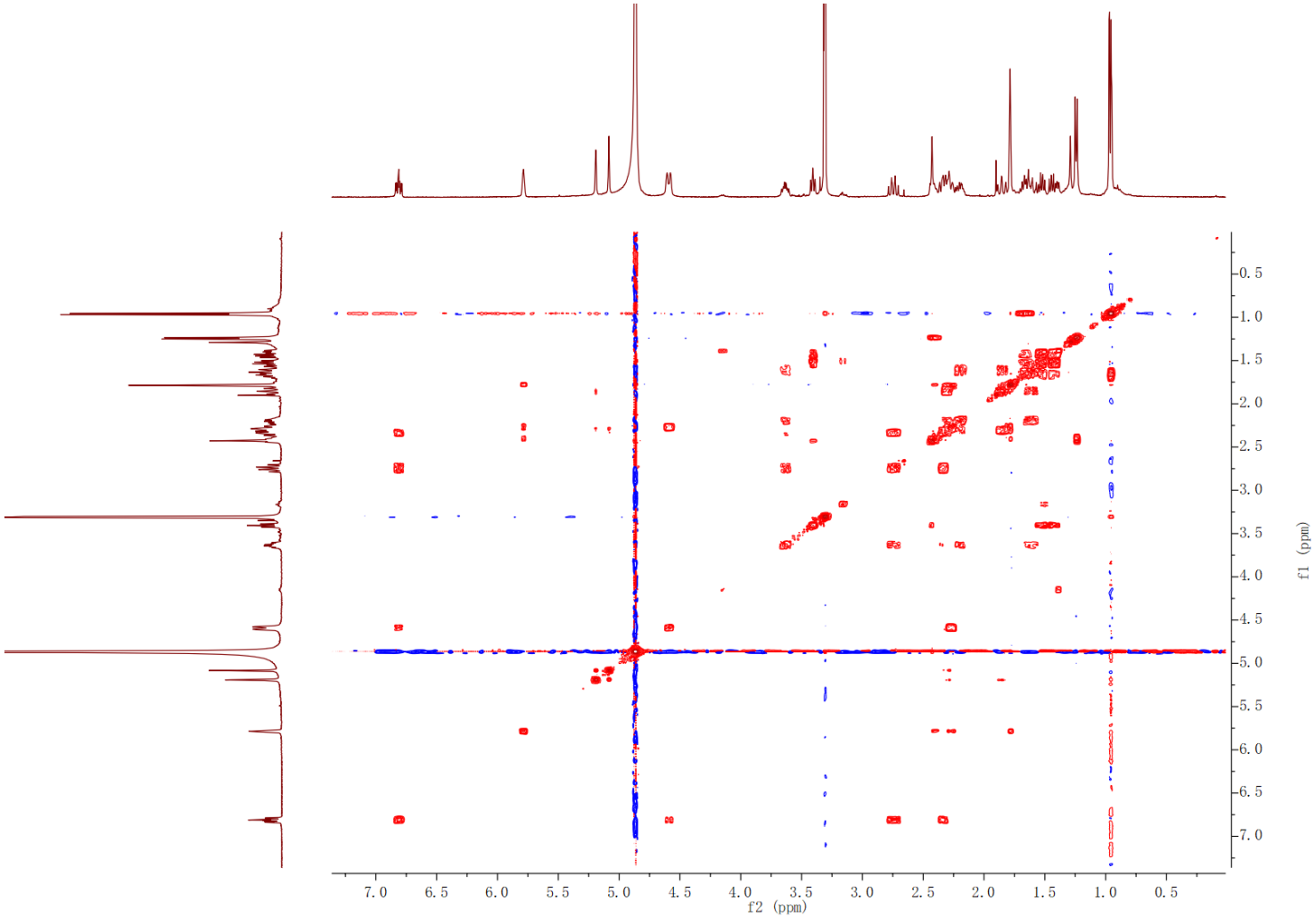

Figure S43. ^{1}H–^{1}H COSY of compound **4** (in CD_3OD)

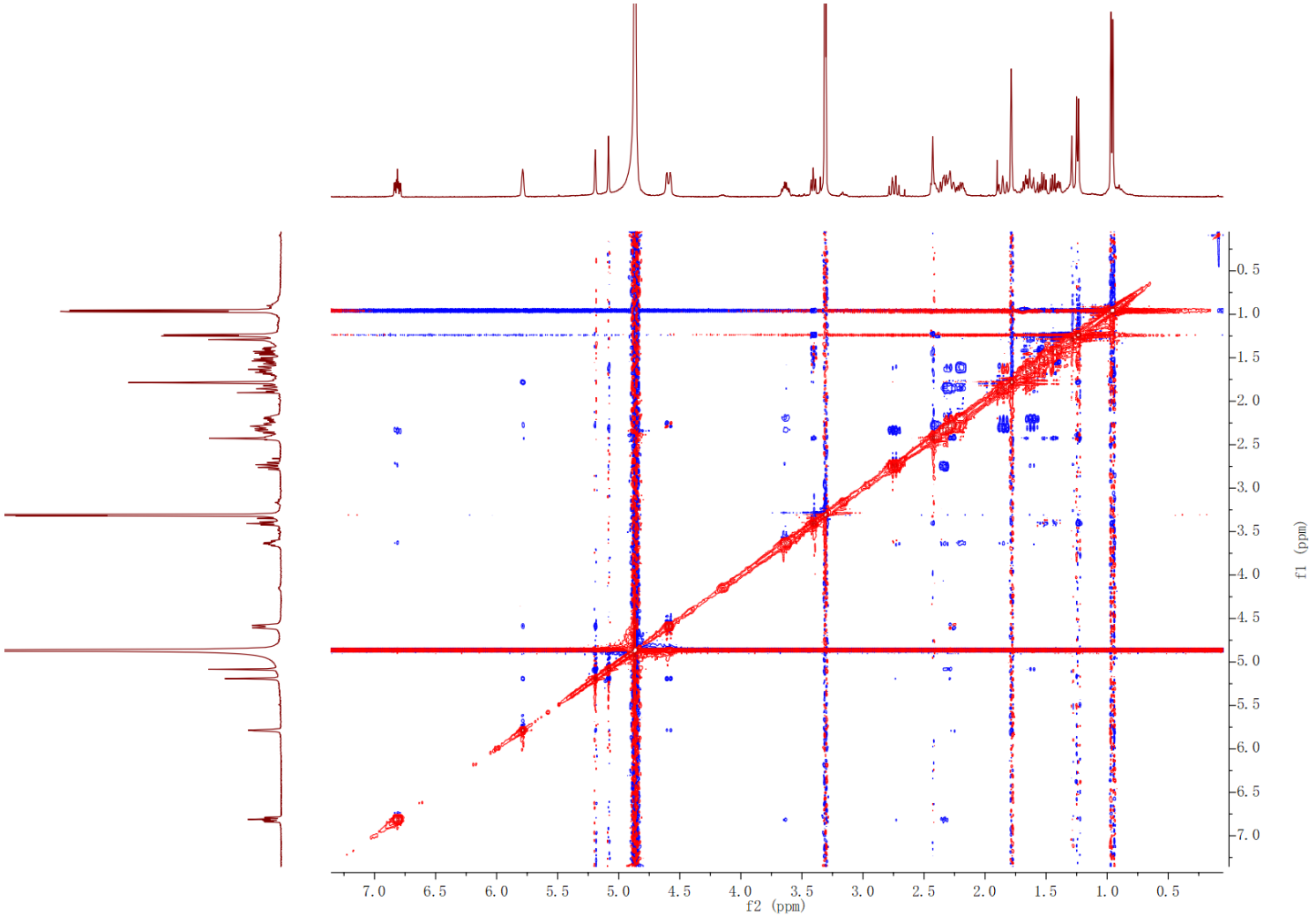

Figure S44. NOESY of compound **4** (in CD_3OD)

