Supporting Information

Bipolaquinones A–J, Immunosuppressive Meroterpenoids from a Soil-Derived *Bipolaris zeicola*

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Contents of Supporting Information

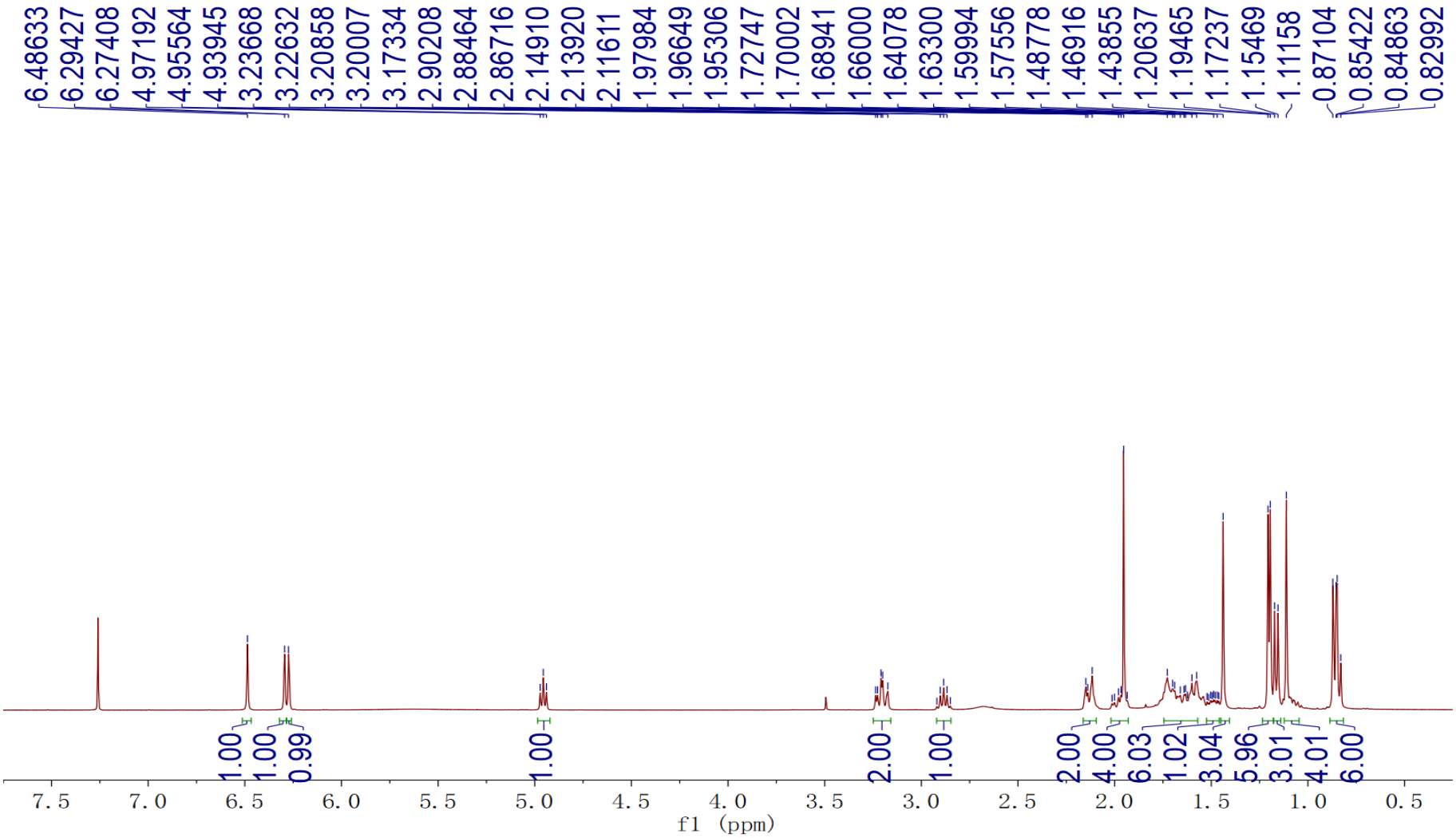


Figure S1. ^{1}H NMR spectrum of compound **1** (Recorded in $CDCl_3$)

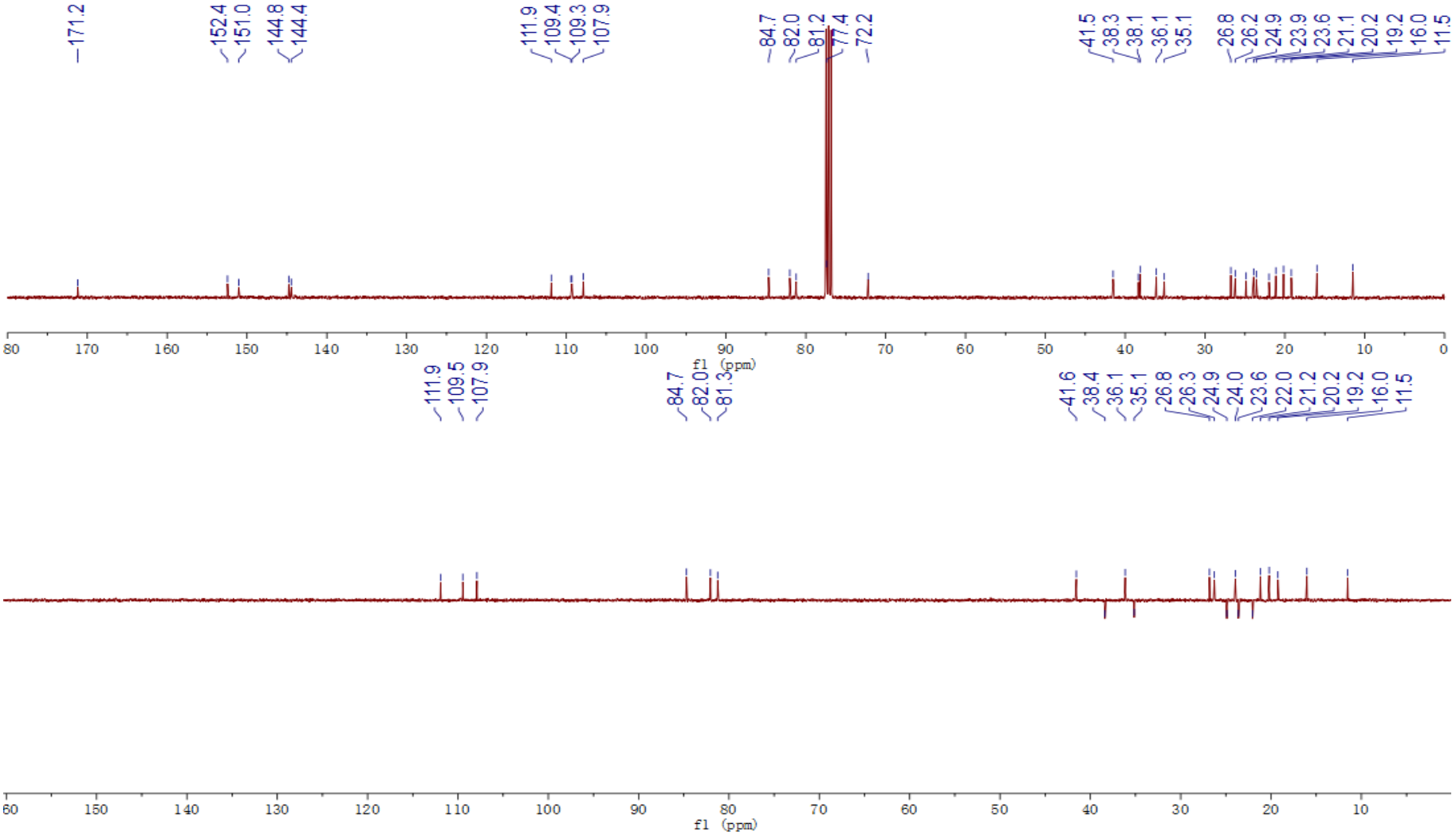


Figure S2. ^{13}C NMR and DEPT spectra of compound **1** (Recorded in $CDCl_3$)

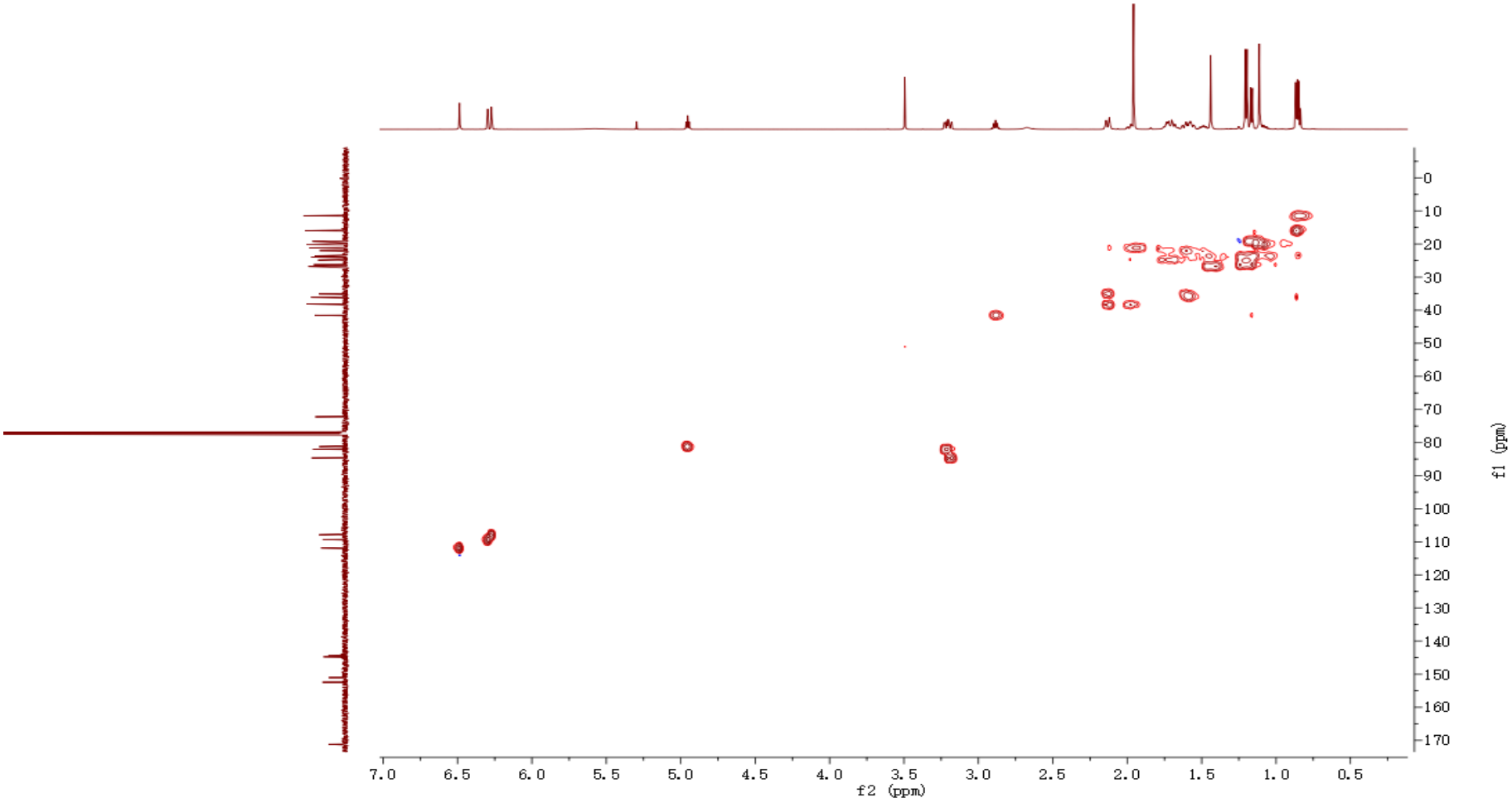


Figure S3. HSQC spectrum of compound **1** (Recorded in $CDCl_3$)

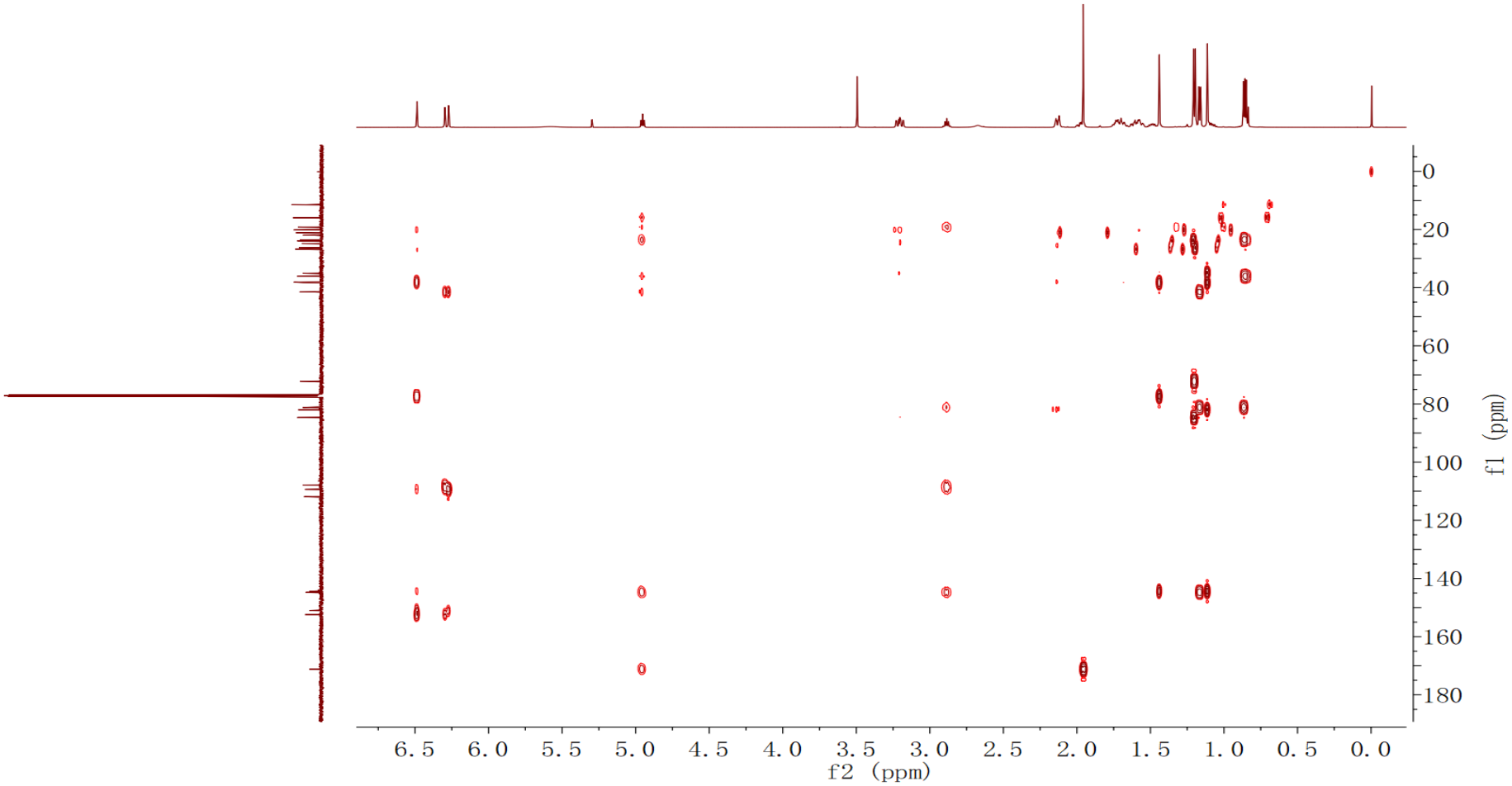


Figure S4. HMBC spectrum of compound **1** (Recorded in $CDCl_3$)

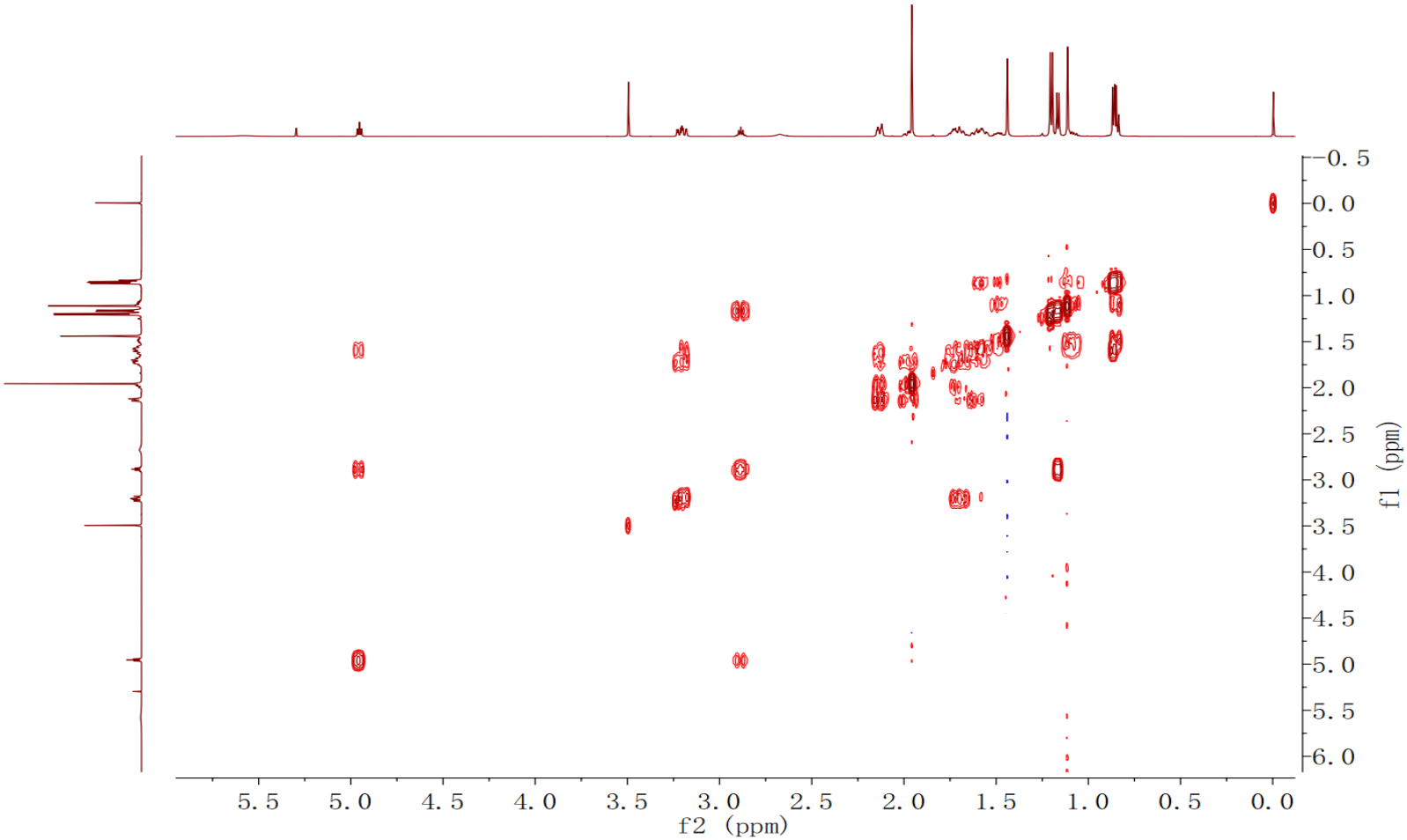


Figure S5. ^{1}H–^{1}H COSY spectrum of compound **1** (Recorded in $CDCl_3$)

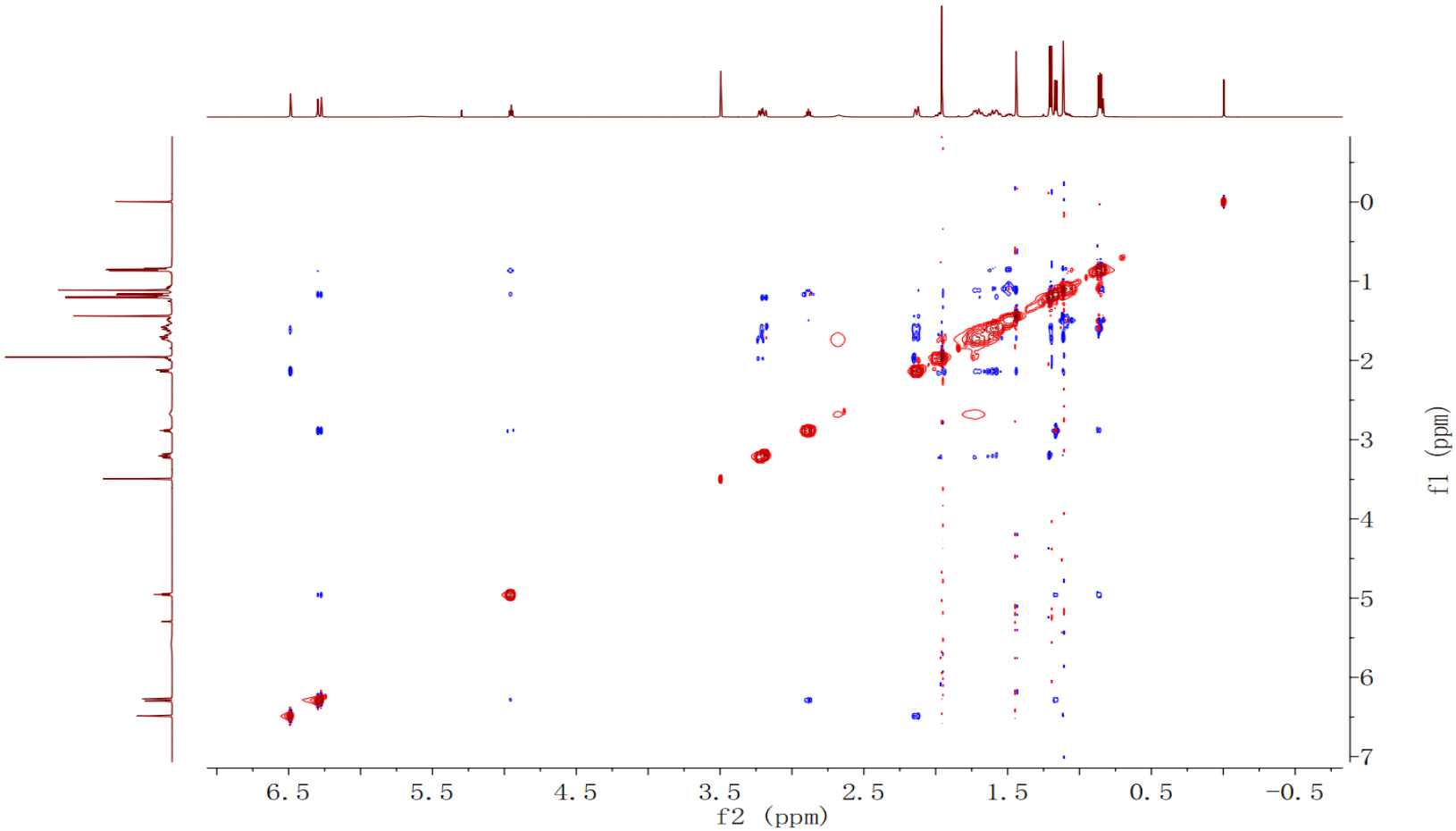


Figure S6. NOESY spectrum spectrum of compound **1** (Recorded in $CDCl_3$)

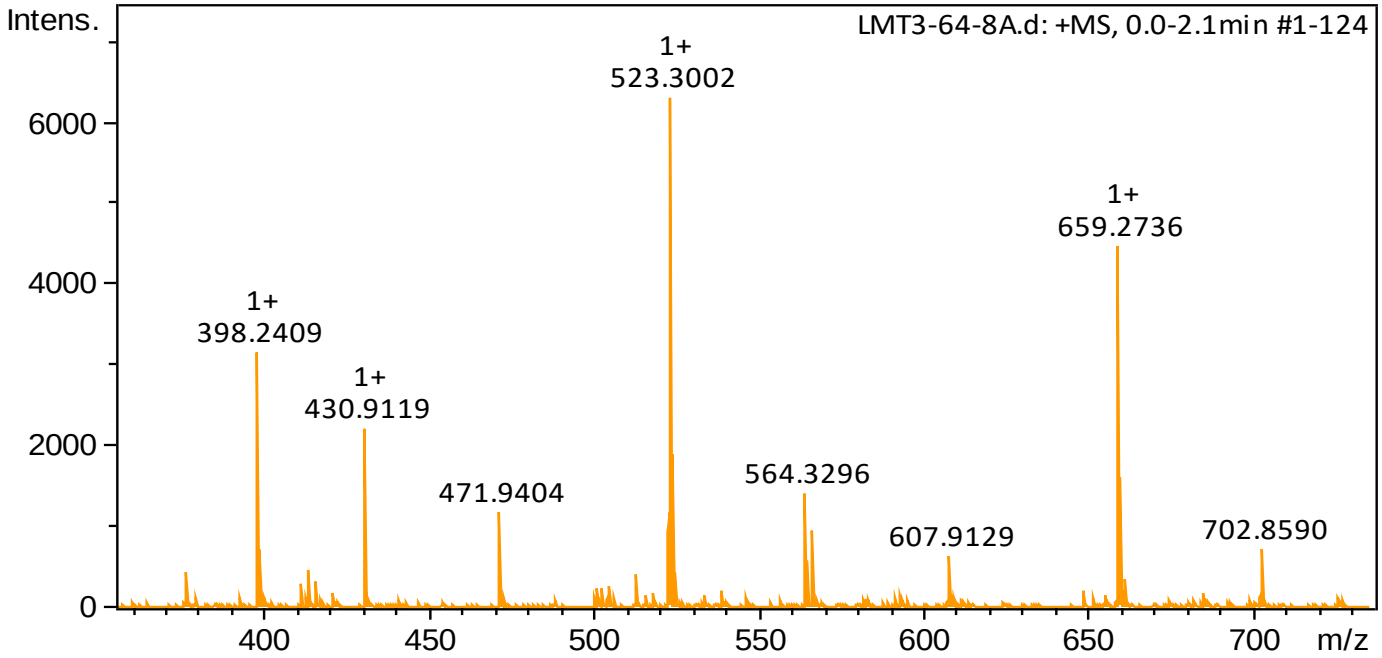


Figure S7. HRESIMS spectrum of compound **1**

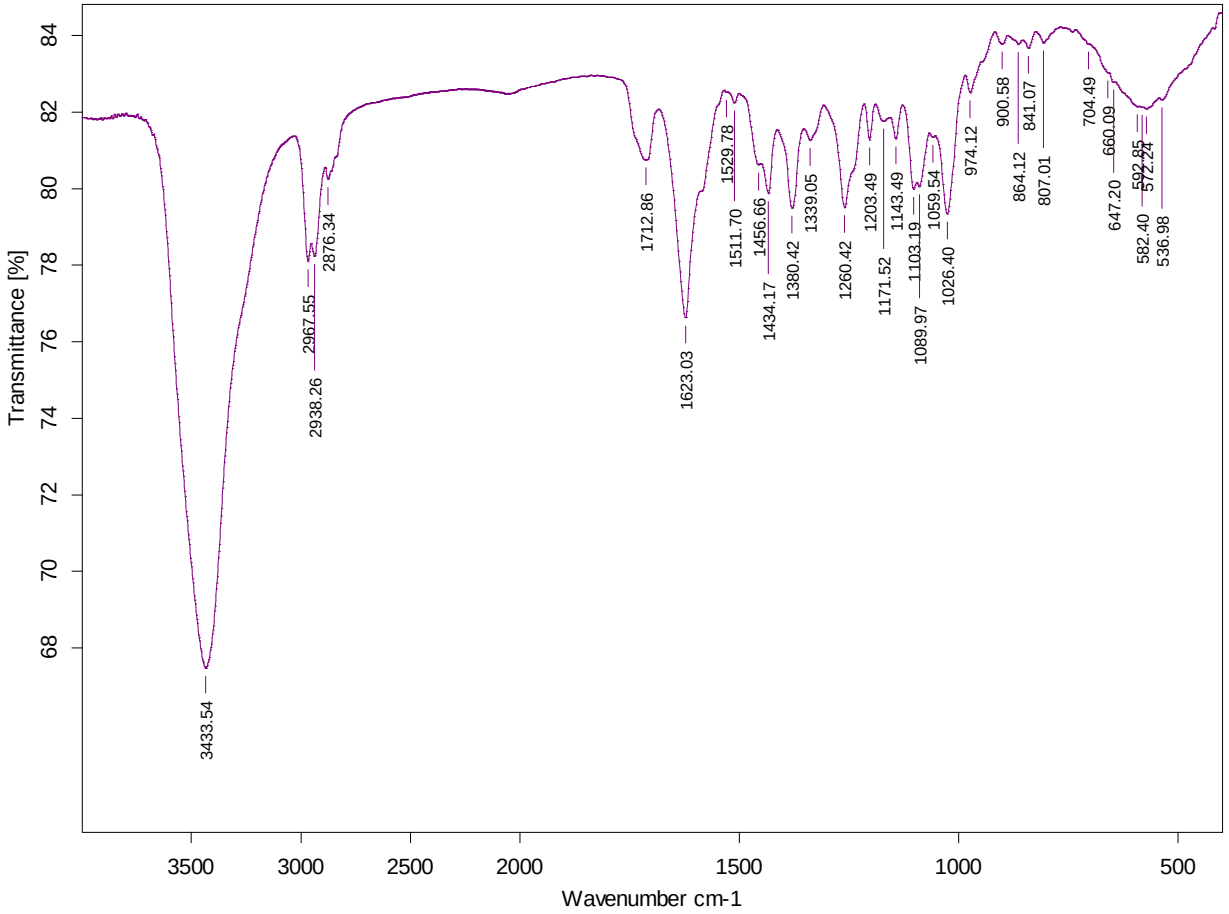


Figure S8. IR spectrum of compound **1**

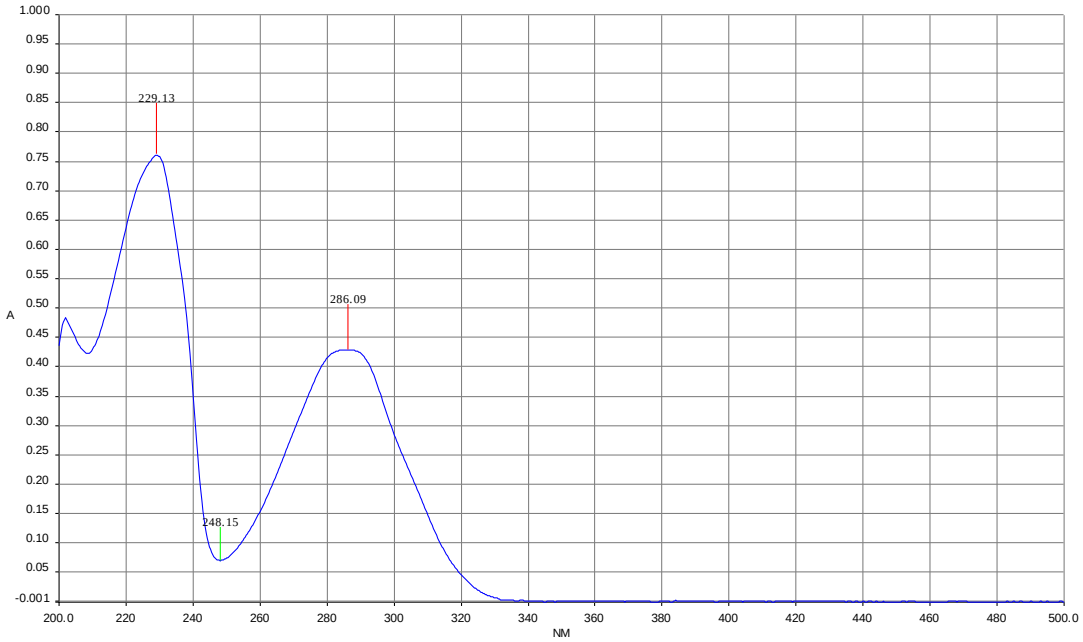


Figure S9. UV spectrum of compound **1**

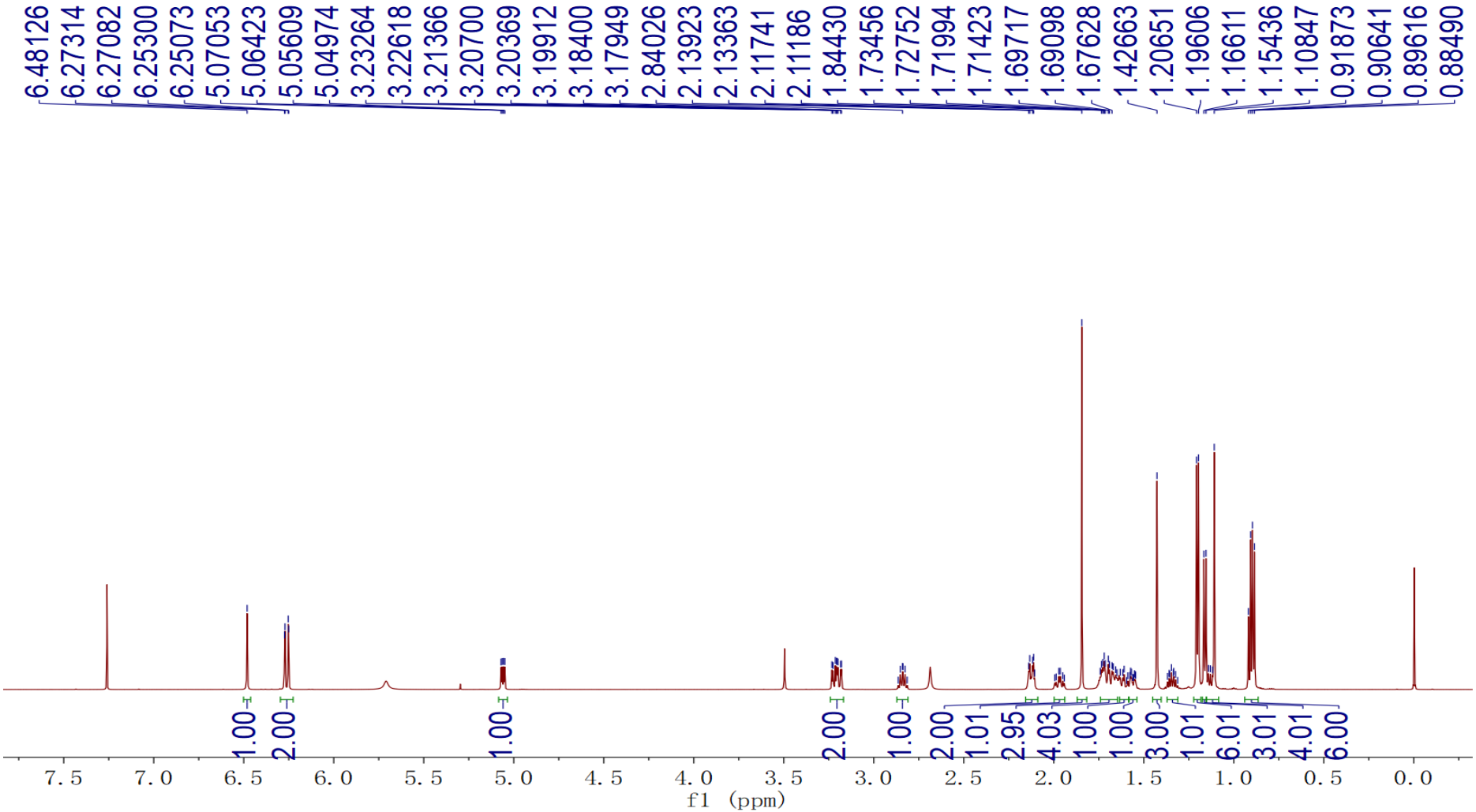


Figure S10. ^{1}H NMR spectrum of compound **2** (Recorded in $CDCl_3$)

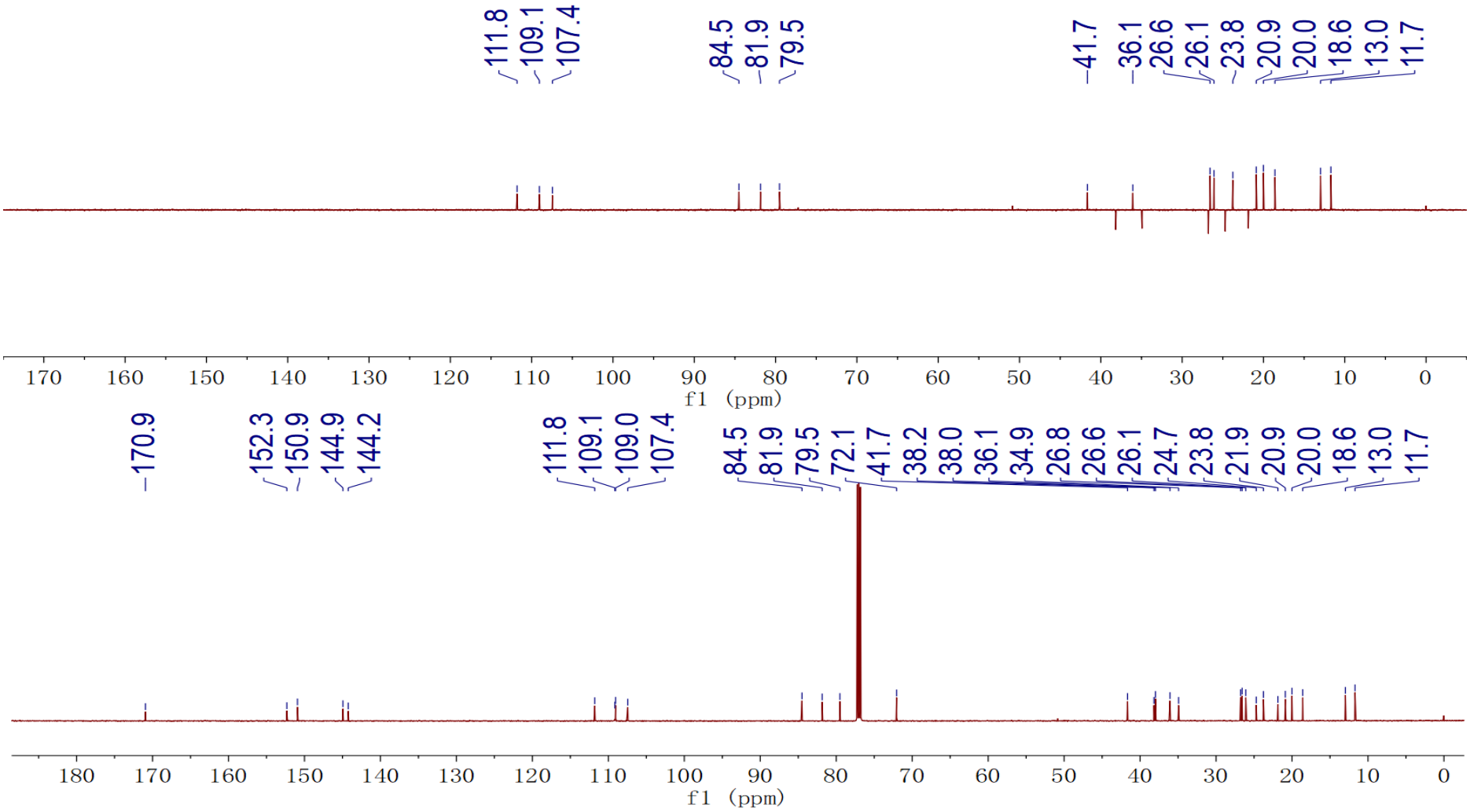


Figure S11. ^{13}C NMR and DEPT spectra of compound **2** (Recorded in $CDCl_3$)

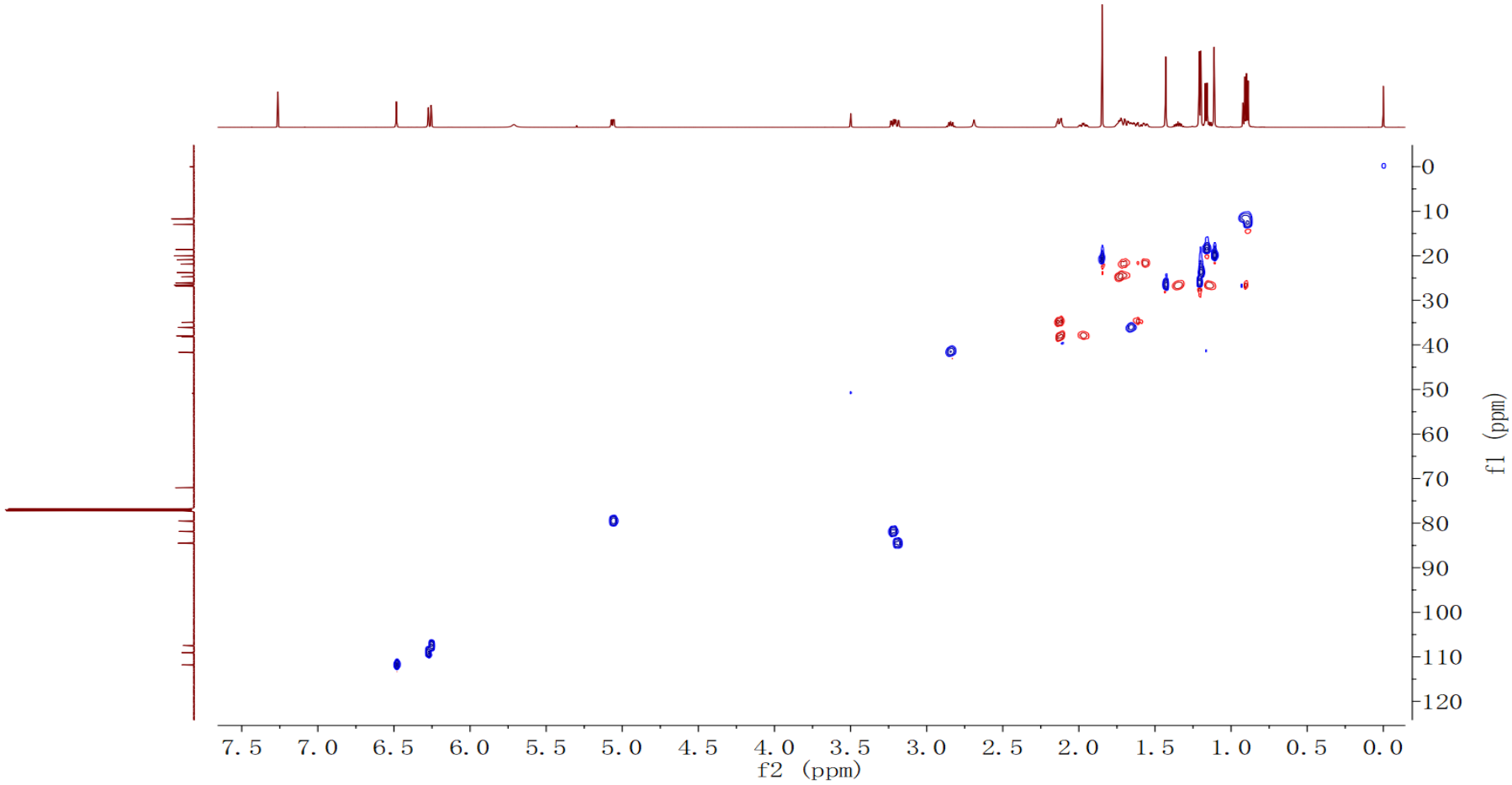


Figure S12. HSQC spectrum of compound **2** (Recorded in $CDCl_3$)