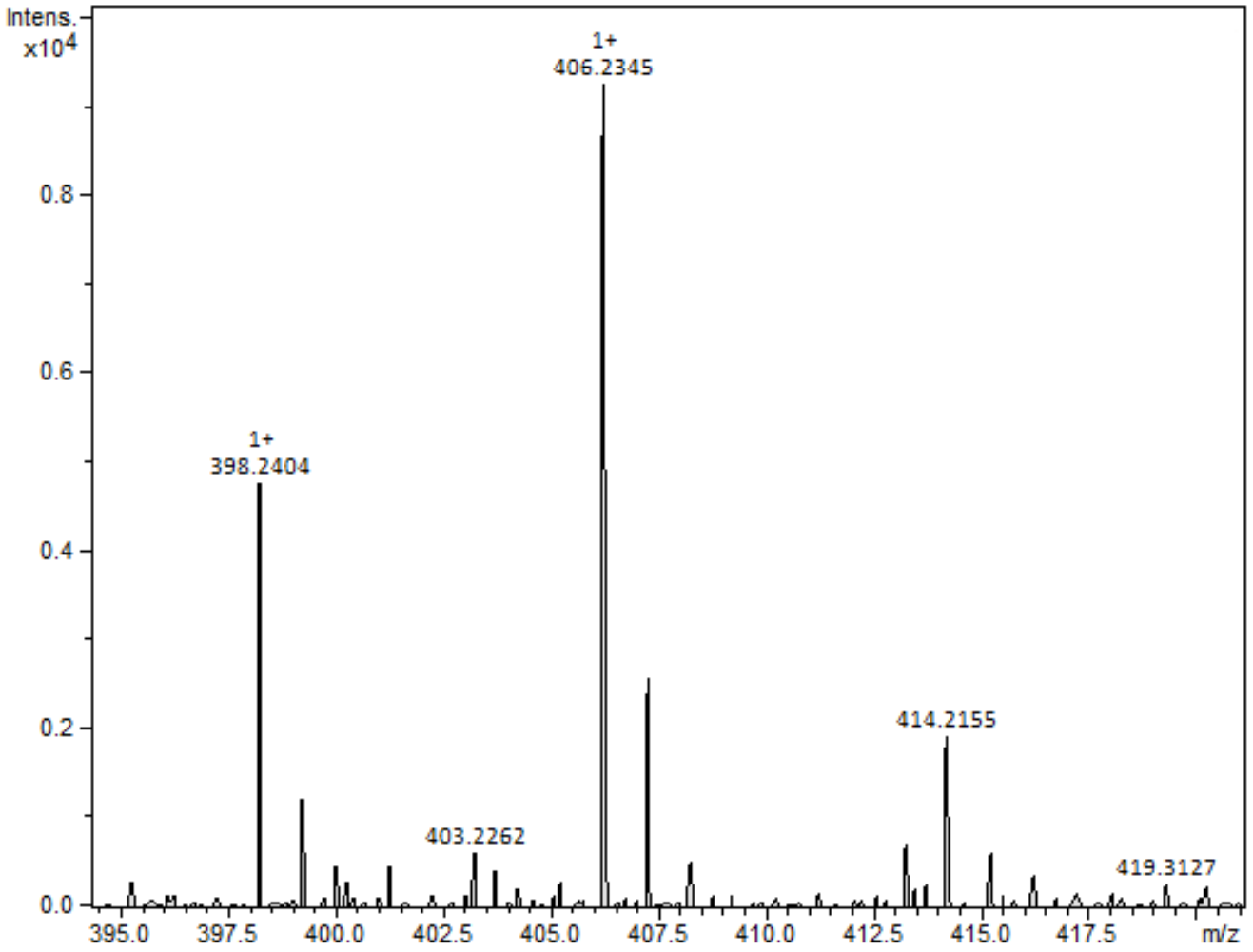

Figure S45. HRESIMS of compound **4**

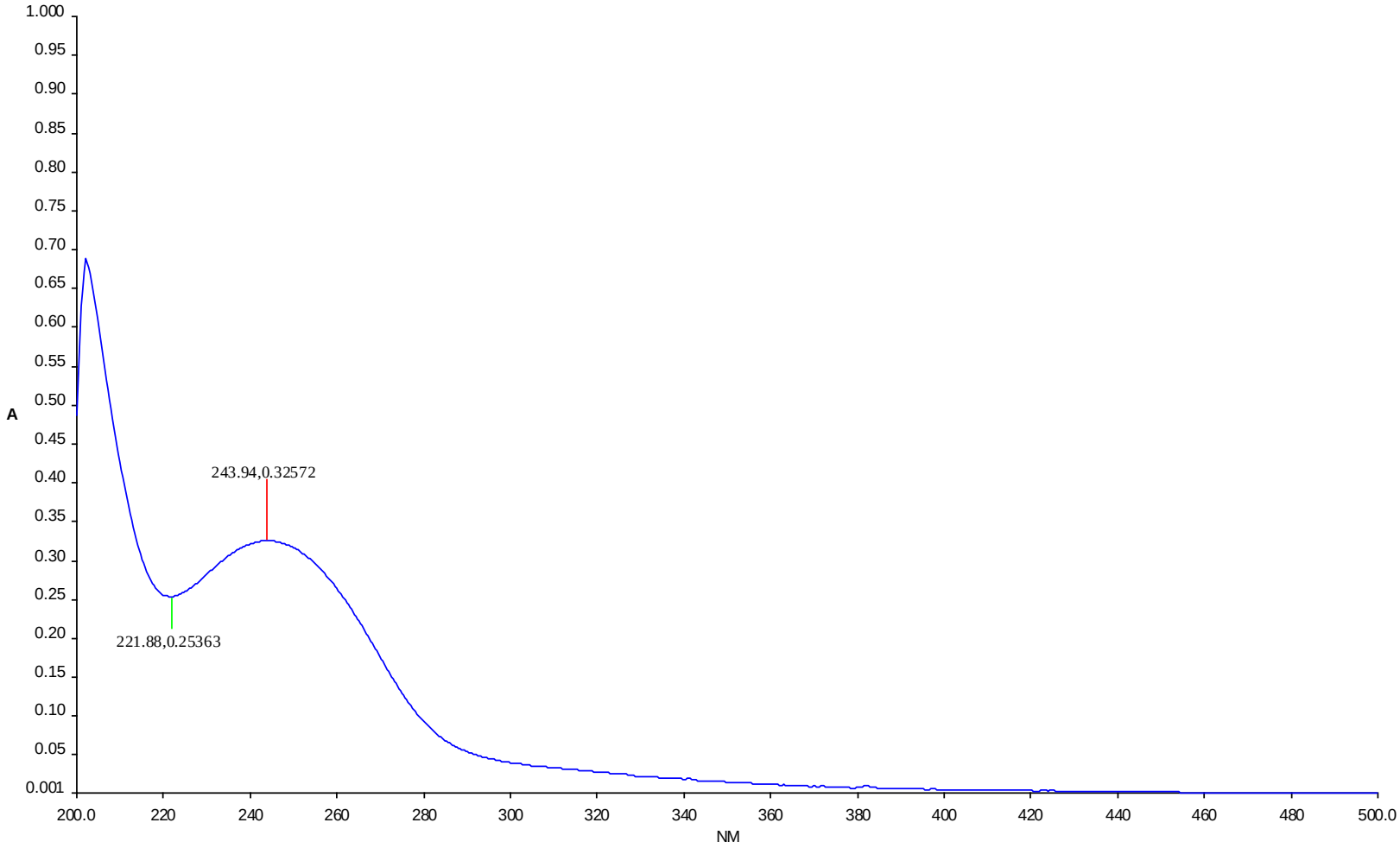

Figure S46. UV of compound **4**

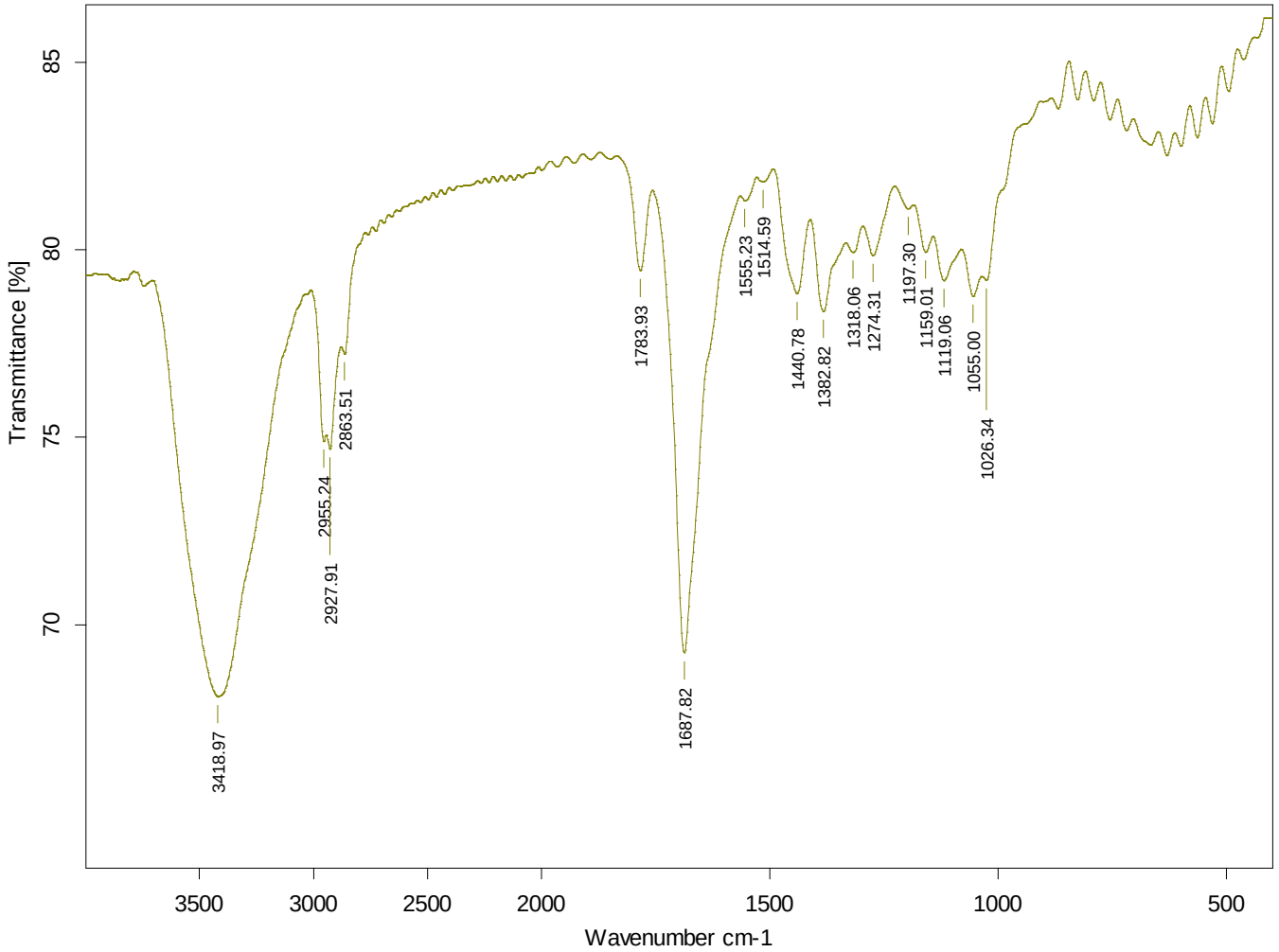

Figure S47. IR of compound **4**

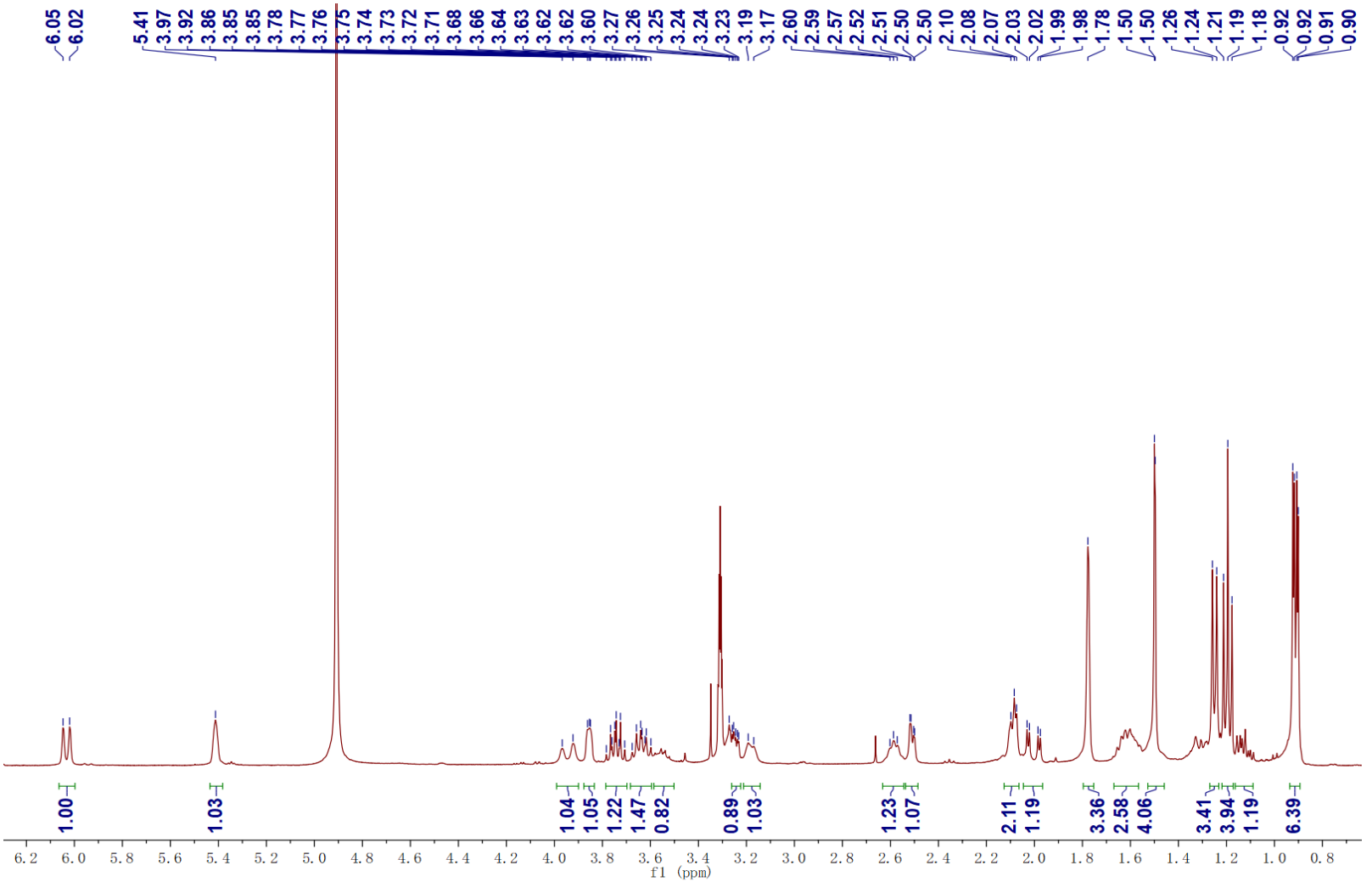

Figure S48. ^{1}H NMR of compound **5** (in CD_3OD)

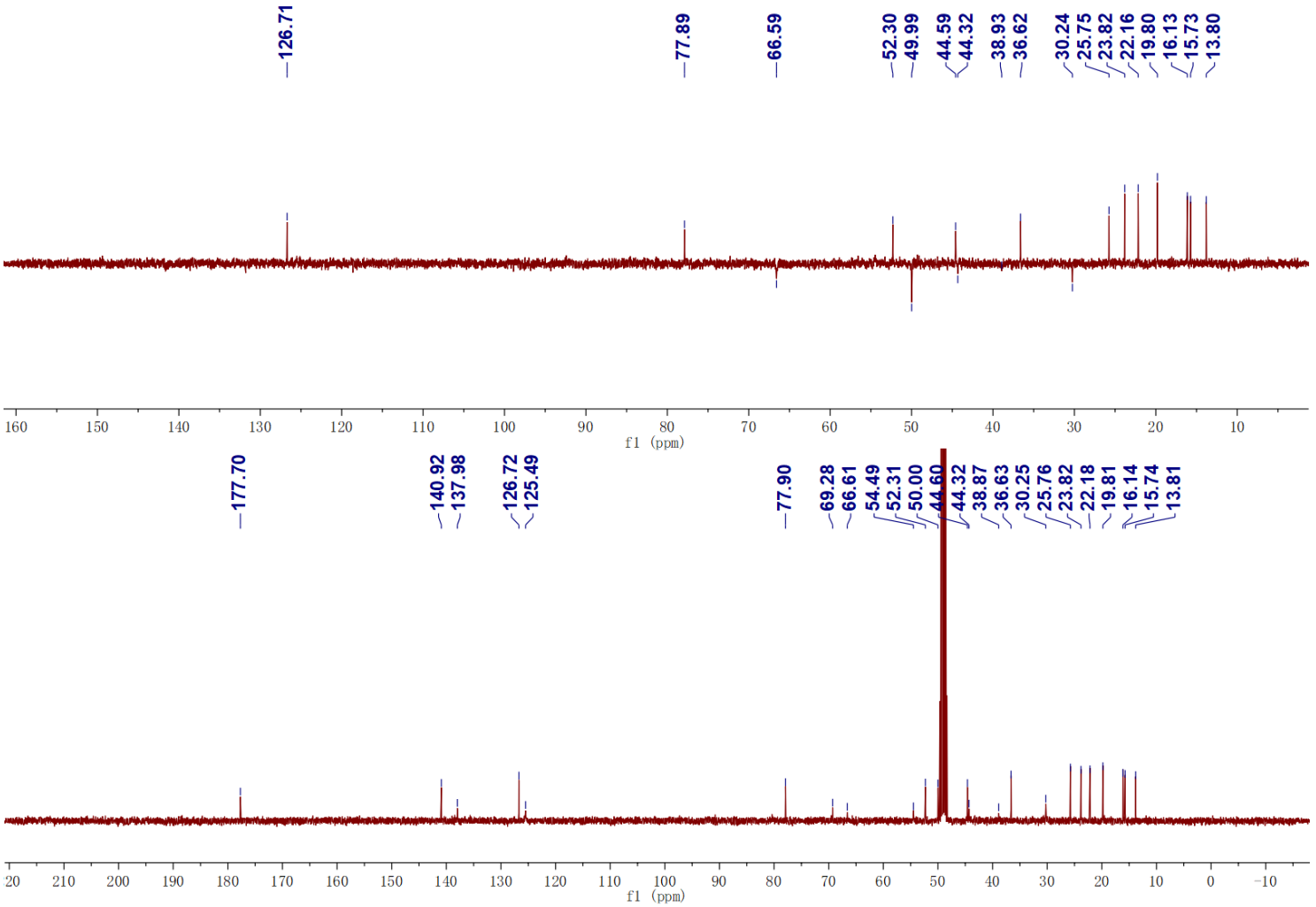

Figure S49. ^{13}C NMR of compound **5** (in CD_3OD)

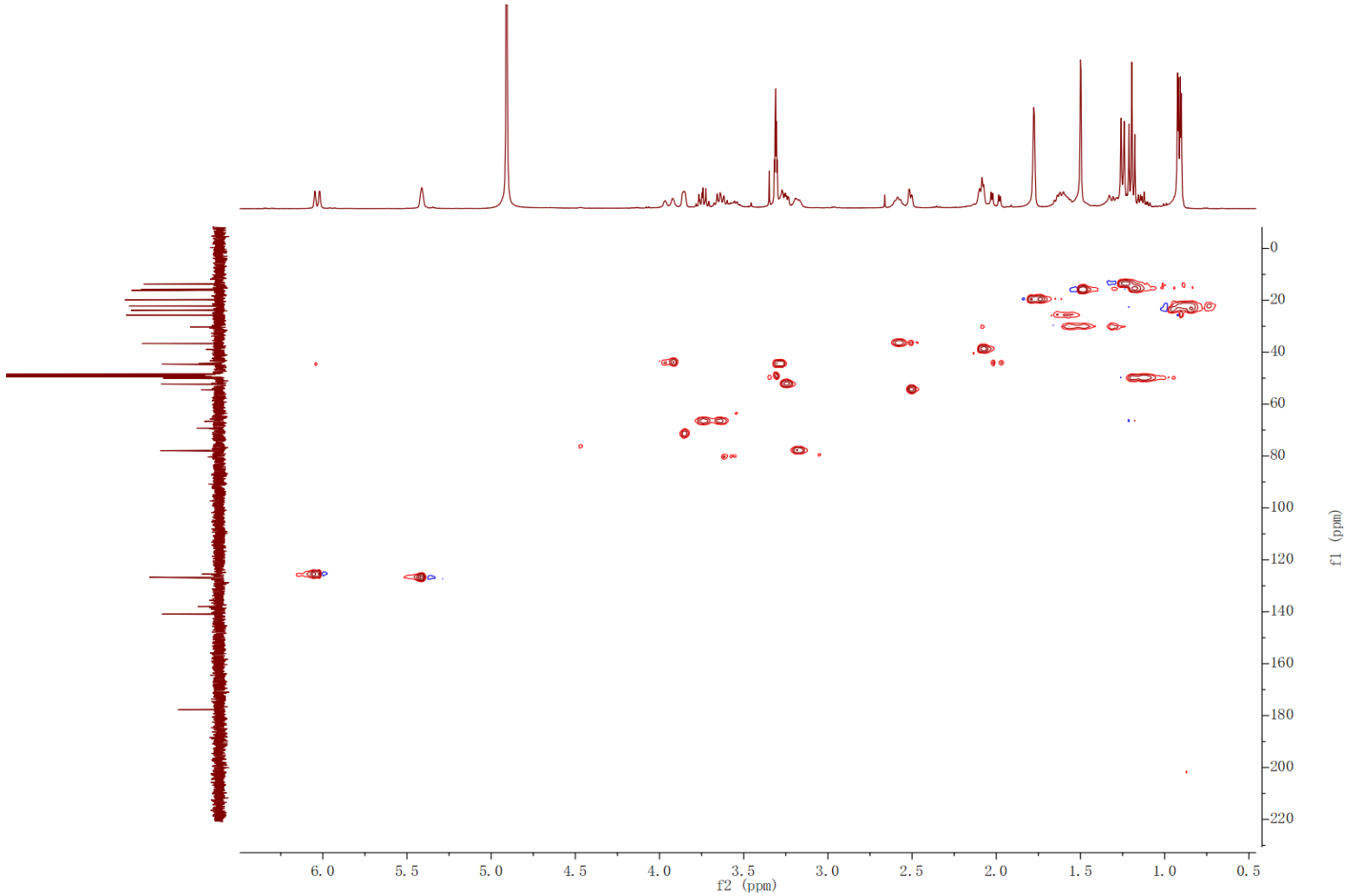

Figure S50. HSQC of compound **5** (in CD_3OD)

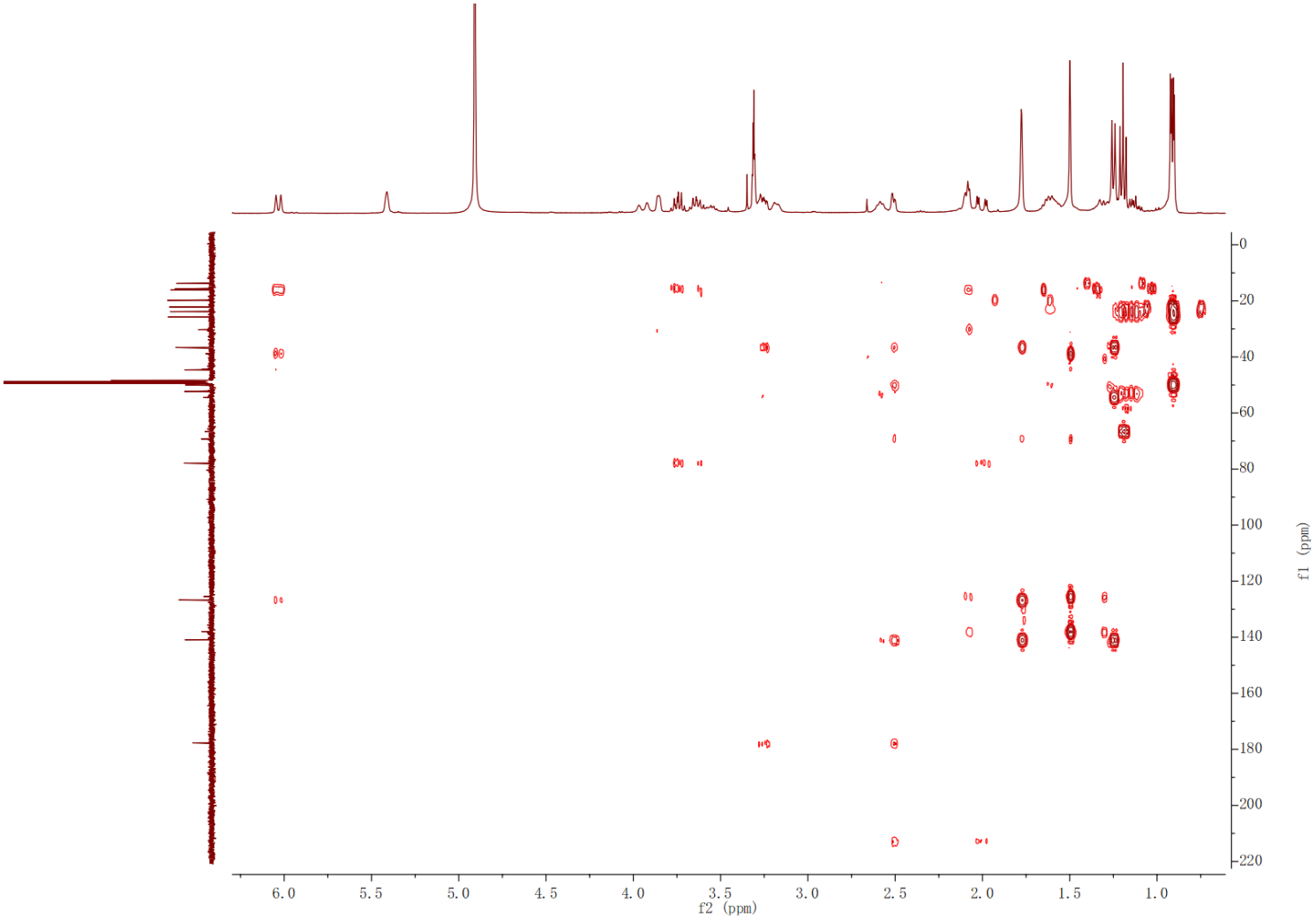

Figure S51. HMBC of compound **5** (in CD_3OD)

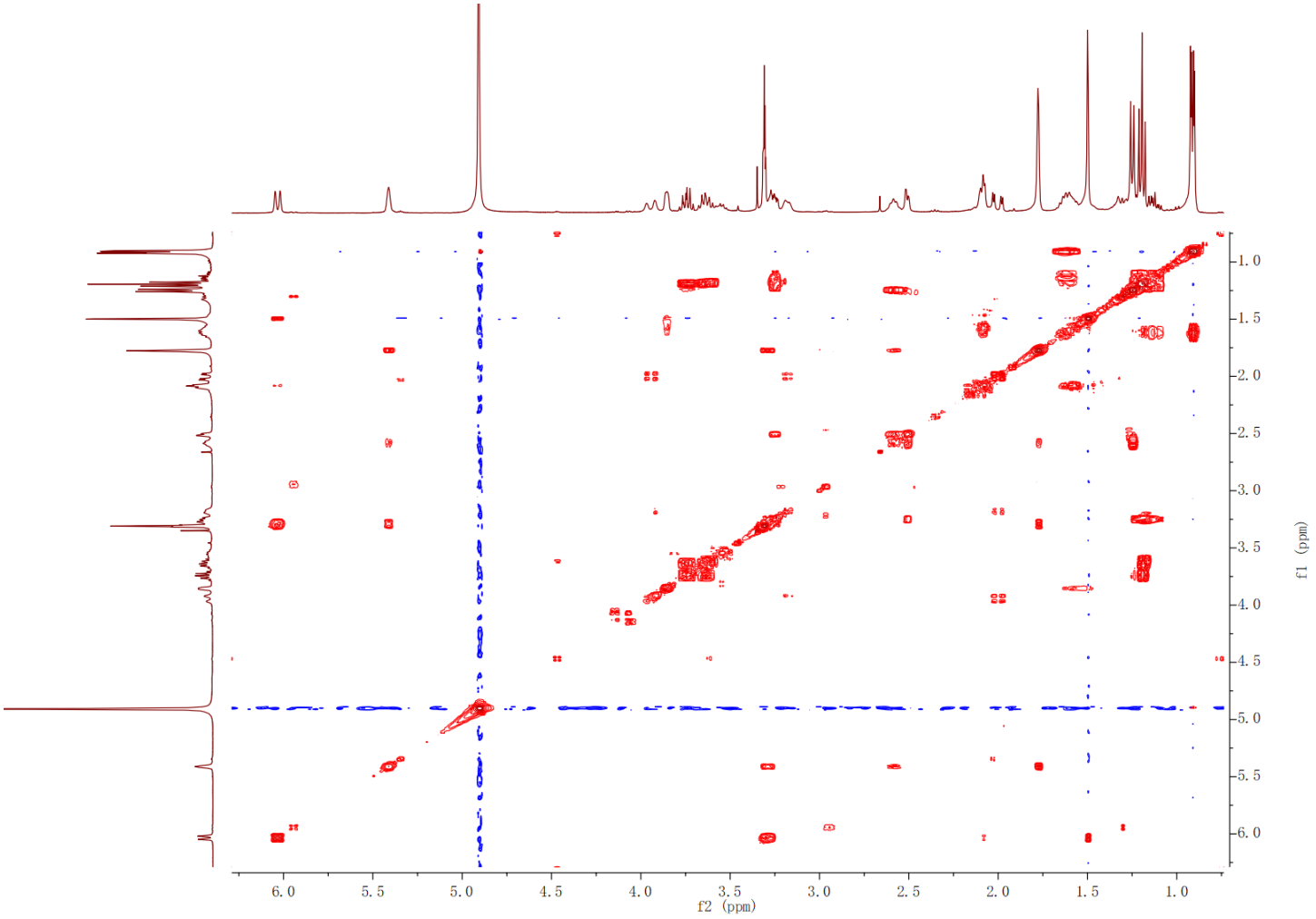

Figure S52. ^{1}H–^{1}H COSY of compound **5** (in CD_3OD)

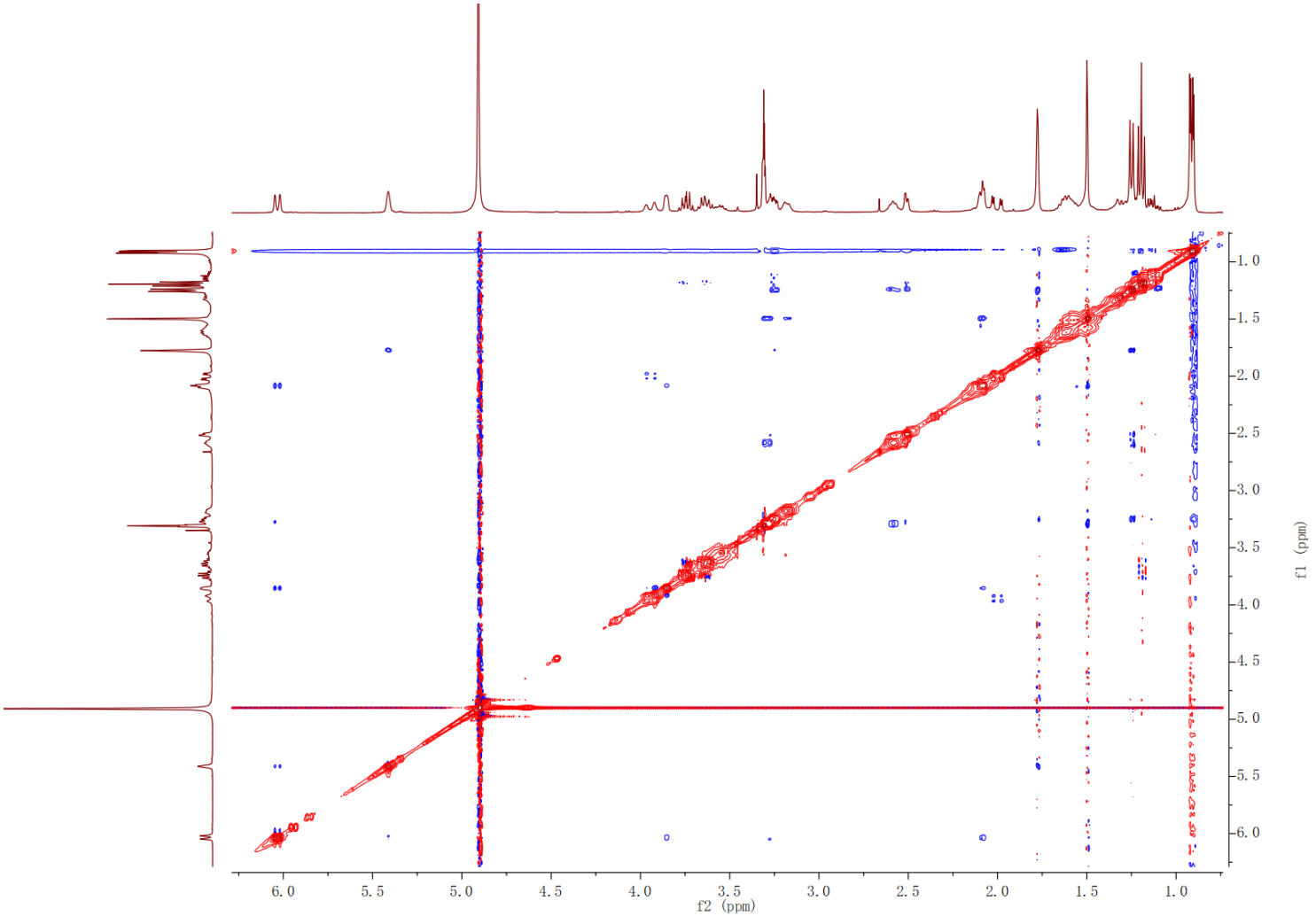

Figure S53. NOESY of compound **5** (in CD_3OD)

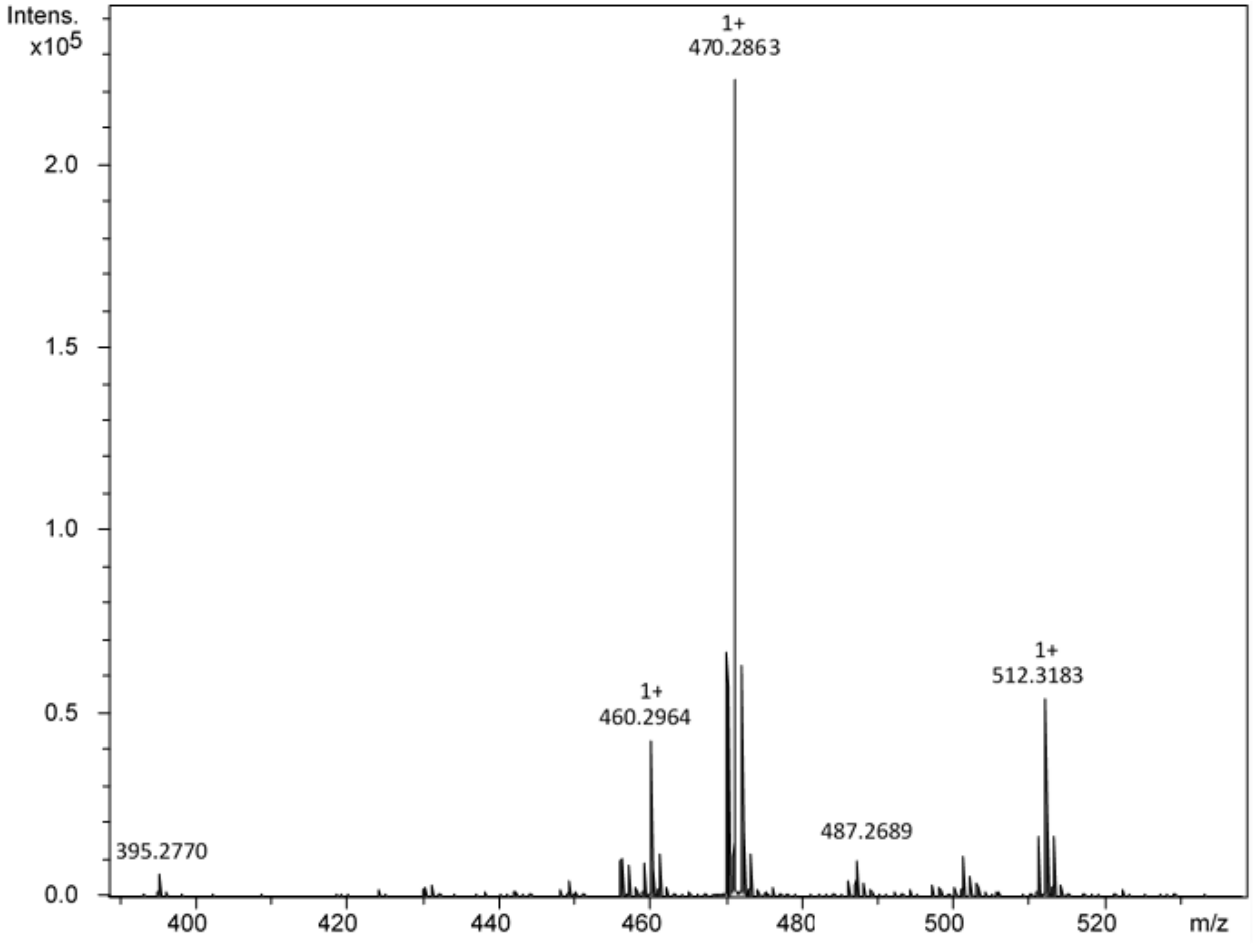

Figure S54. HRESIMS of compound **5**

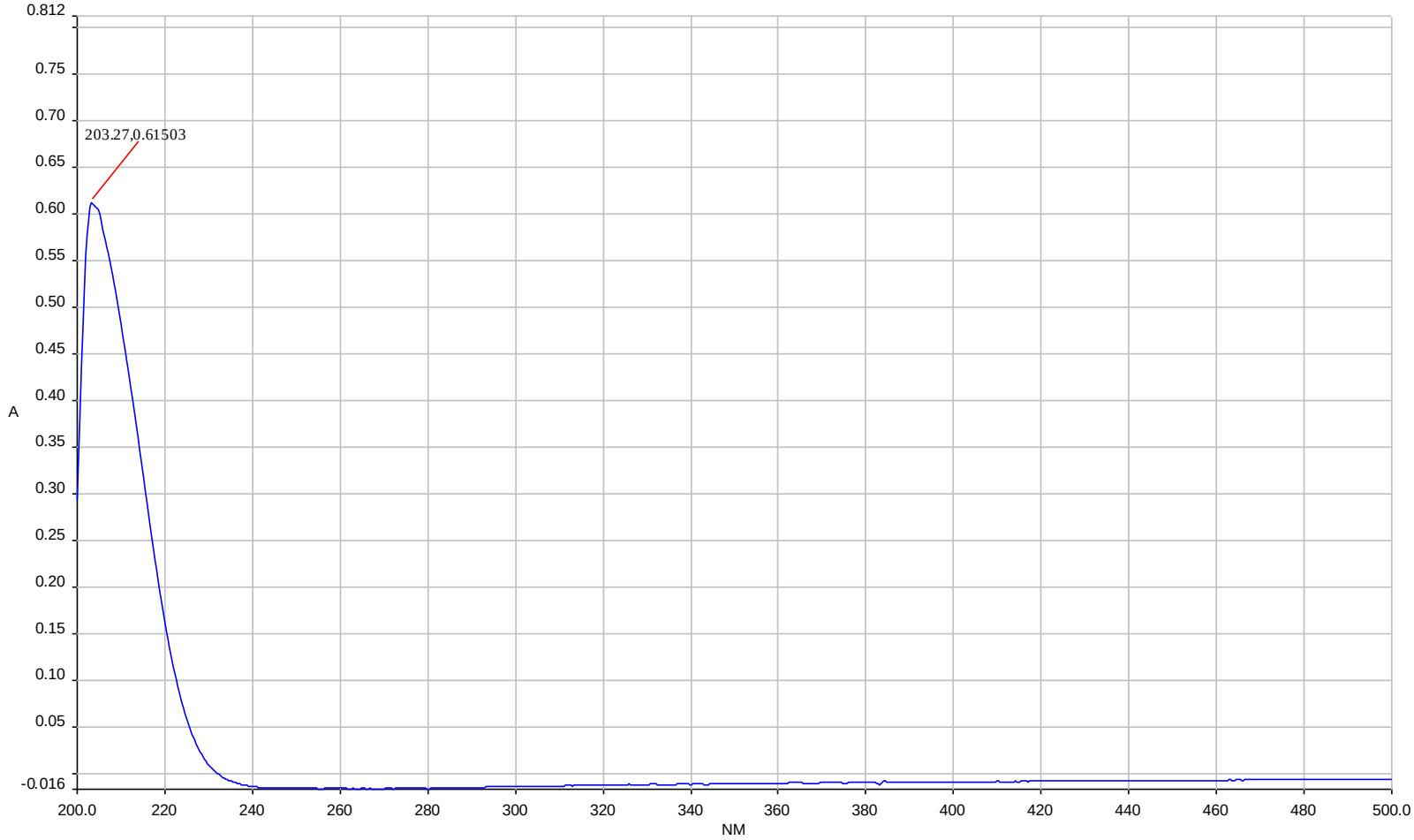

Figure S55. UV of compound **5**

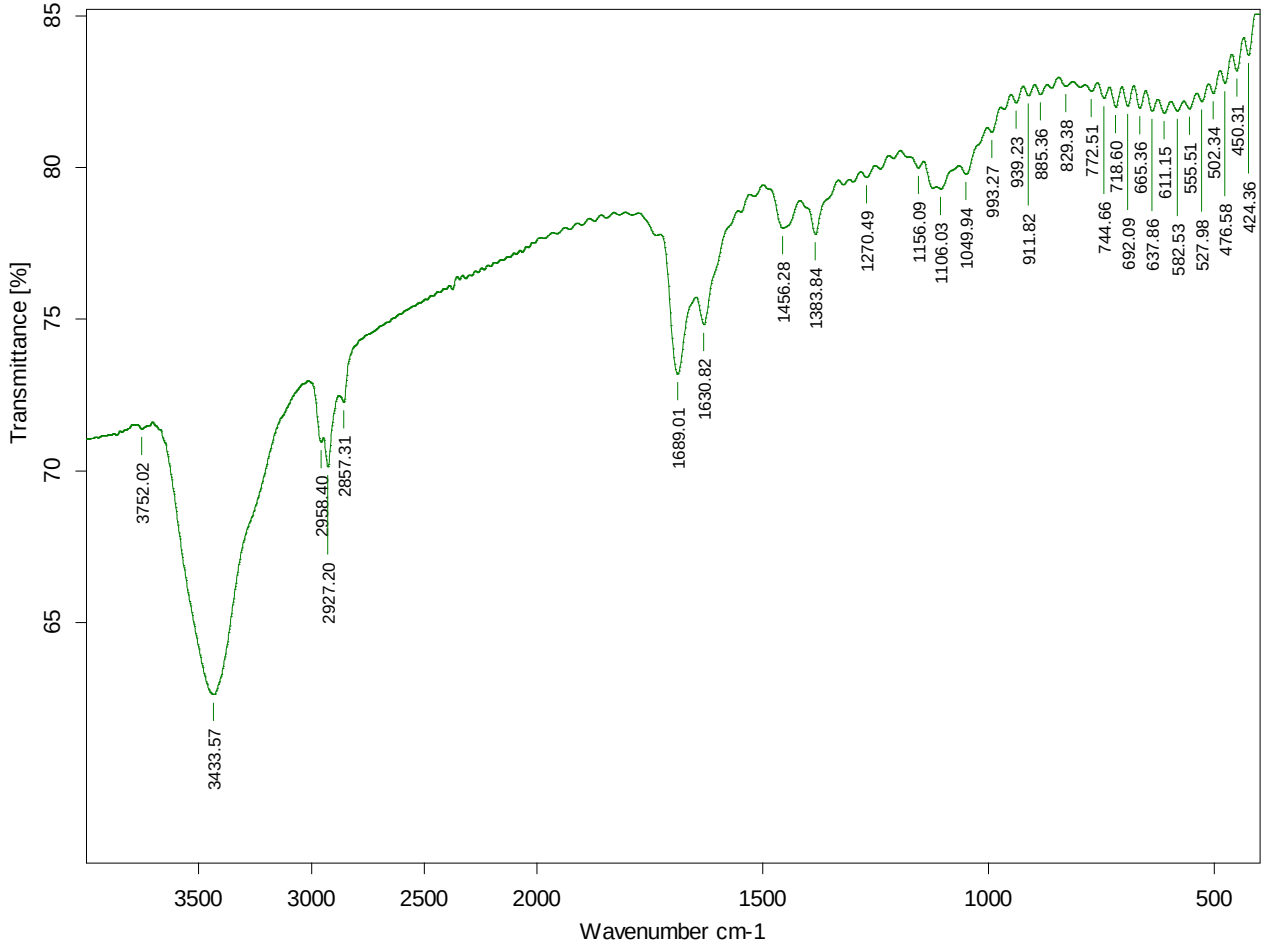

Figure S56. IR of compound **5**

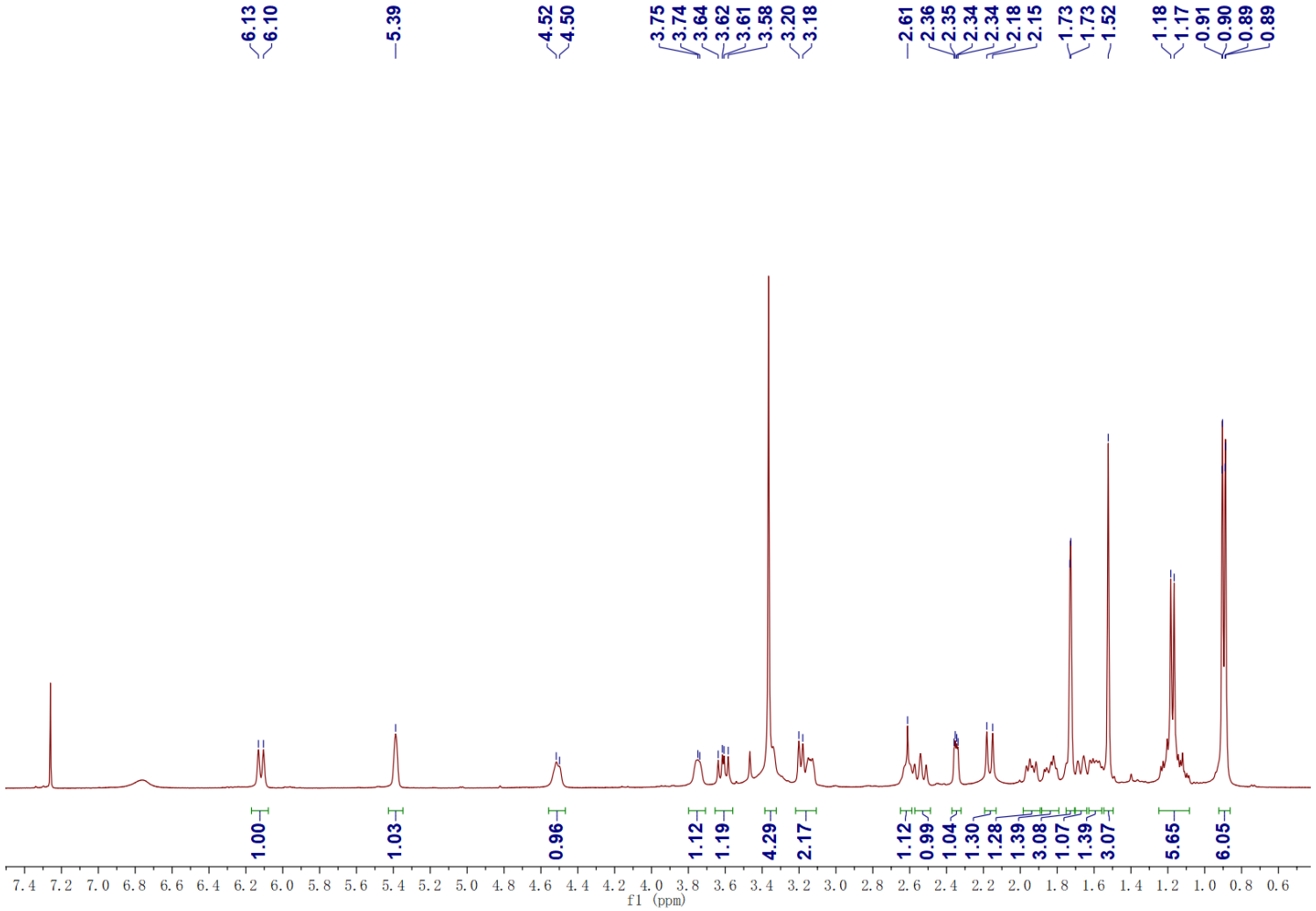

Figure S57. ^{1}H NMR of compound **6** (in $CDCl_3$)