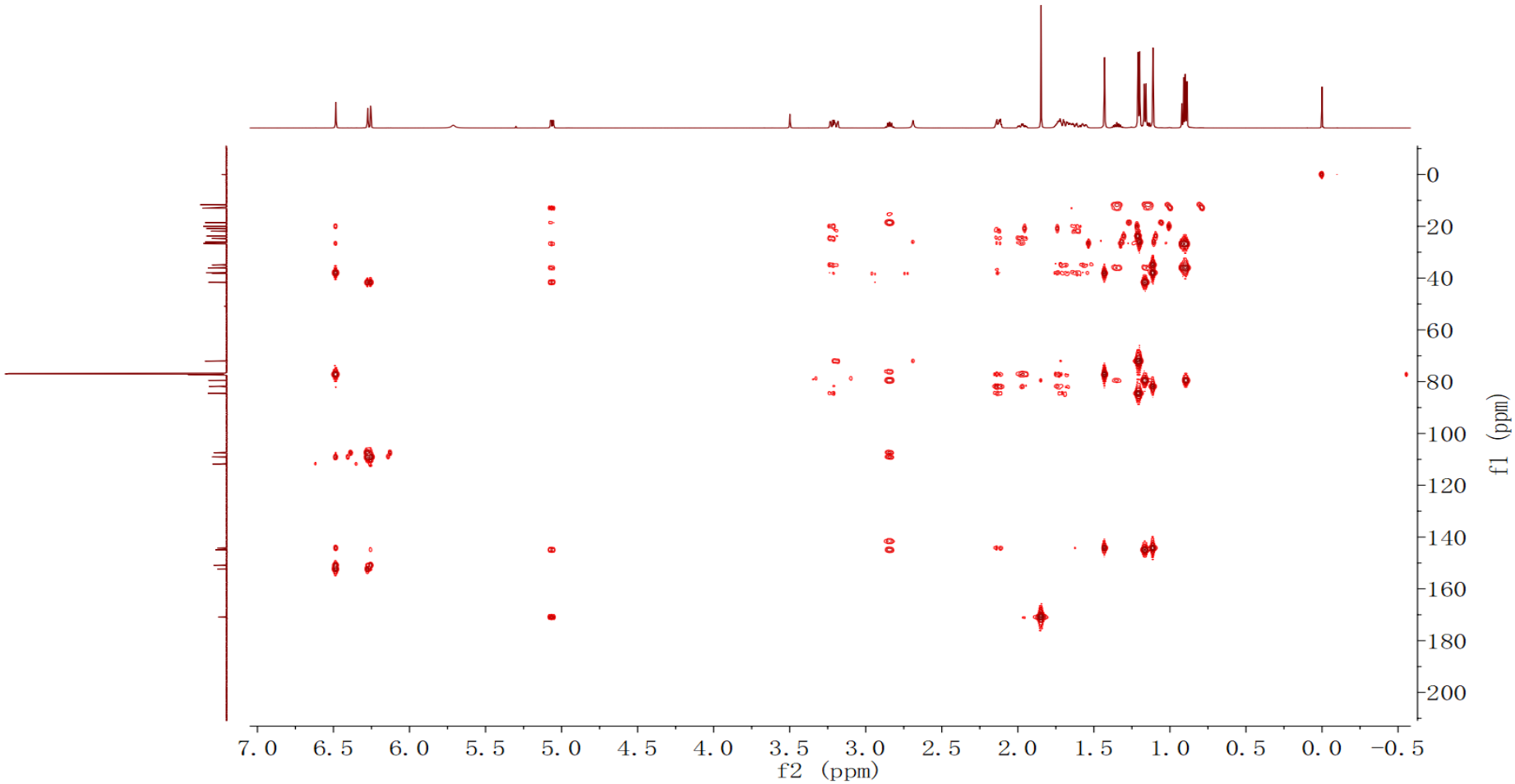


Figure S13. HMBC spectrum of compound **2** (Recorded in $CDCl_3$)

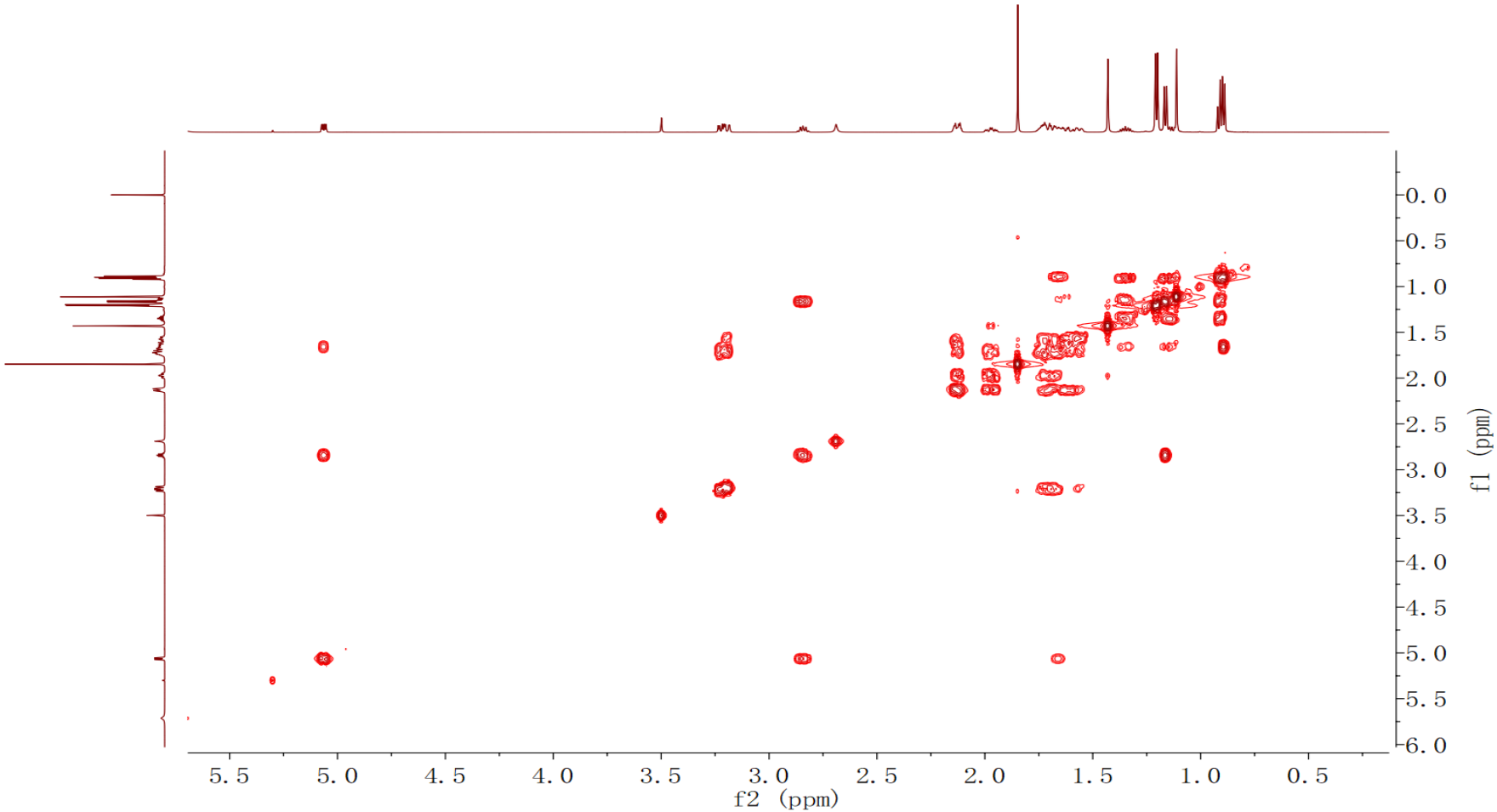


Figure S14. ^{1}H–^{1}H COSY spectrum of compound **2** (Recorded in $CDCl_3$)

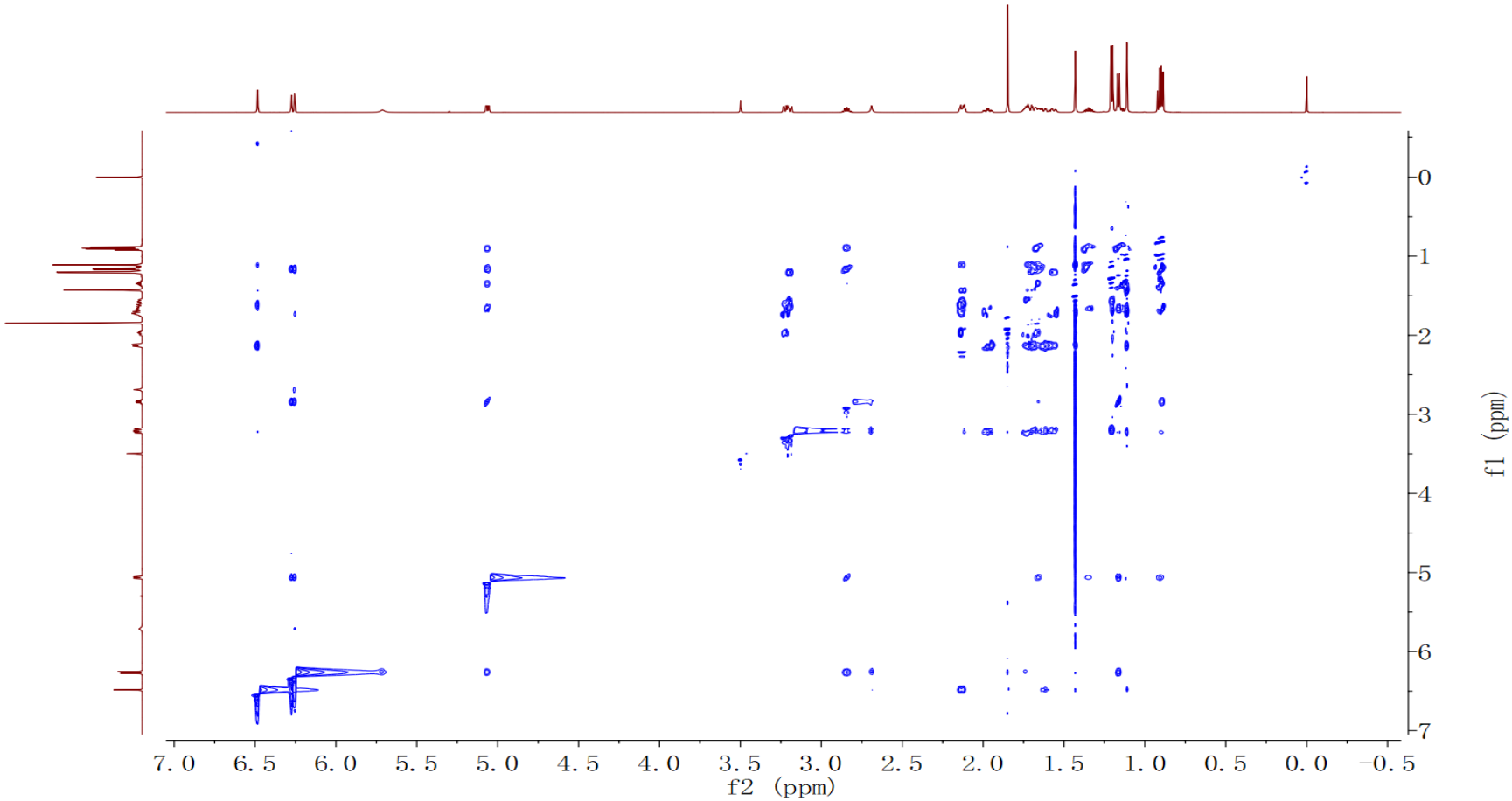


Figure S15. ROESY spectrum of compound **2** (Recorded in $CDCl_3$)

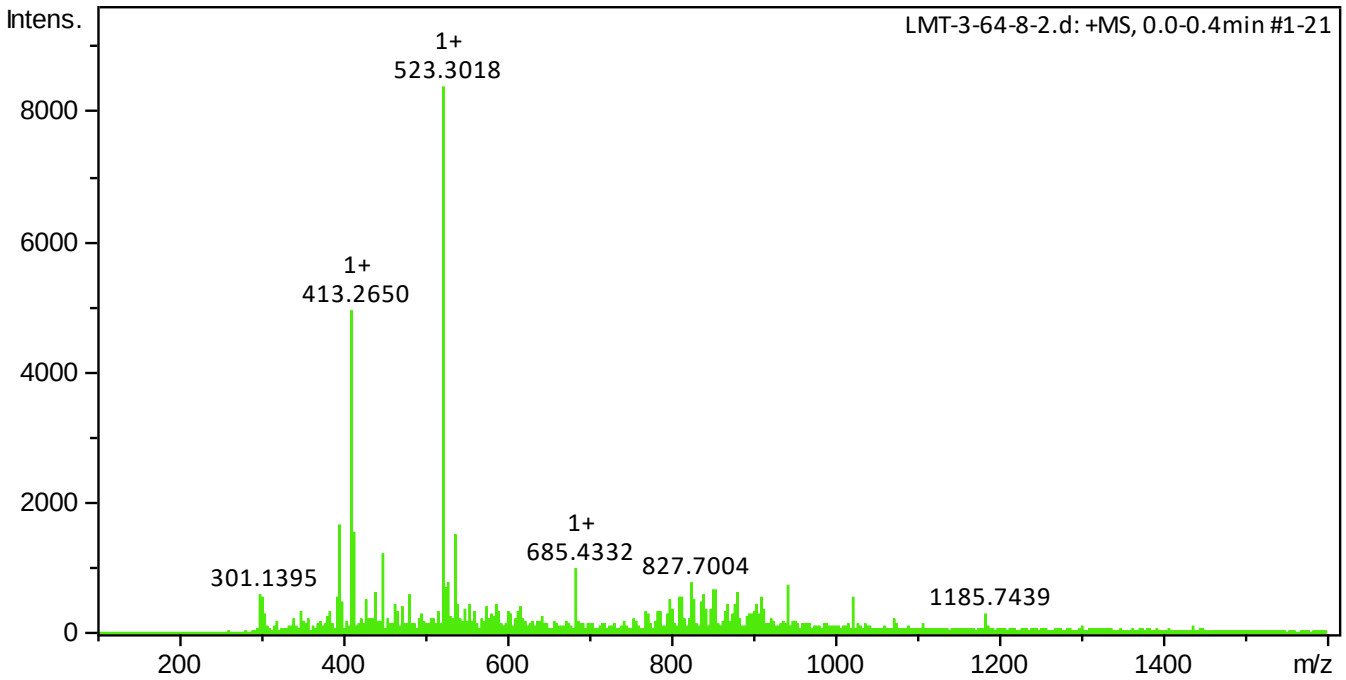
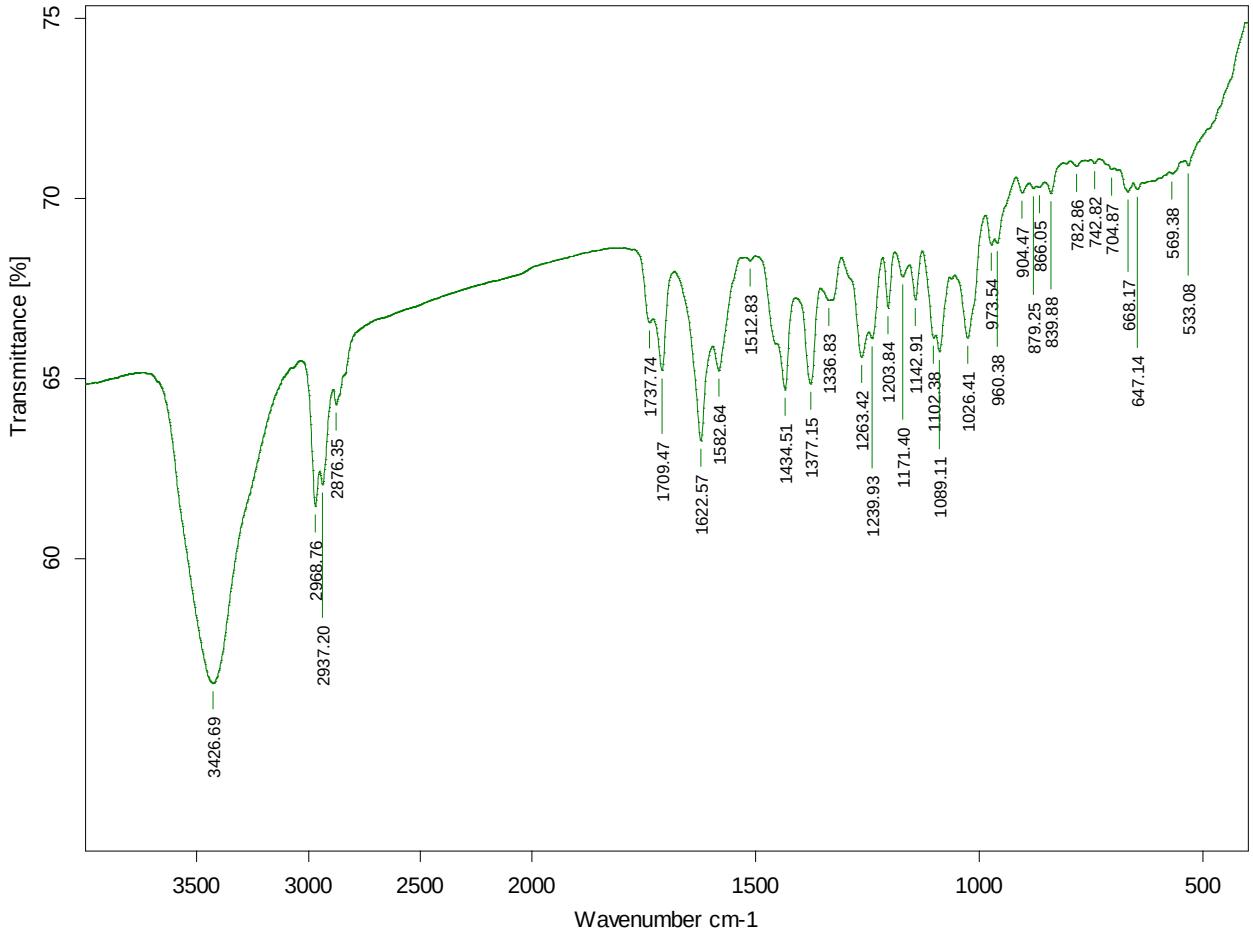


Figure S16. HRESIMS spectrum of compound **2**



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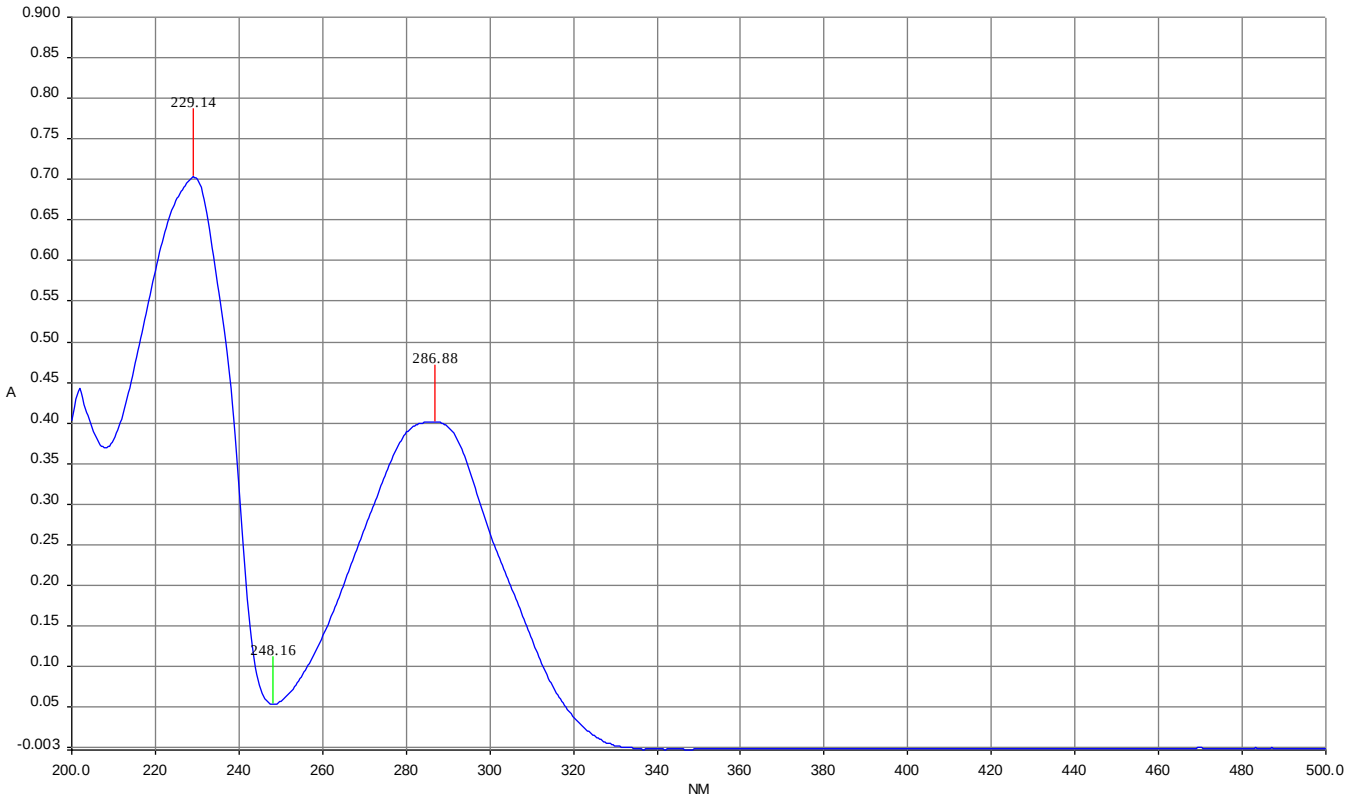

Figure S18. UV spectrum of compound **2**

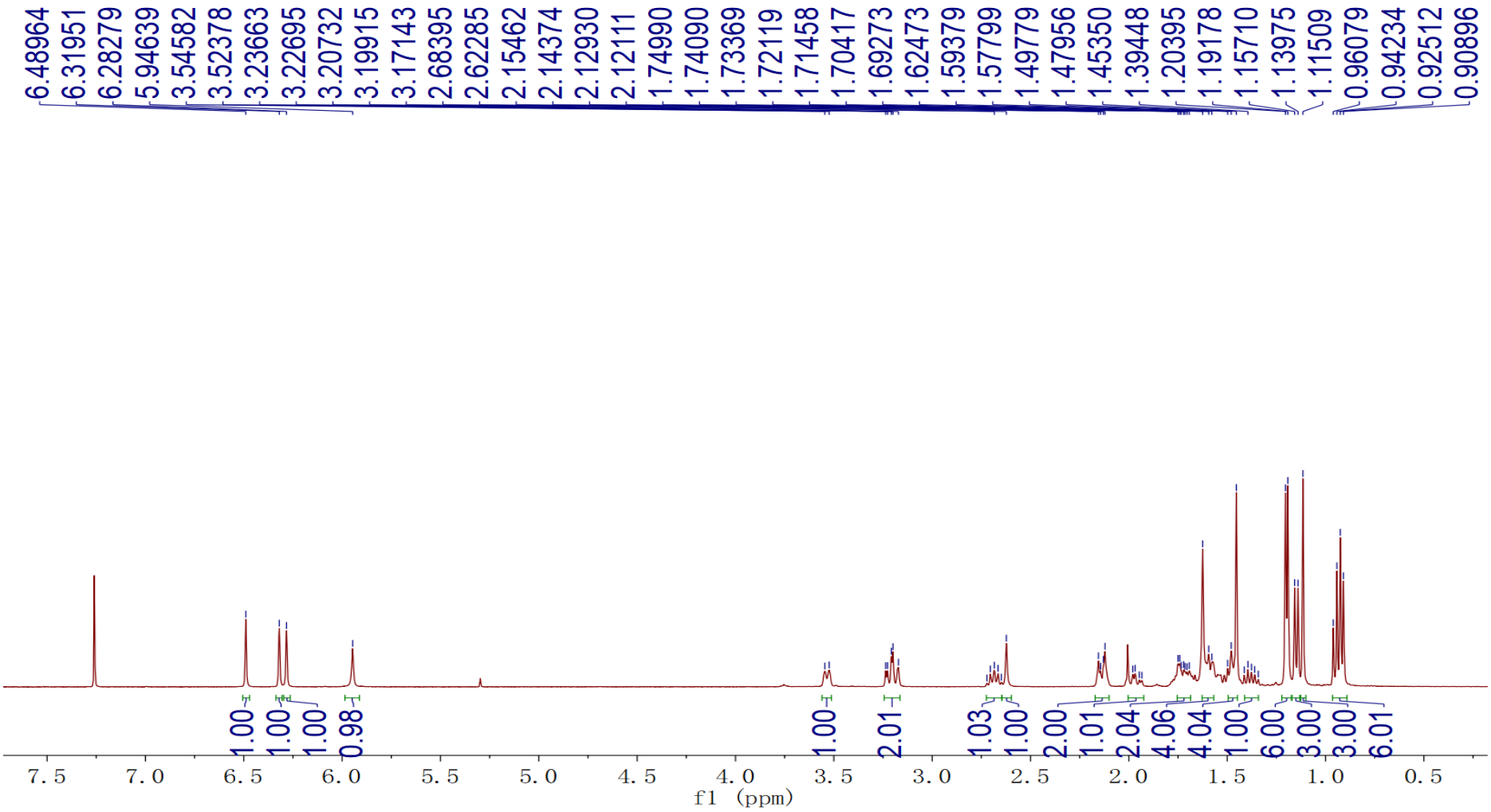

Figure S19. ^{1}H NMR spectrum of compound **3** (Recorded in $CDCl_3$)

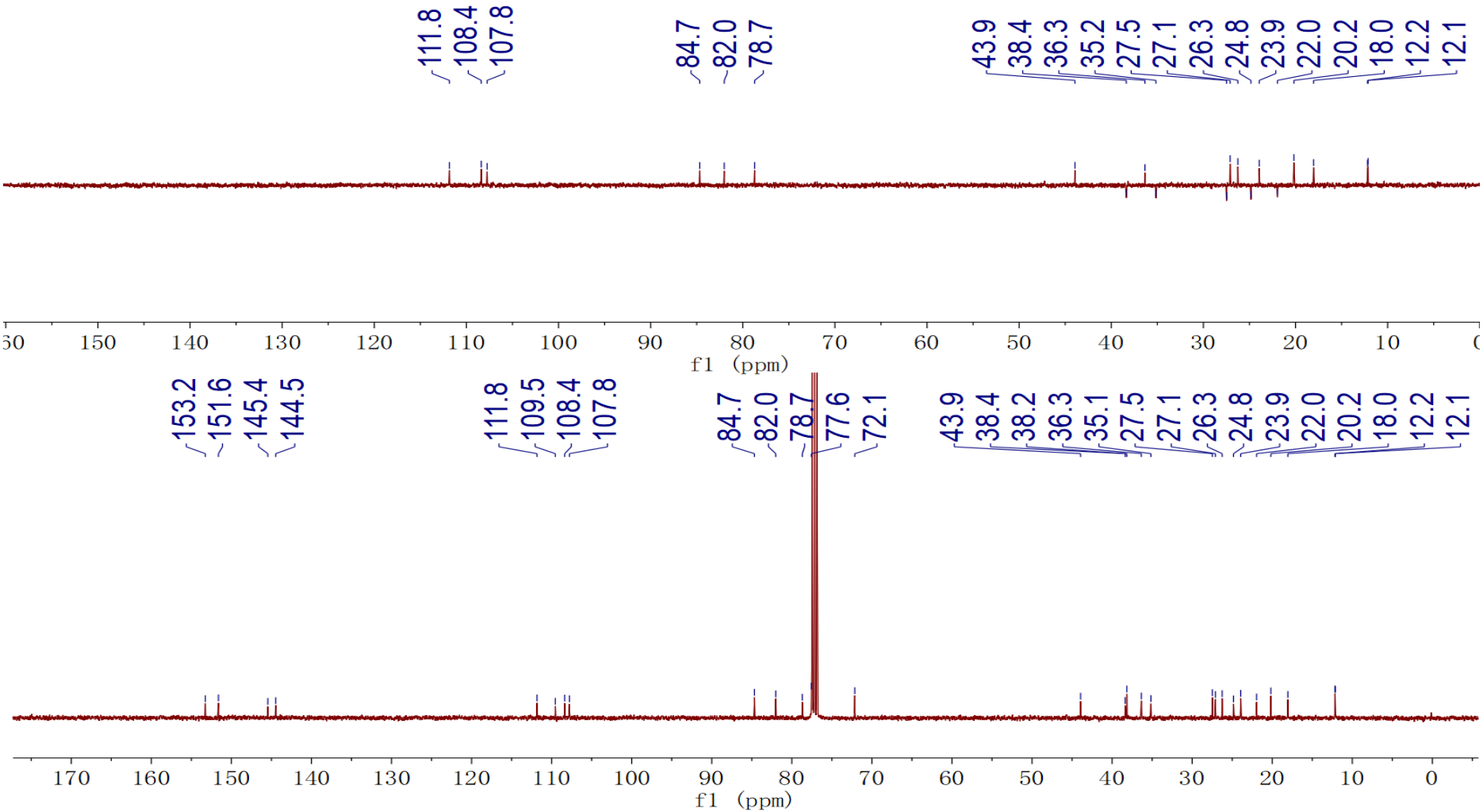

Figure S20. ^{13}C NMR and DEPT spectra of compound **3** (Recorded in $CDCl_3$)

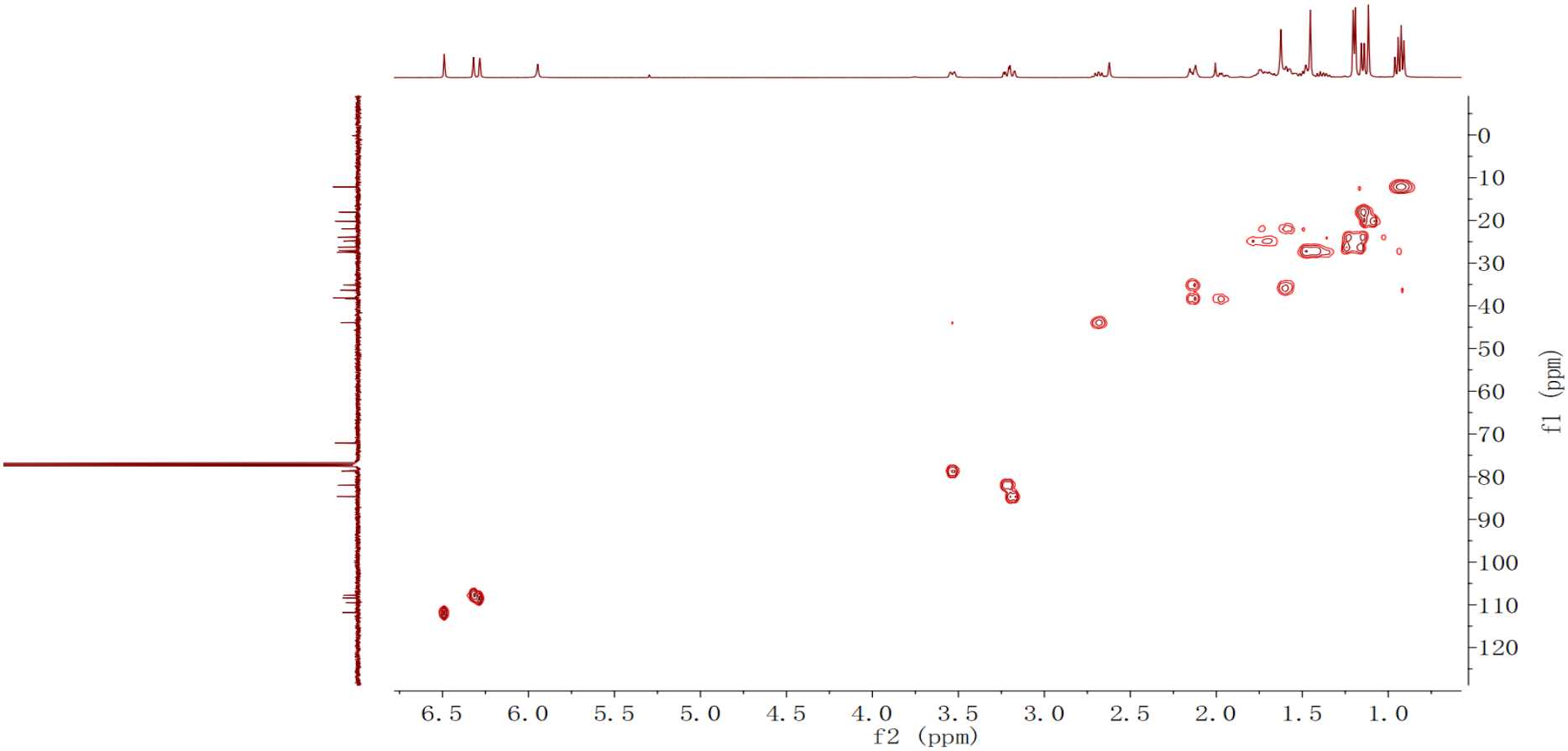

Figure S21. HSQC spectrum of compound **3** (Recorded in $CDCl_3$)

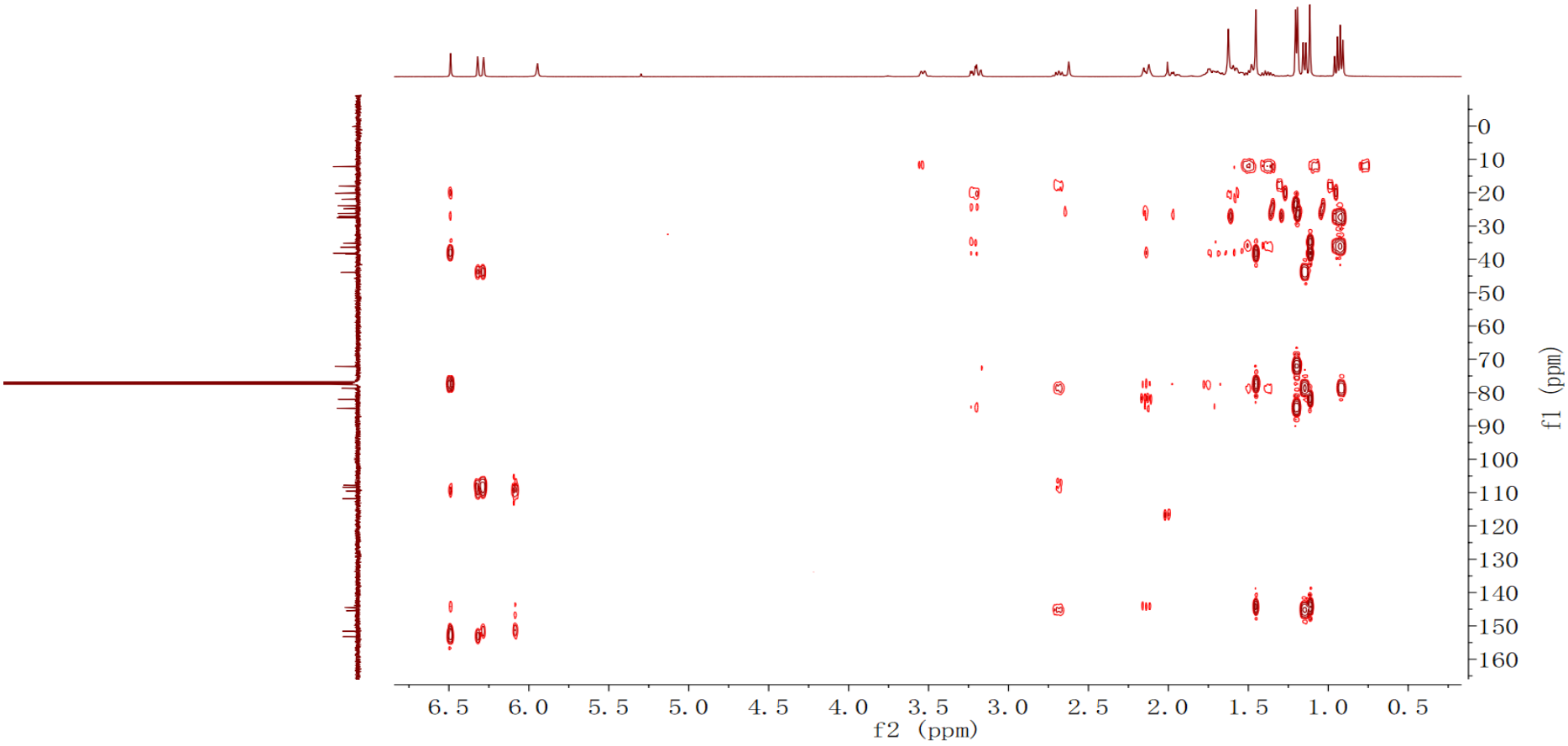

Figure S22. HMBC spectrum of compound **3** (Recorded in $CDCl_3$)

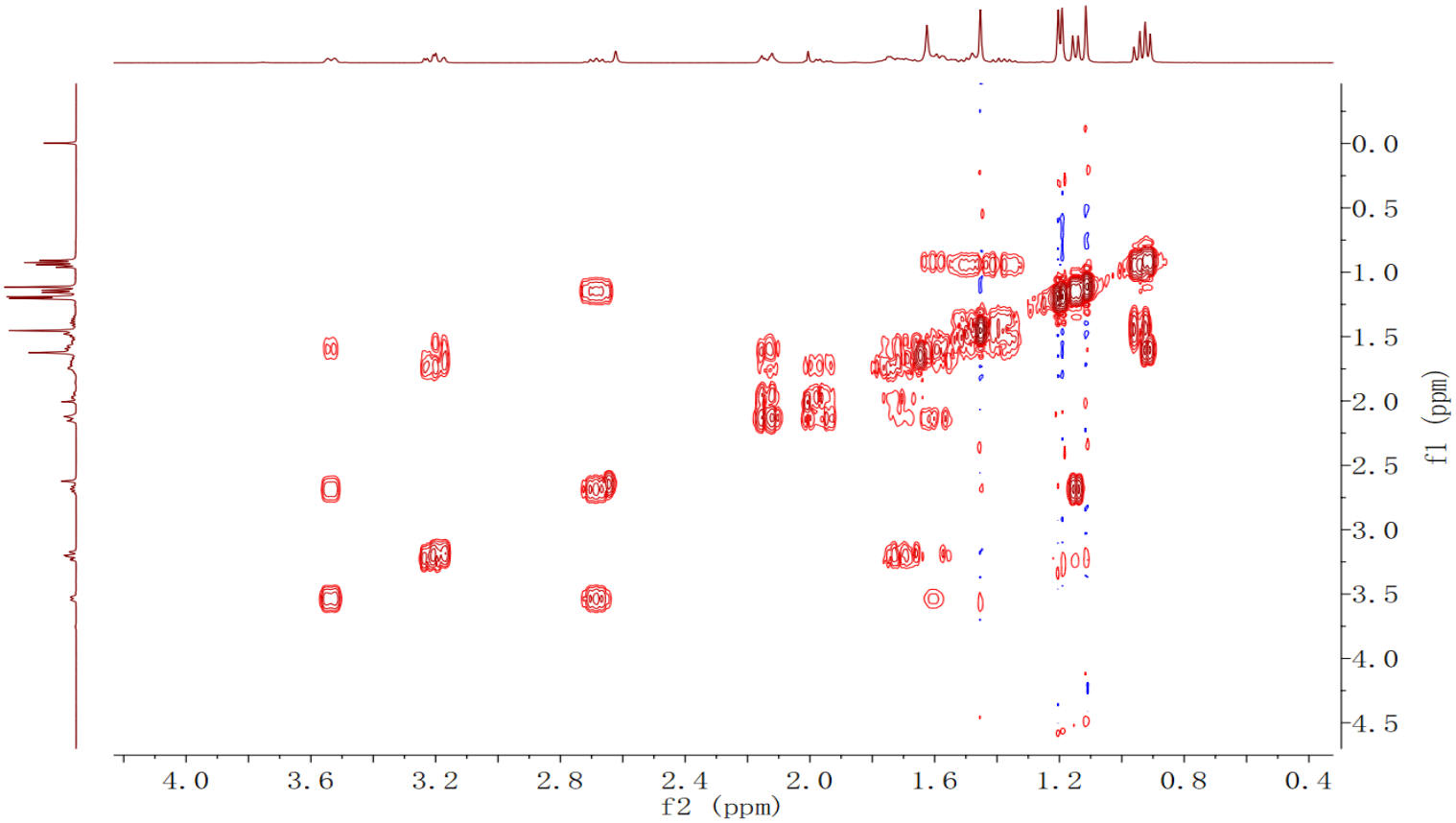

Figure S23. ^{1}H–^{1}H COSY spectrum of compound **3** (Recorded in $CDCl_3$)