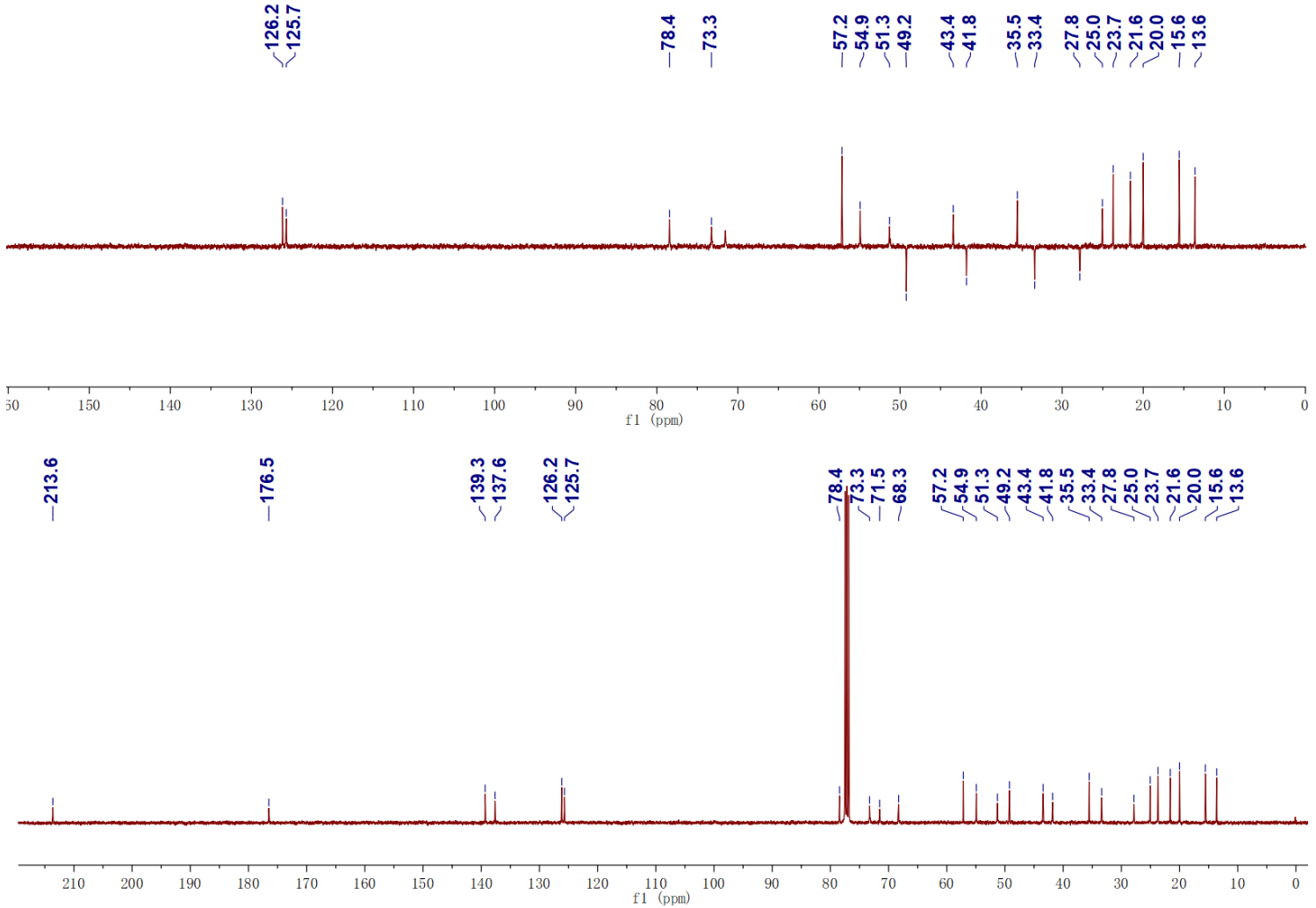

Figure S58. ^{13}C NMR of compound **6** (in $CDCl_3$)

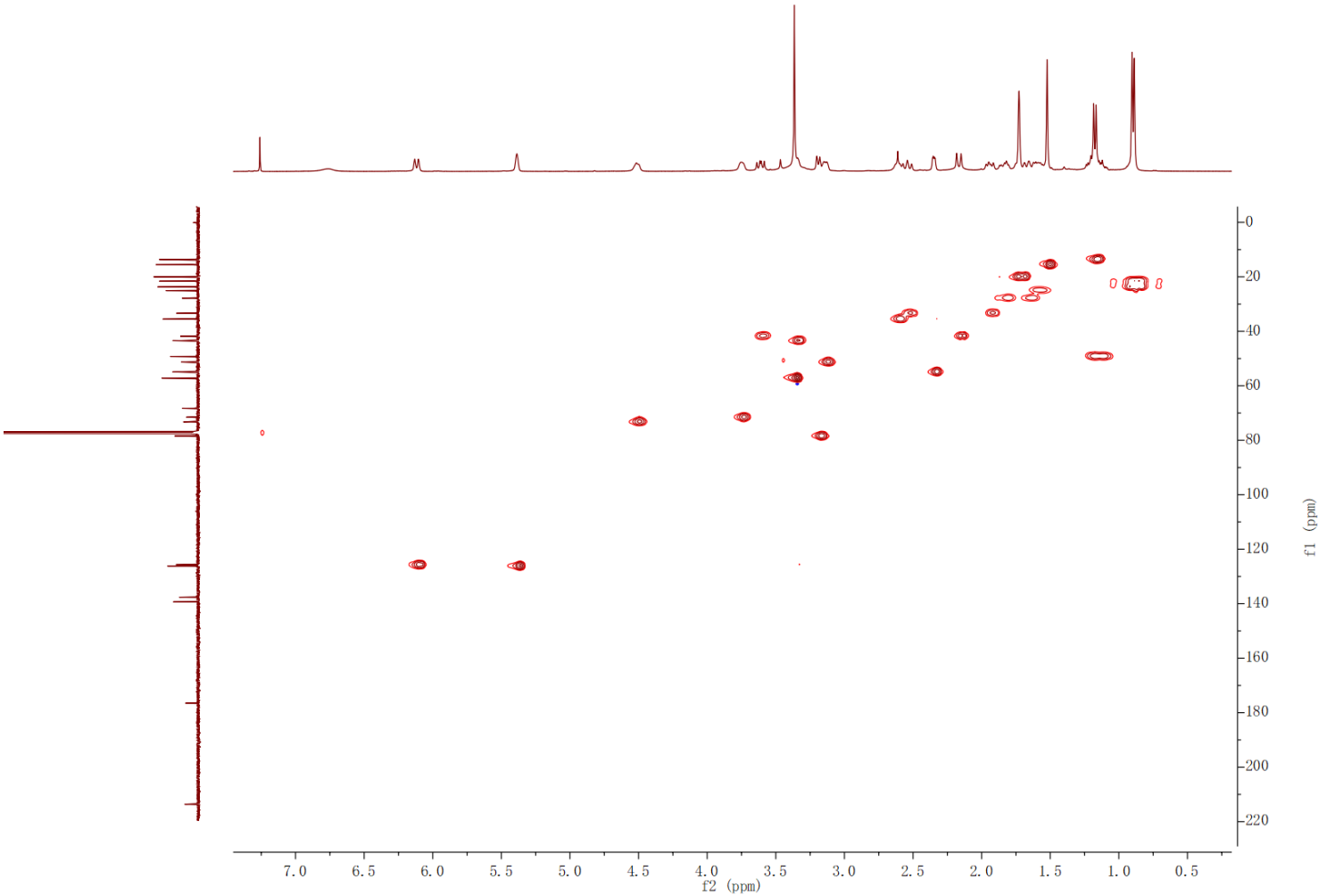

Figure S59. HSQC of compound **6** (in $CDCl_3$)

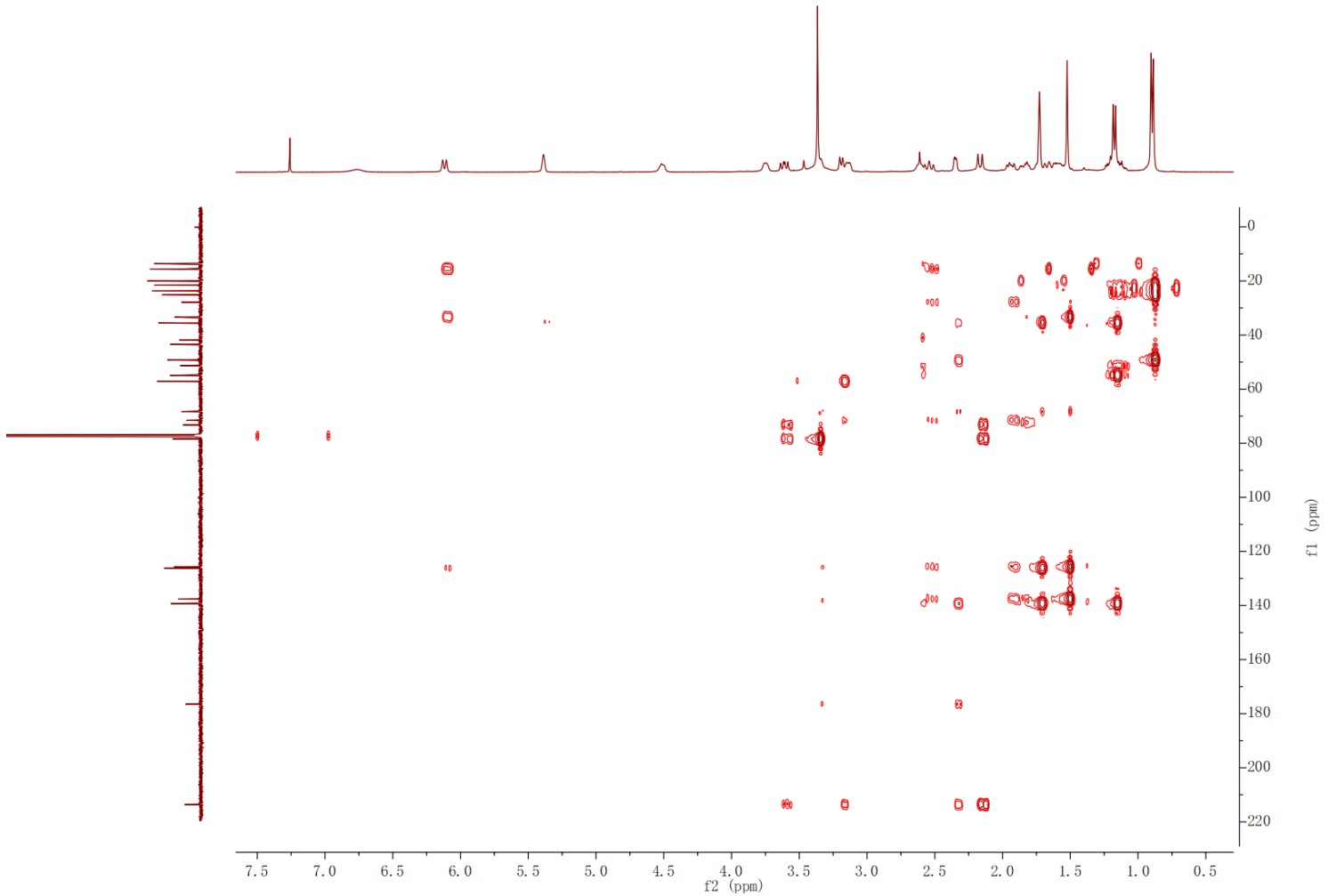

Figure S60. HMBC of compound **6** (in $CDCl_3$)

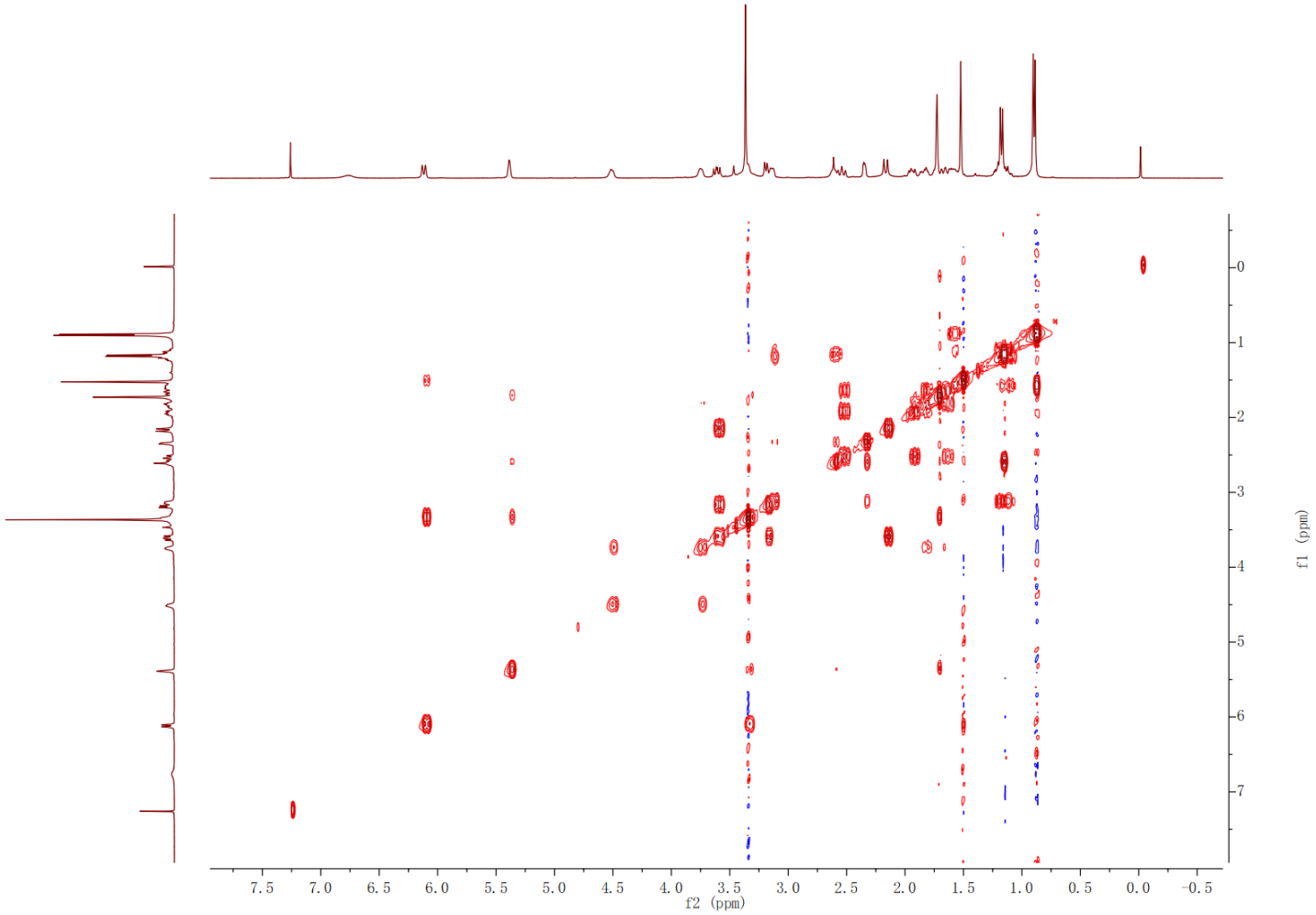

Figure S61. ^{1}H–^{1}H COSY of compound **6** (in $CDCl_3$)

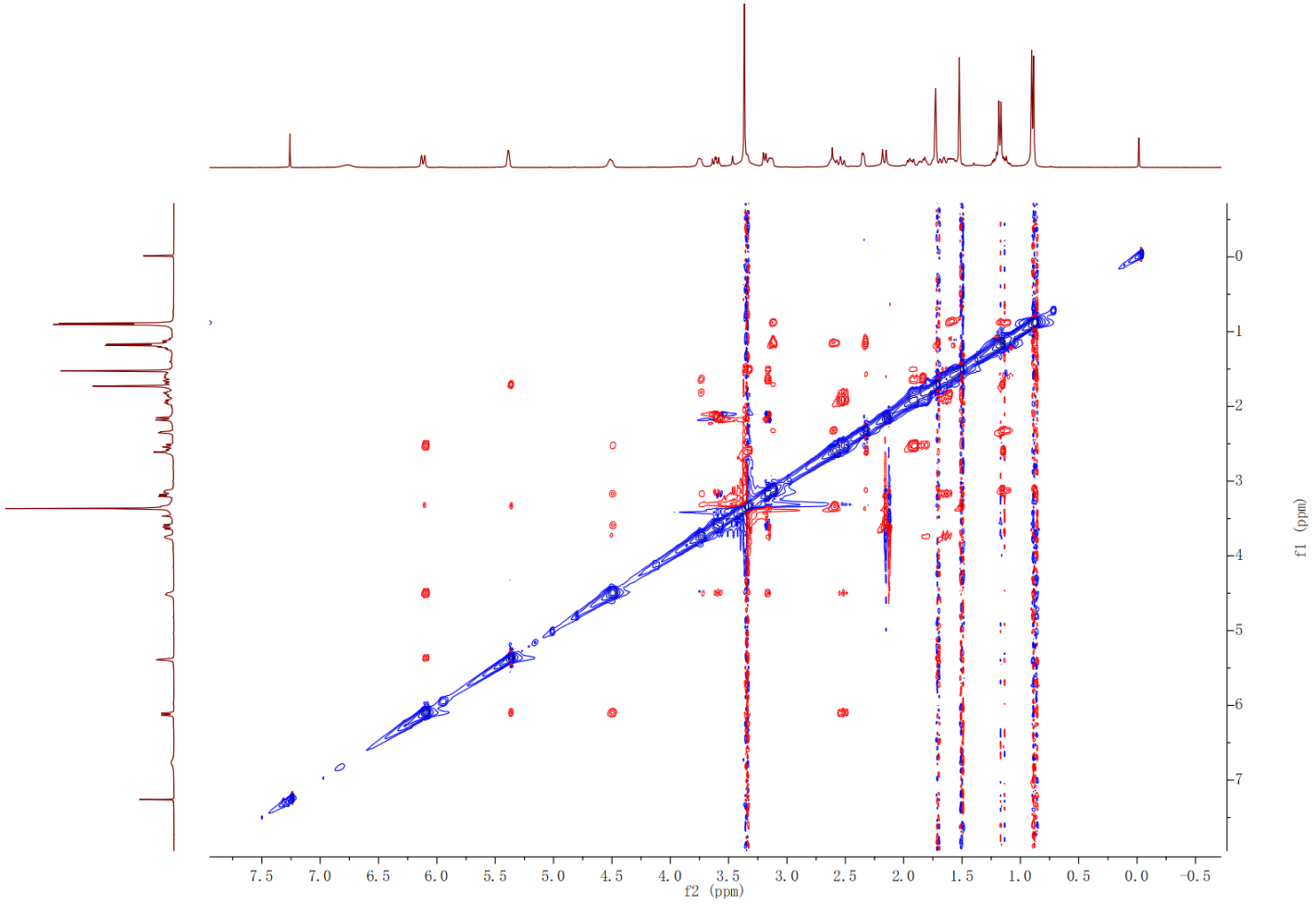

Figure S62. NOESY of compound **6** (in $CDCl_3$)

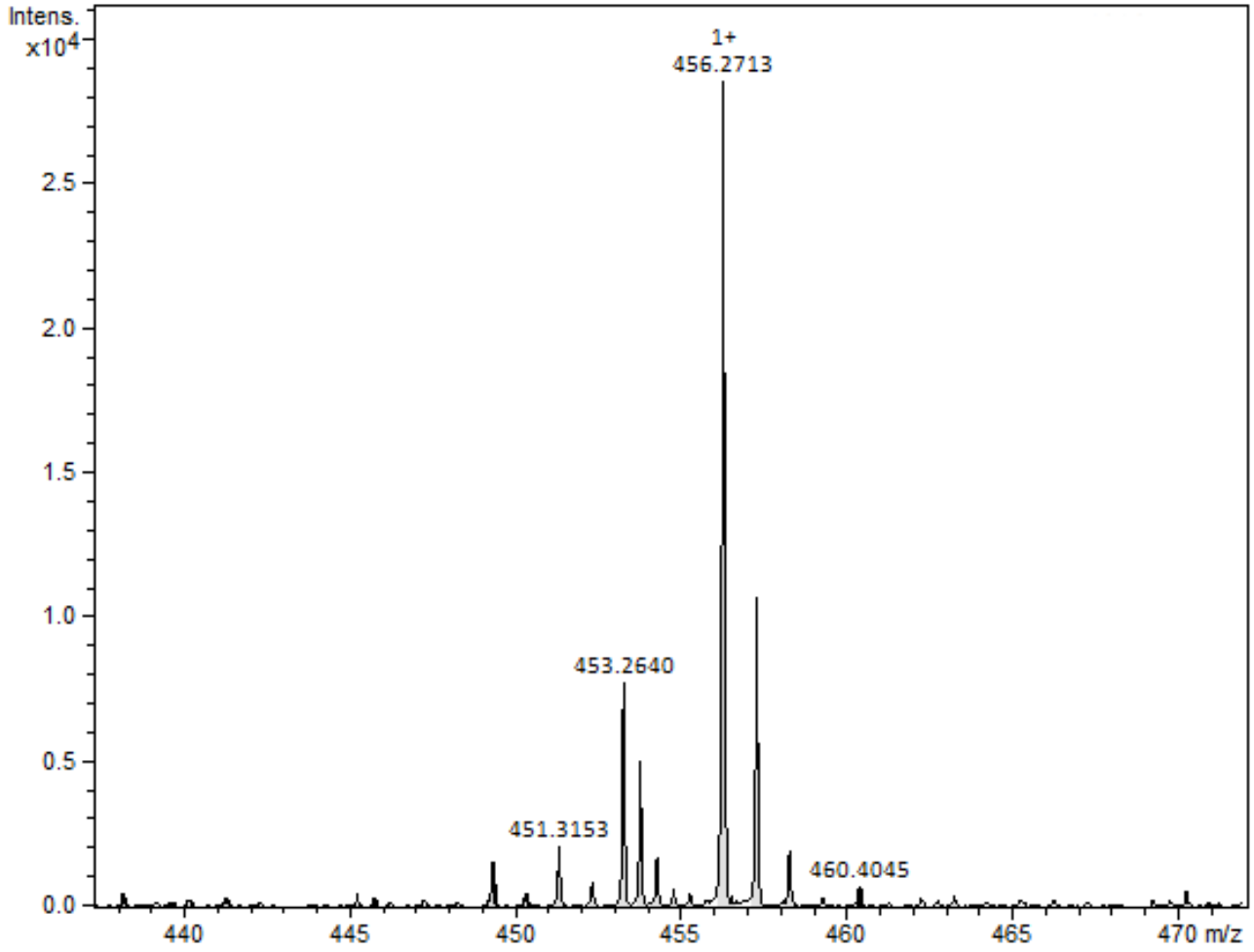

Figure S63. HRESIMS of compound **6**

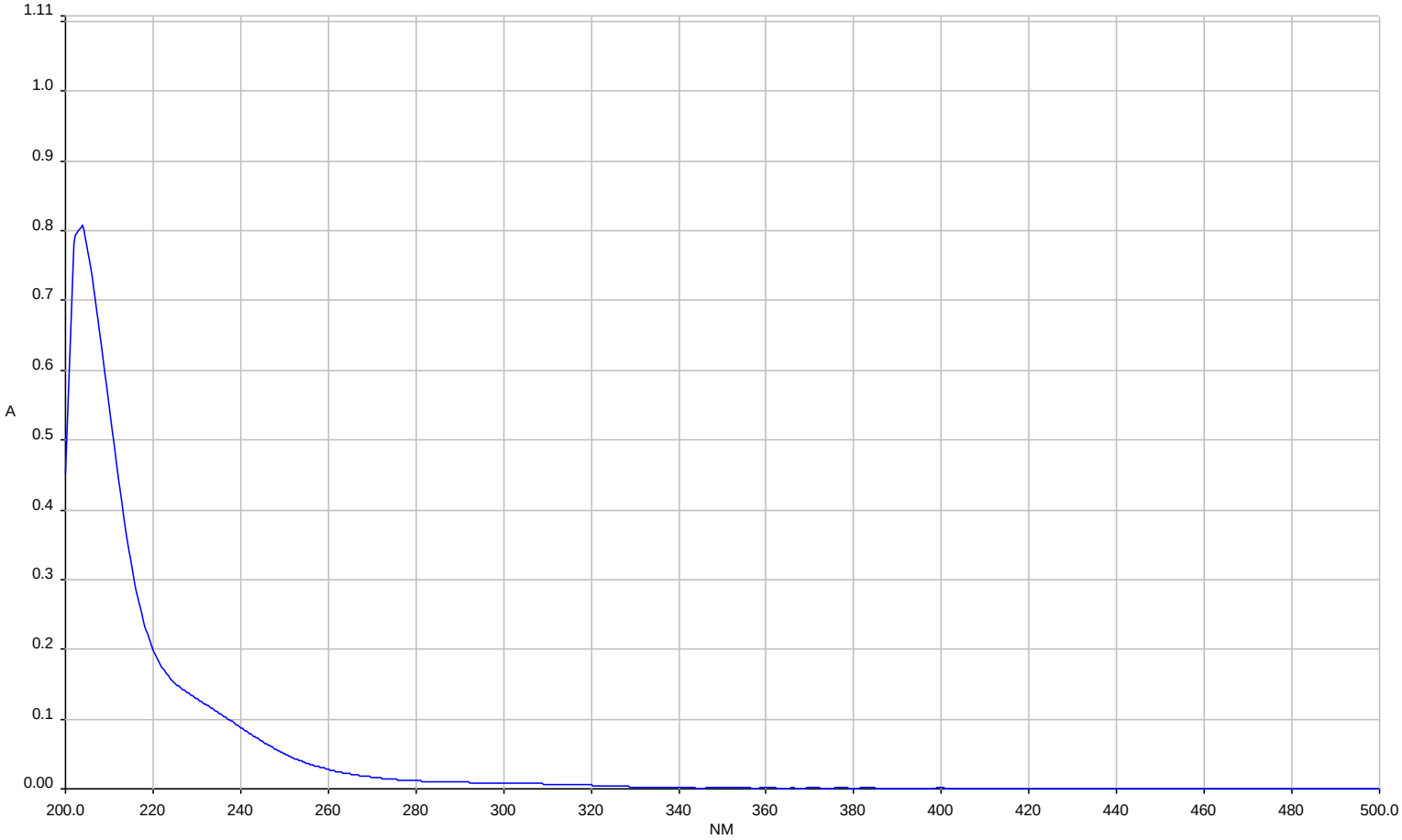

Figure S64. UV of compound **6**

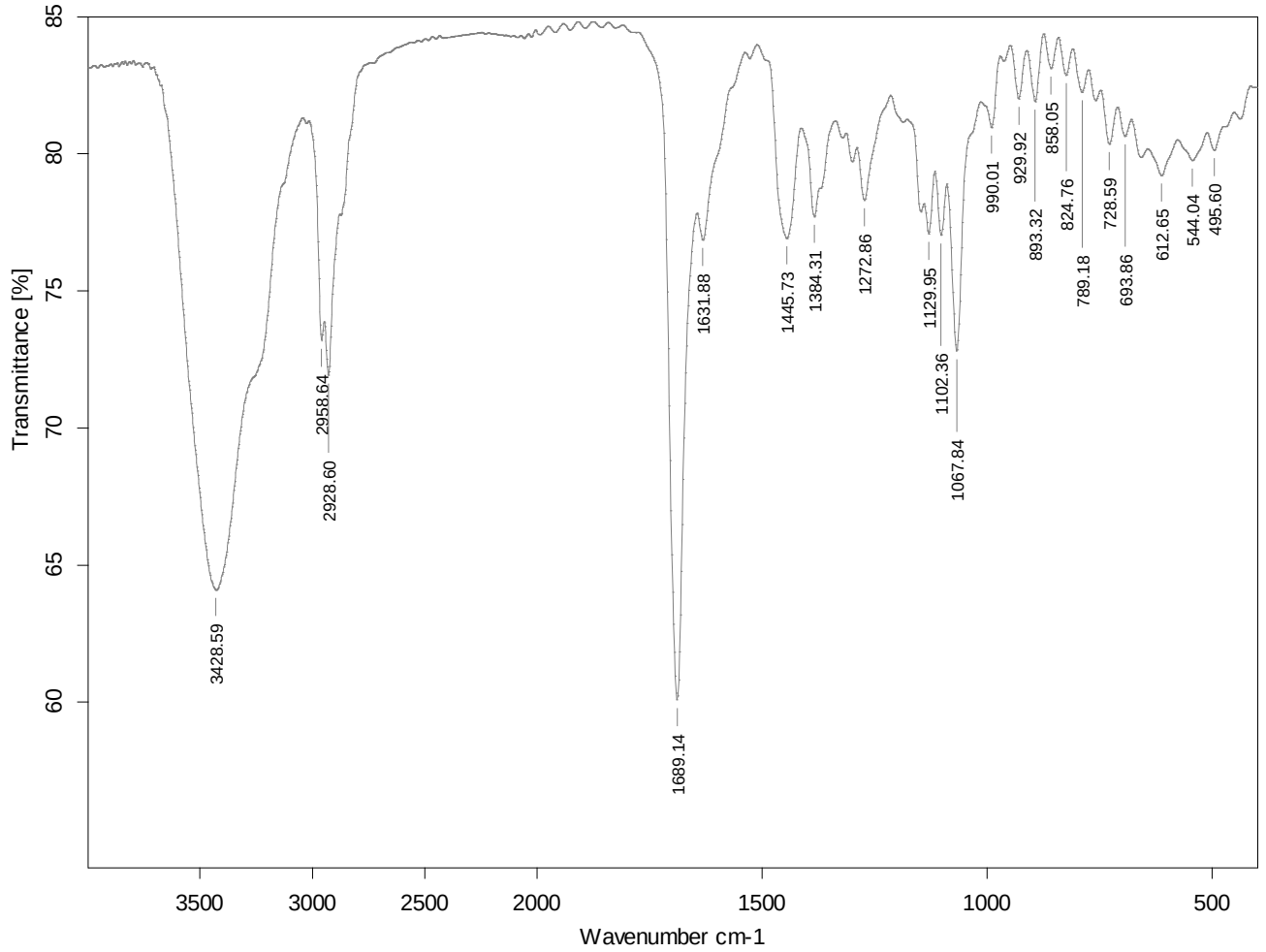

Figure S65. IR of compound **6**

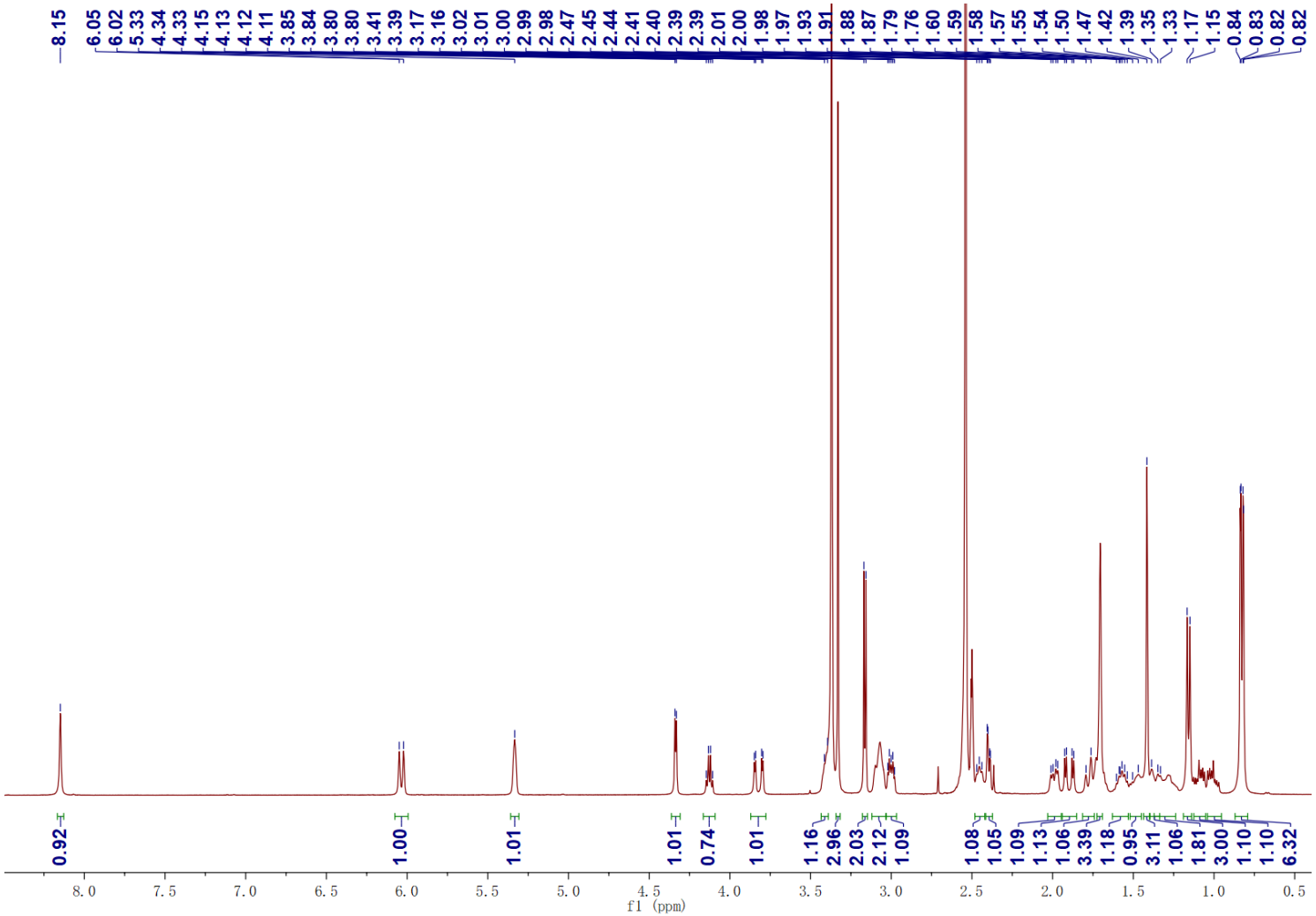

Figure S66. ^{1}H NMR of compound **7** (in DMSO-d_6)

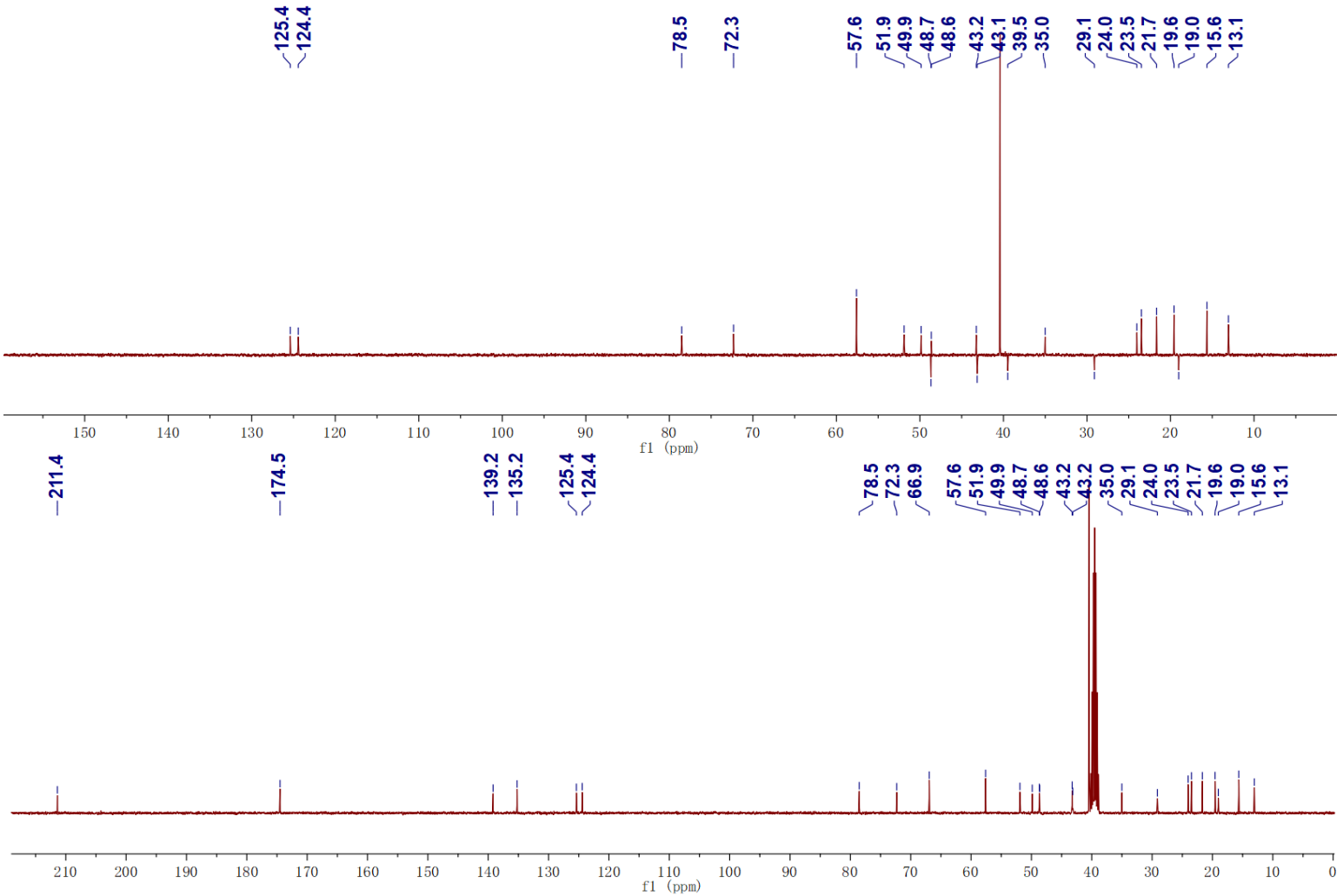

Figure S67. ^{13}C NMR of compound **7** (in DMSO-d_6)