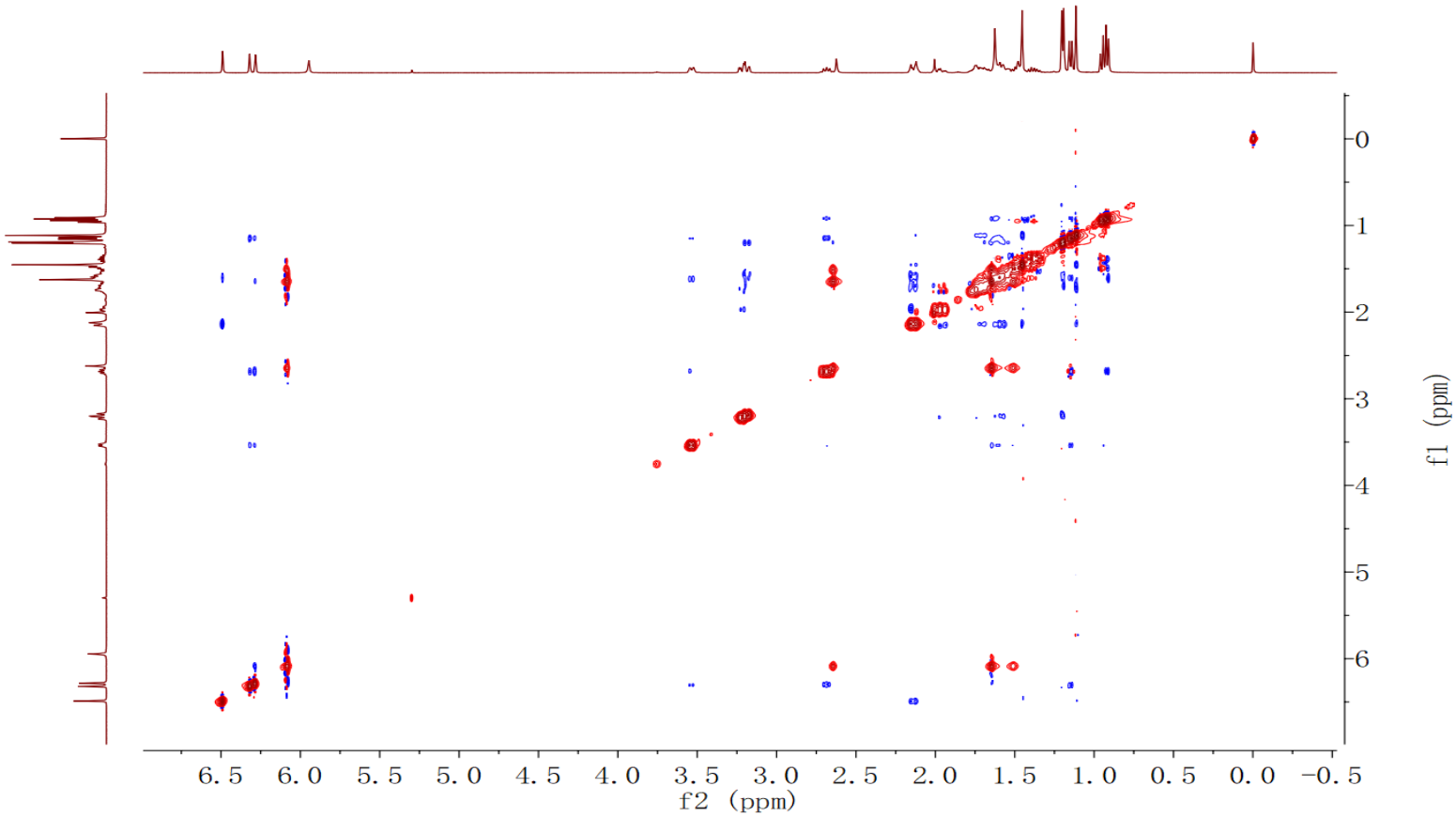

Figure S24. NOESY spectrum of compound **3** (Recorded in $CDCl_3$)

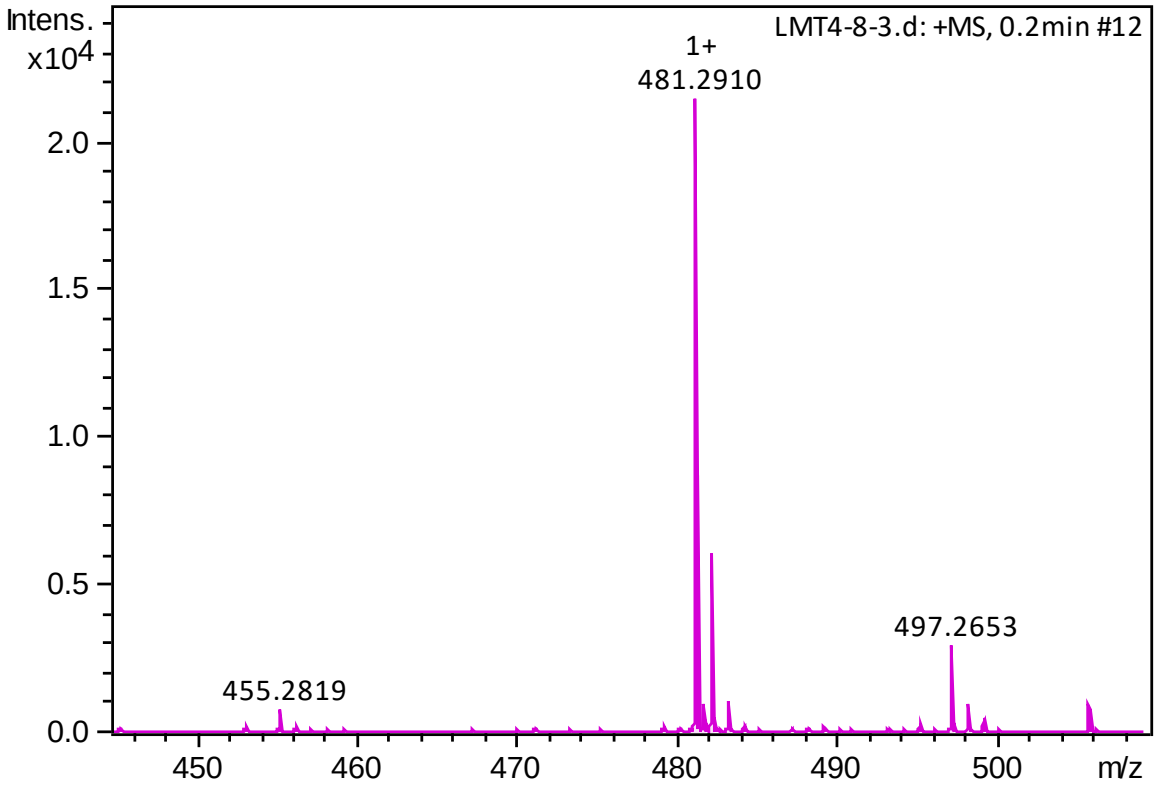

Figure S25. HRESIMS spectrum of compound **3**

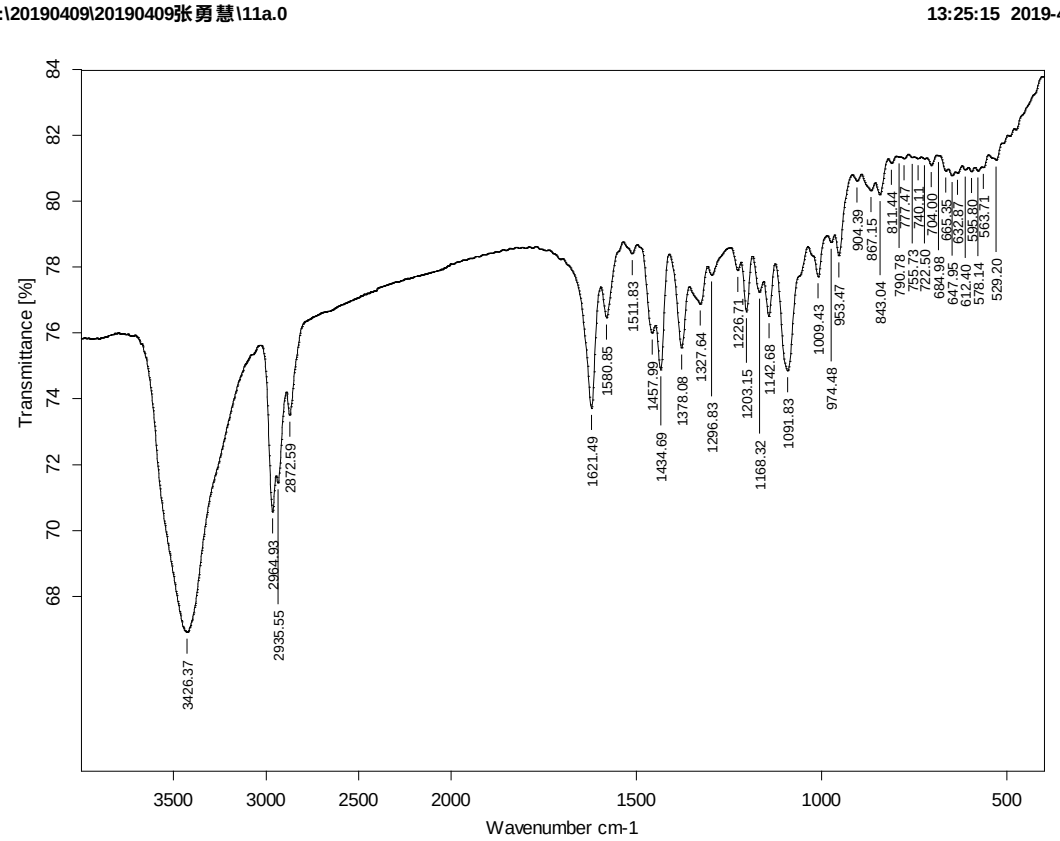

Figure S26. IR spectrum of compound **3**

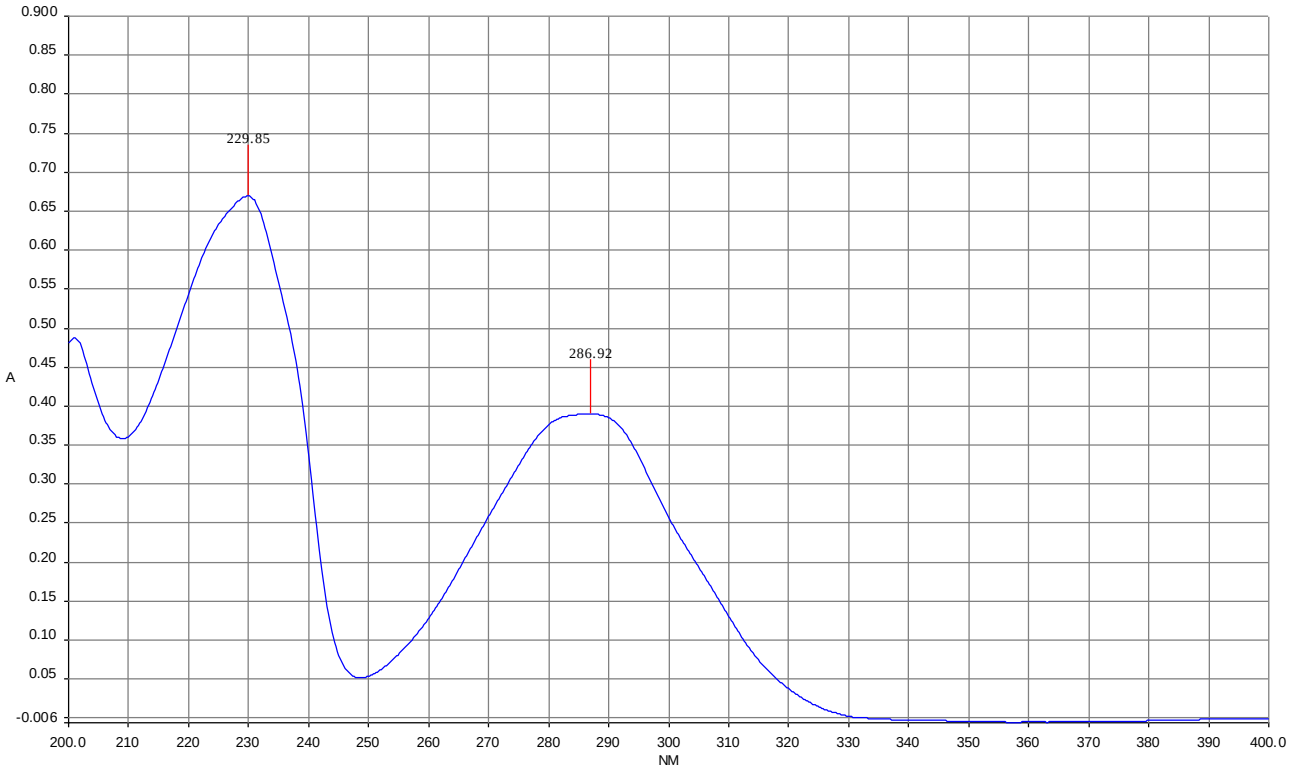

Figure S27. UV spectrum of compound **3**

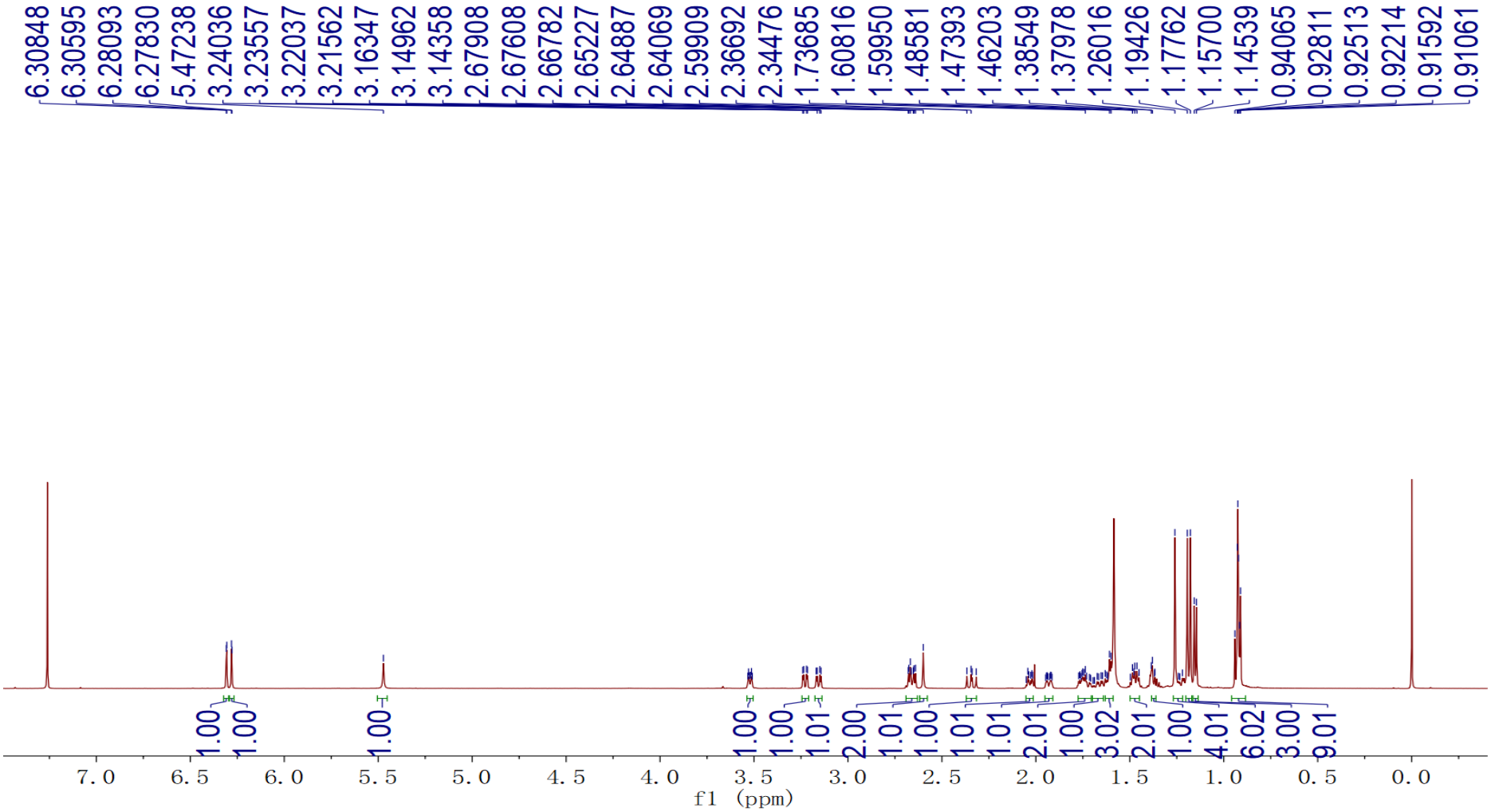

Figure S28. ^{1}H NMR spectrum of compound **4** (Recorded in $CDCl_3$)

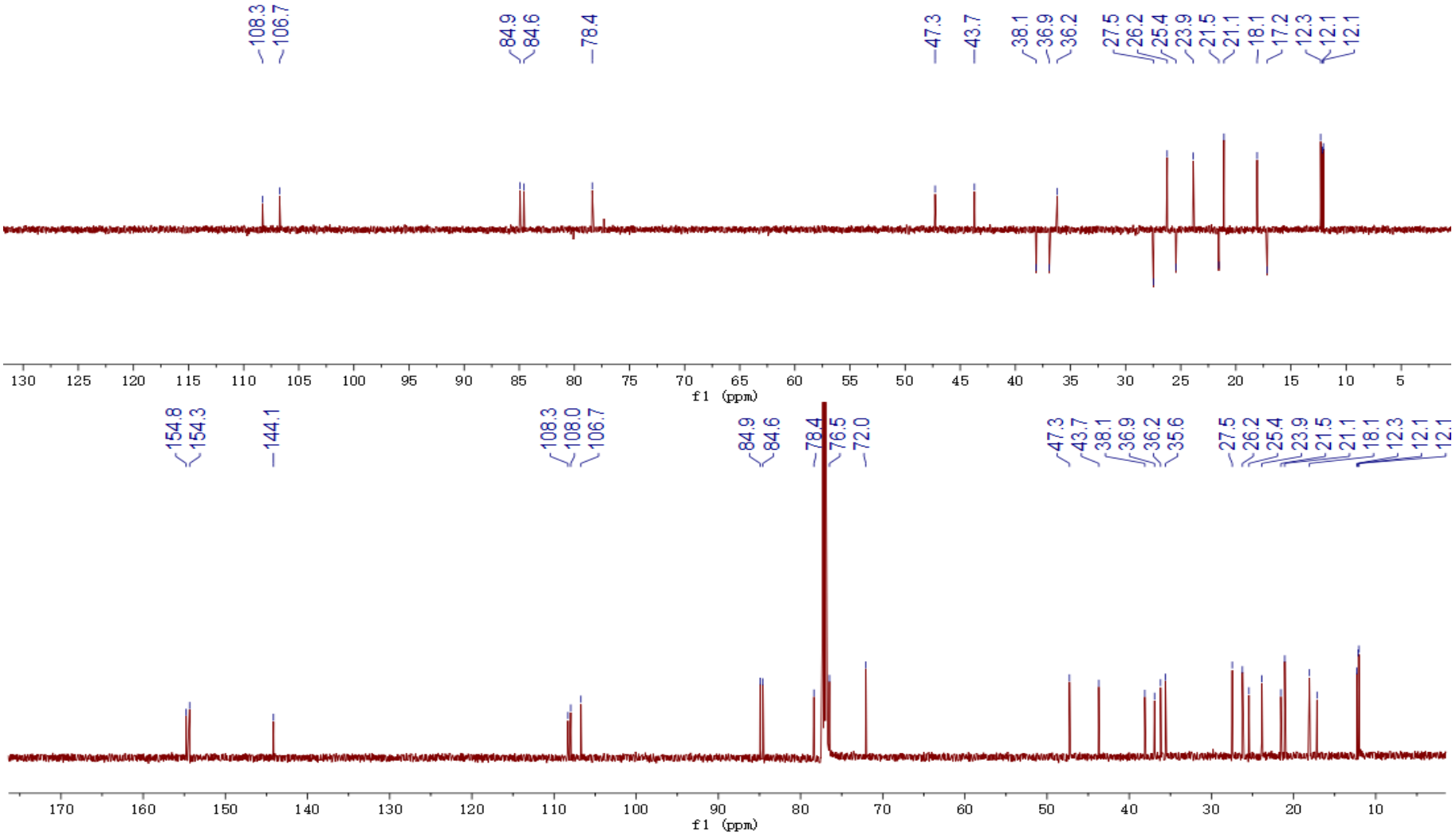

Figure S29. ^{13}C NMR and DEPT spectra of compound **4** (Recorded in $CDCl_3$)

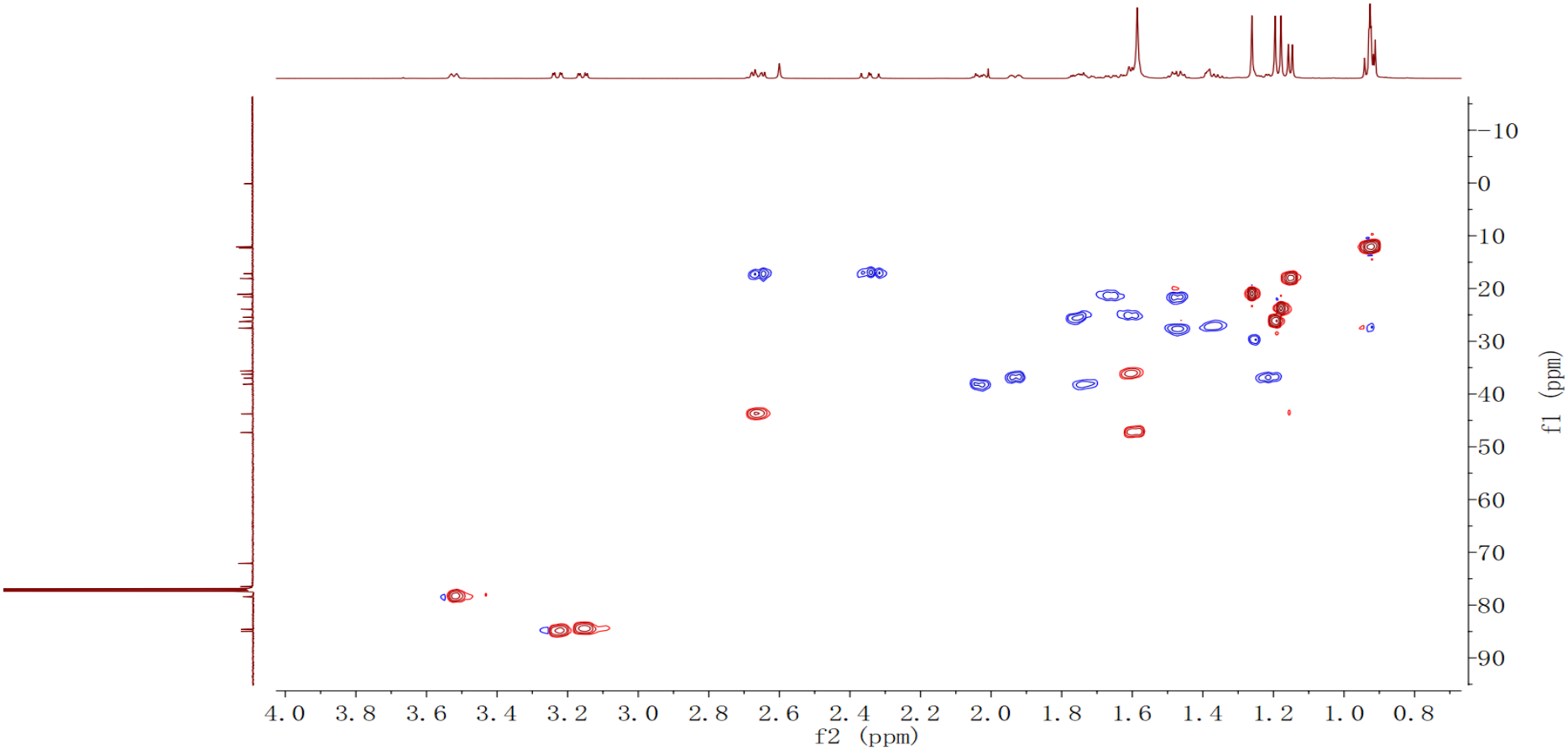

Figure S30. HSQC spectrum of compound **4** (Recorded in $CDCl_3$)

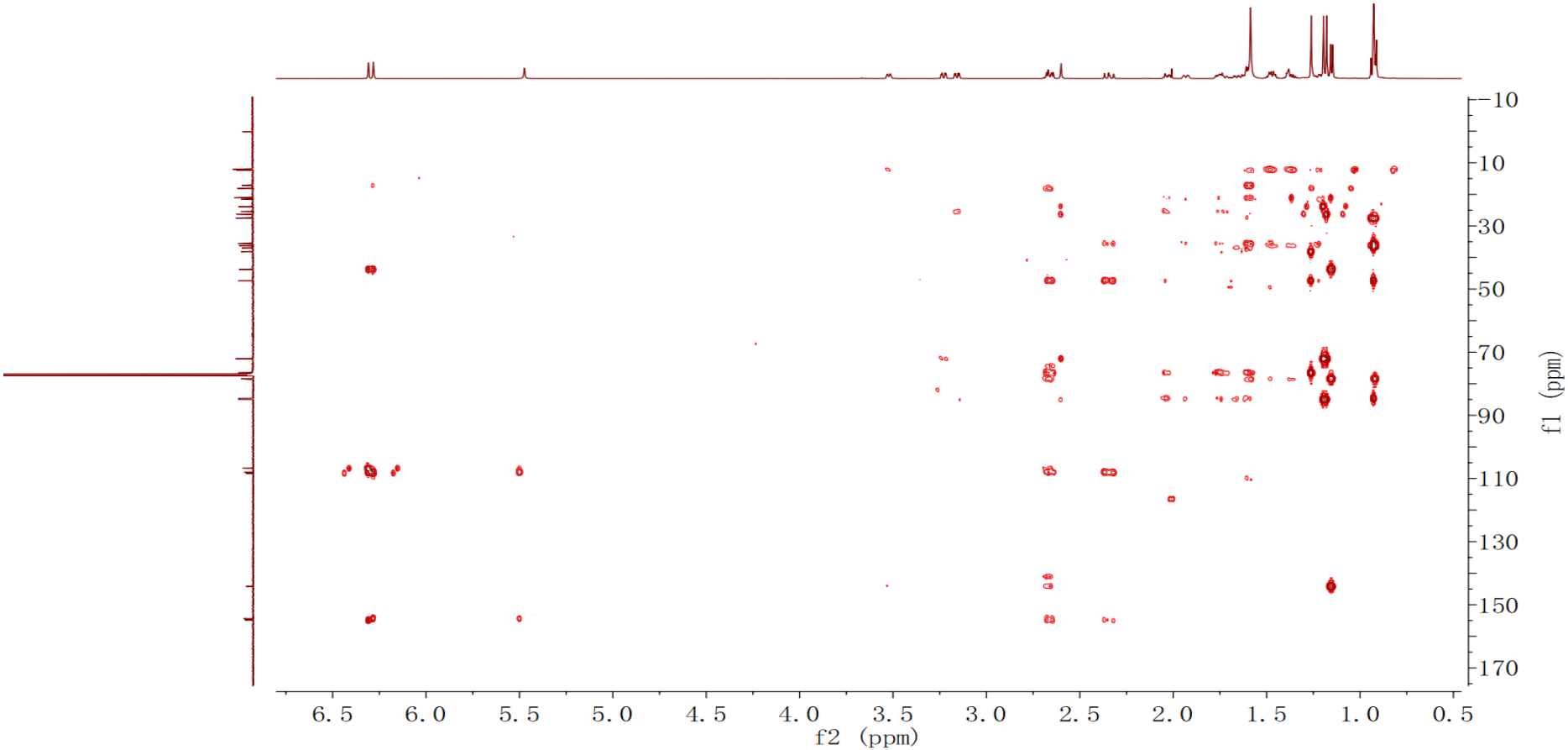

Figure S31. HMBC spectrum of compound **4** (Recorded in $CDCl_3$)

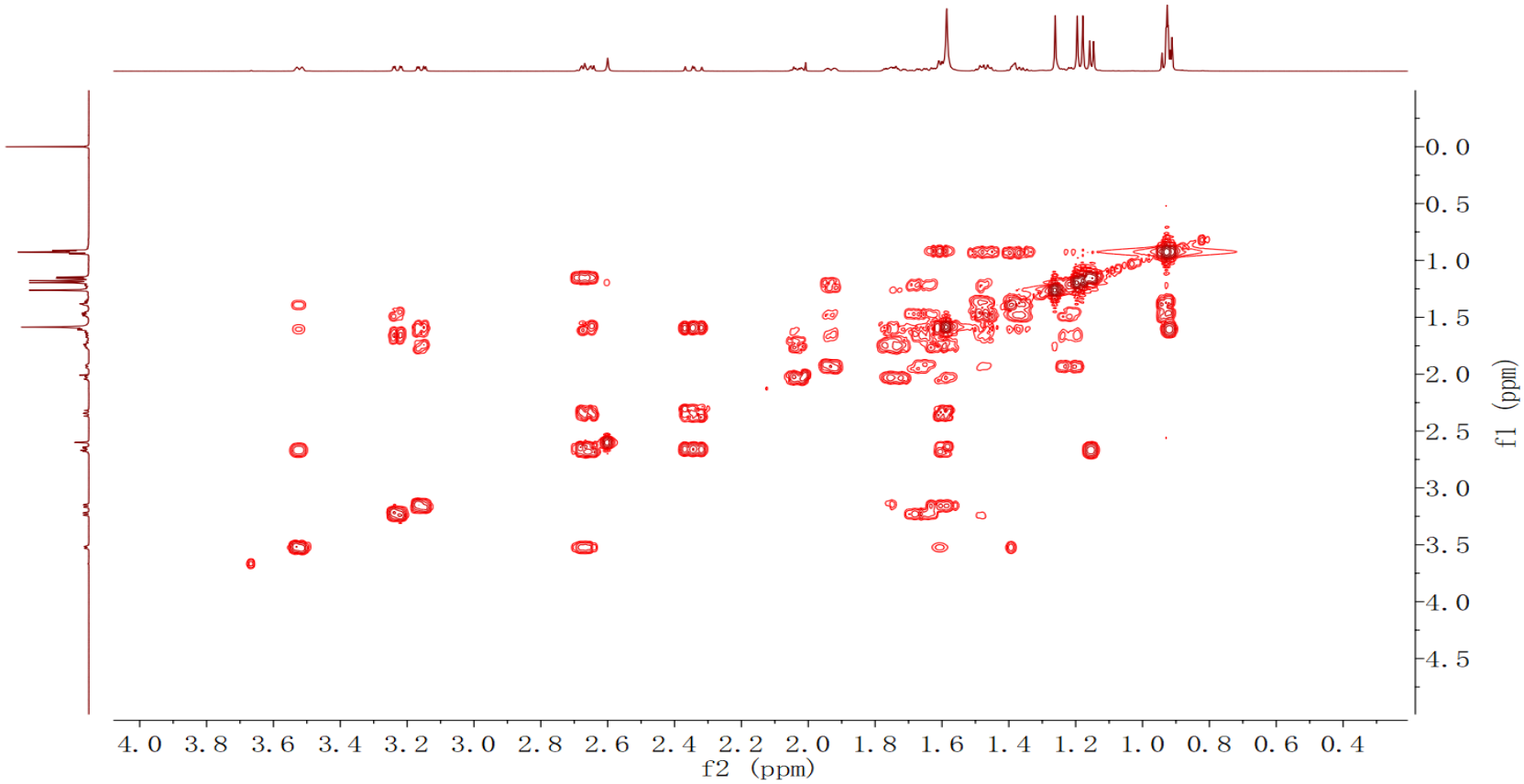

Figure S32. ^{1}H–^{1}H COSY spectrum of compound **4** (Recorded in $CDCl_3$)

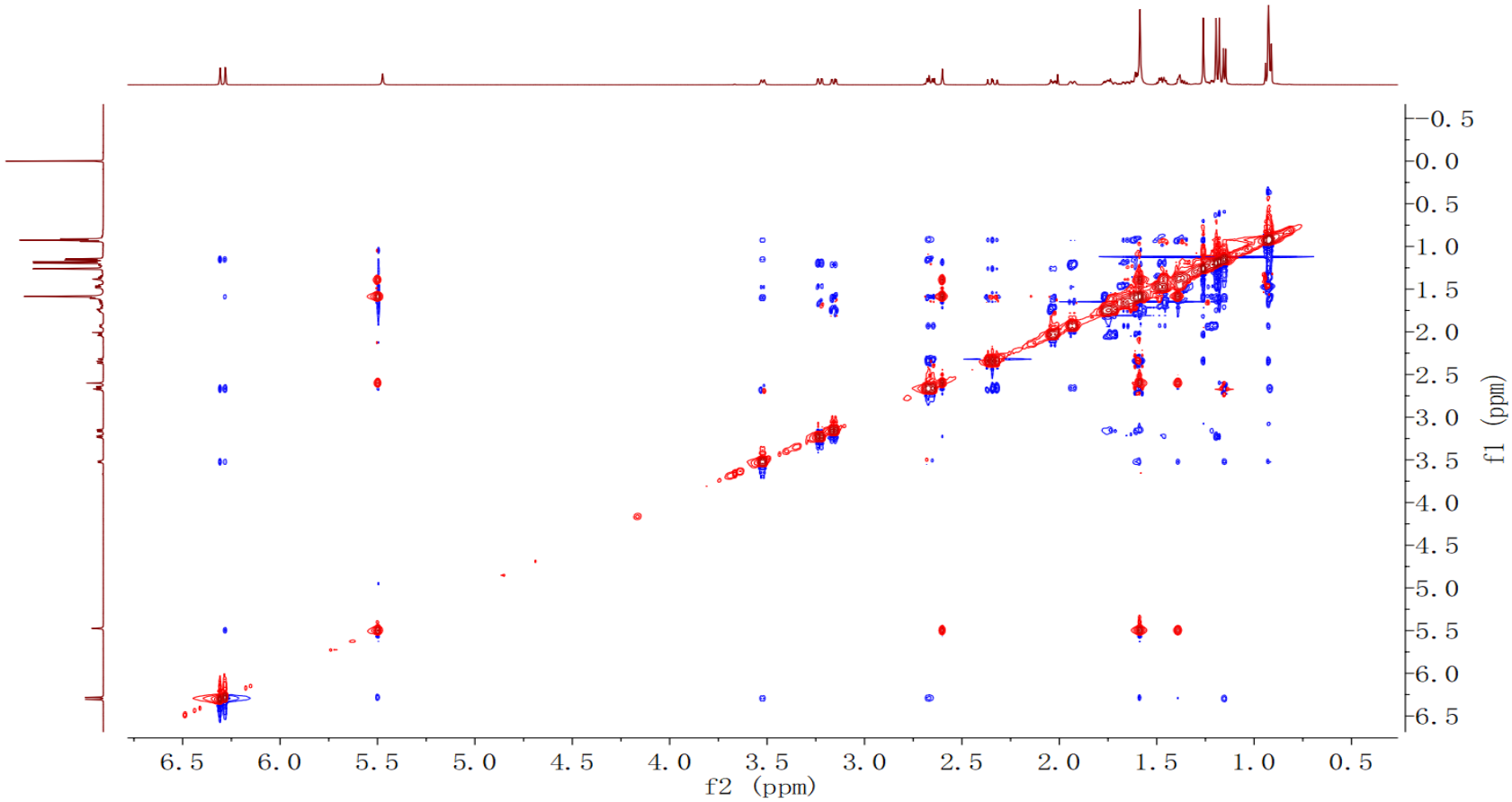

Figure S33. ROESY spectrum of compound **4** (Recorded in $CDCl_3$)