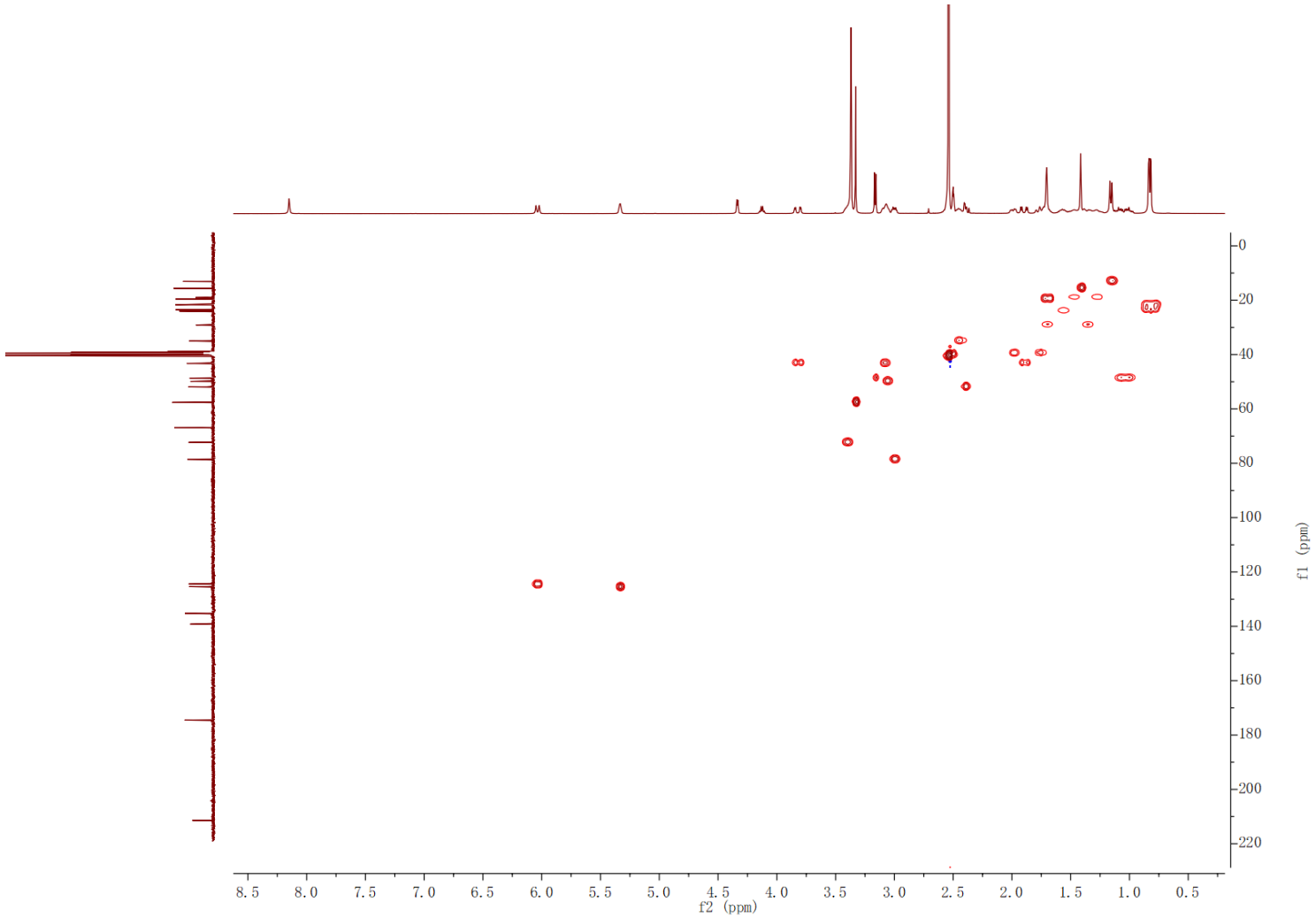

Figure S68. HSQC of compound **7** (in DMSO-d_6)

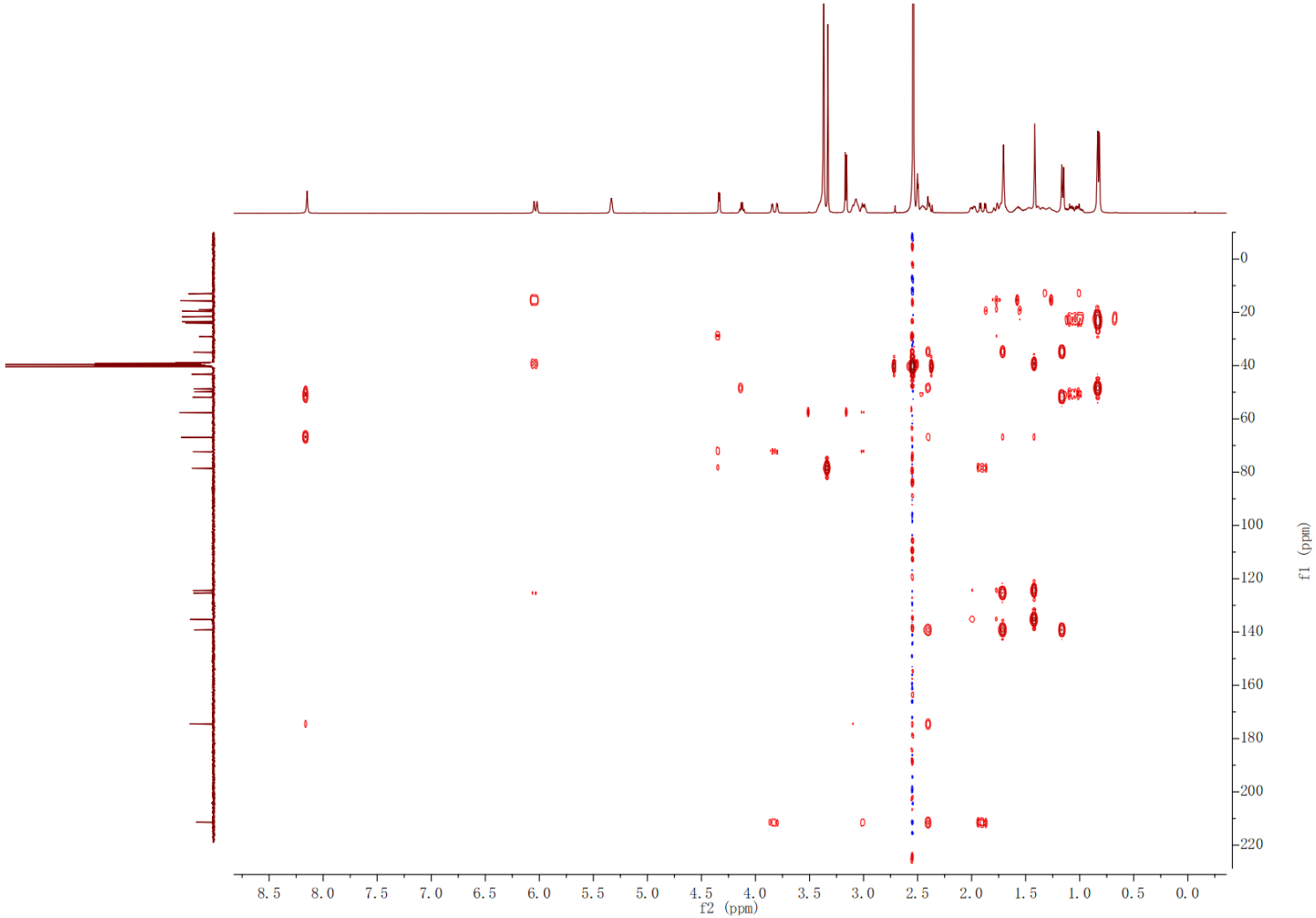

Figure S69. HMBC of compound **7** (in DMSO-d_6)

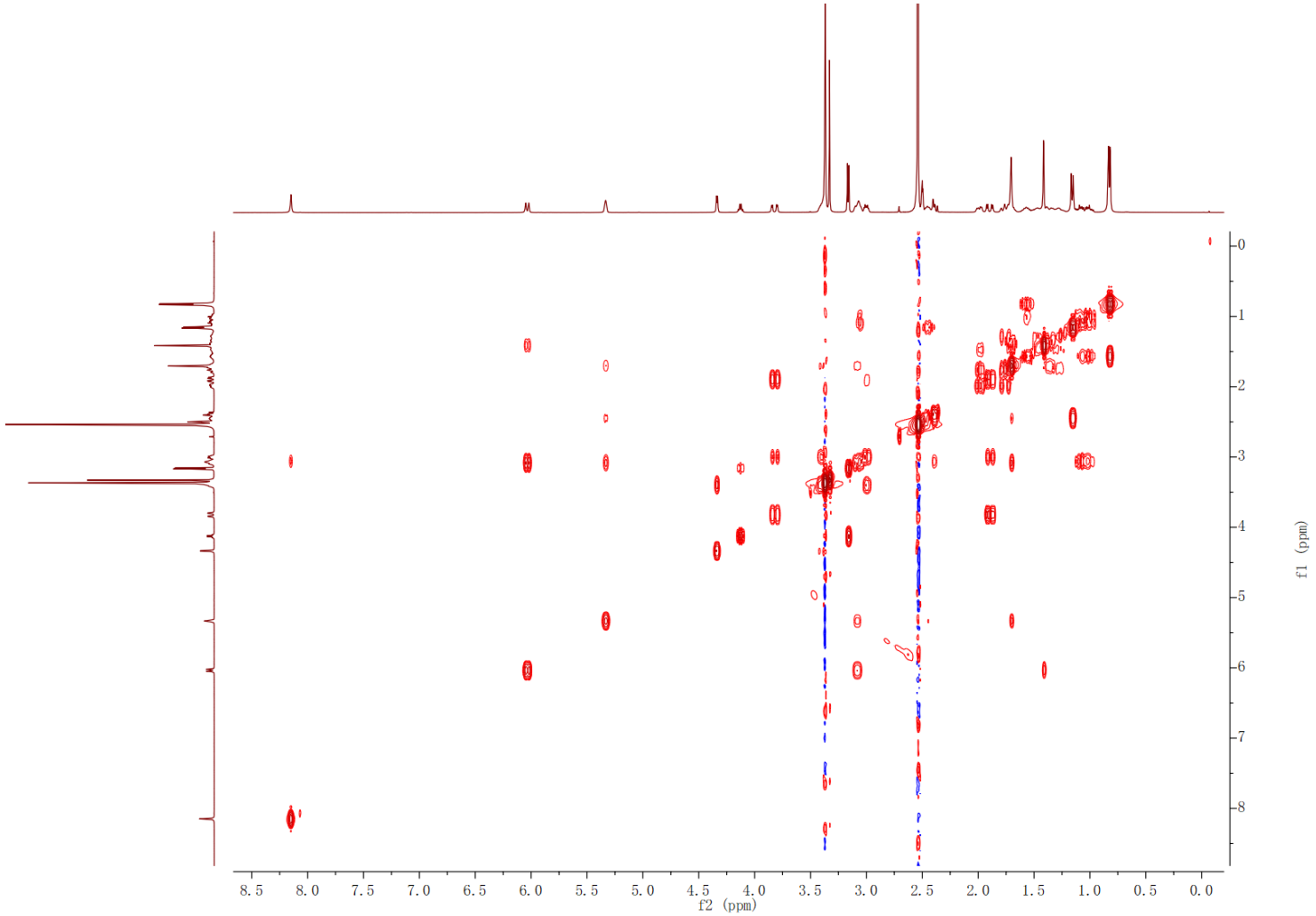

Figure S70. ^{1}H-^{1}H COSY of compound **7** (in DMSO-d_6)

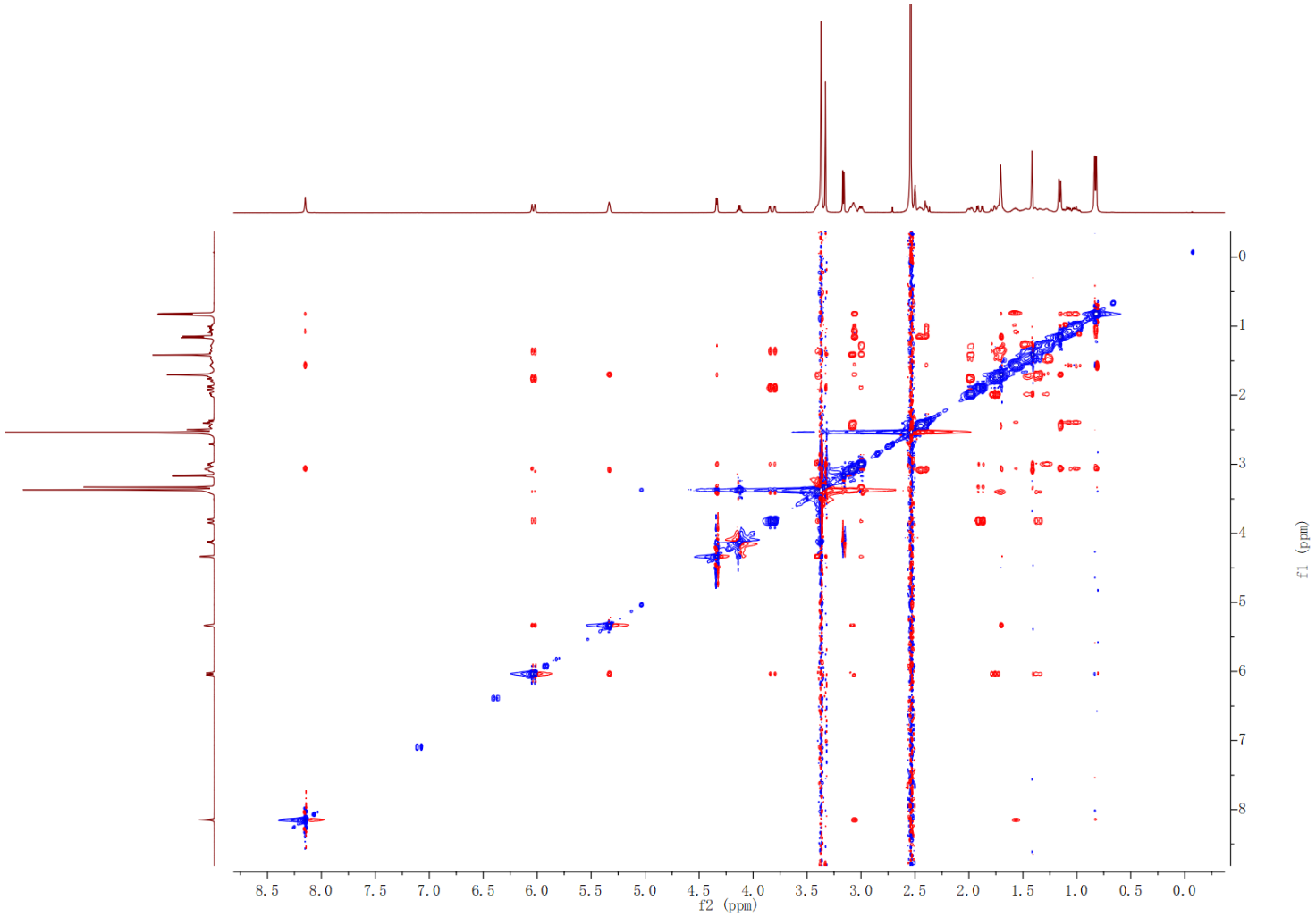

Figure S71. NOESY of compound **7** (in DMSO-d_6)

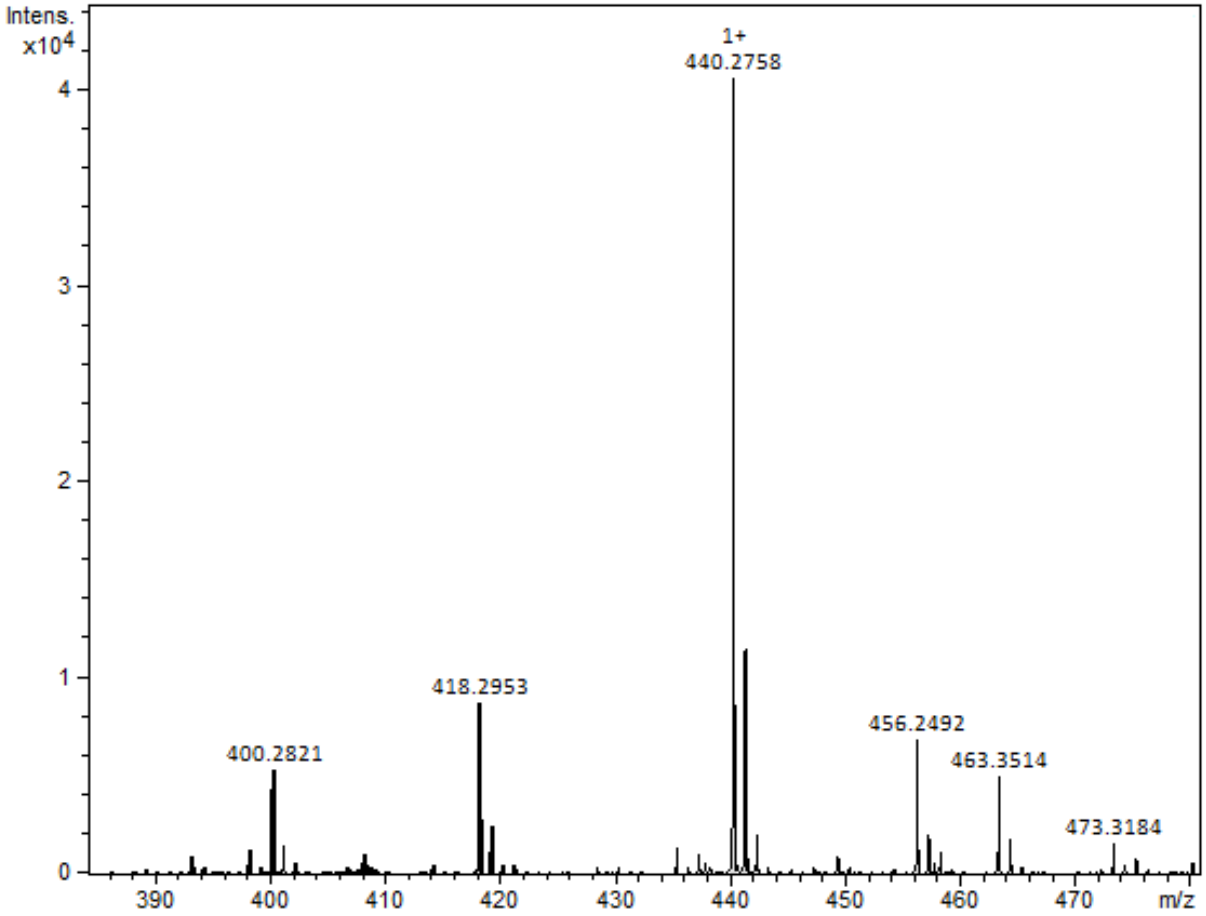

Figure S72. HRESIMS of compound **7**

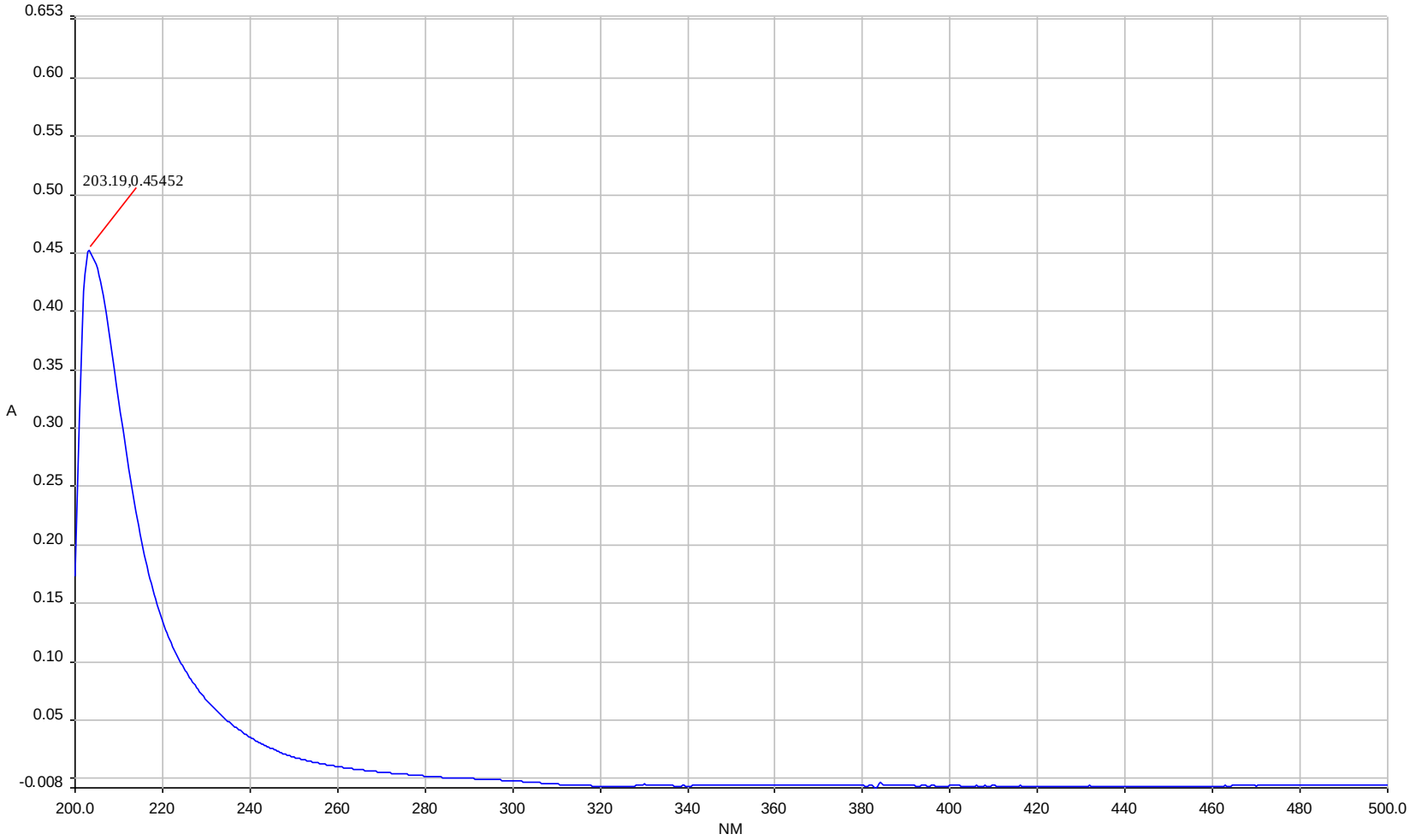

Figure S73. UV of compound **7**

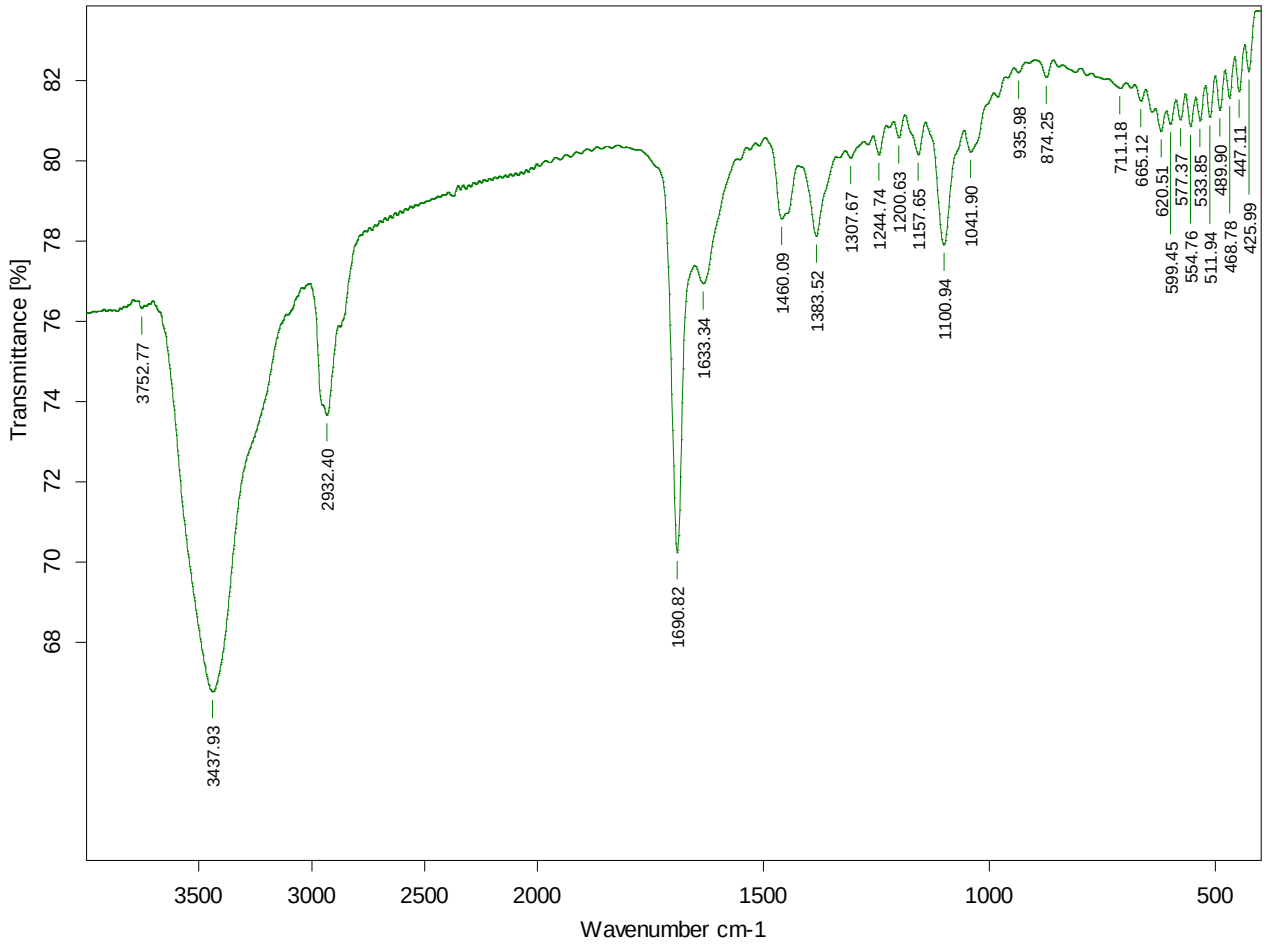

Figure S74. IR of compound **7**

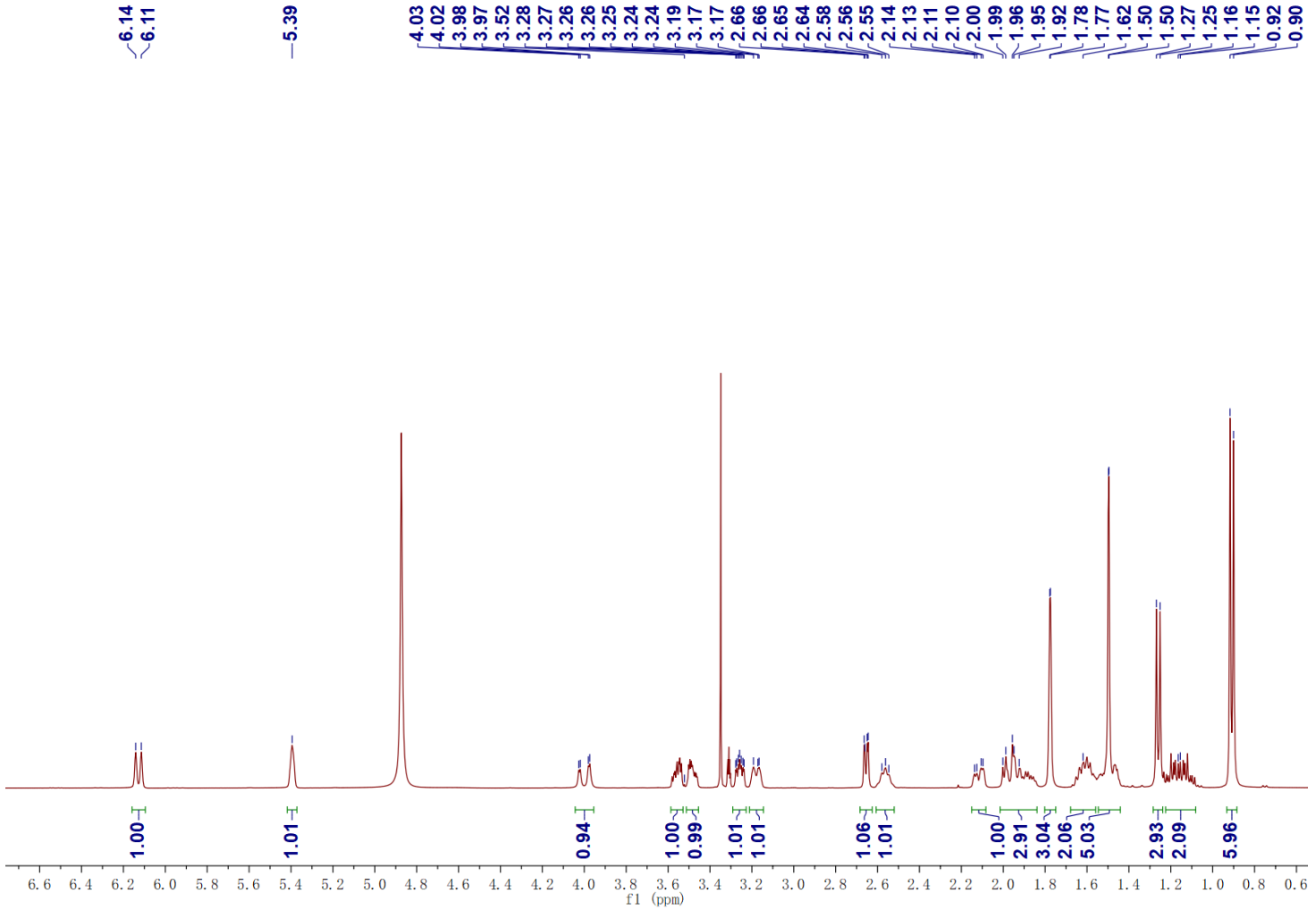

Figure S75. ^{1}H NMR of compound **8** (in CD_3OD)

Figure S76. ^{13}C NMR of compound **8** (in CD_3OD)

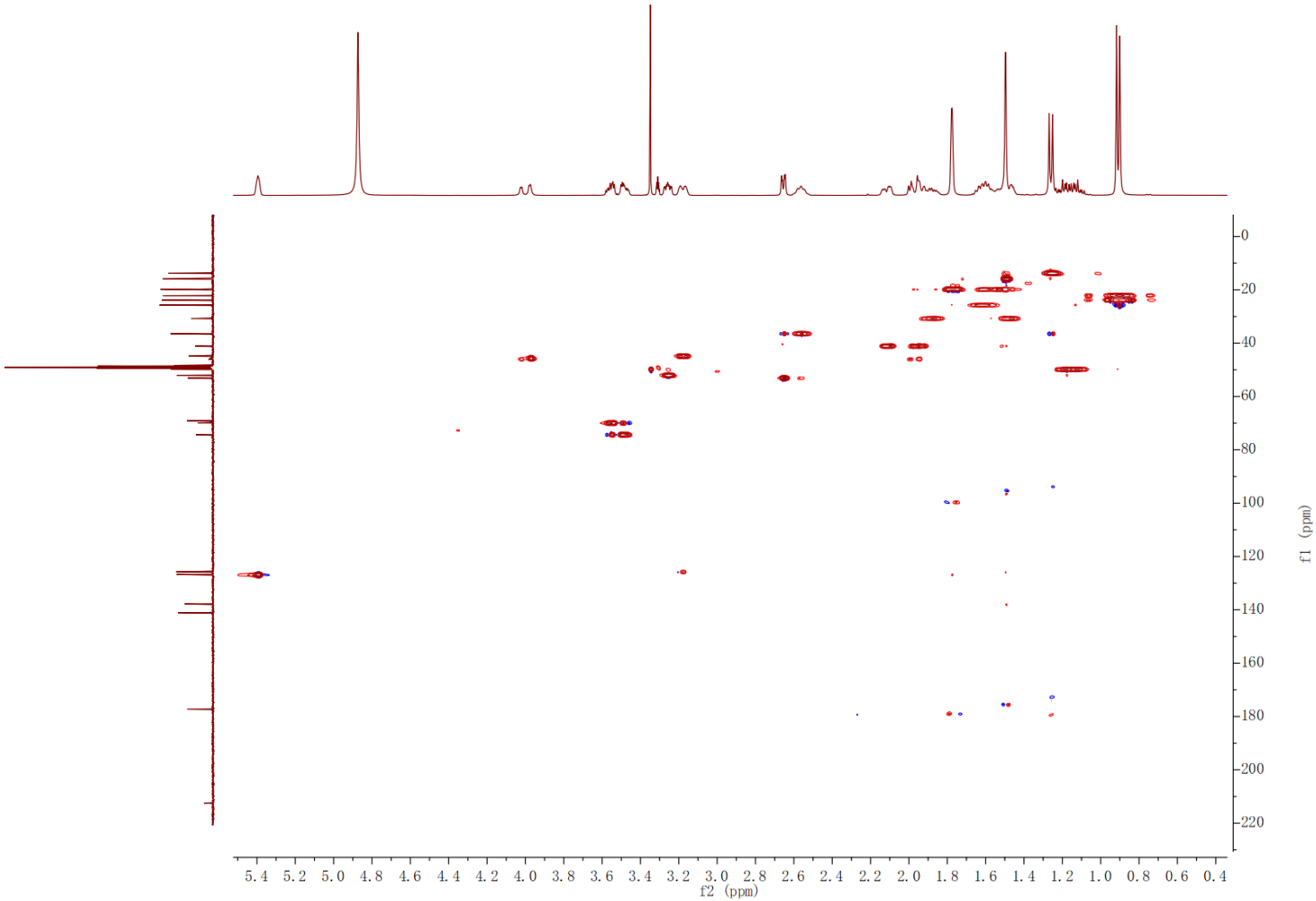

Figure S77. HSQC of compound **8** (in CD_3OD)

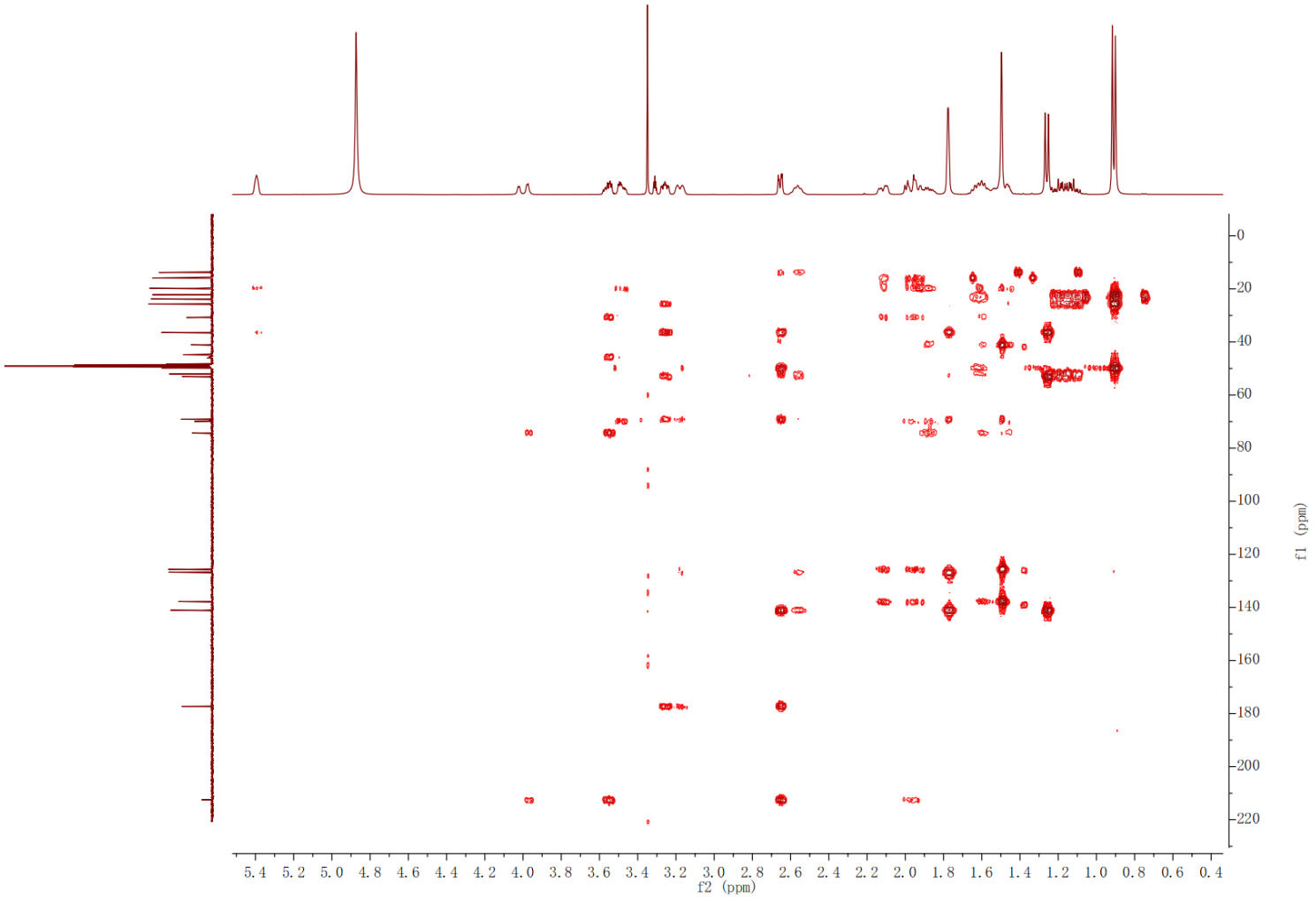

Figure S78. HMBC of compound **8** (in CD_3OD)

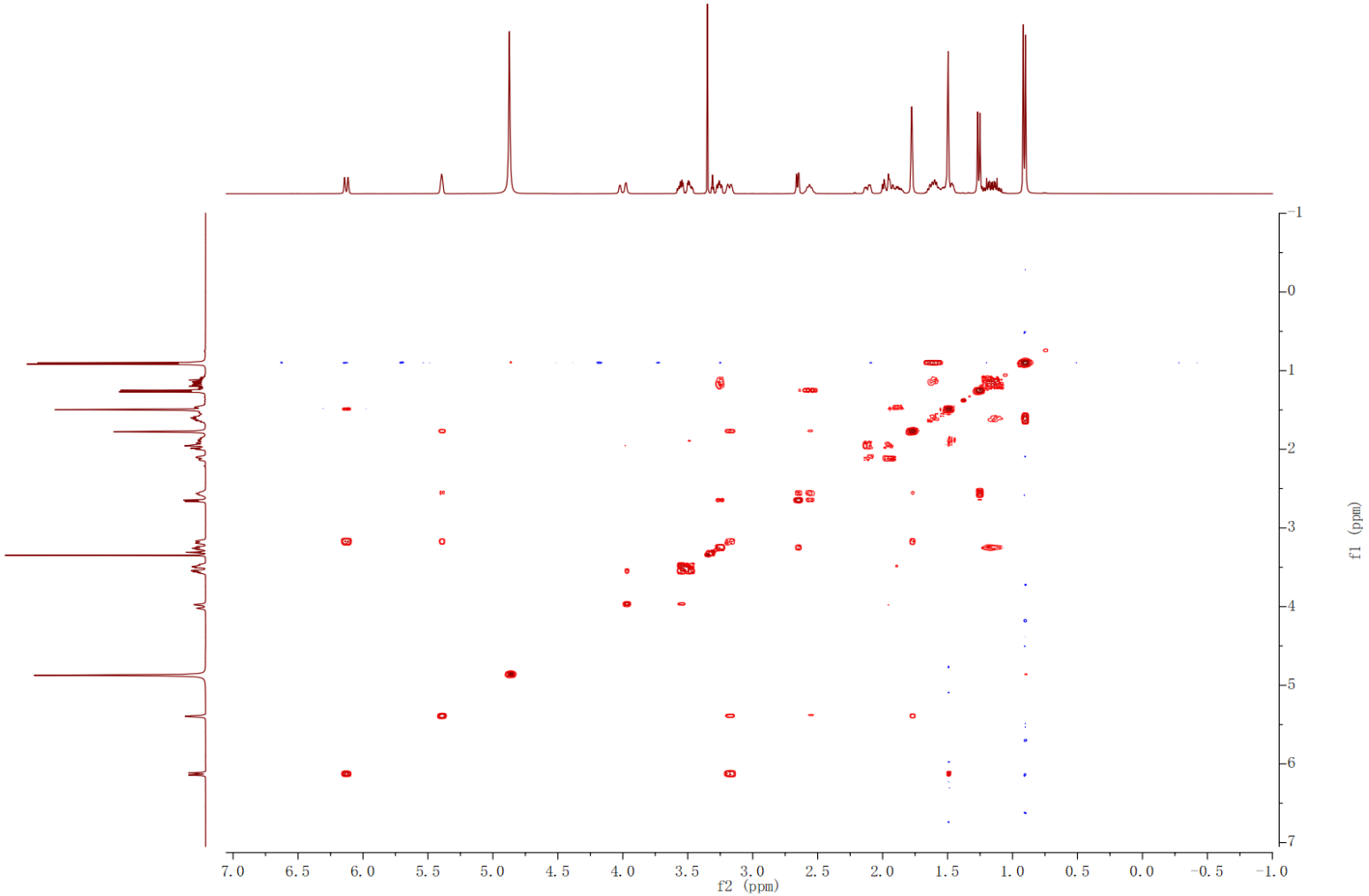

Figure S79. ^{1}H-^{1}H COSY of compound **8** (in CD_3OD)