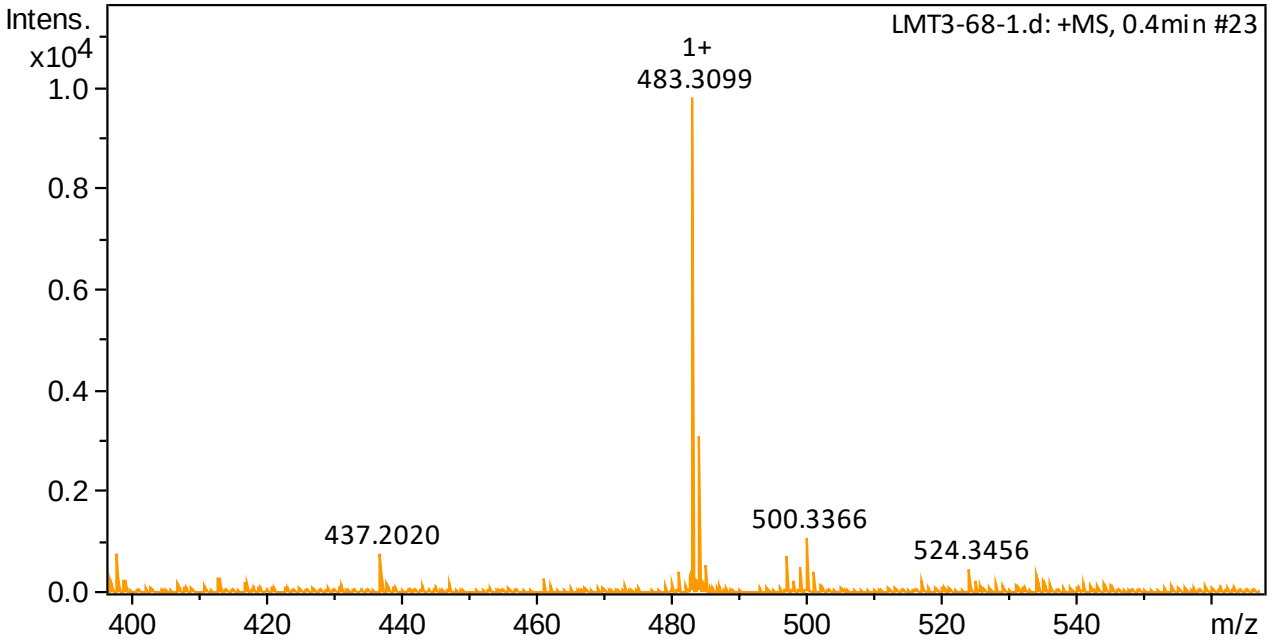

Figure S34. HRESIMS spectrum of compound **4**

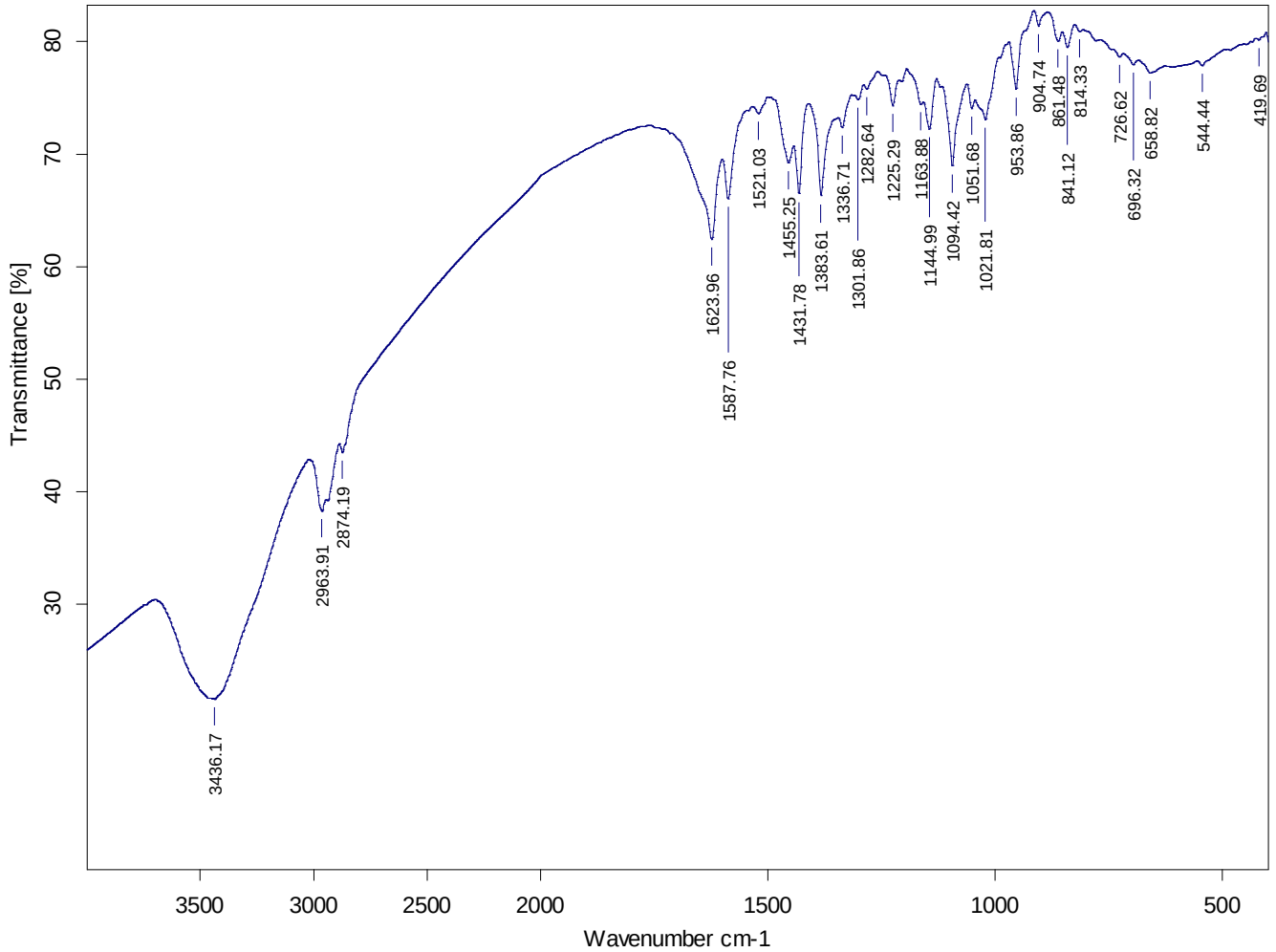

Figure S35. IR spectrum of compound **4**

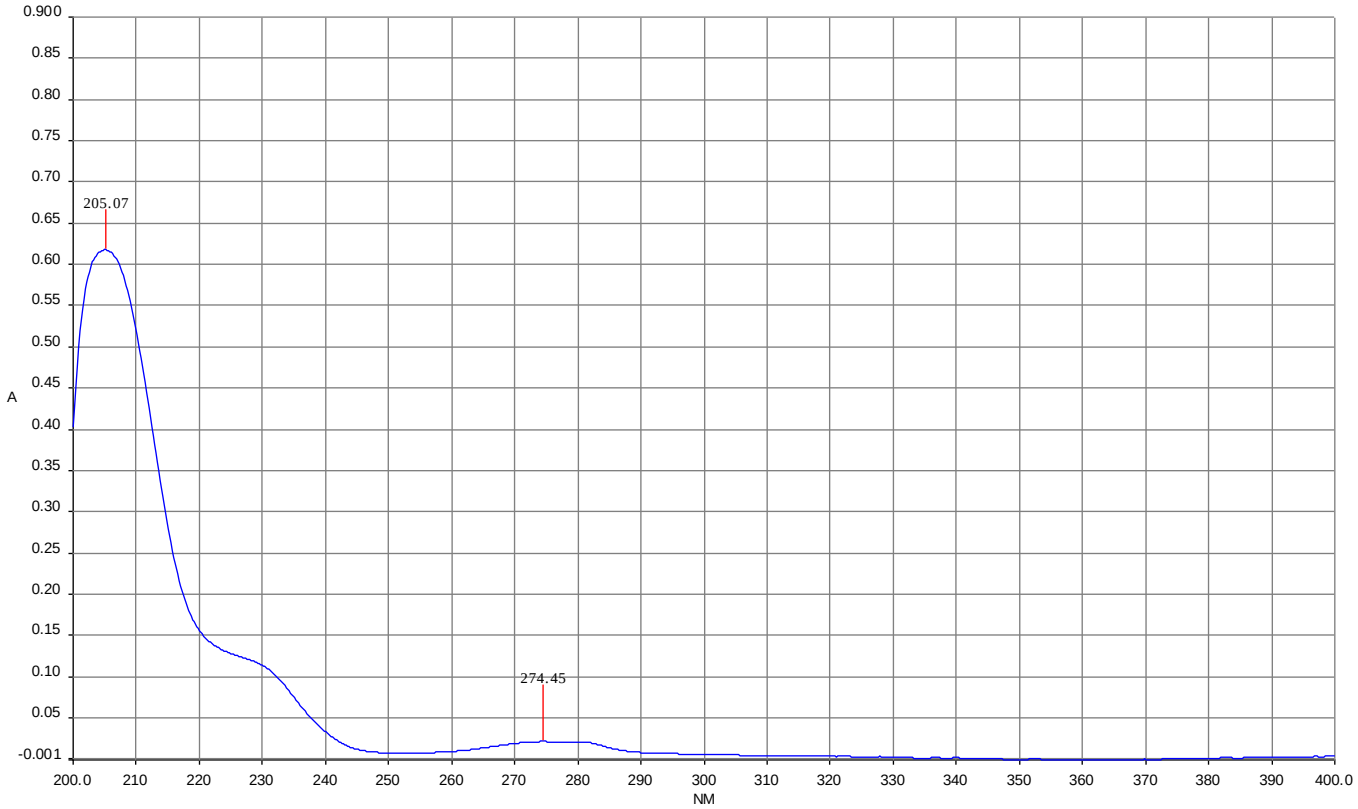

Figure S36. UV spectrum of compound **4**

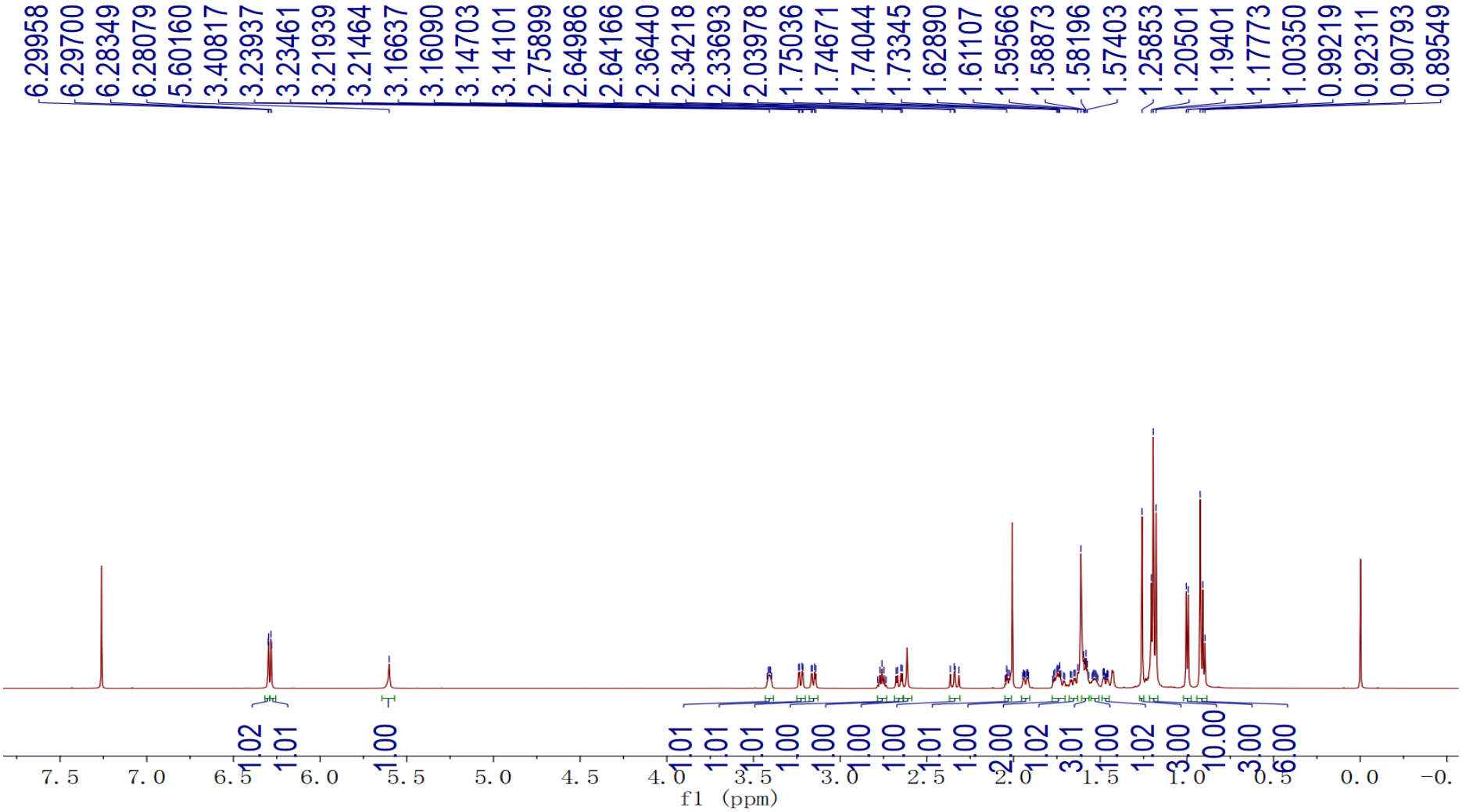

Figure S37. ^{1}H NMR spectrum of compound **5** (Recorded in $CDCl_3$)

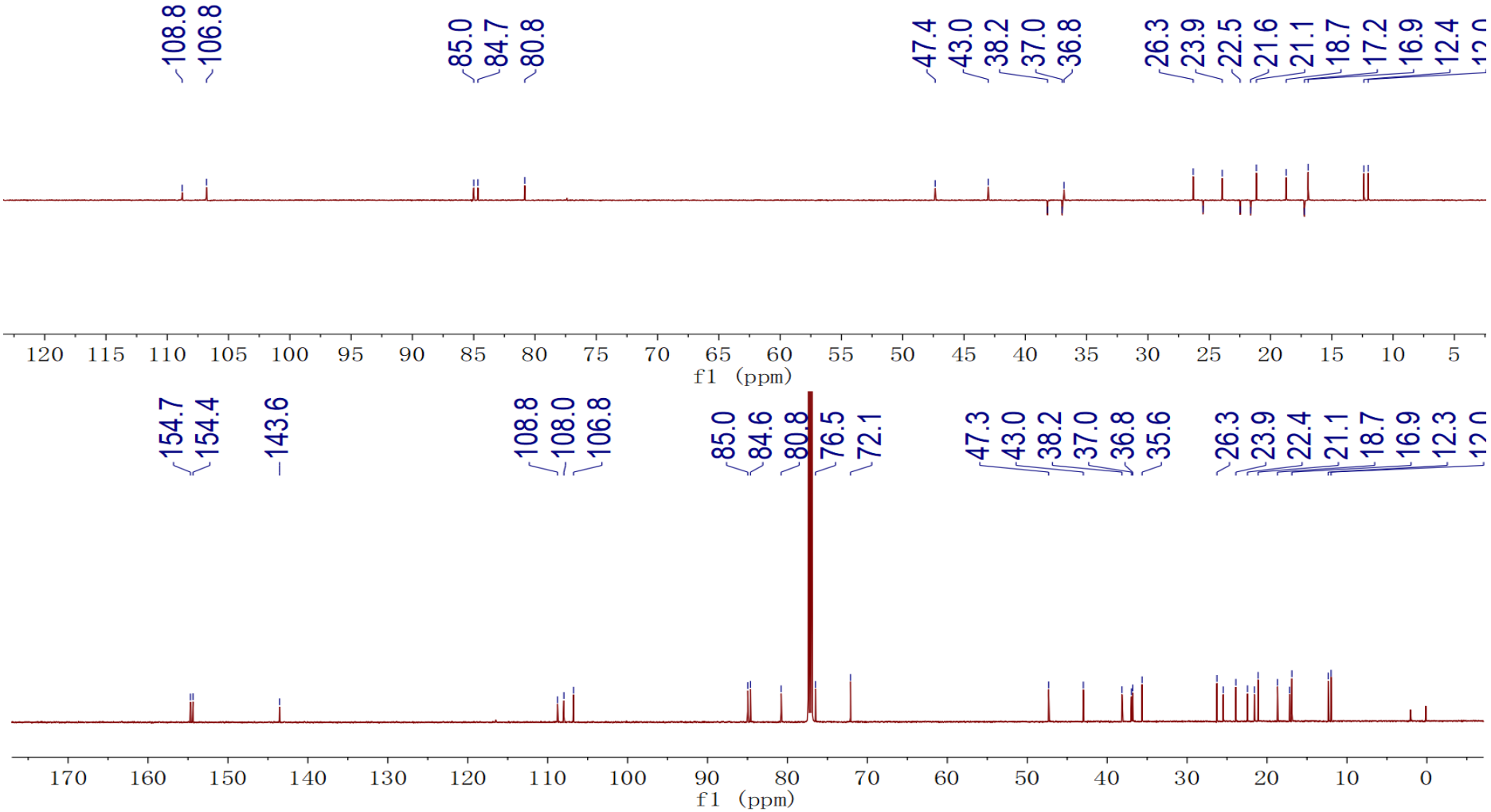

Figure S38. ^{13}C NMR and DEPT spectra of compound **5** (Recorded in $CDCl_3$)

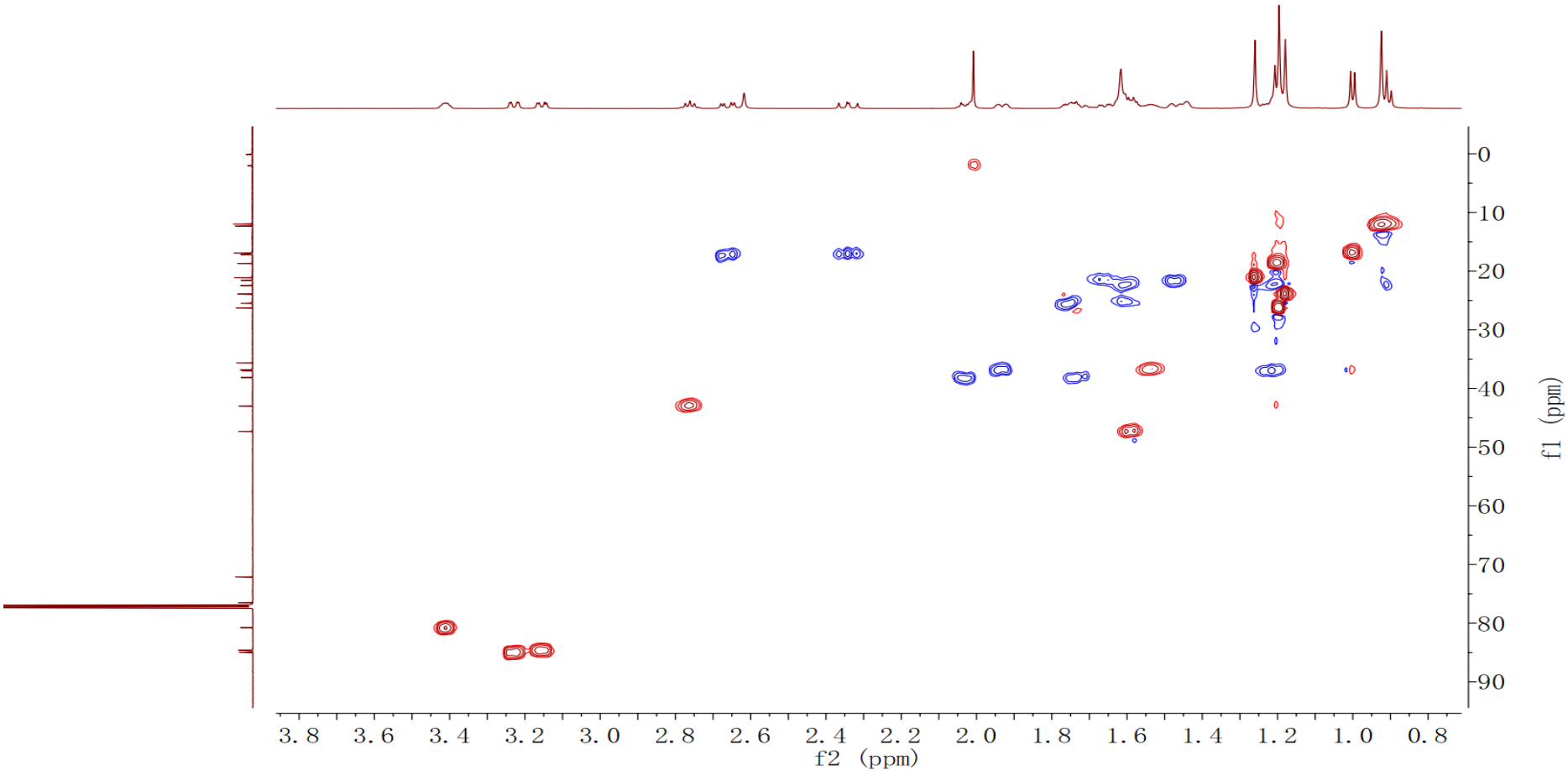

Figure S39. HSQC spectrum of compound **5** (Recorded in $CDCl_3$)

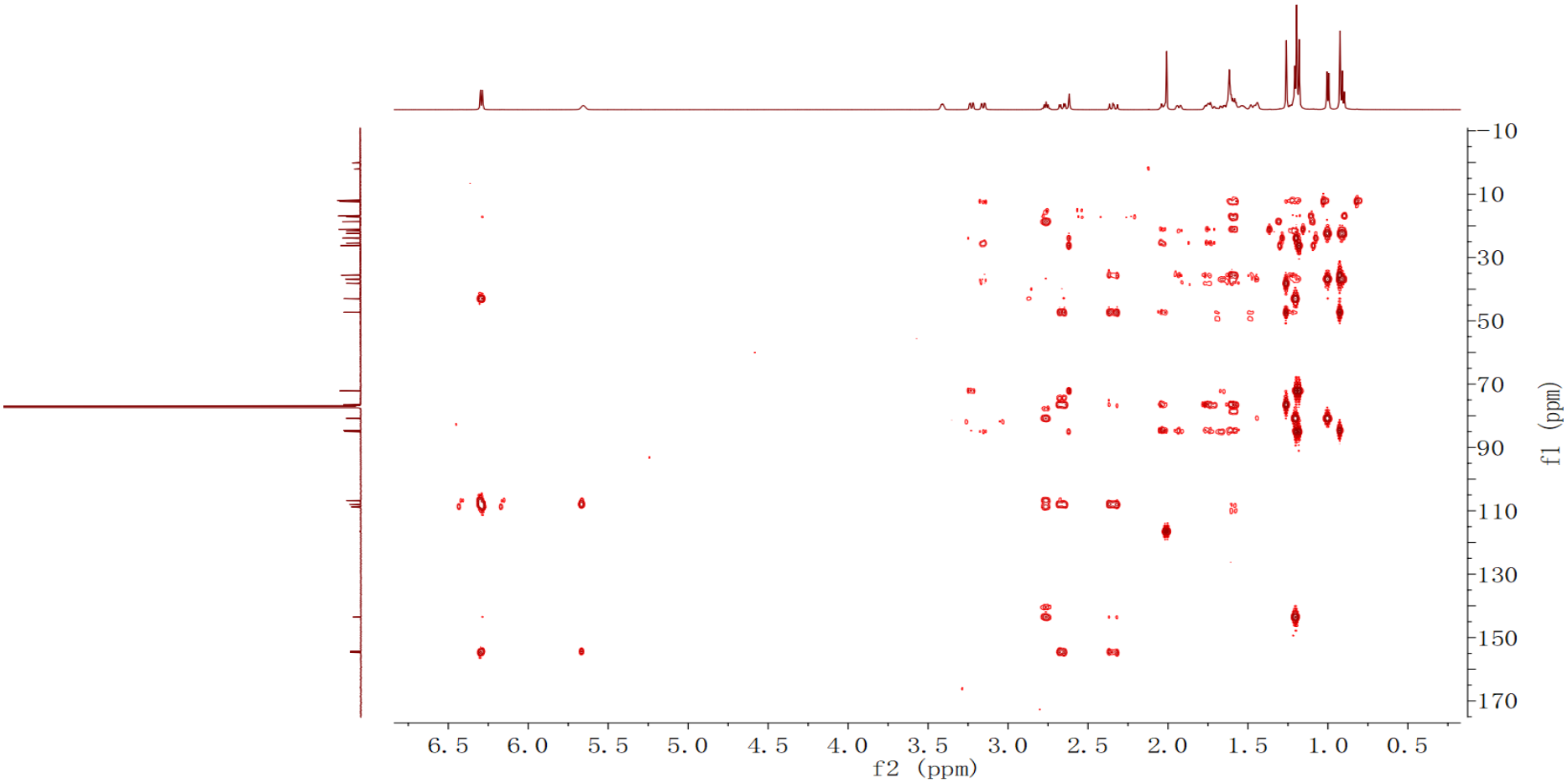

Figure S40. HMBC spectrum of compound **5** (Recorded in $CDCl_3$)

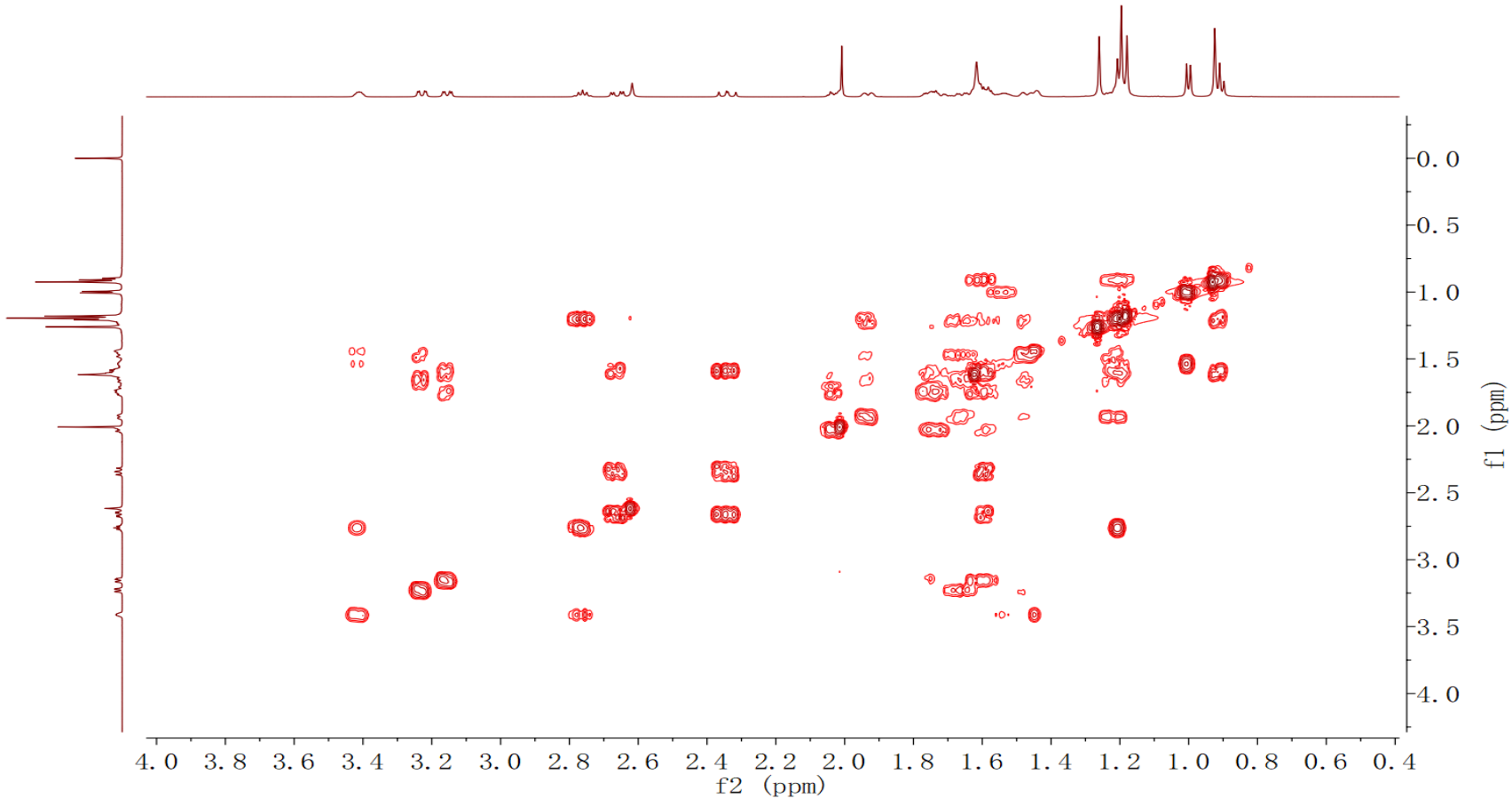

Figure S41. ^{1}H–^{1}H COSY spectrum of compound **5** (Recorded in $CDCl_3$)

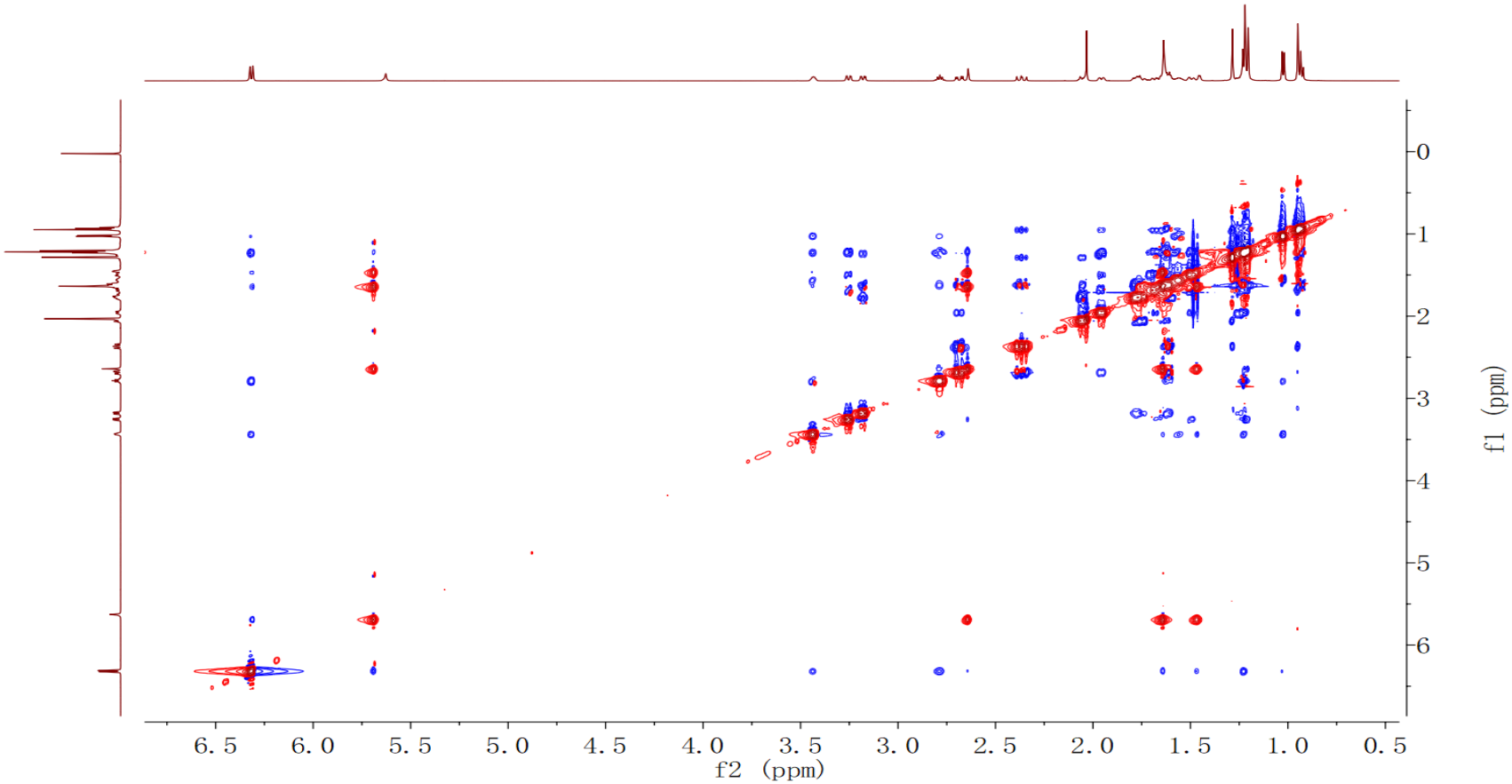

Figure S42. ROESY spectrum of compound **5** (Recorded in $CDCl_3$)

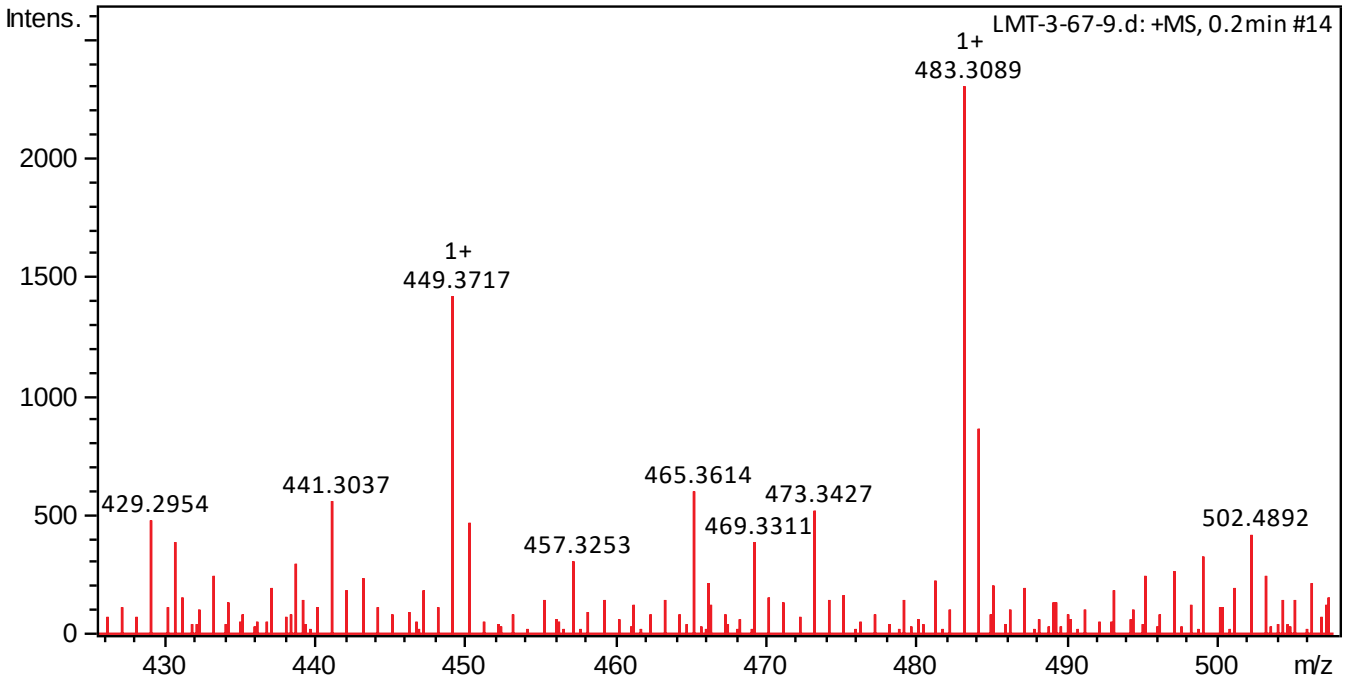

Figure S43. HRESIMS spectrum of compound **5**

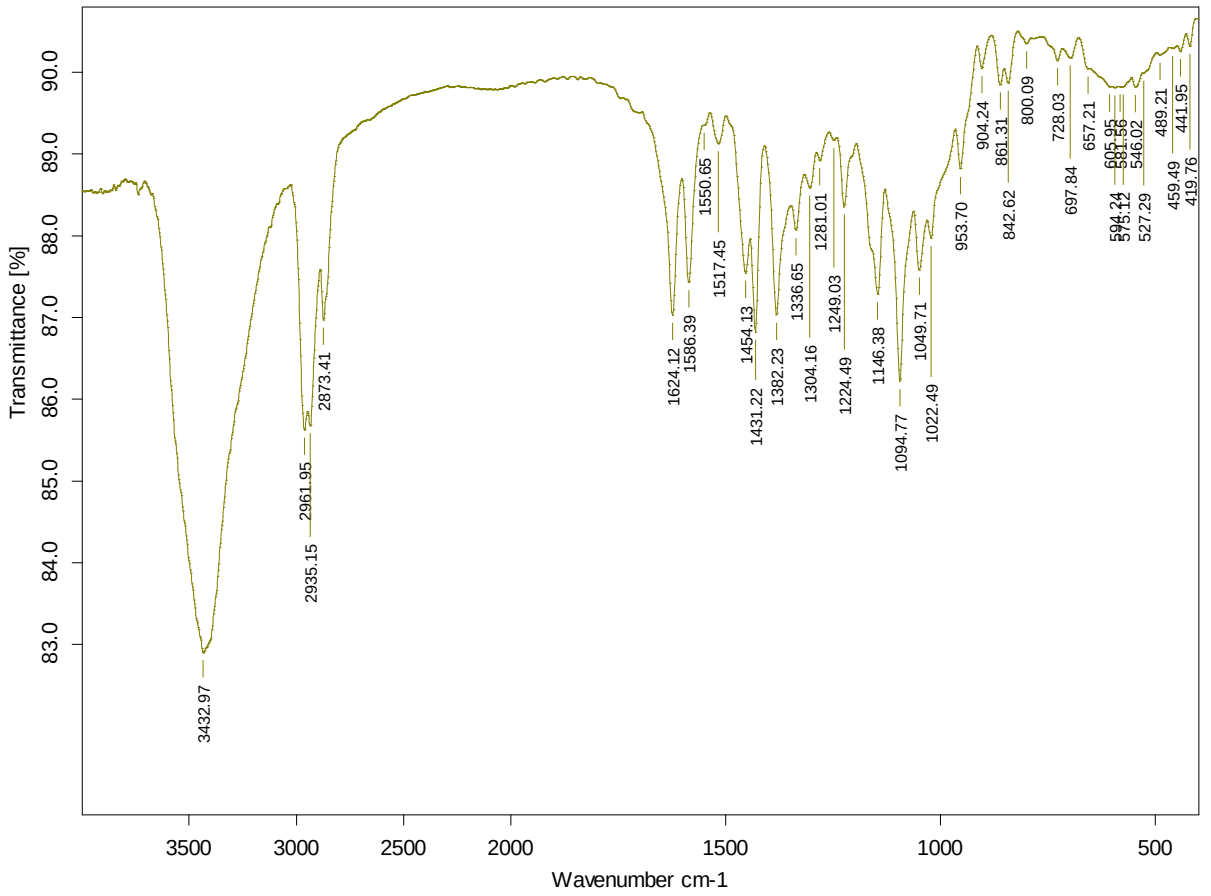

Figure S44. IR spectrum of compound **5**

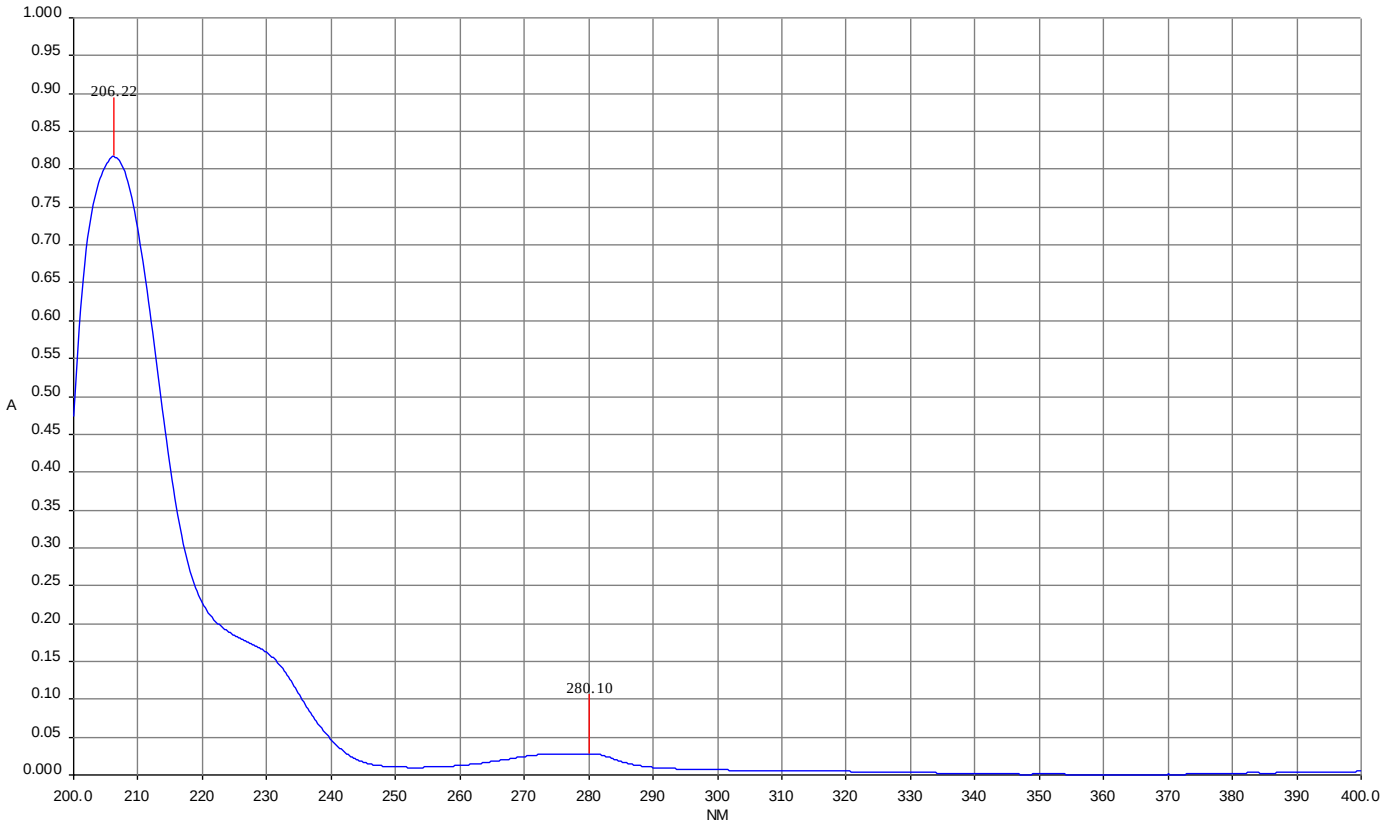

Figure S45. UV spectrum of compound **5**

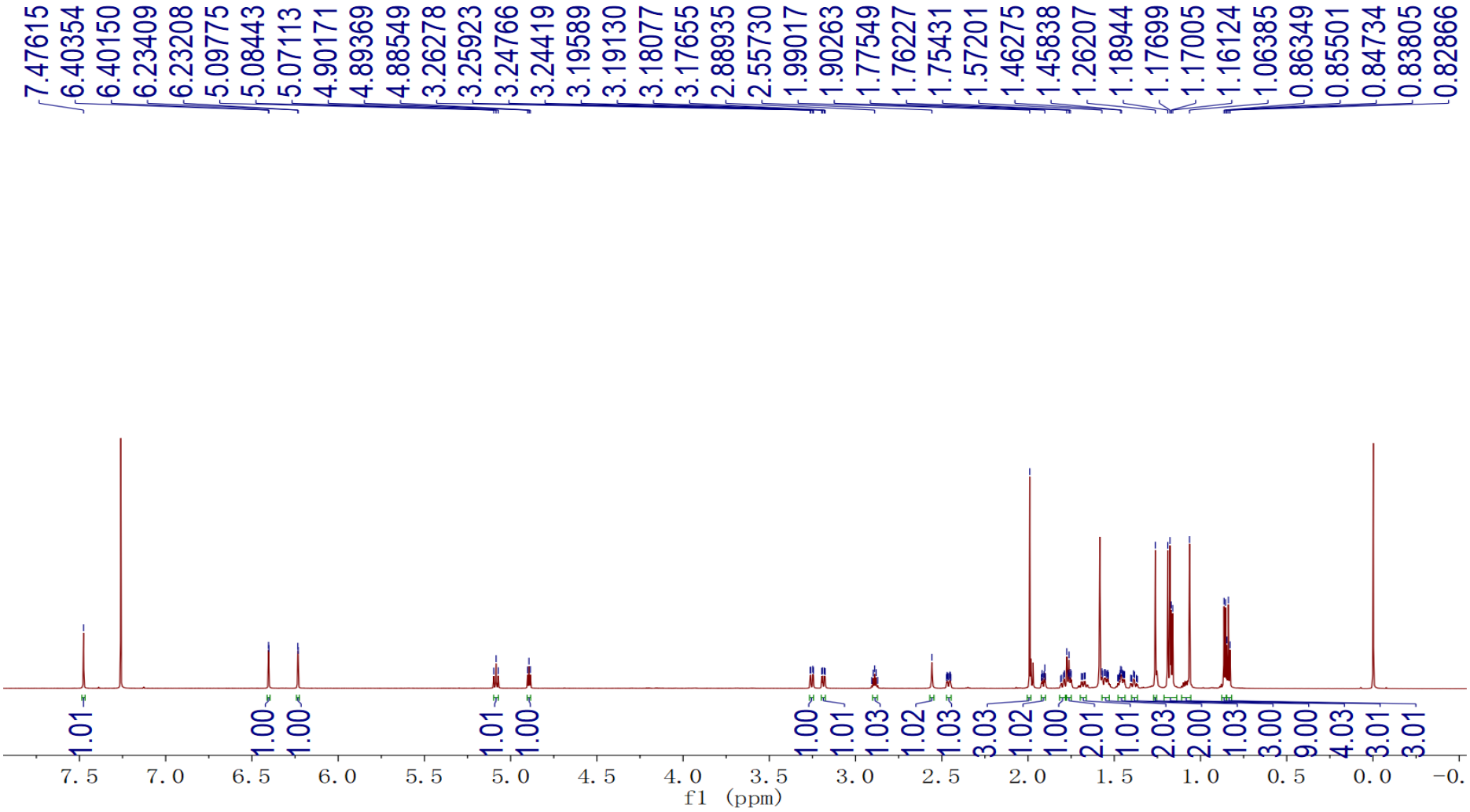

Figure S46. ^{1}H NMR spectrum of compound **6** (Recorded in $CDCl_3$)

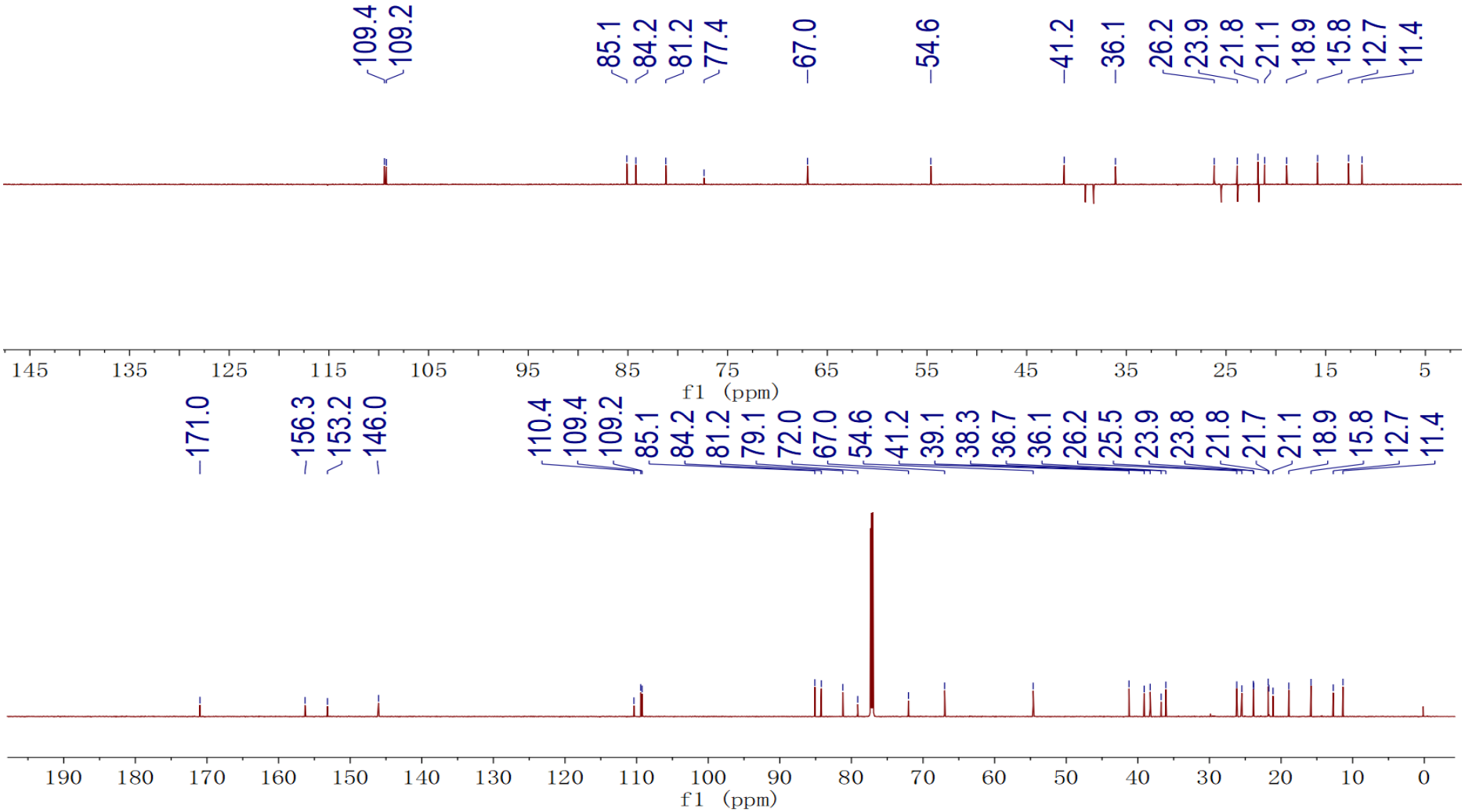

Figure S47. ^{13}C NMR and DEPT spectra of compound **6** (Recorded in $CDCl_3$)

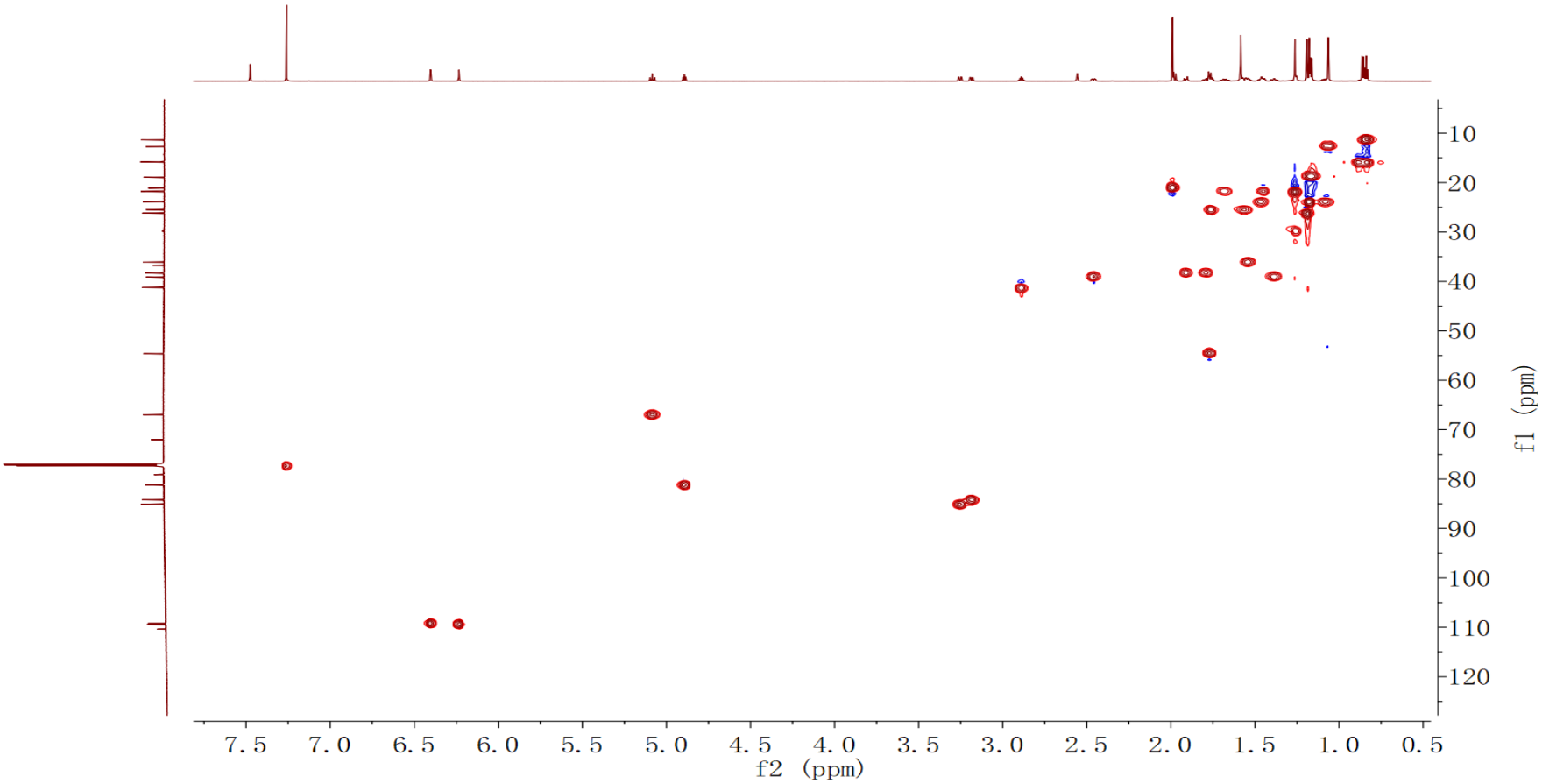

Figure S48. HSQC spectrum of compound **6** (Recorded in $CDCl_3$)

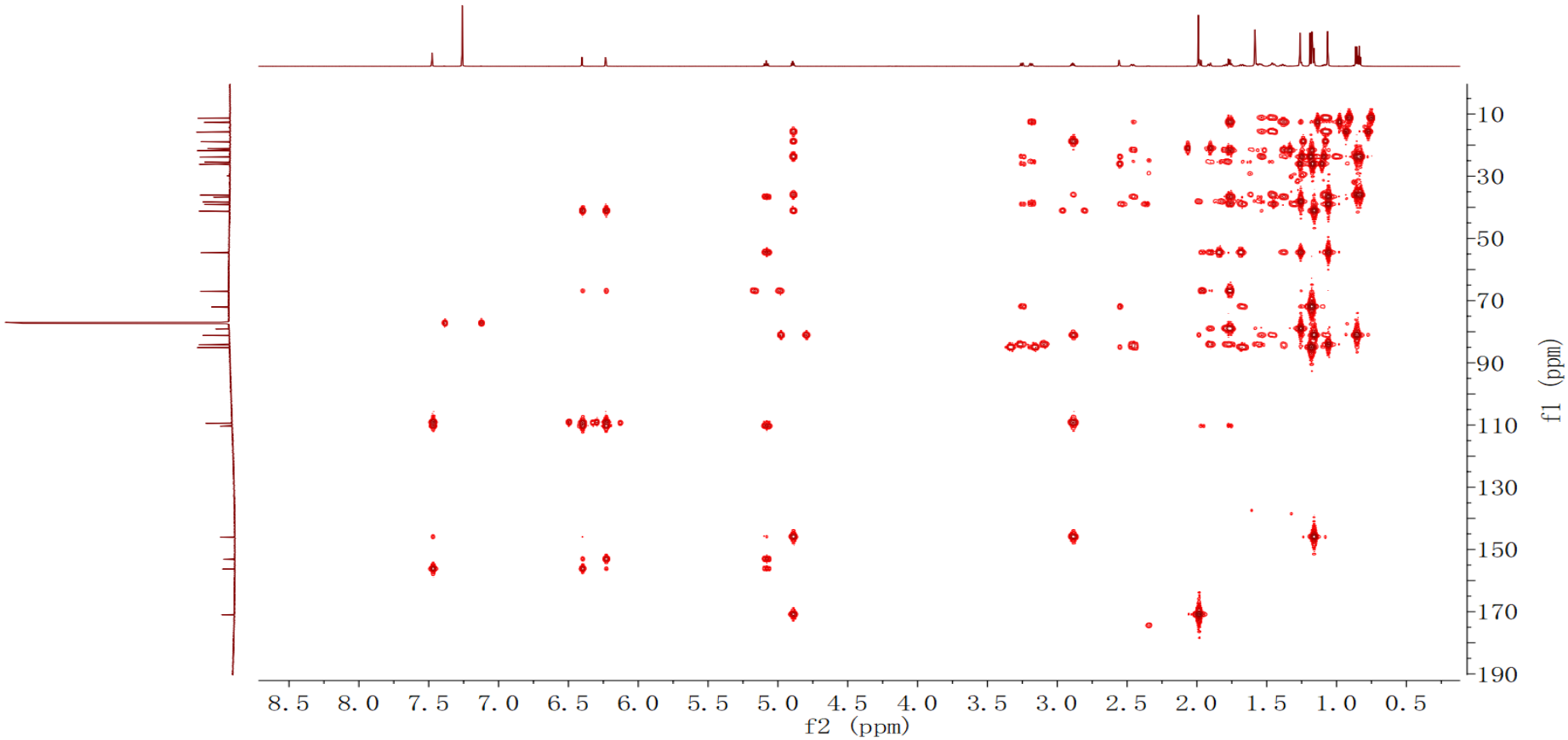

Figure S49. HMBC spectrum of compound **6** (Recorded in $CDCl_3$)

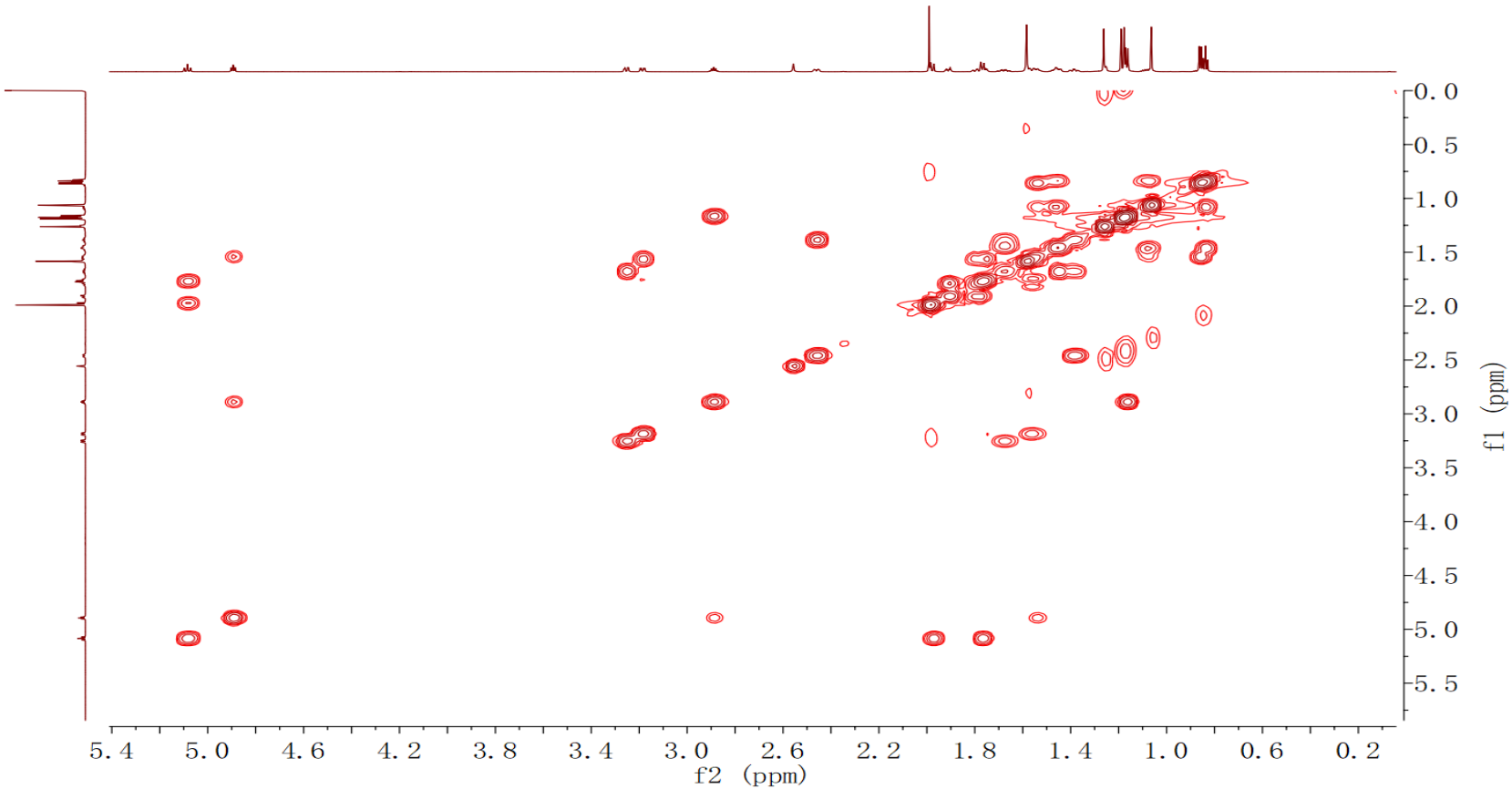

Figure S50. ^{1}H–^{1}H COSY spectrum of compound **6** (Recorded in $CDCl_3$)

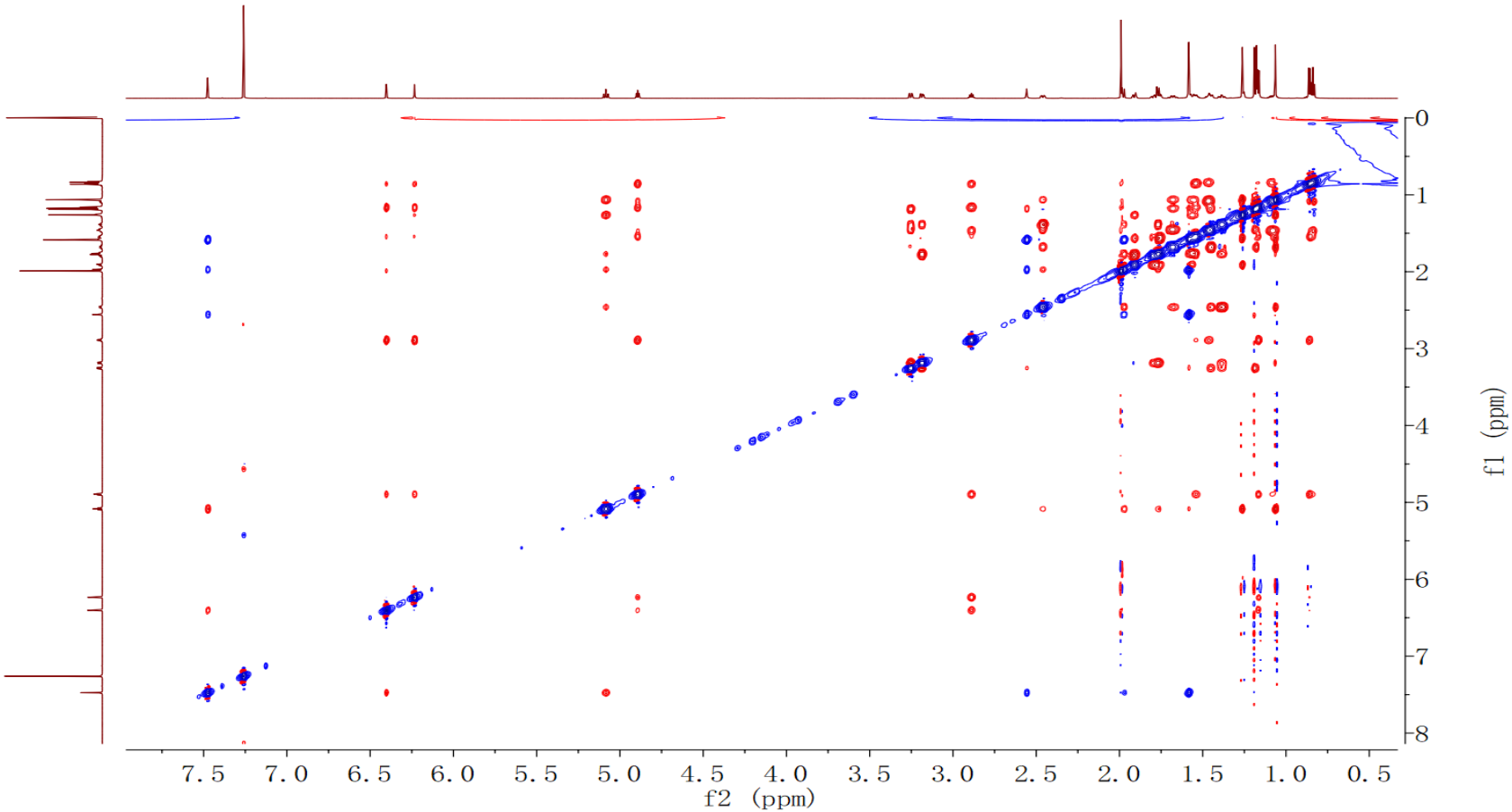

Figure S51. ROESY spectrum of compound **6** (Recorded in $CDCl_3$)

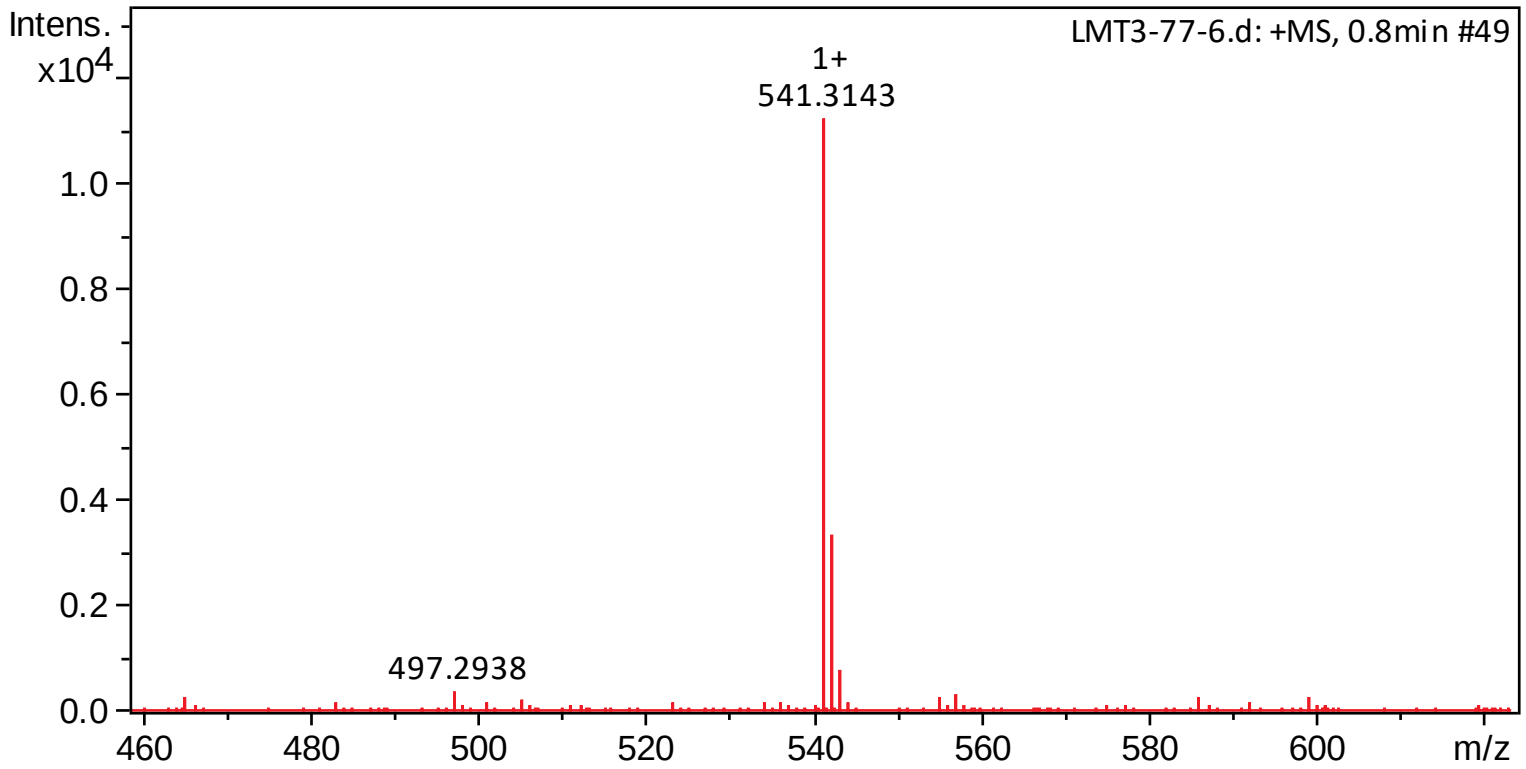

Figure S52. HRESIMS spectrum of compound **6**

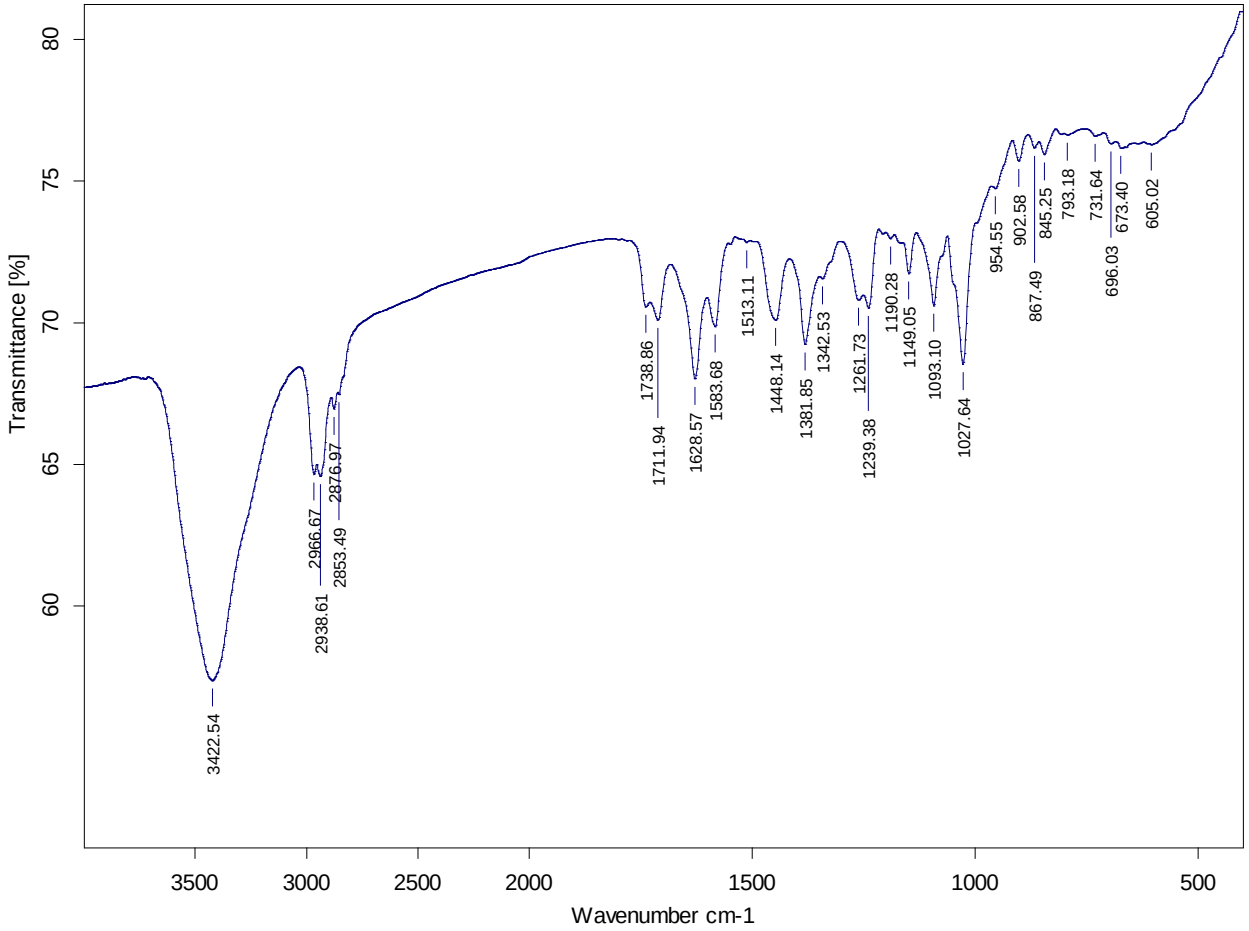

Figure S53. IR spectrum of compound **6**

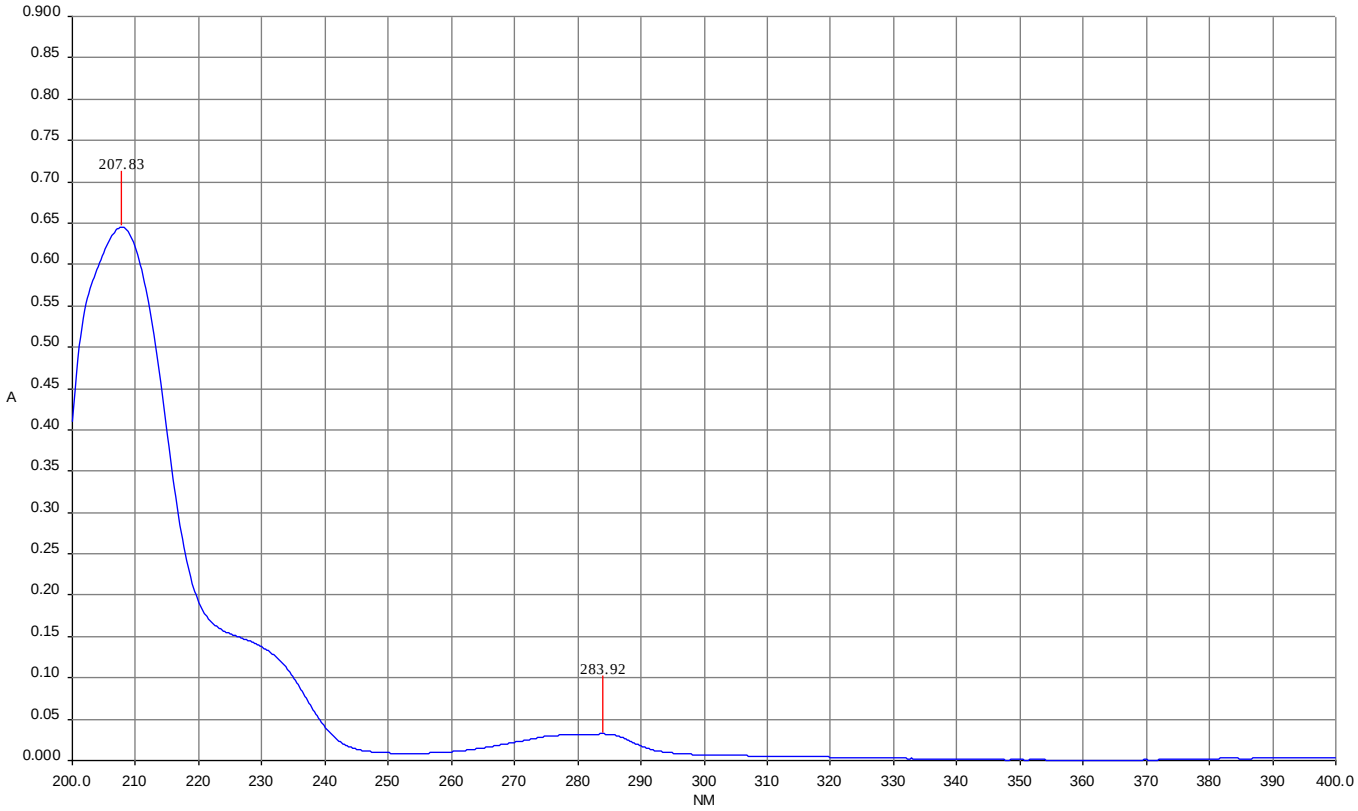

Figure S54. UV spectrum of compound **6**

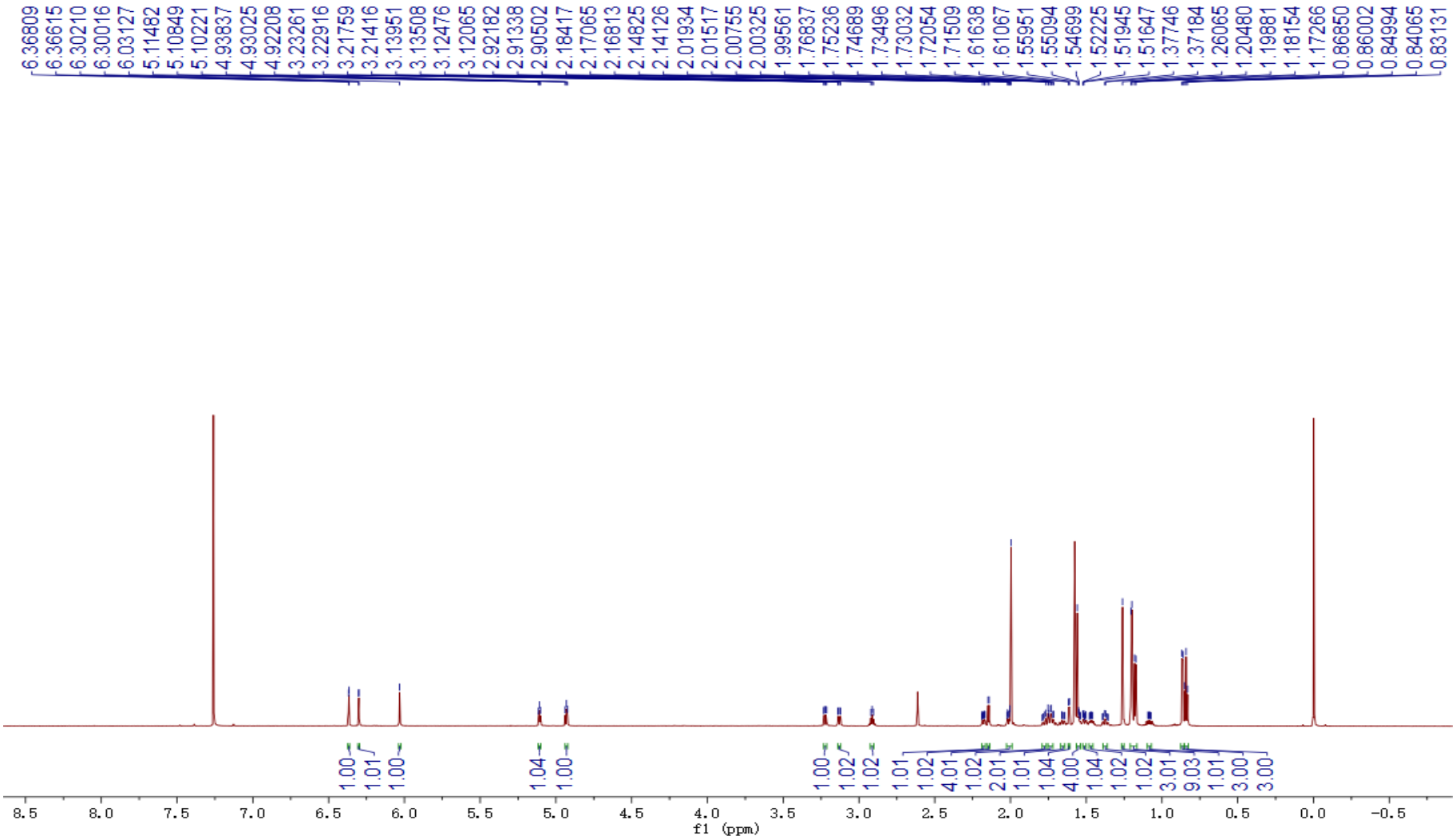

Figure S55. ^{1}H NMR spectrum of compound **7** (Recorded in $CDCl_3$)

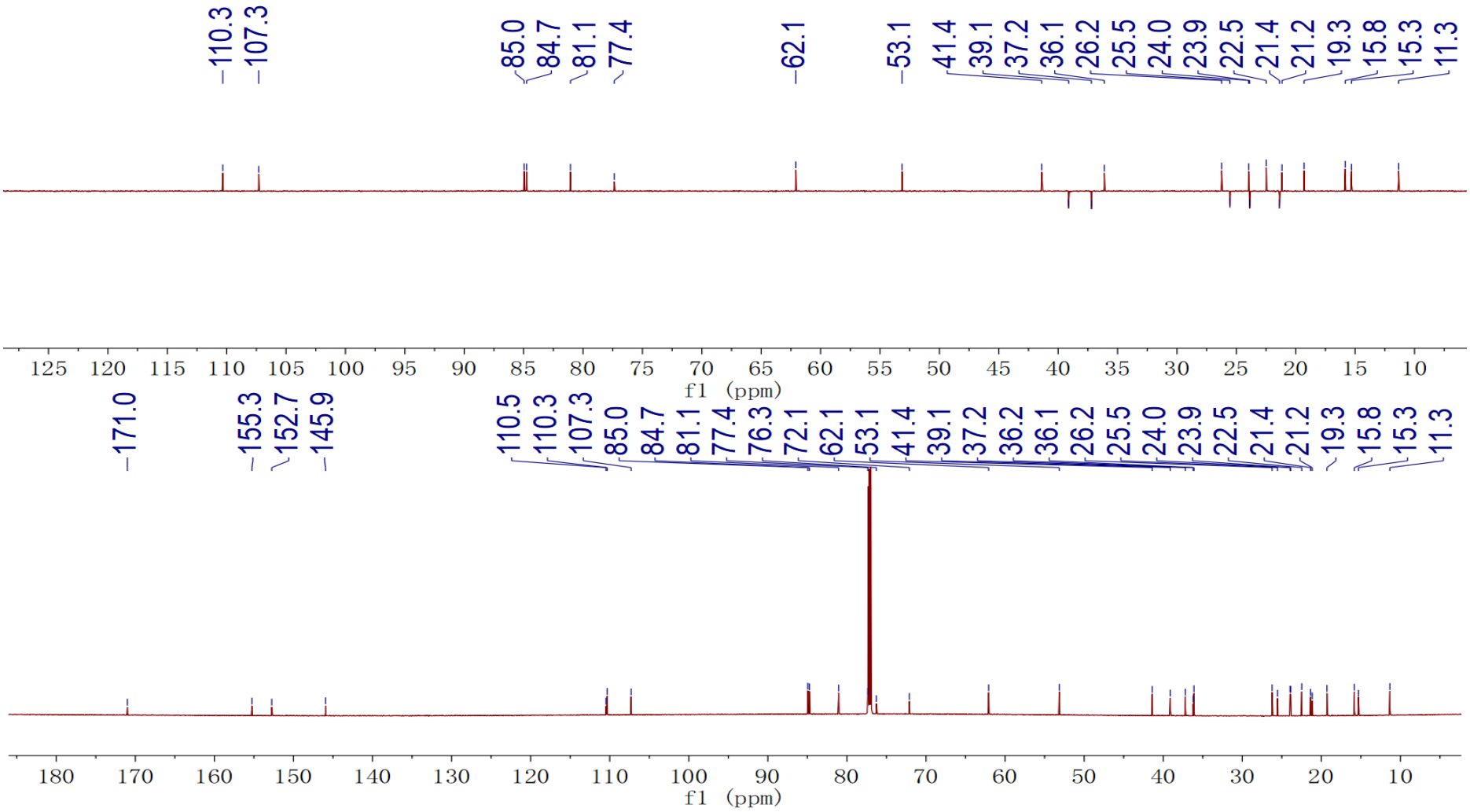

Figure S56. ^{13}C NMR and DEPT spectra of compound **7** (Recorded in $CDCl_3$)

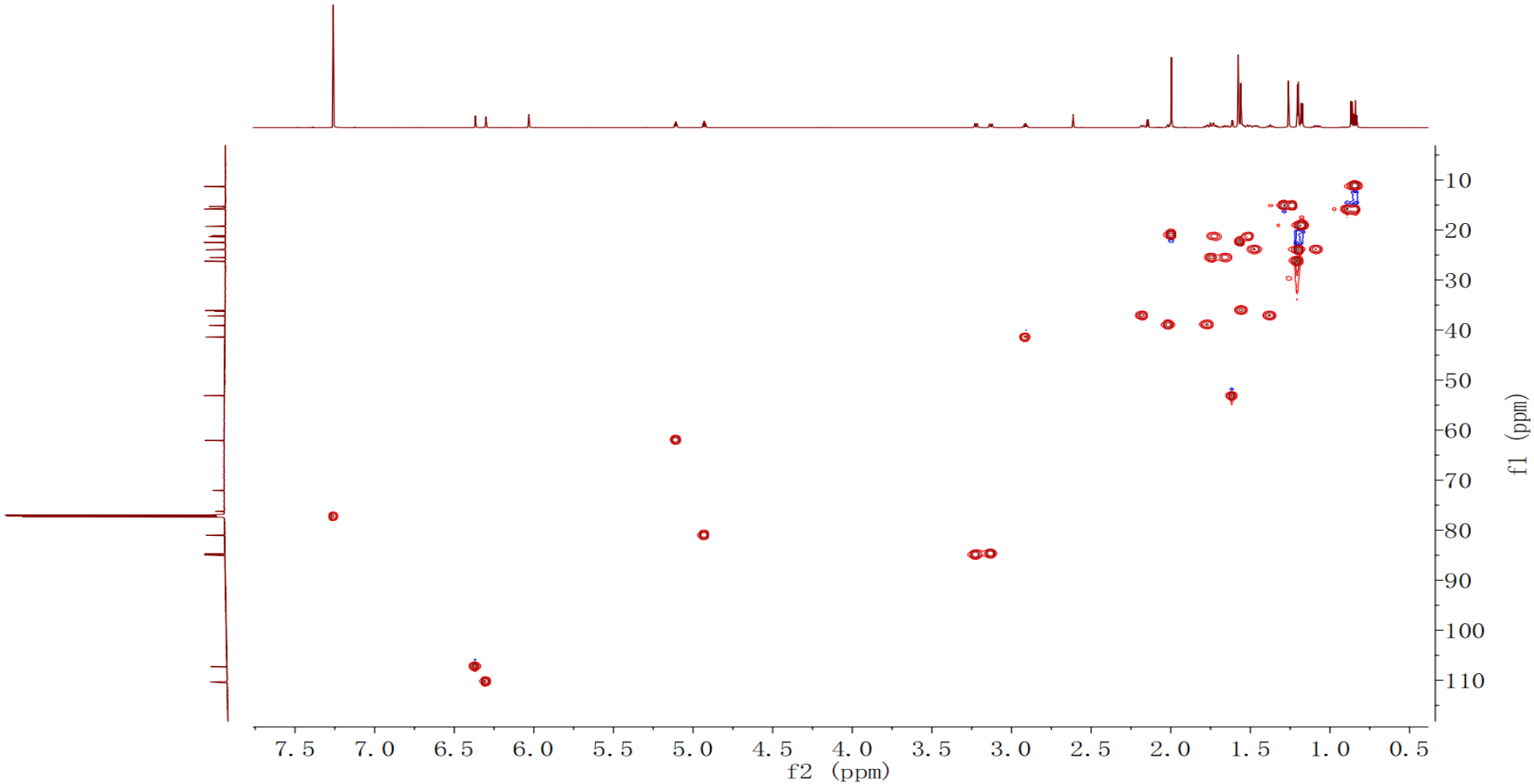

Figure S57. HSQC spectrum of compound **7** (Recorded in $CDCl_3$)