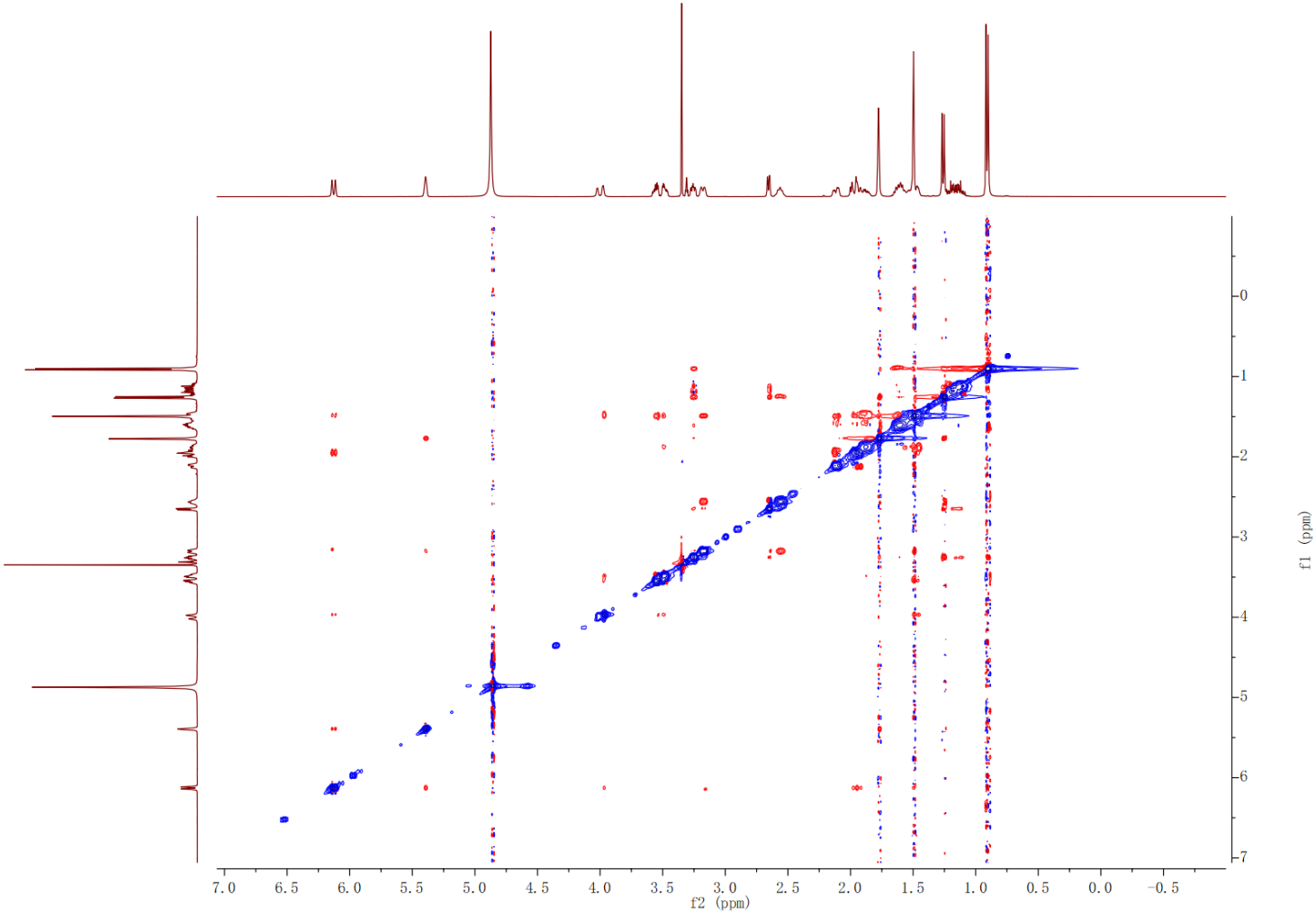

Figure S80. NOESY of compound **8** (in CD_3OD)

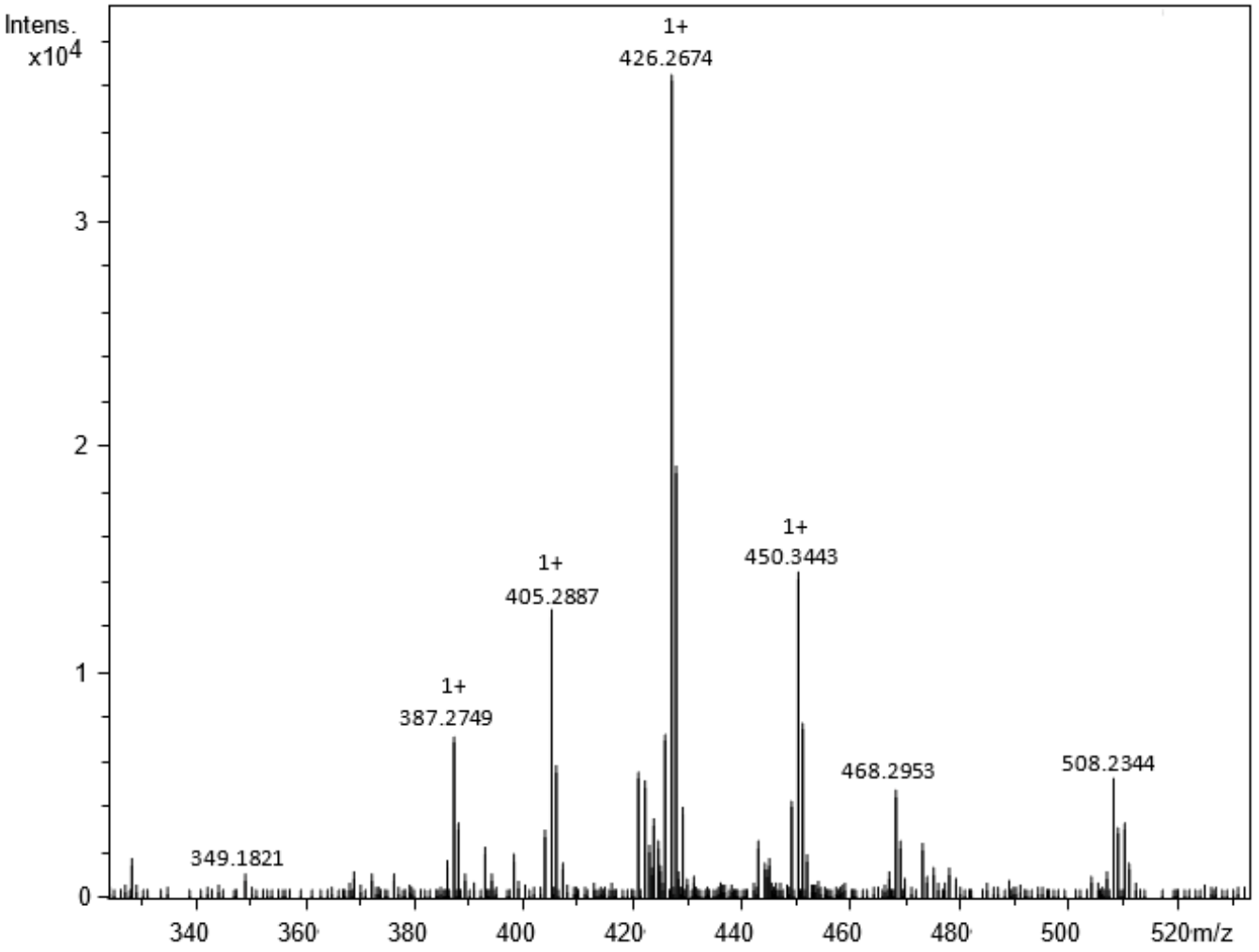

Figure S81. HRESIMS of compound **8**

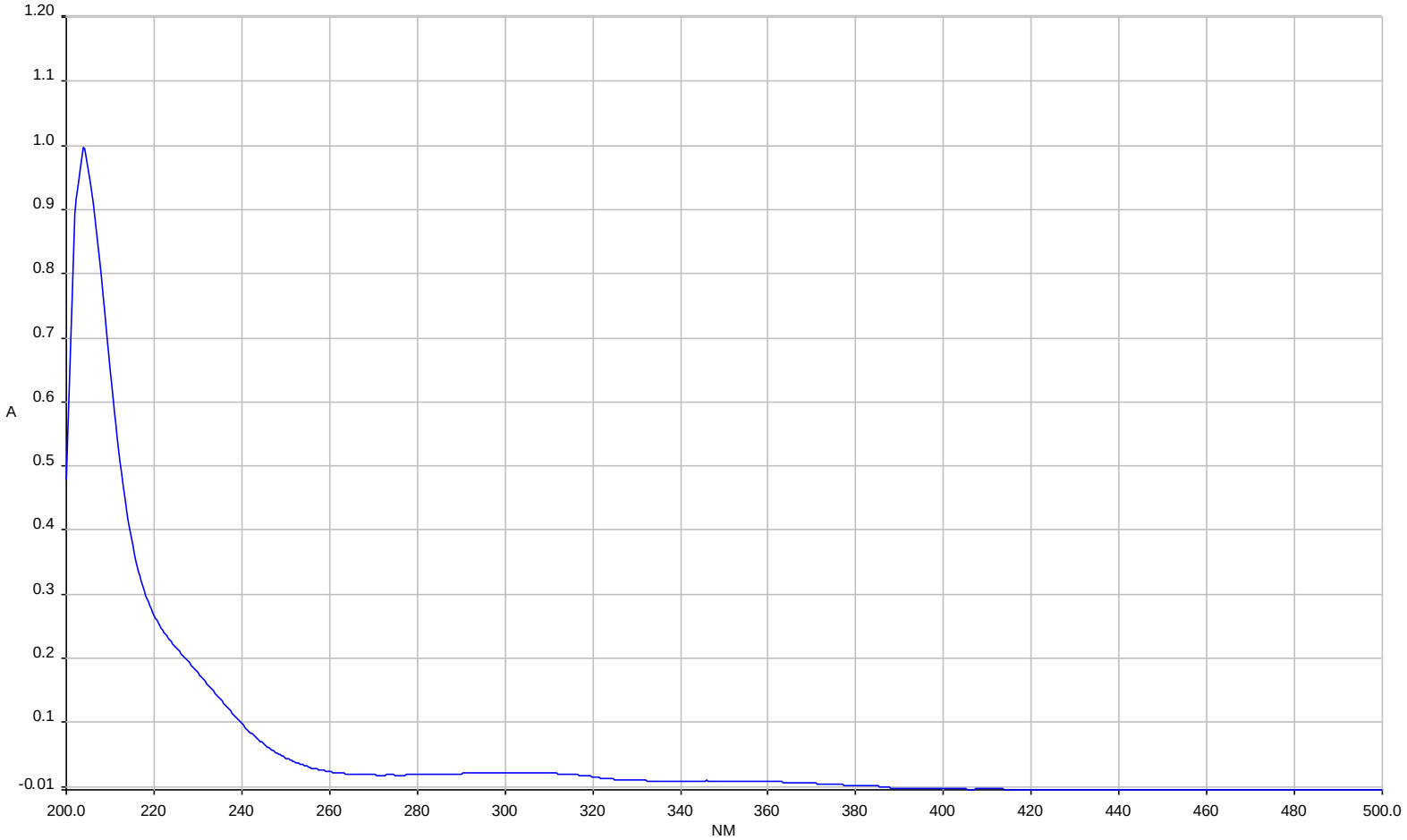

Figure S82. UV of compound **8**

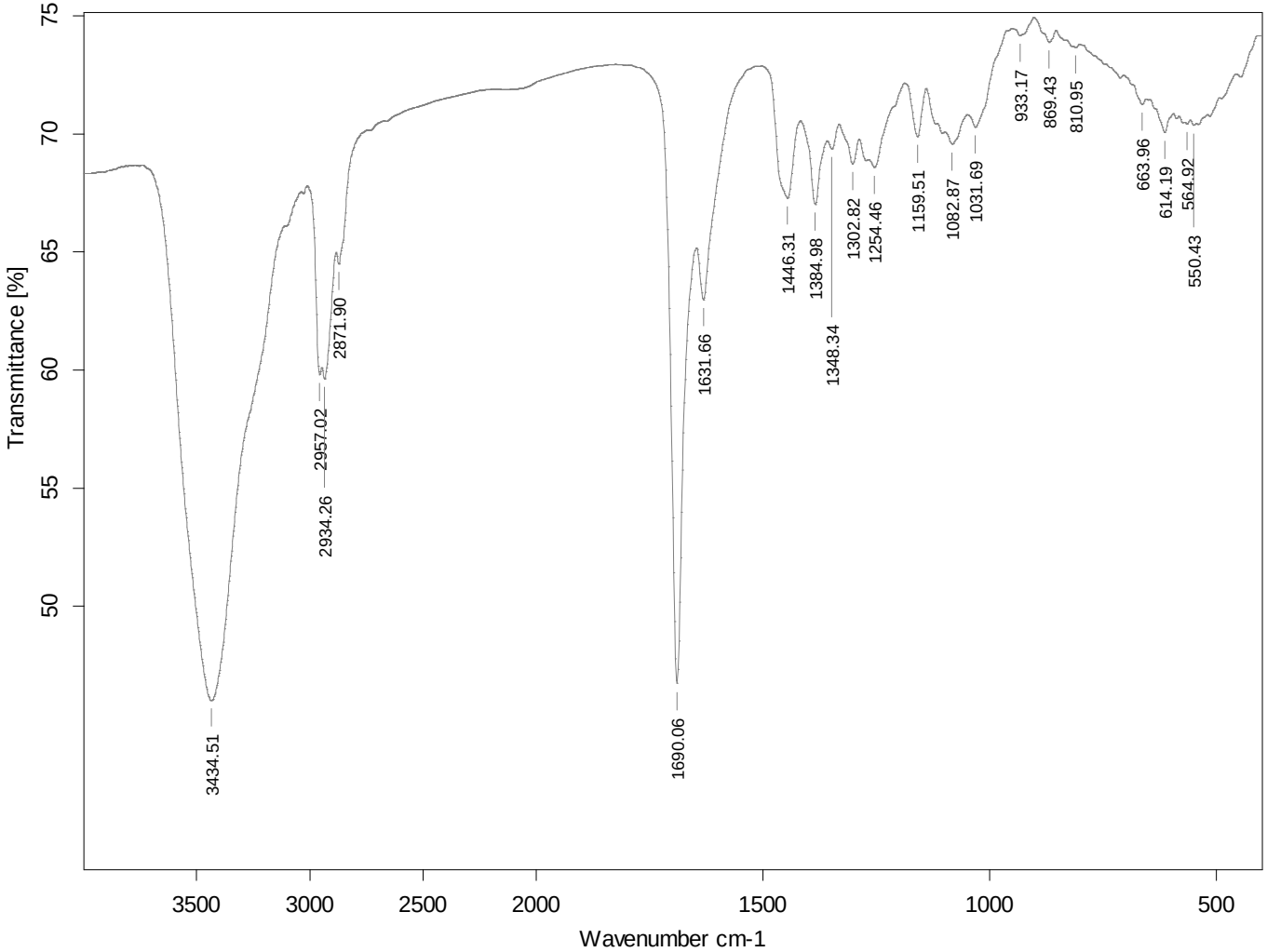

Figure S83. IR of compound **8**

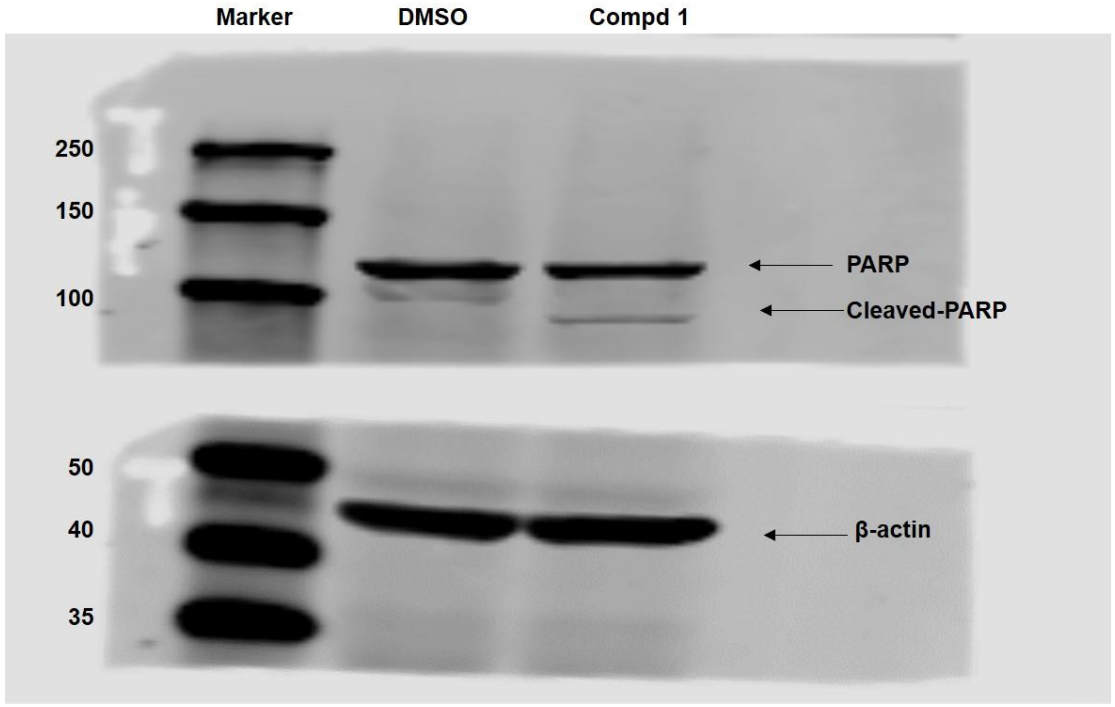

Figure S84. Complete western blotting pictures.