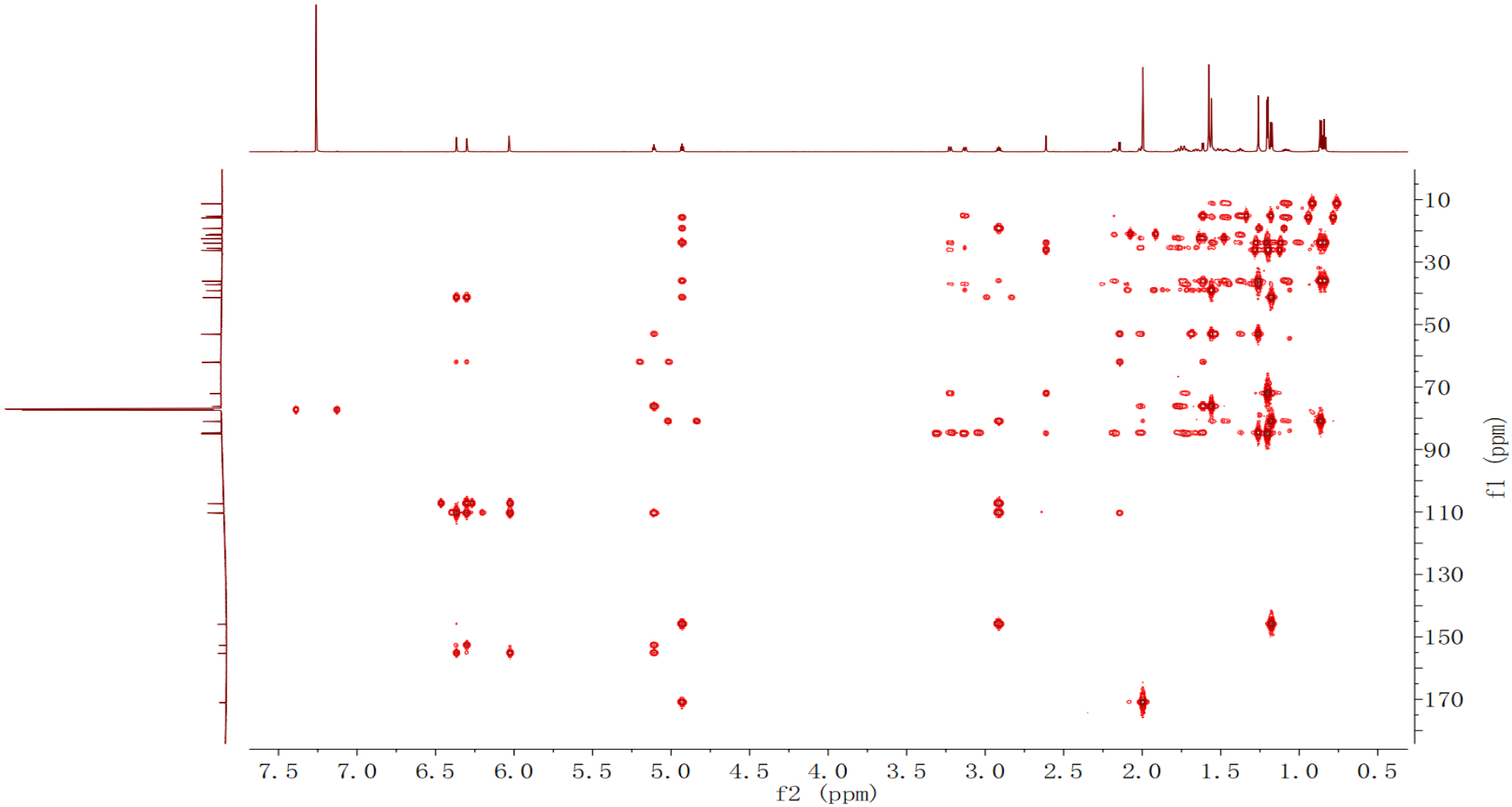

Figure S58. HMBC spectrum of compound **7** (Recorded in $CDCl_3$)

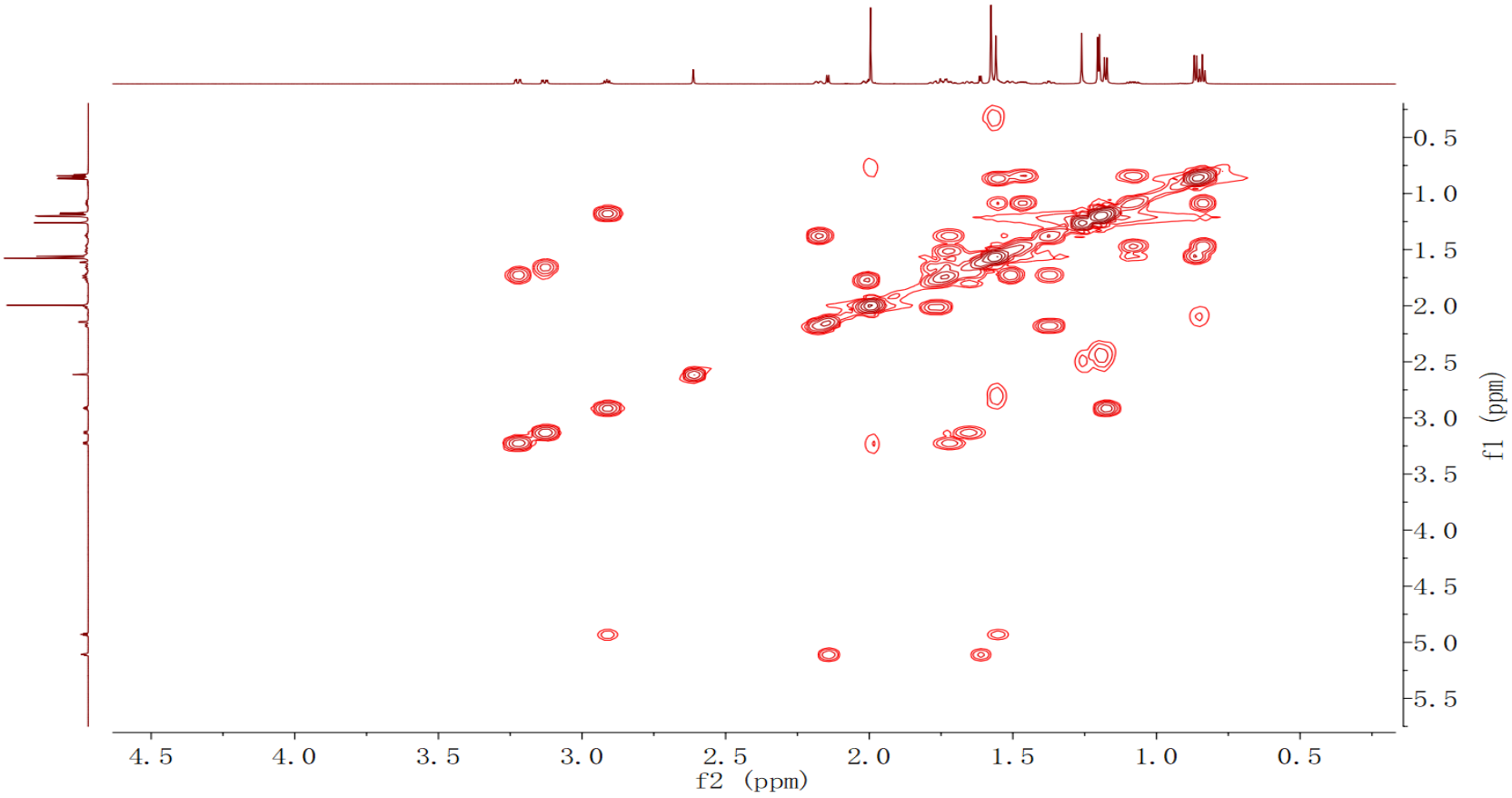

Figure S59. ^{1}H–^{1}H COSY spectrum of compound **7** (Recorded in $CDCl_3$)

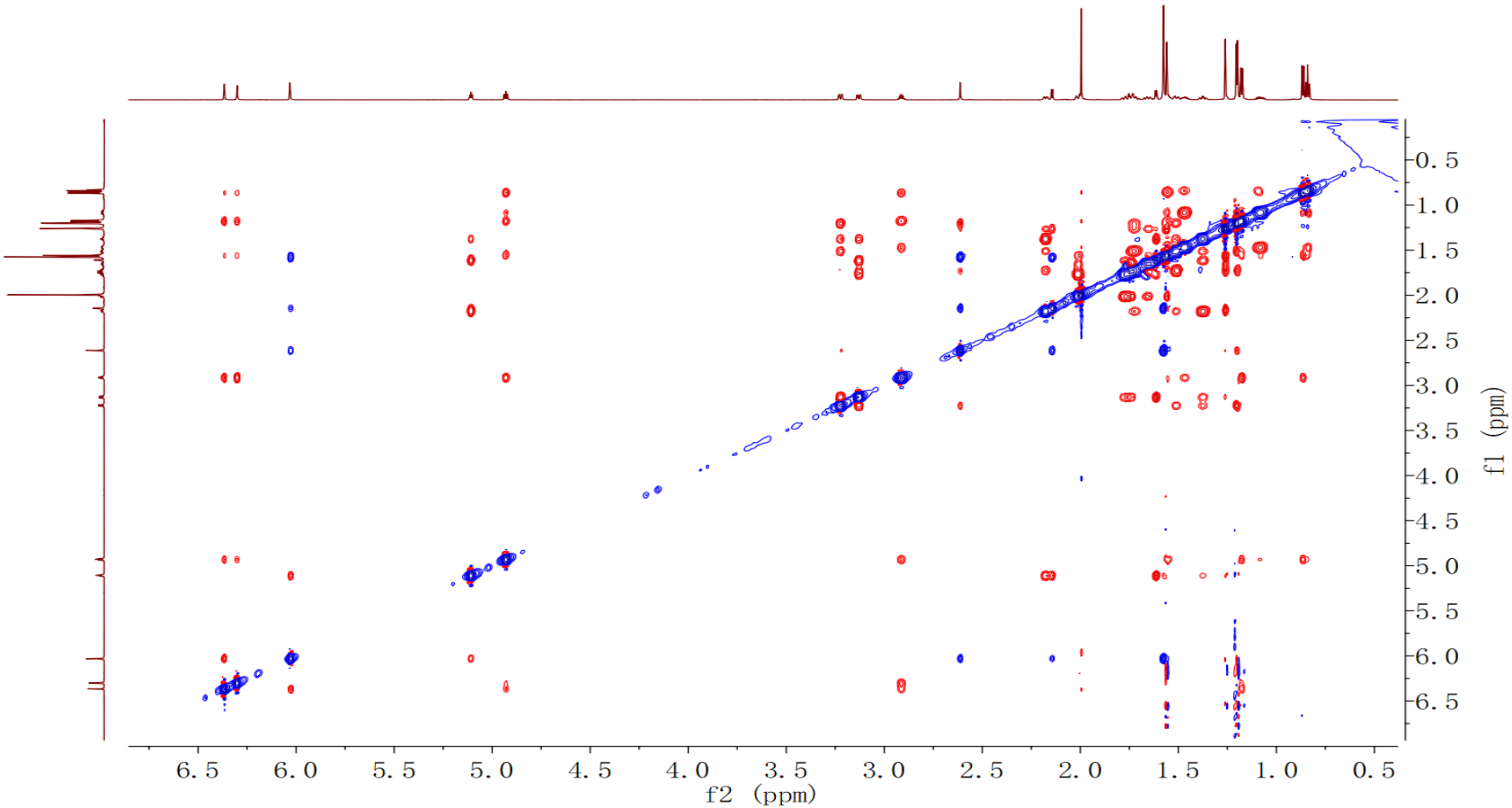

Figure S60. ROESY spectrum of compound **7** (Recorded in $CDCl_3$)

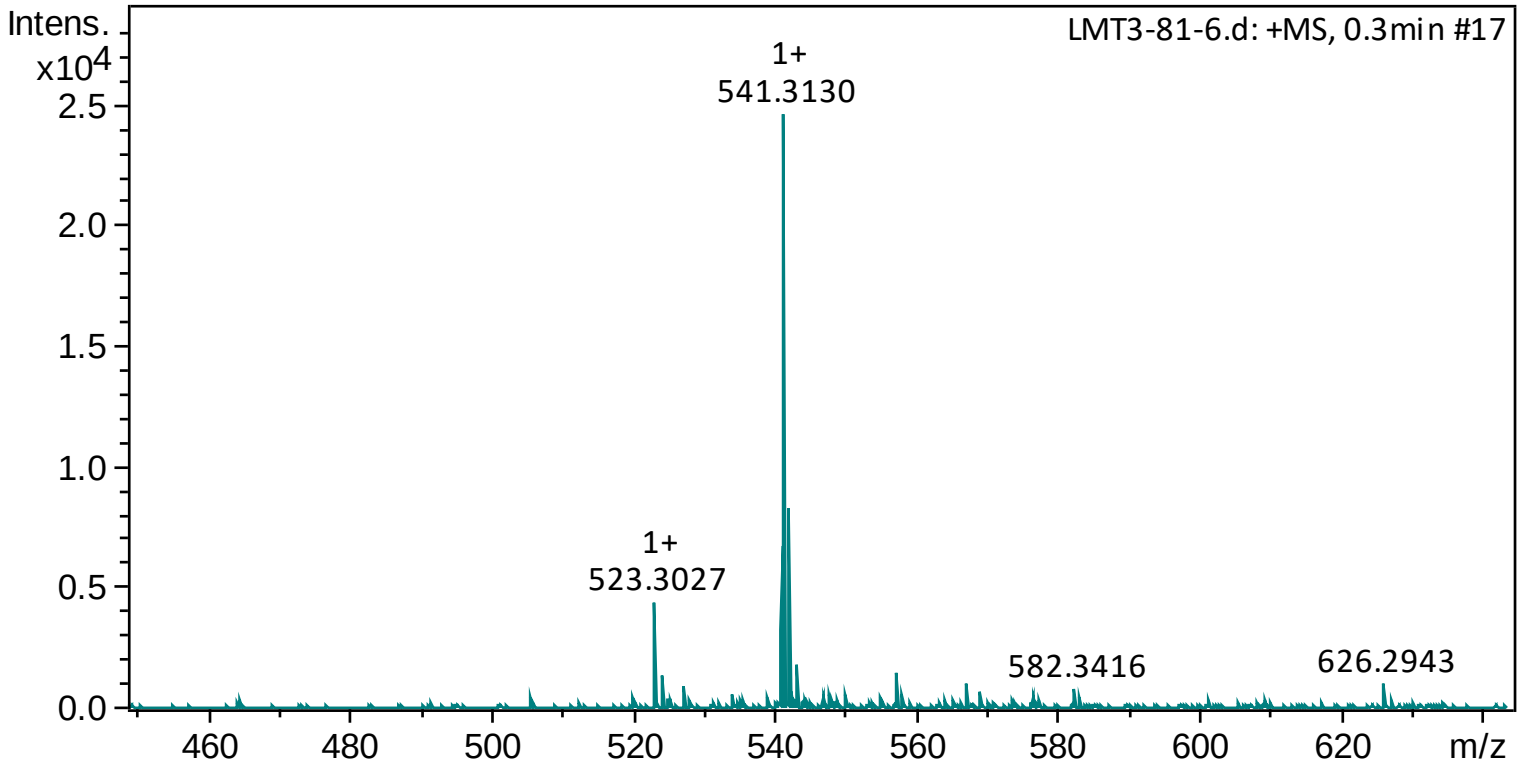

Figure S61. HRESIMS spectrum of compound **7**

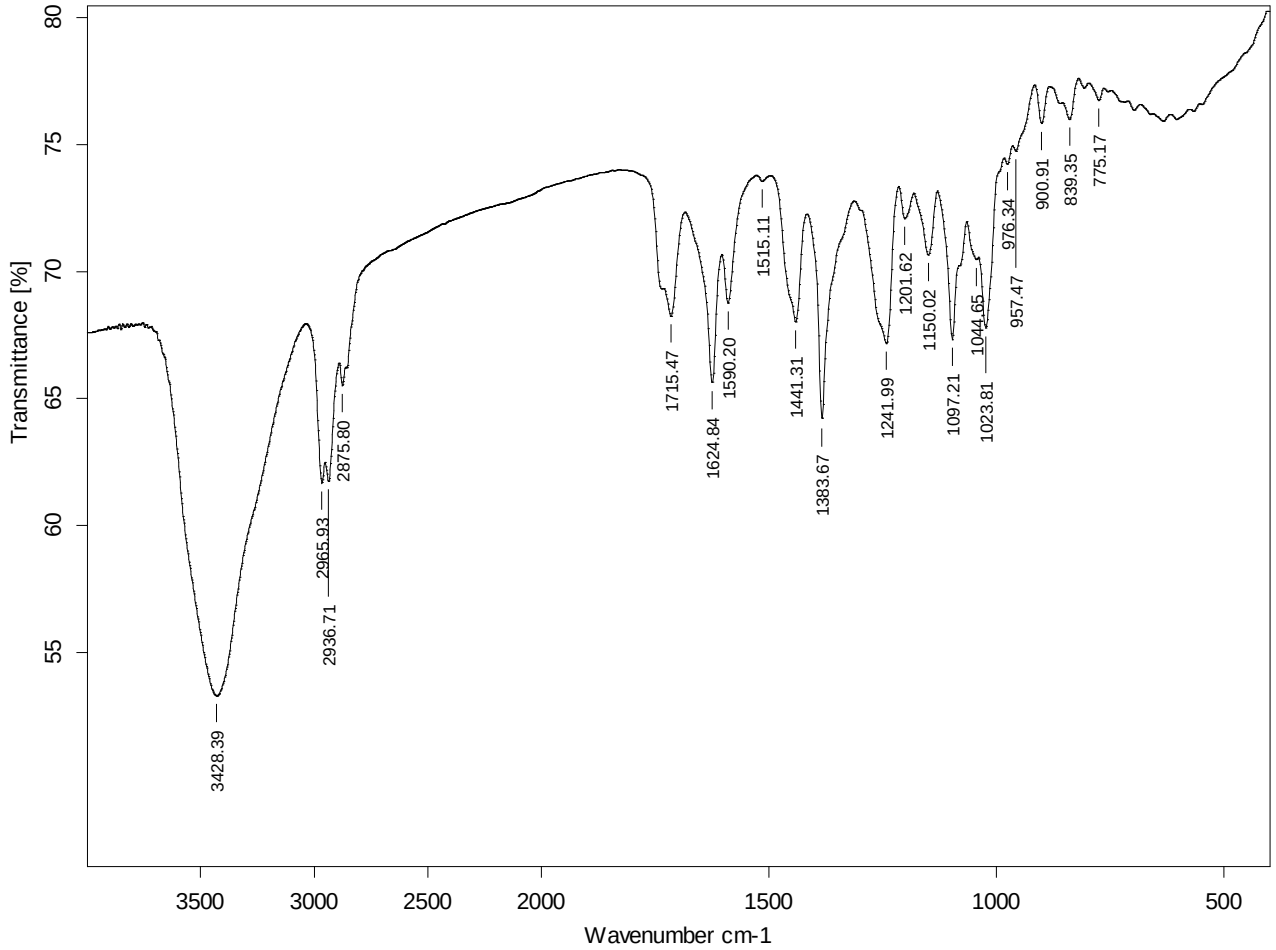

Figure S62. IR spectrum of compound **7**

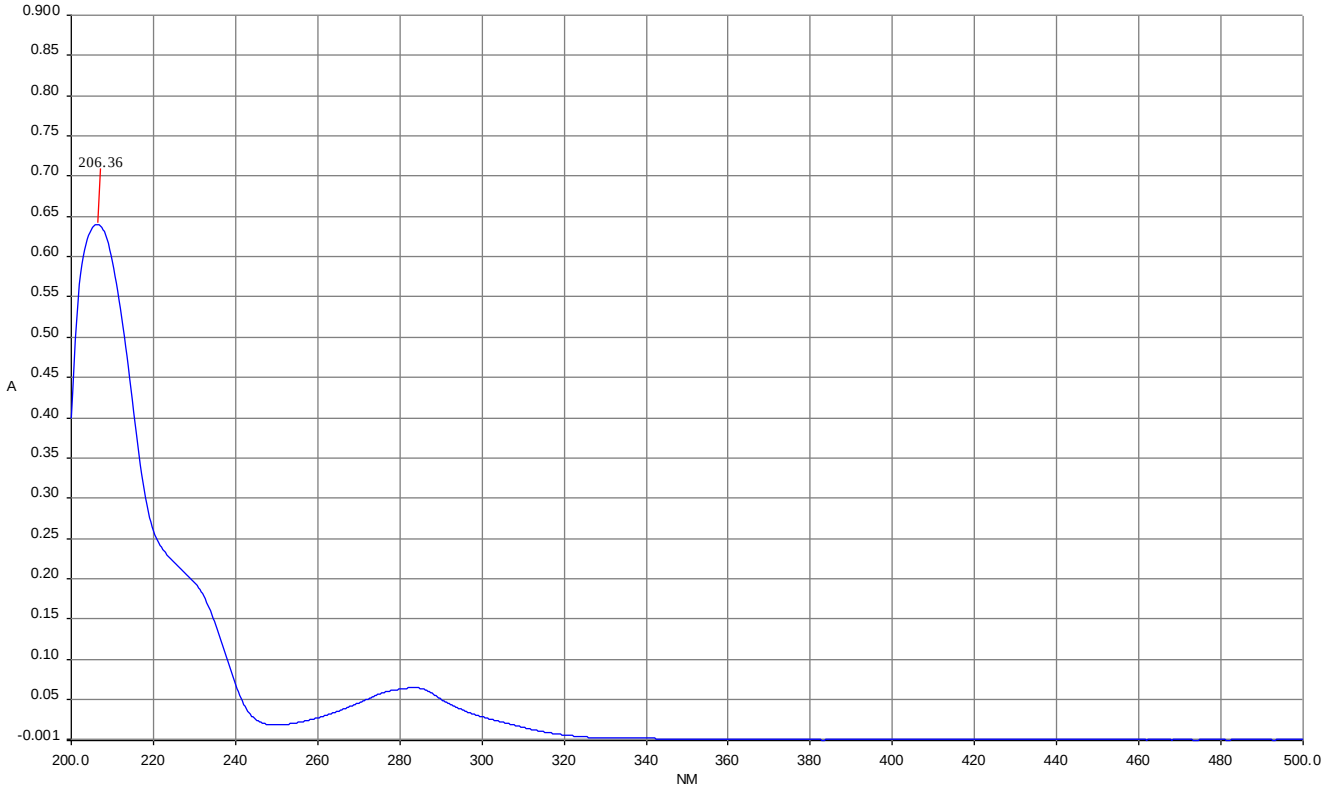

Figure S63. UV spectrum of compound **7**

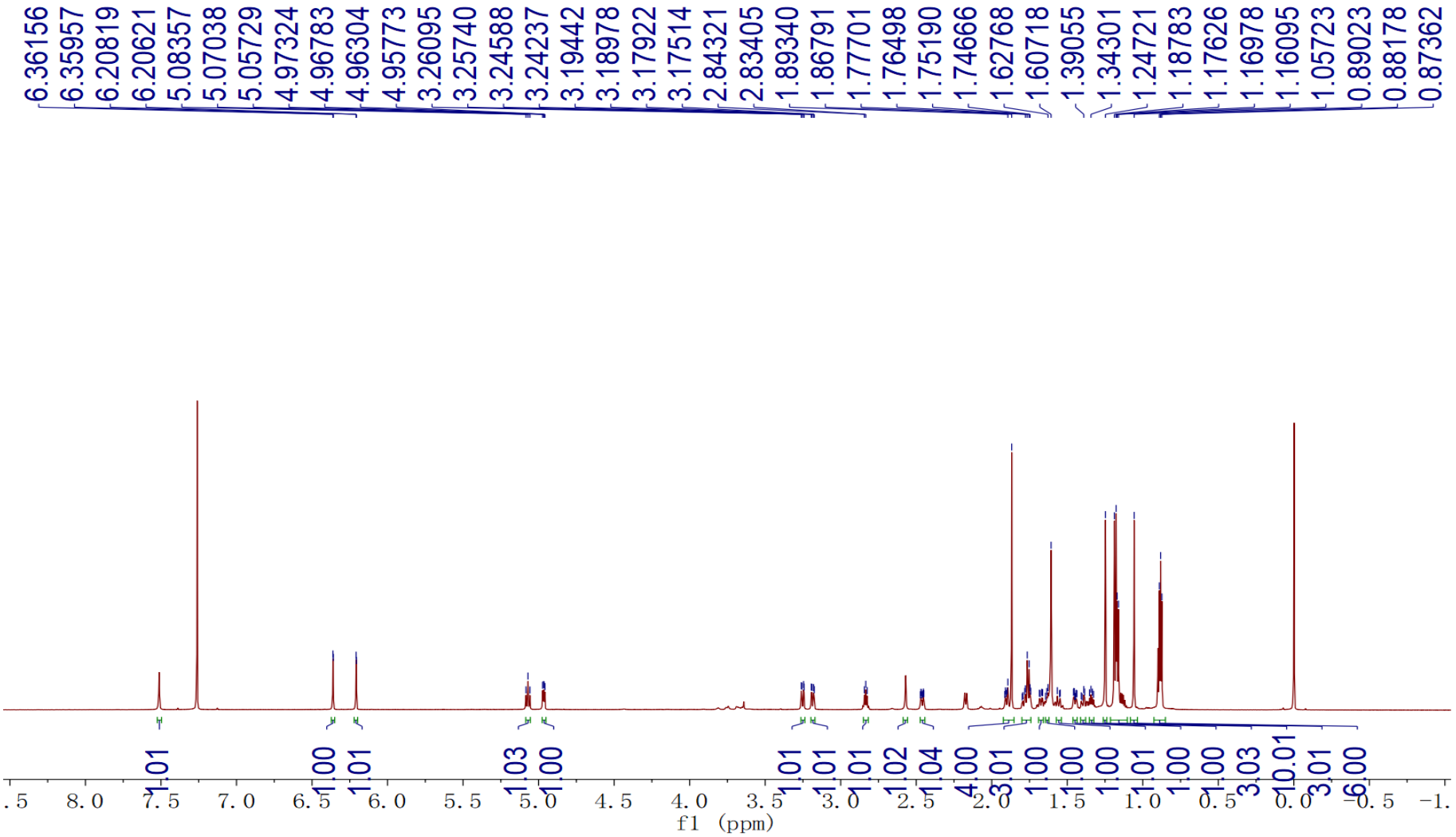

Figure S64. ^{1}H NMR spectrum of compound **8** (Recorded in $CDCl_3$)

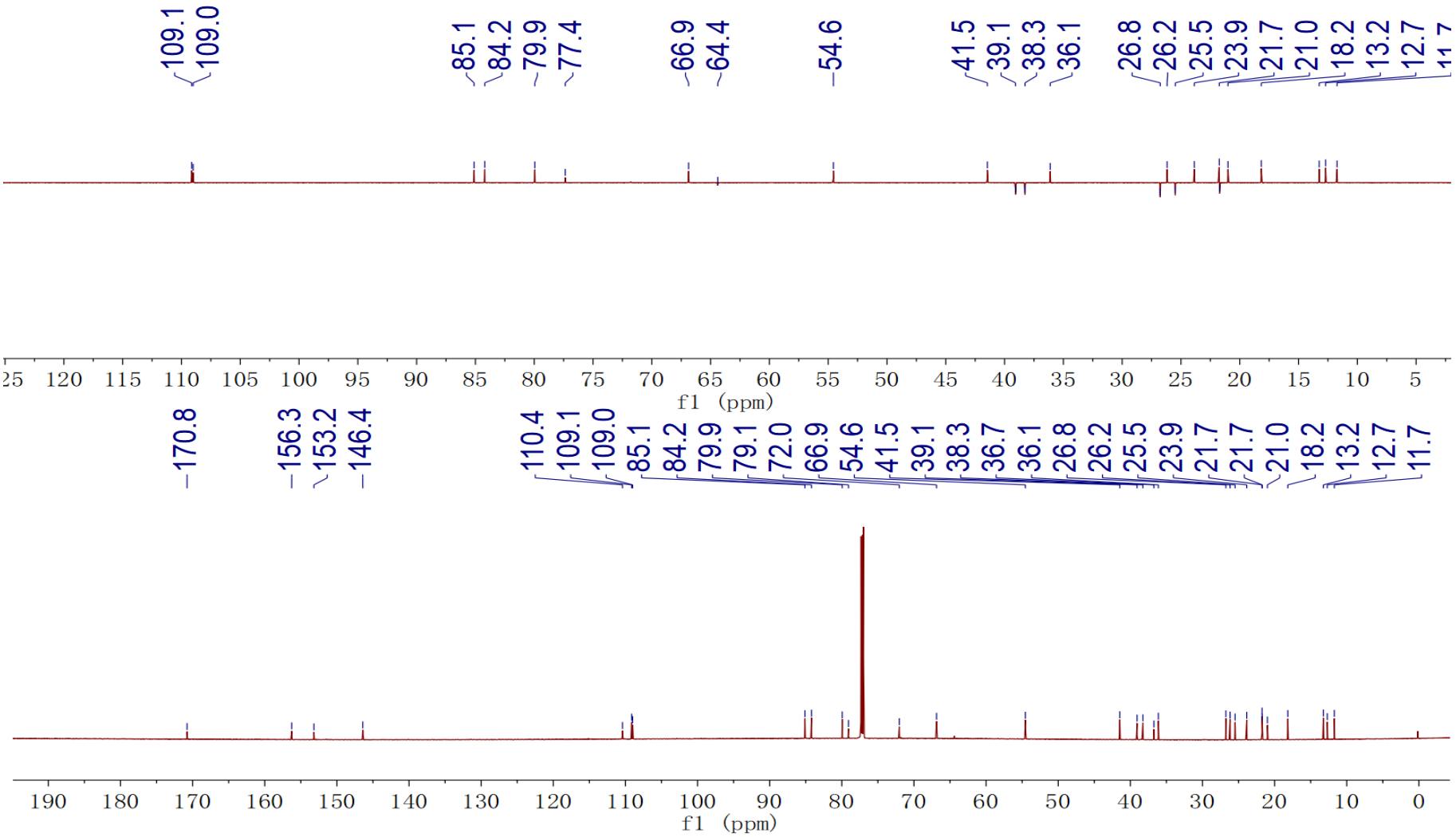

Figure S65. ^{13}C NMR and DEPT spectra of compound **8** (Recorded in $CDCl_3$)

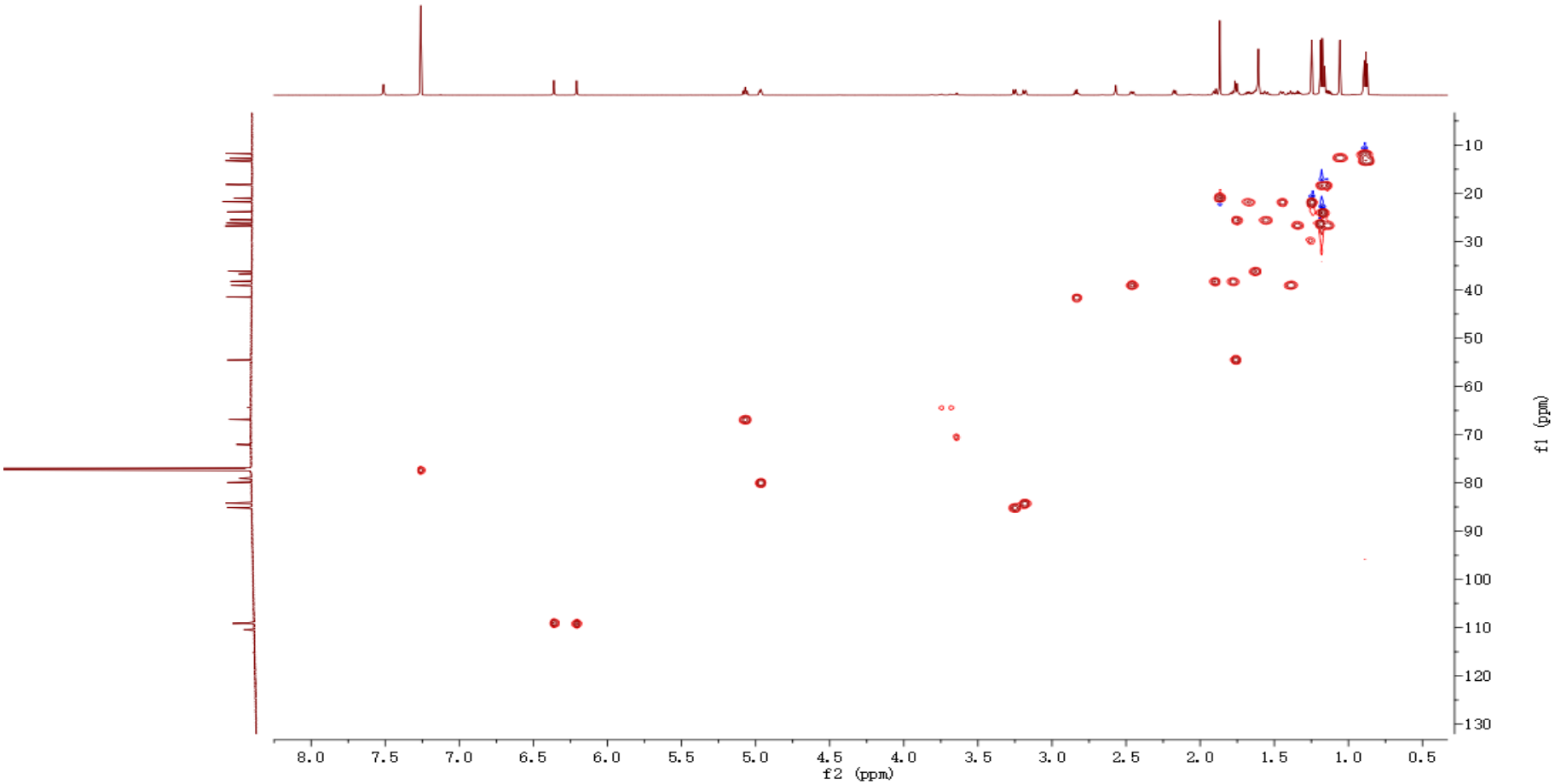

Figure S66. HSQC spectrum of compound **8** (Recorded in $CDCl_3$)

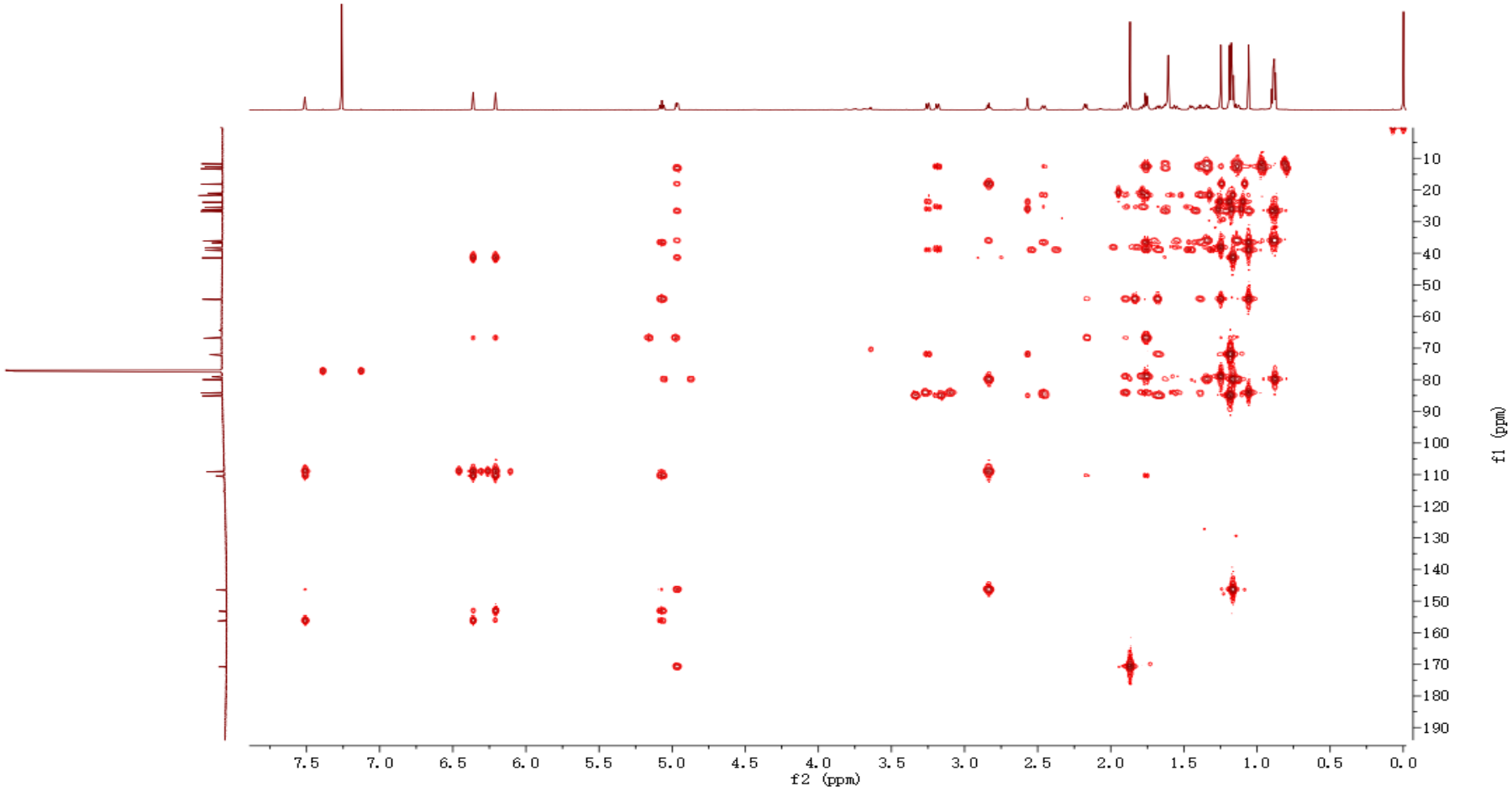

Figure S67. HMBC spectrum of compound **8** (Recorded in $CDCl_3$)

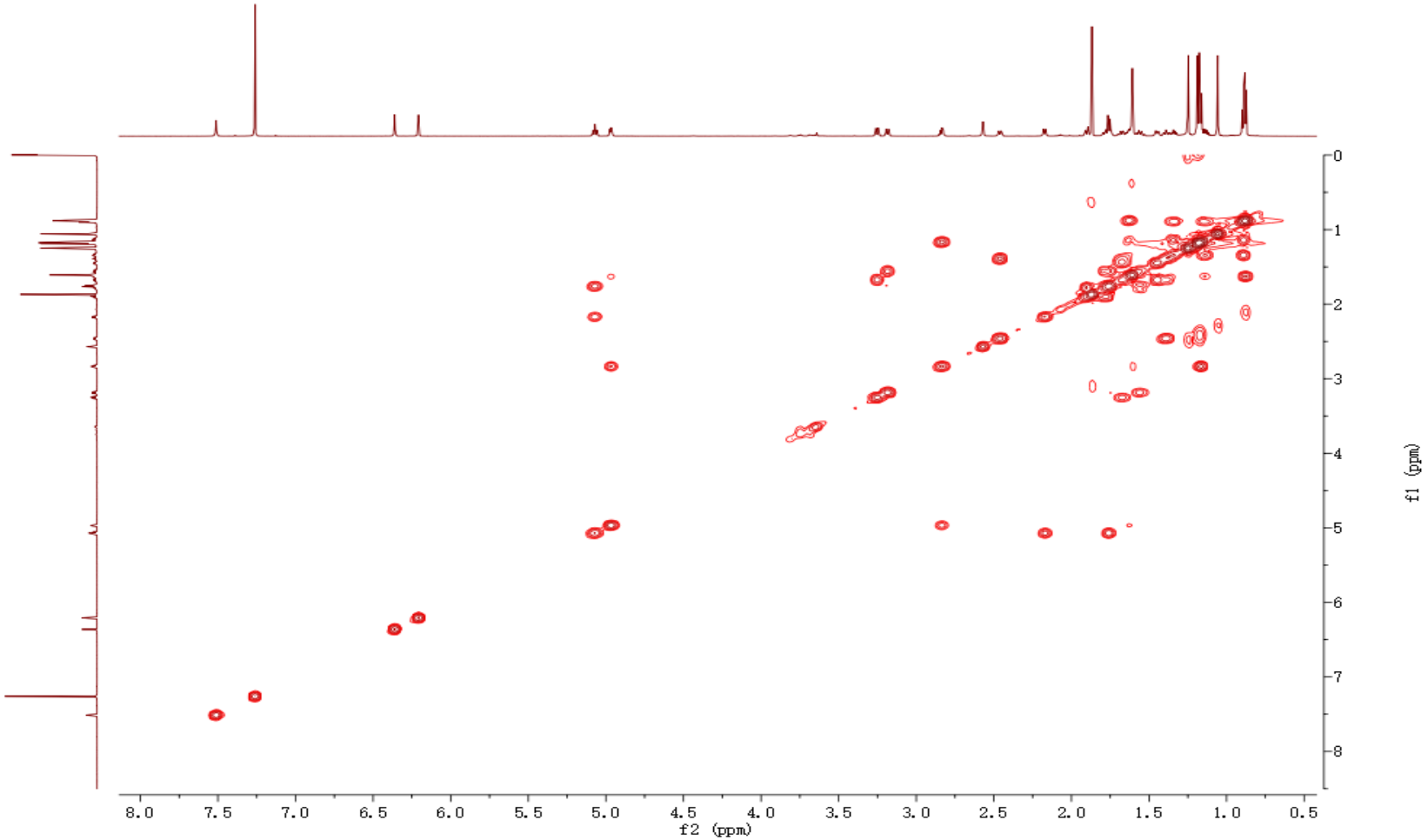

Figure S68. ^{1}H–^{1}H COSY spectrum of compound **8** (Recorded in $CDCl_3$)

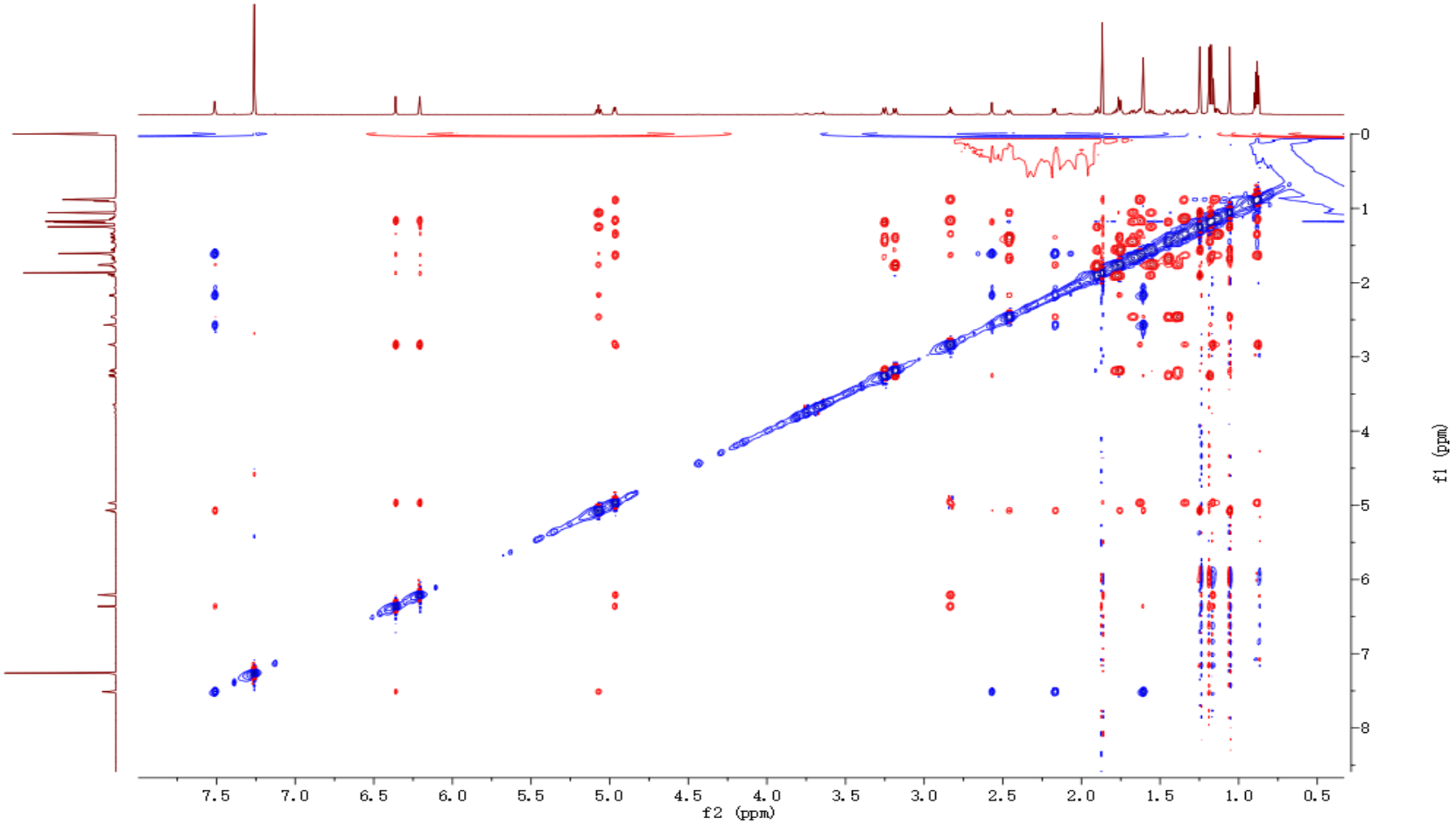

Figure S69. ROESY spectrum of compound **8** (Recorded in $CDCl_3$)

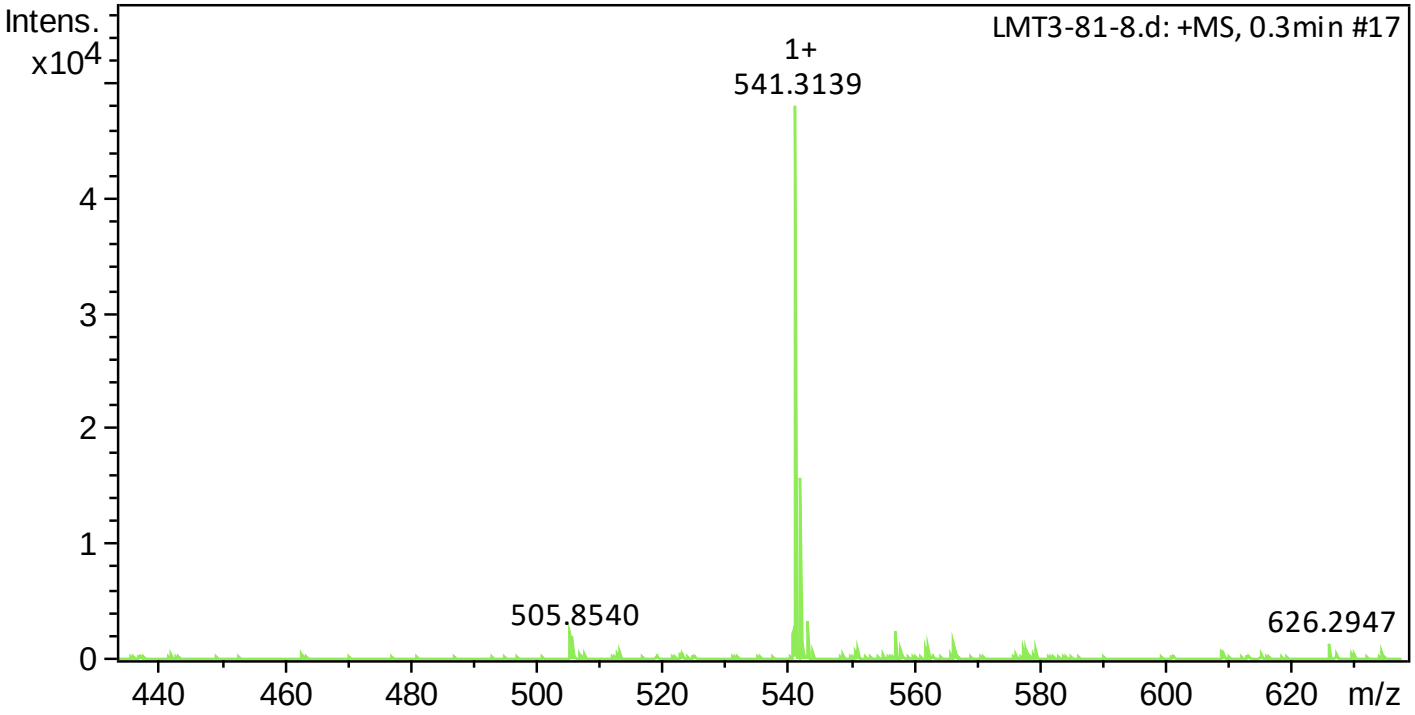

Figure S70. HRESIMS spectrum of compound **8**

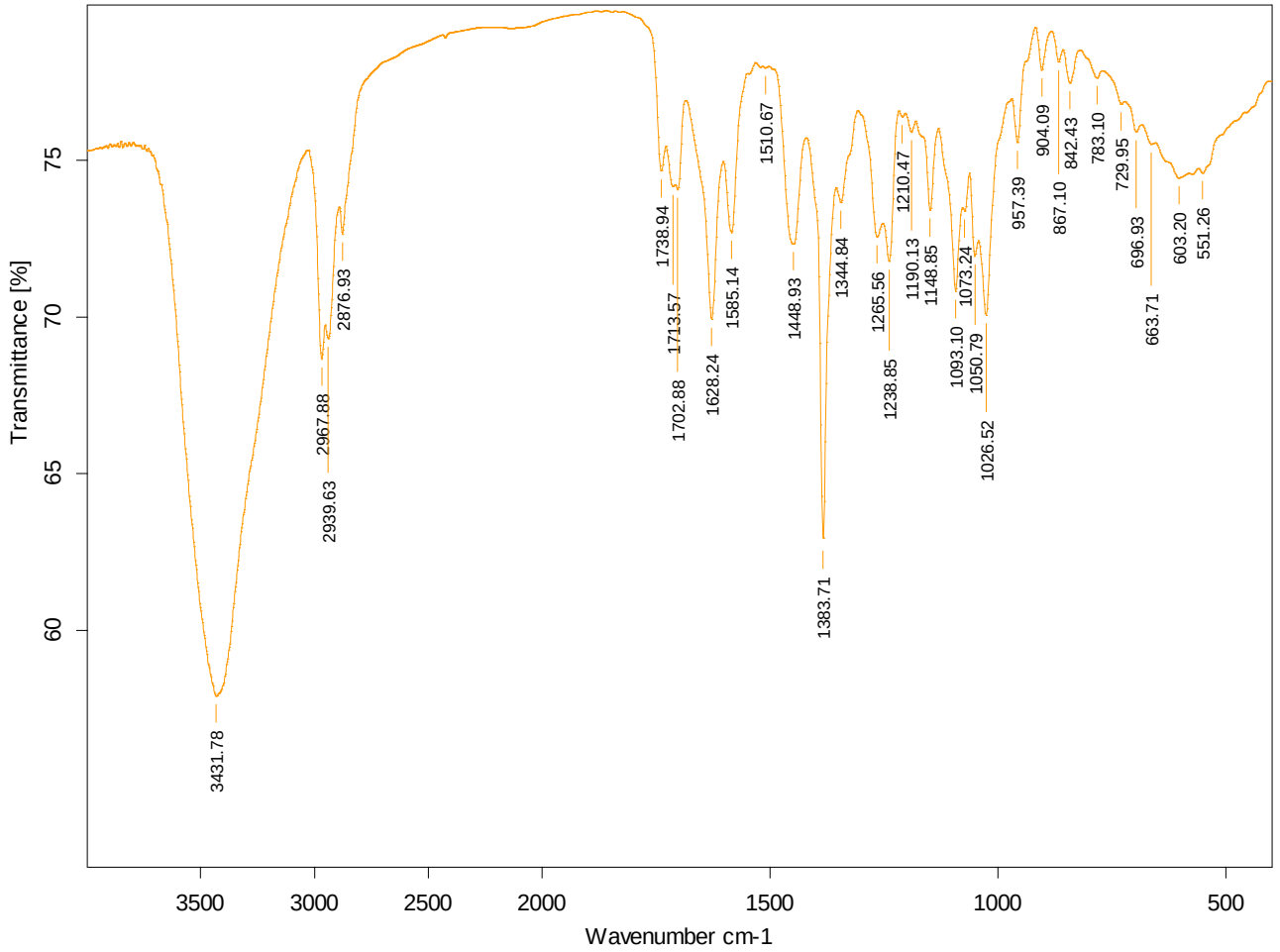

Figure S71. IR spectrum of compound **8**

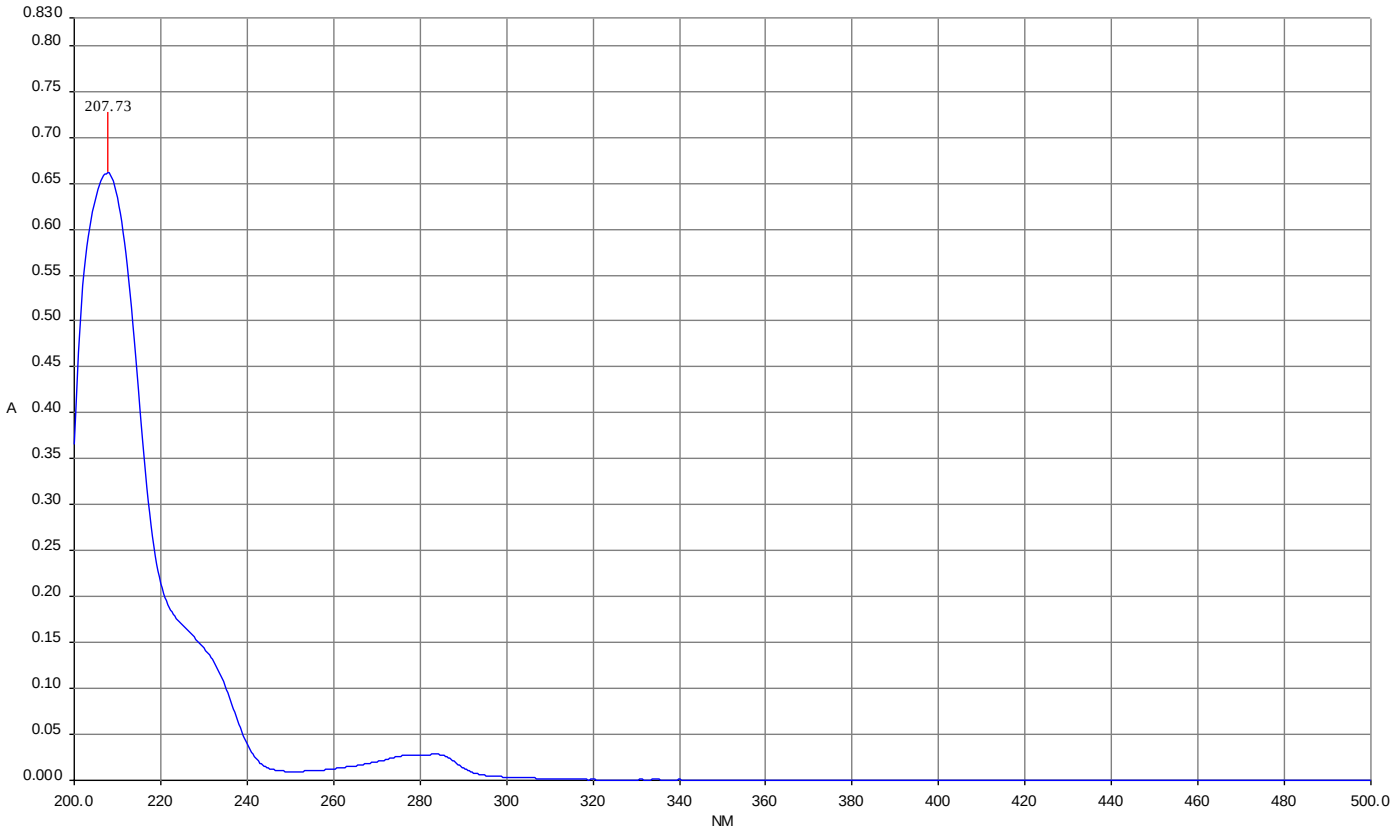

Figure S72. UV spectrum of compound **8**

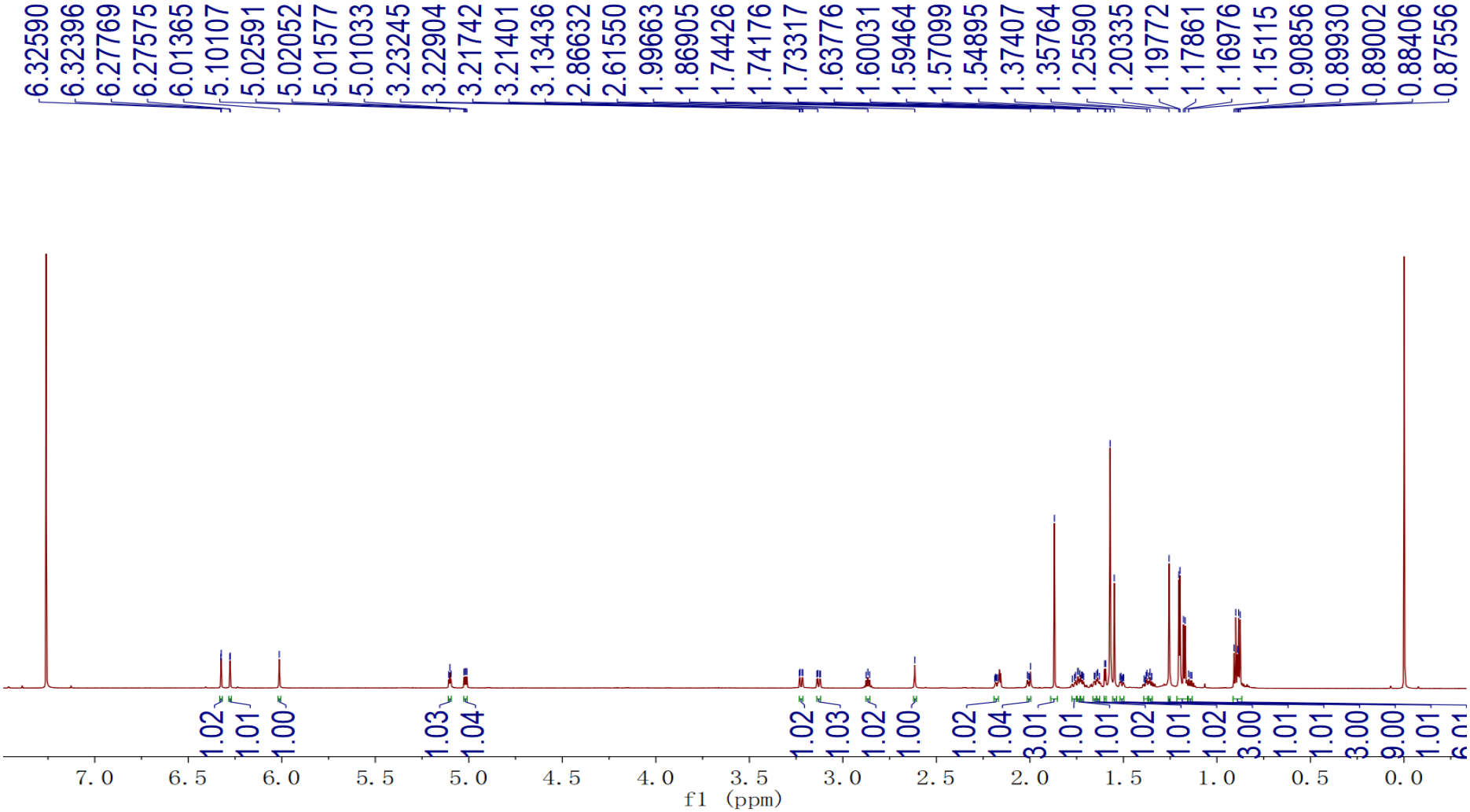

Figure S73. ^{1}H NMR spectrum of compound **9** (Recorded in $CDCl_3$)

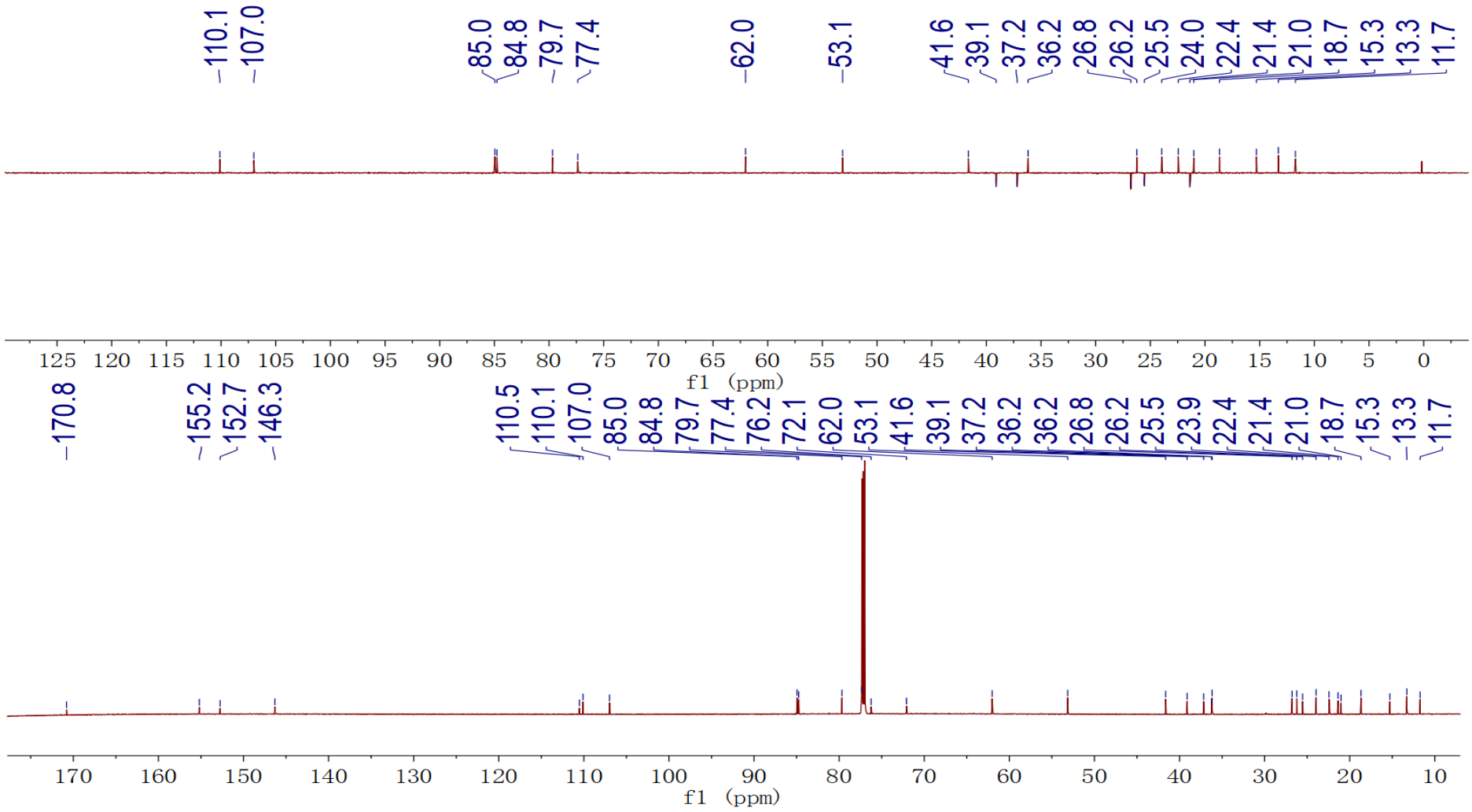

Figure S74. ^{13}C NMR and DEPT spectra of compound **9** (Recorded in $CDCl_3$)

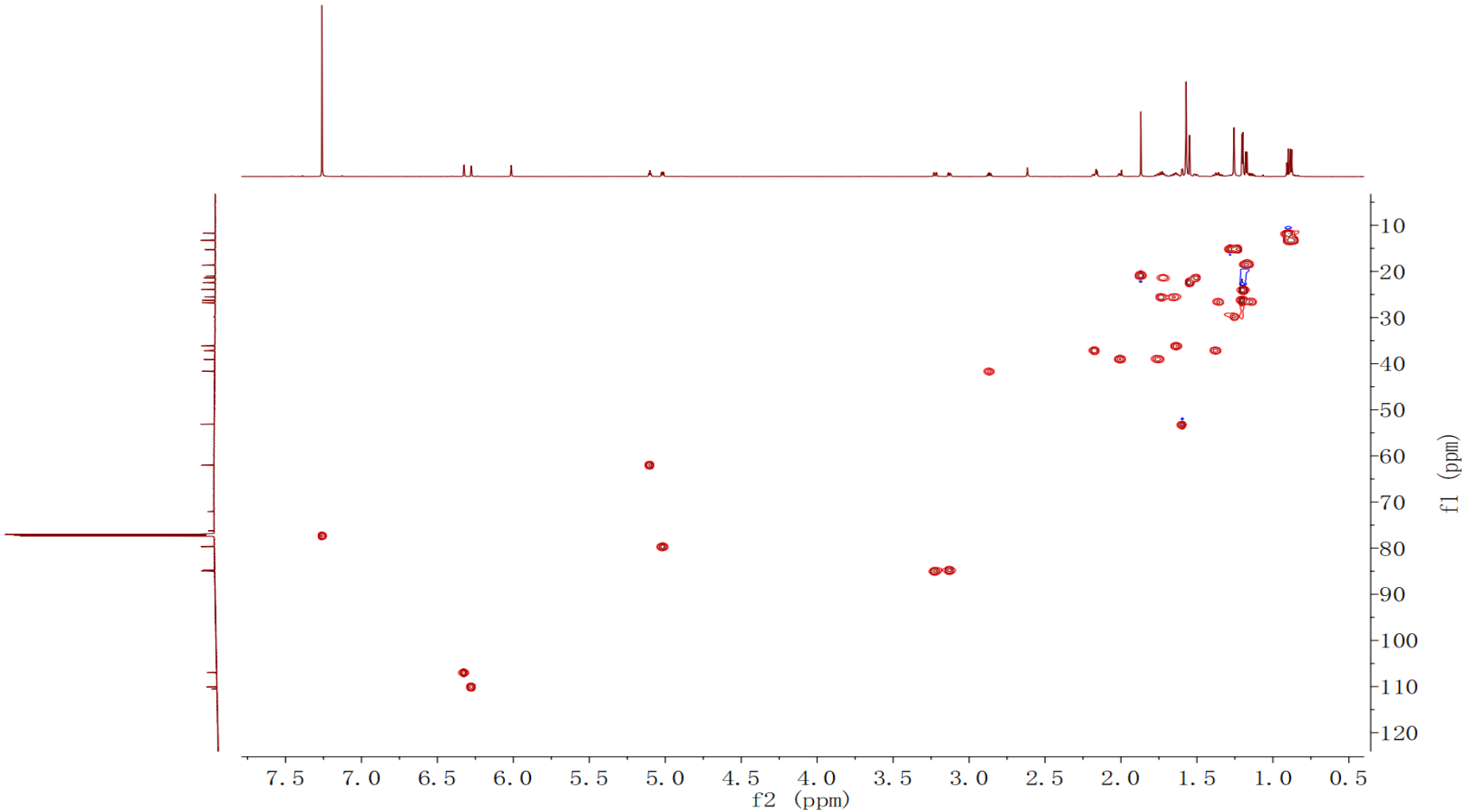

Figure S75. HSQC spectrum of compound **9** (Recorded in $CDCl_3$)

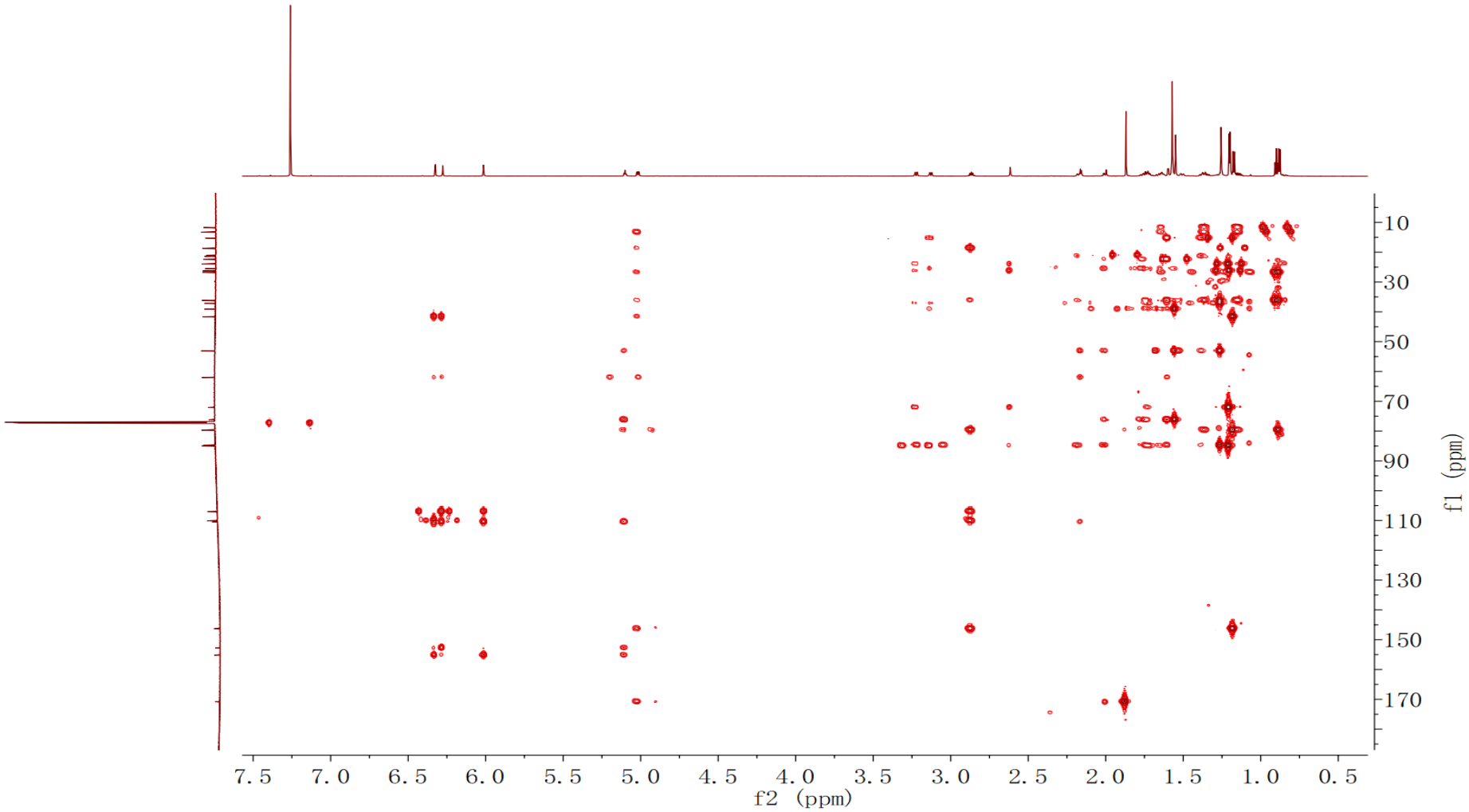

Figure S76. HMBC spectrum of compound **9** (Recorded in $CDCl_3$)

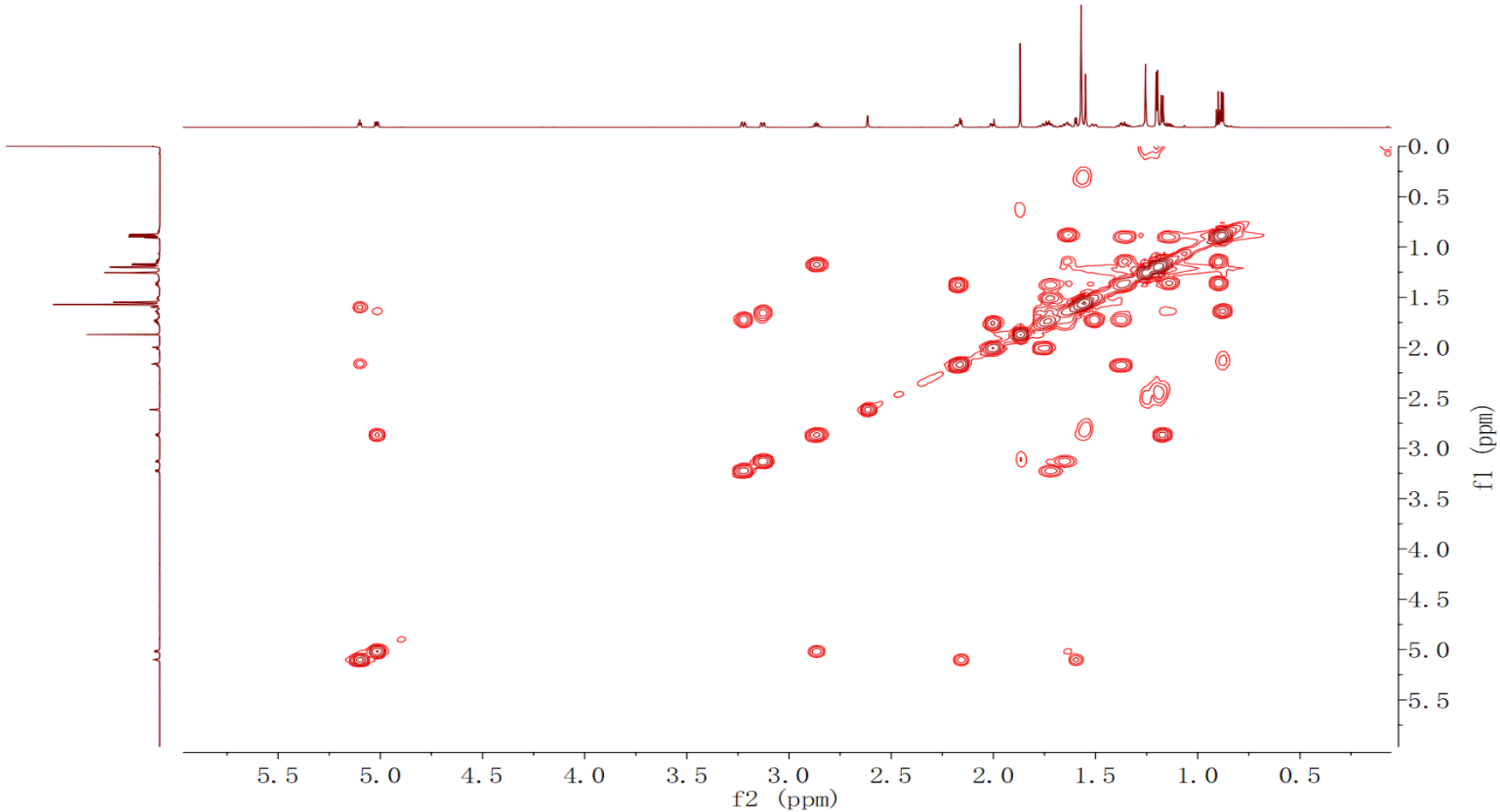

Figure S77. ^{1}H–^{1}H COSY spectrum of compound **9** (Recorded in $CDCl_3$)

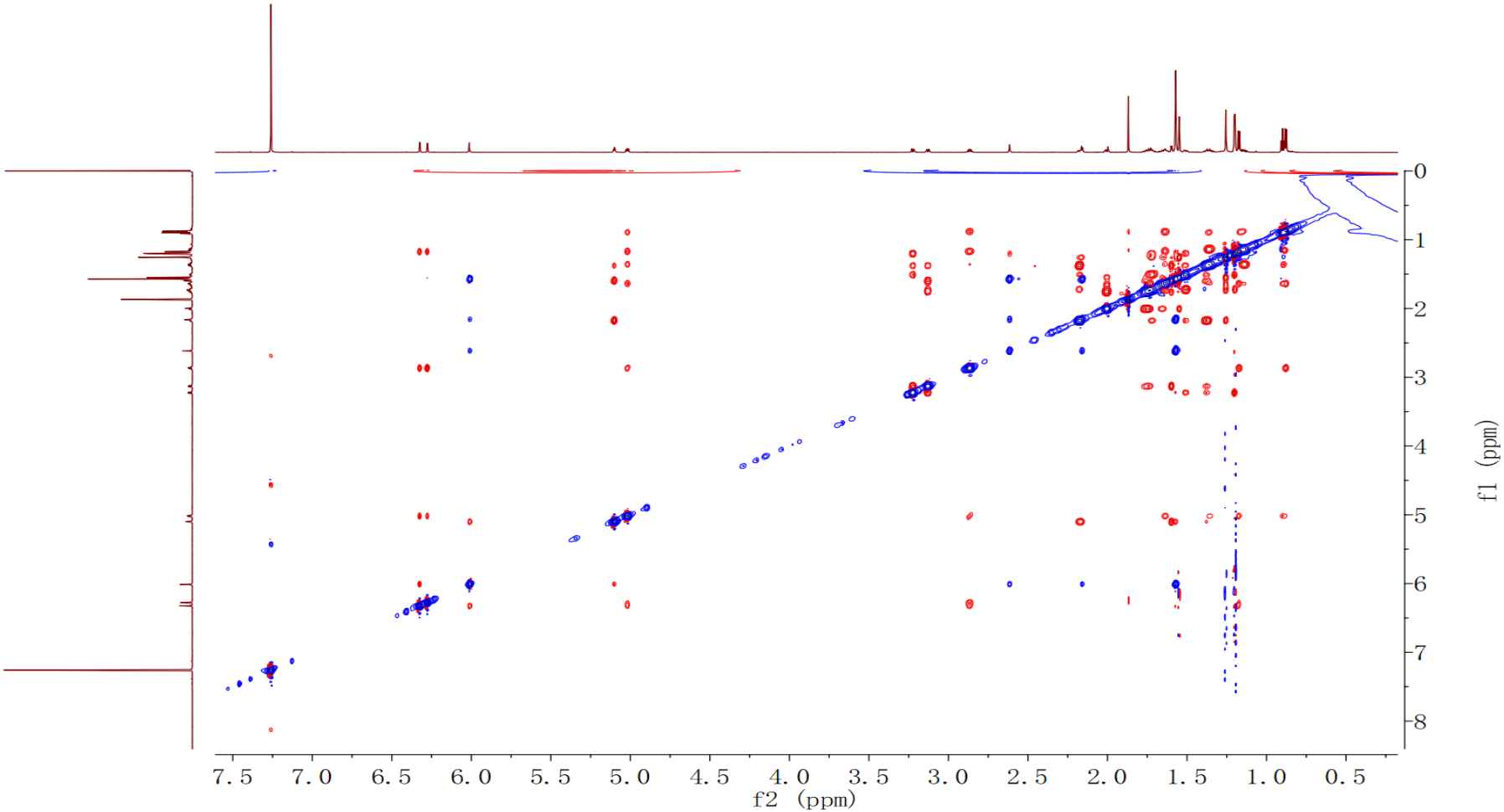

Figure S78. ROESY spectrum of compound **9** (Recorded in $CDCl_3$)

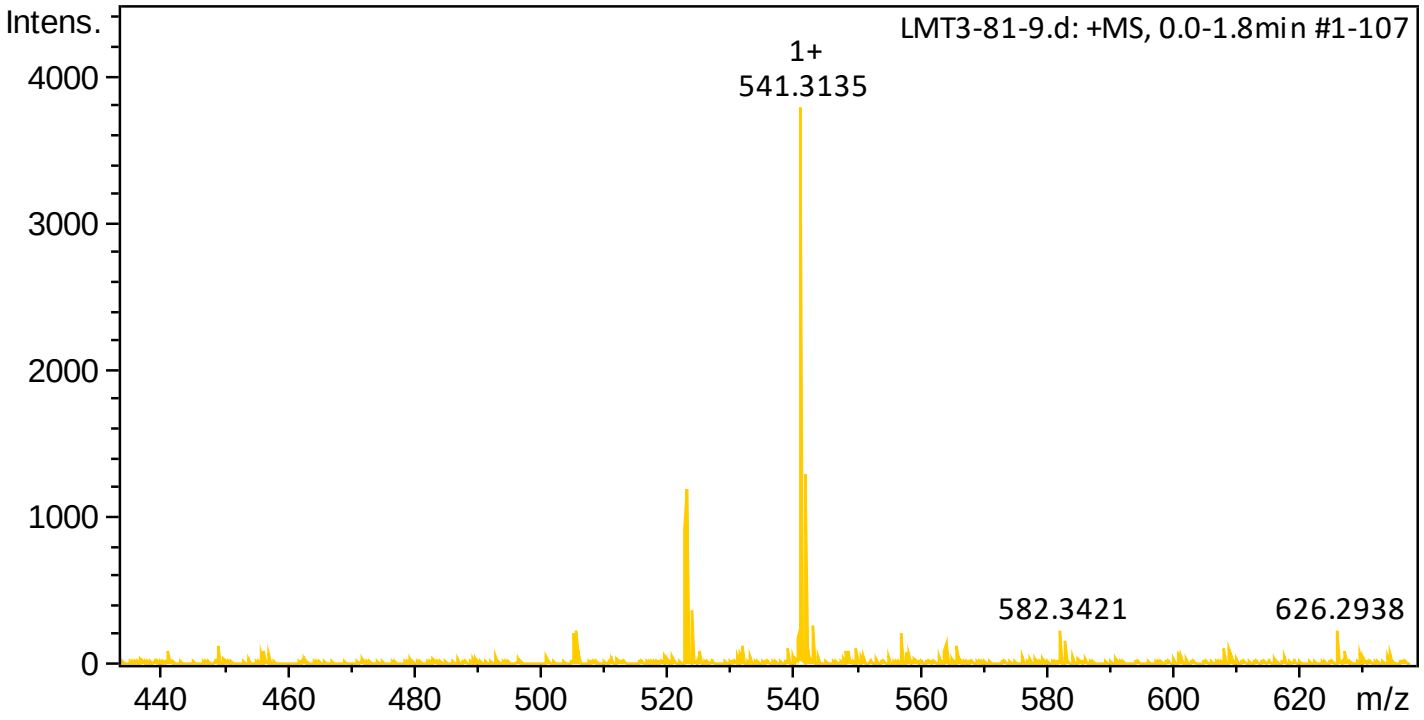

Figure S79. HRESIMS spectrum of compound **9**

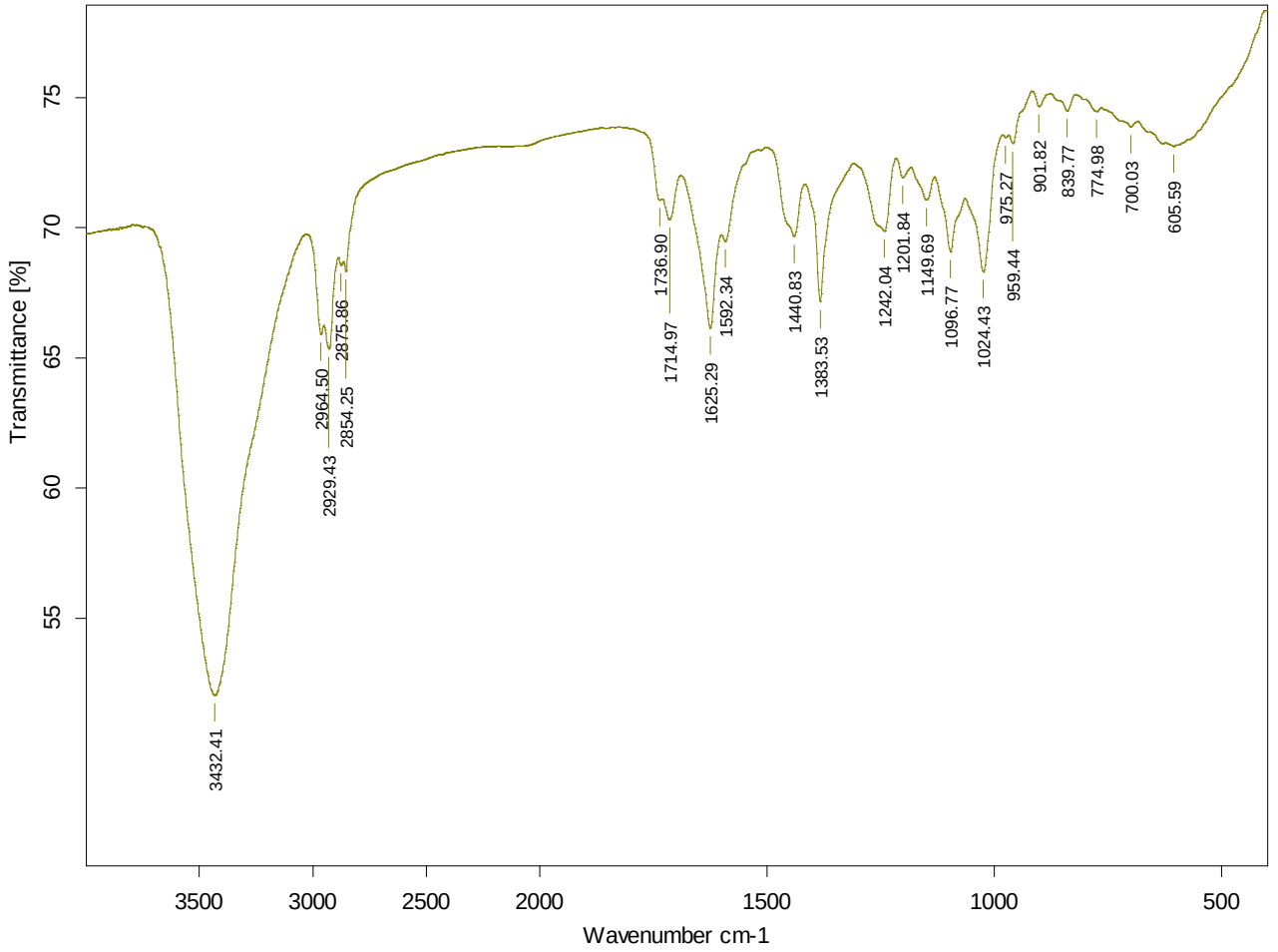

Figure S80. IR spectrum of compound **9**

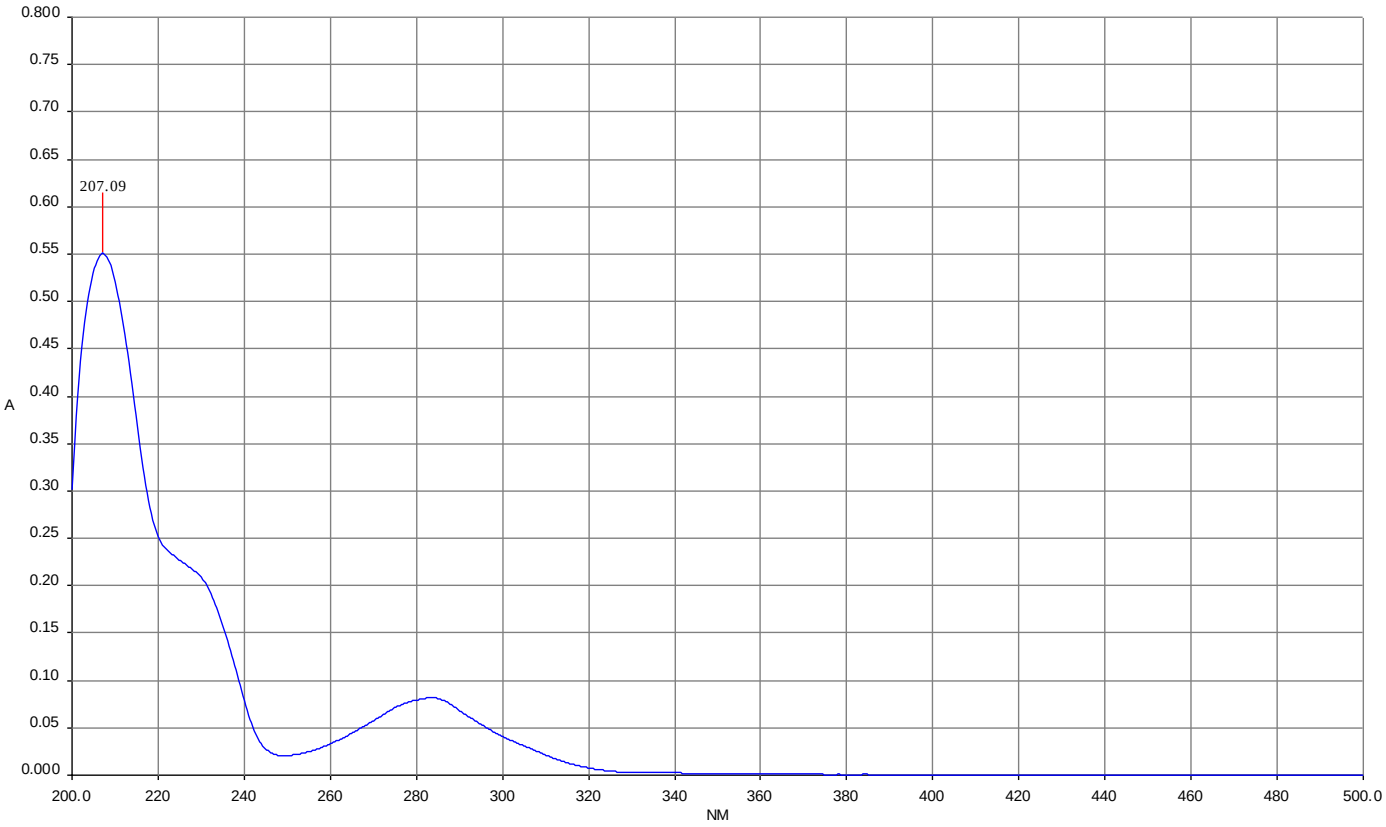

Figure S81. UV spectrum of compound **9**

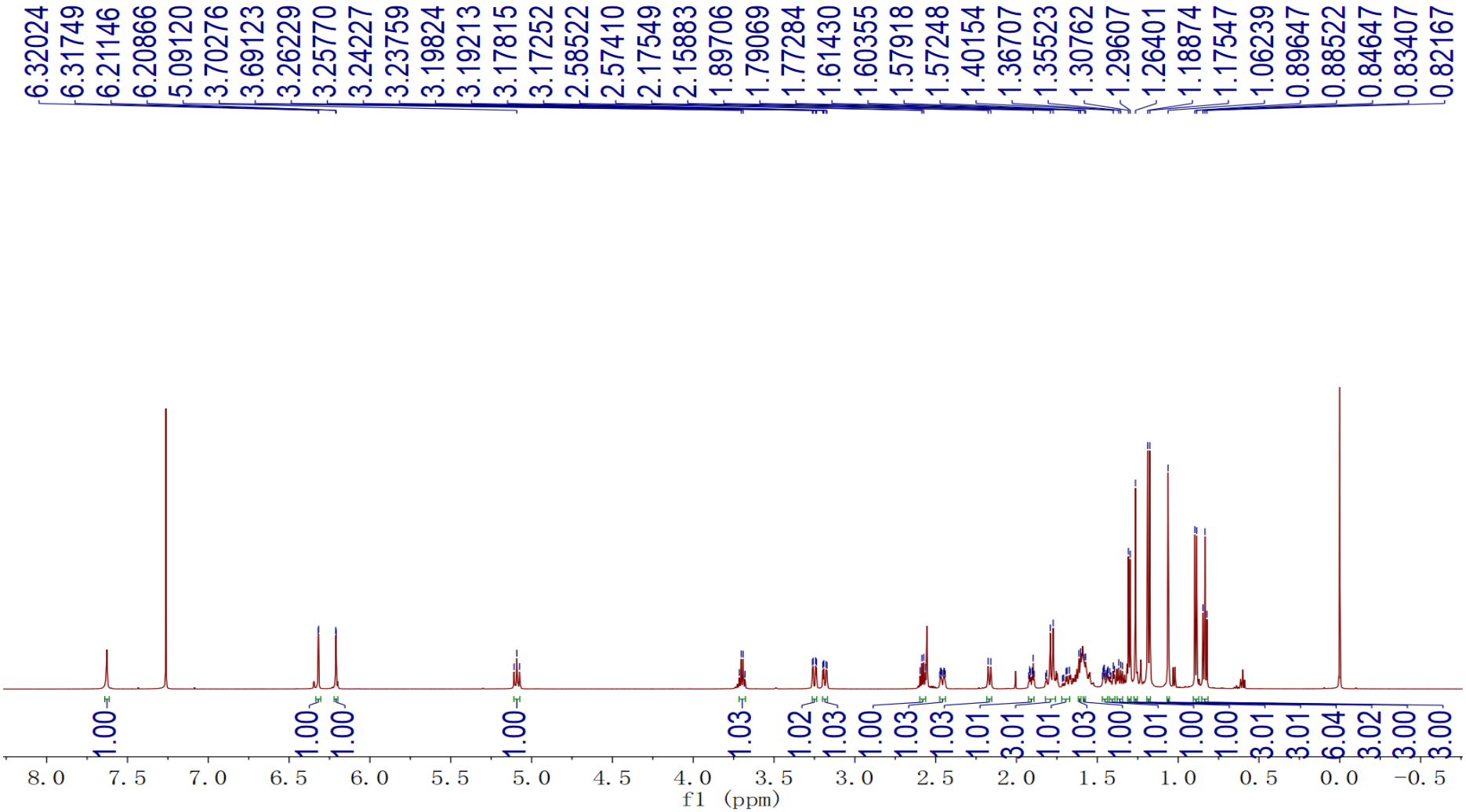

Figure S82. ^{1}H NMR spectrum of compound **10** (Recorded in $CDCl_3$)

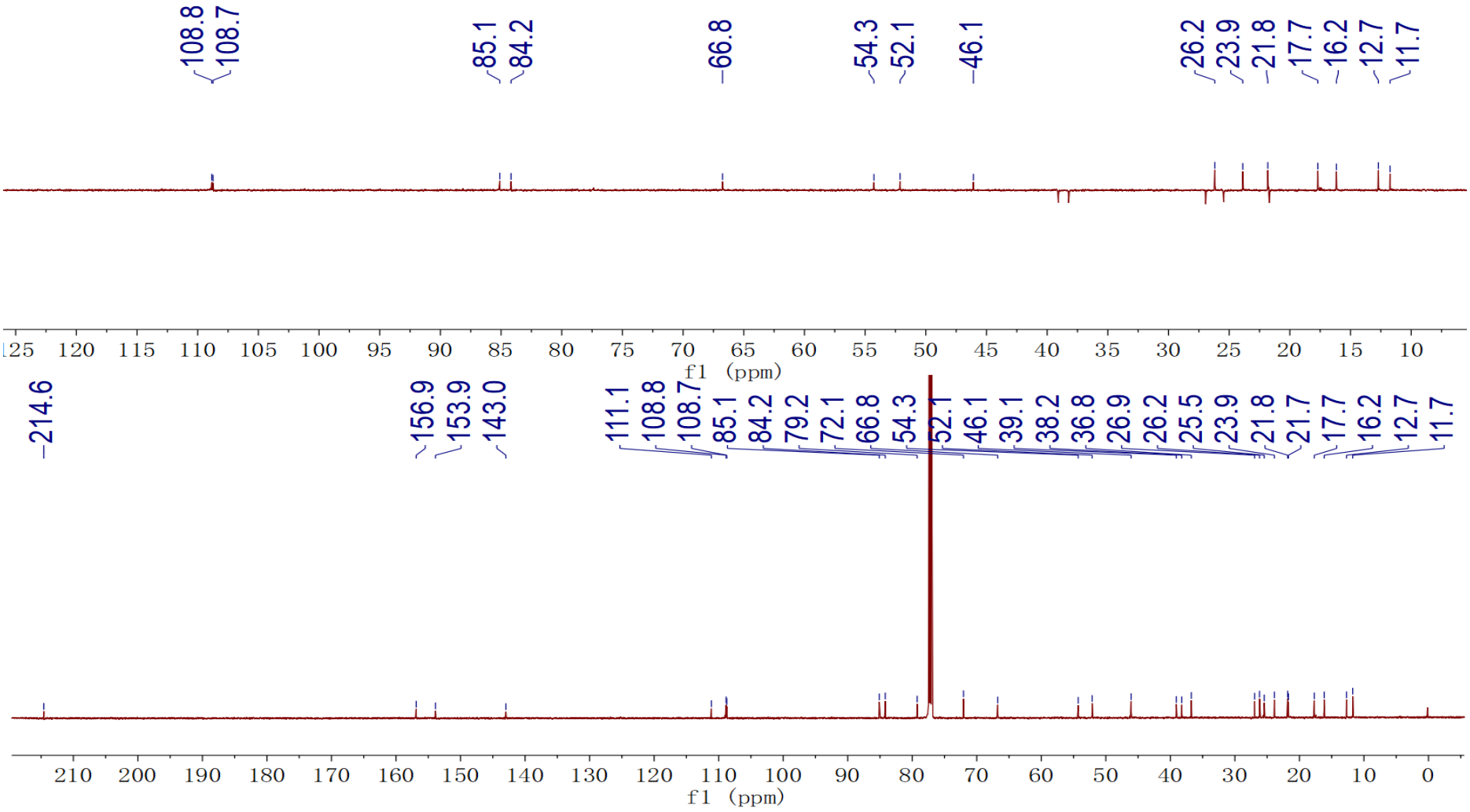

Figure S83. ^{13}C NMR and DEPT spectra of compound **10** (Recorded in $CDCl_3$)

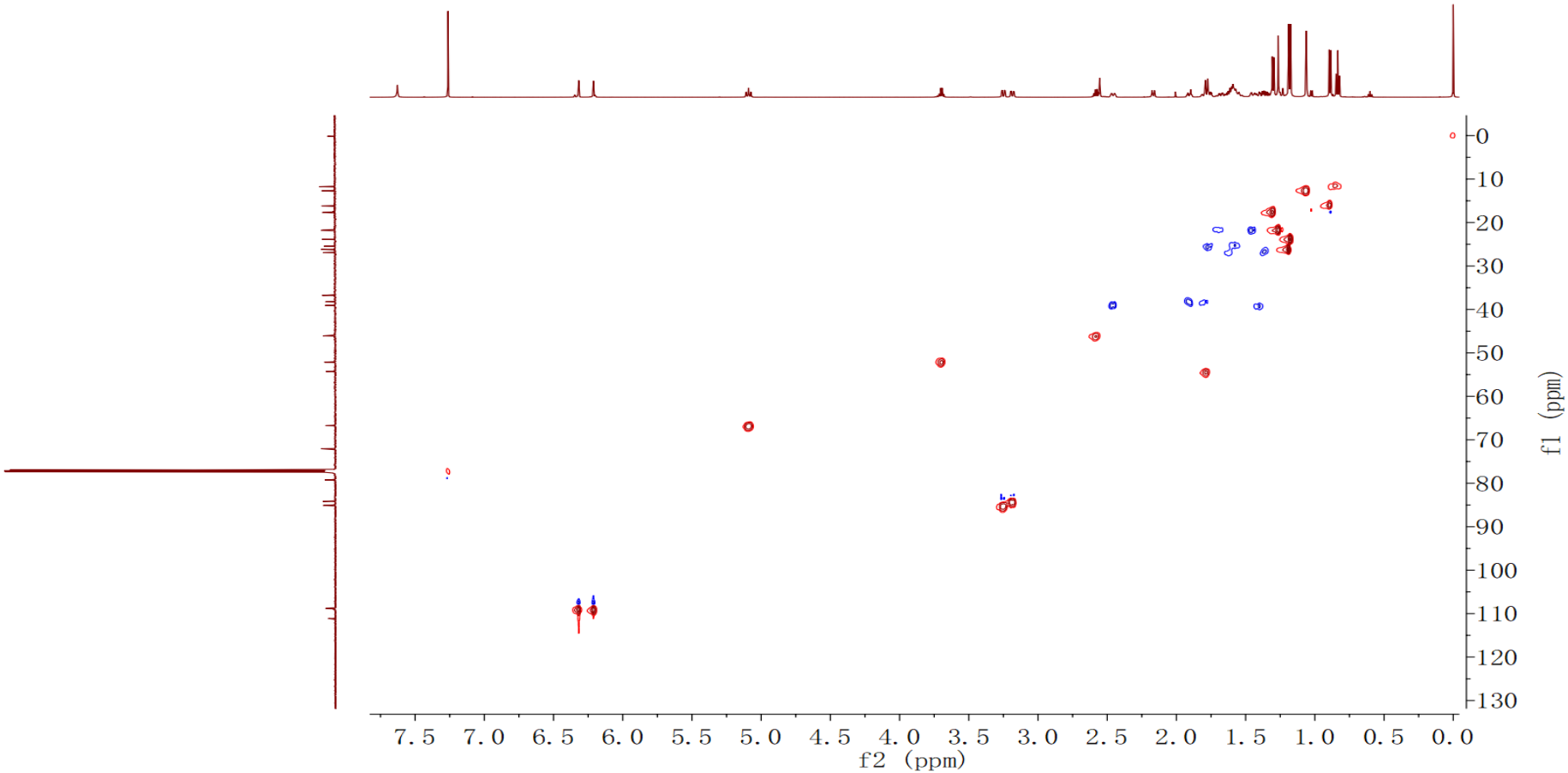

Figure S84. HSQC spectrum of compound **10** (Recorded in $CDCl_3$)

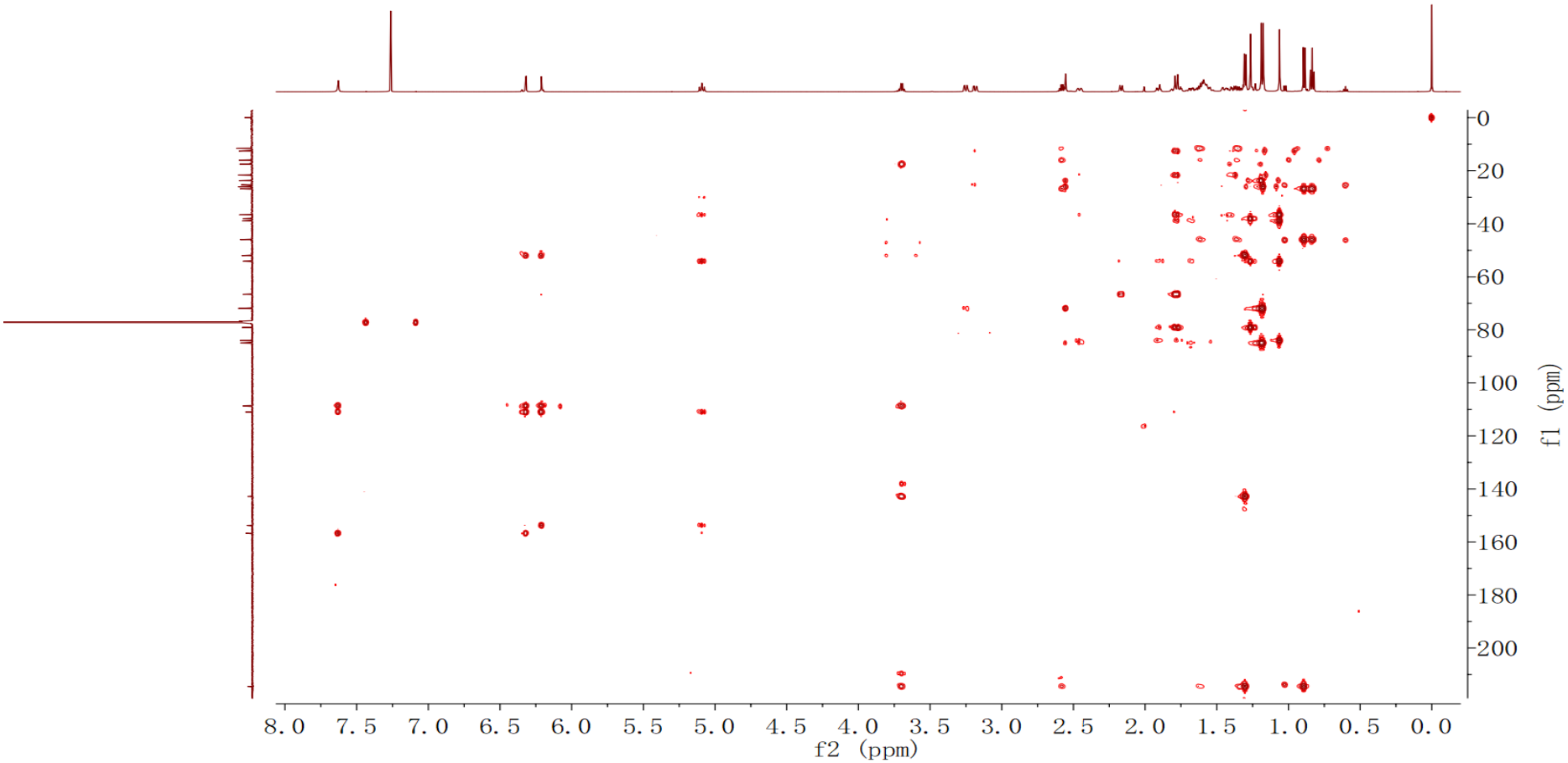

Figure S85. HMBC spectrum of compound **10** (Recorded in $CDCl_3$)

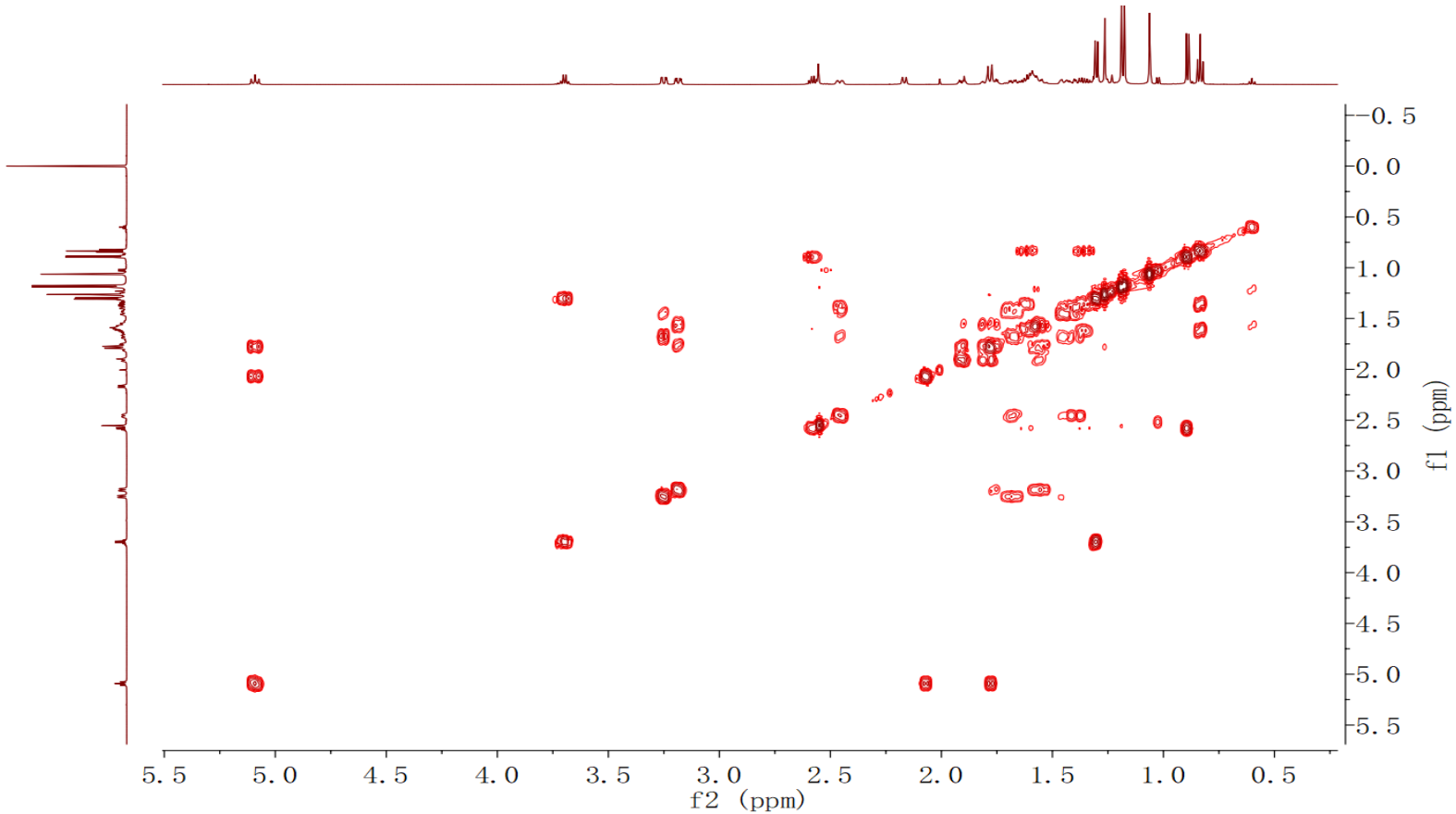

Figure S86. ^{1}H–^{1}H COSY spectrum of compound **10** (Recorded in $CDCl_3$)

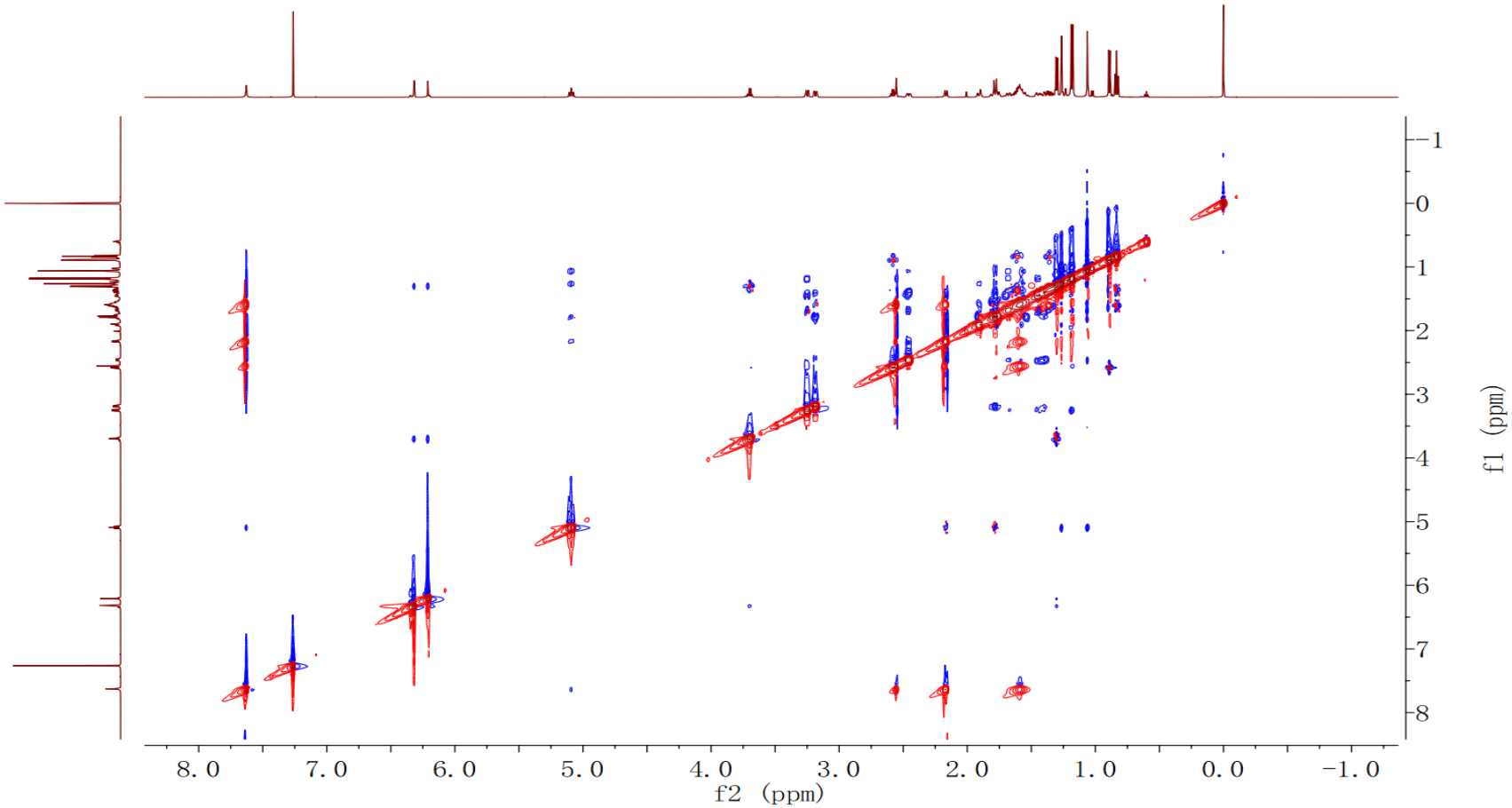

Figure S87. ROESY spectrum of compound **10** (Recorded in $CDCl_3$)

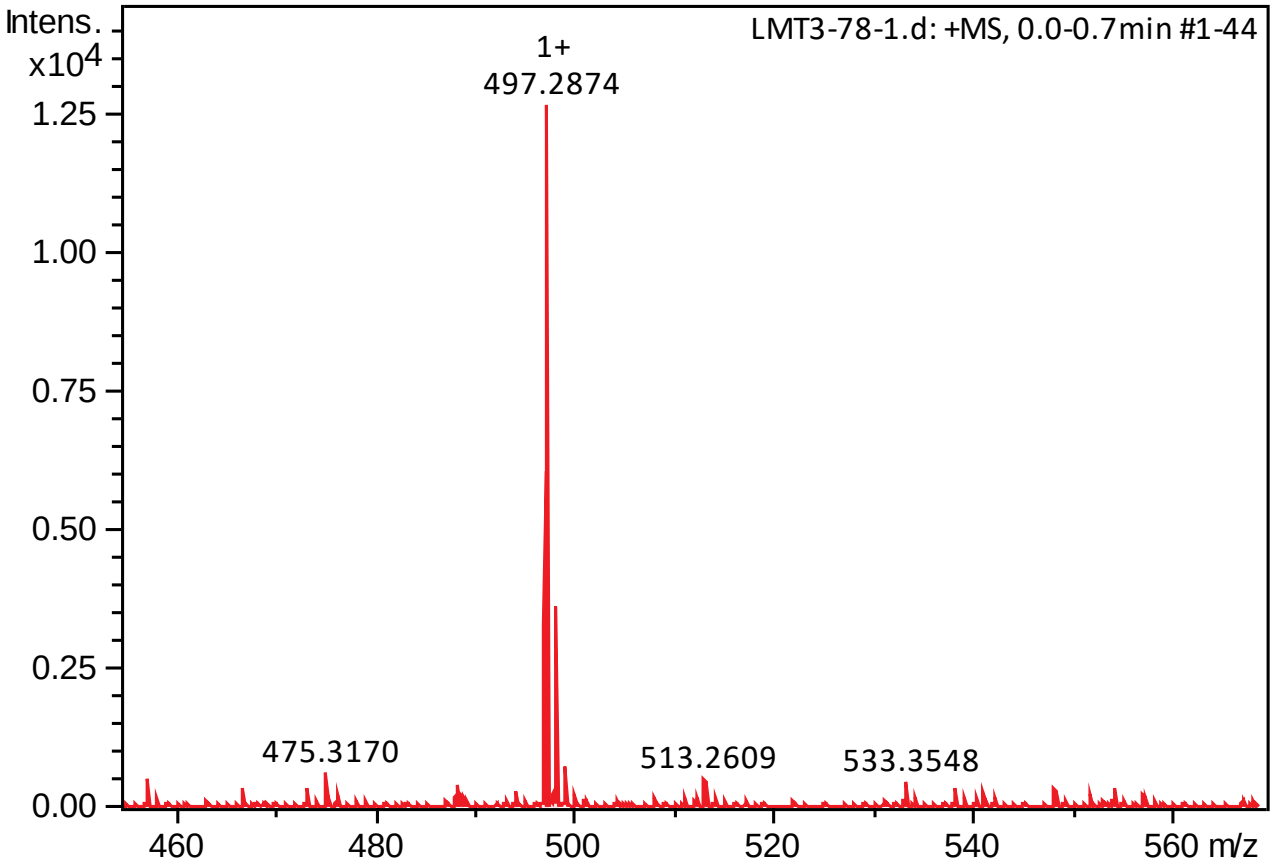

Figure S88. HRESIMS spectrum of compound **10**

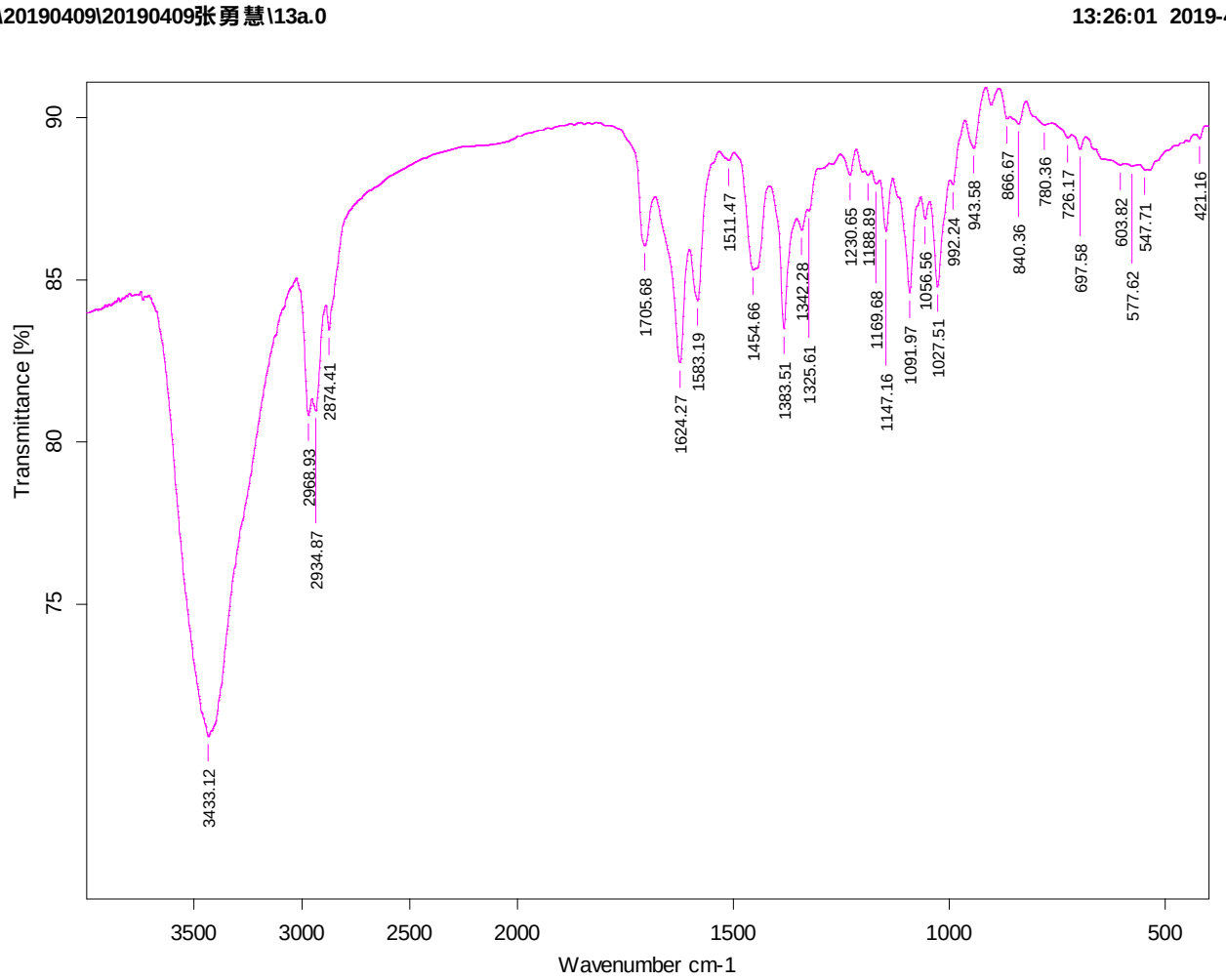

Figure S89. IR spectrum of compound **10**

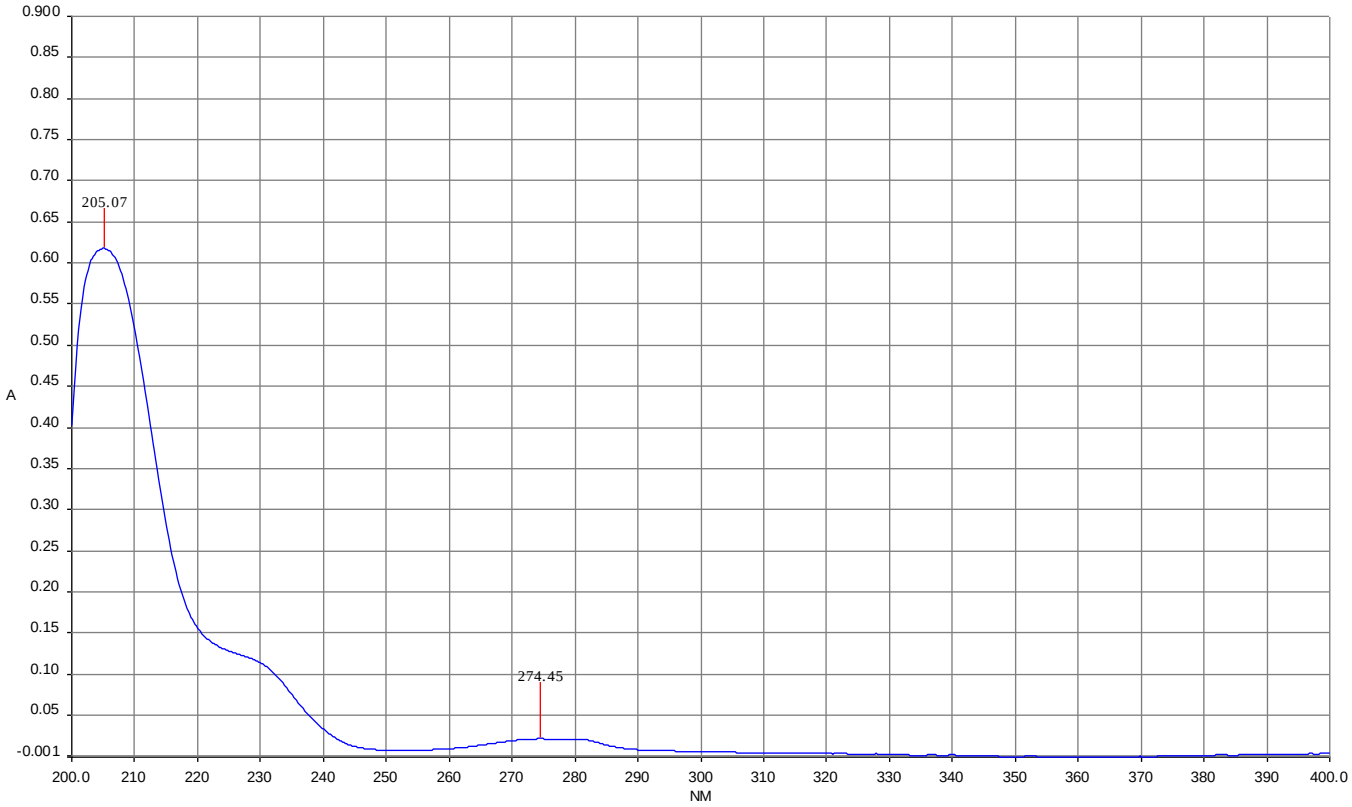

Figure S90. UV spectrum of compound **10**

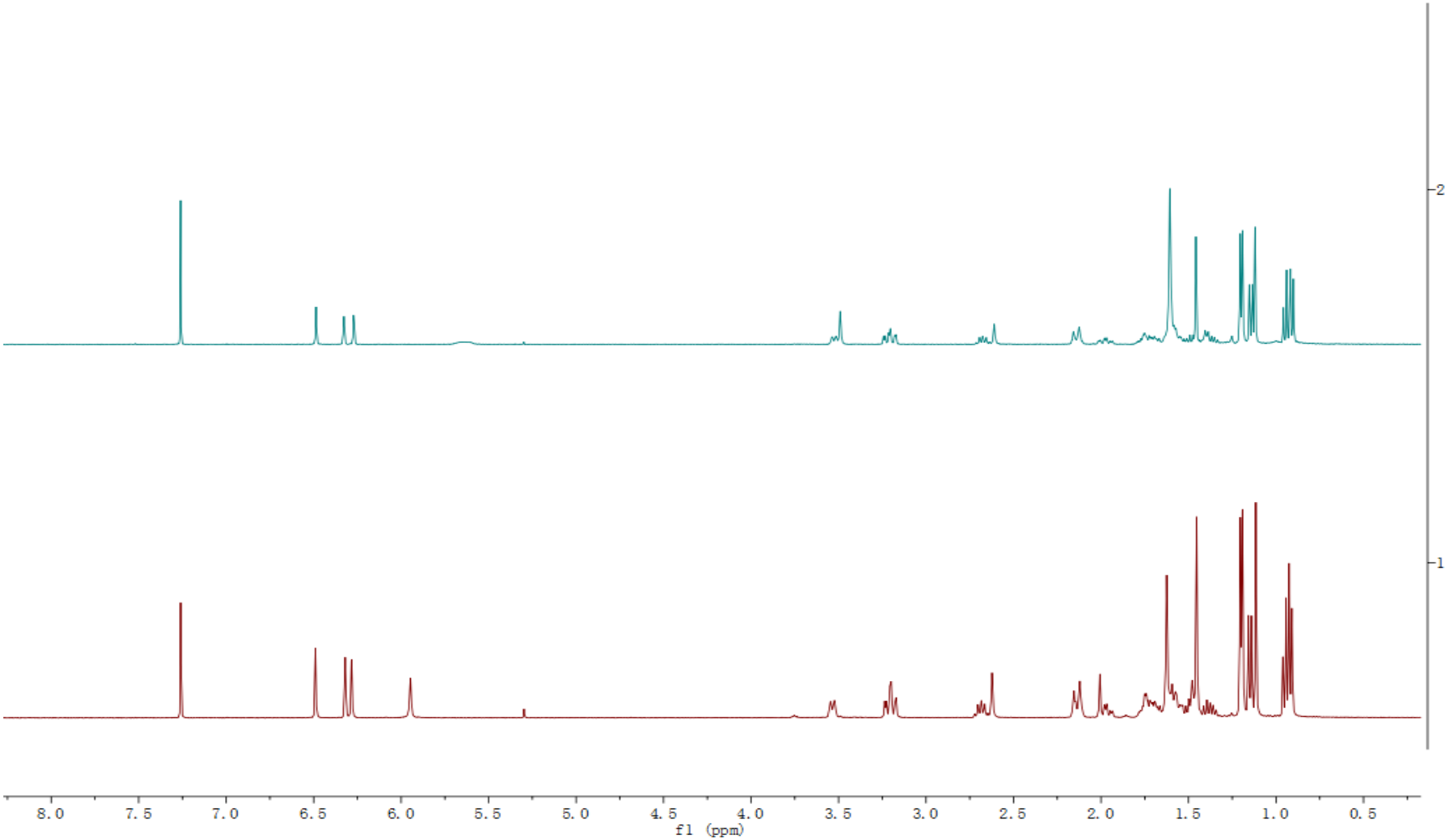

Figure S91. Comparison of ^{1}H NMR spectra of compounds **2a** (up) and **3** (down) (Recorded in $CDCl_3$)

Calculated ECD data of 4

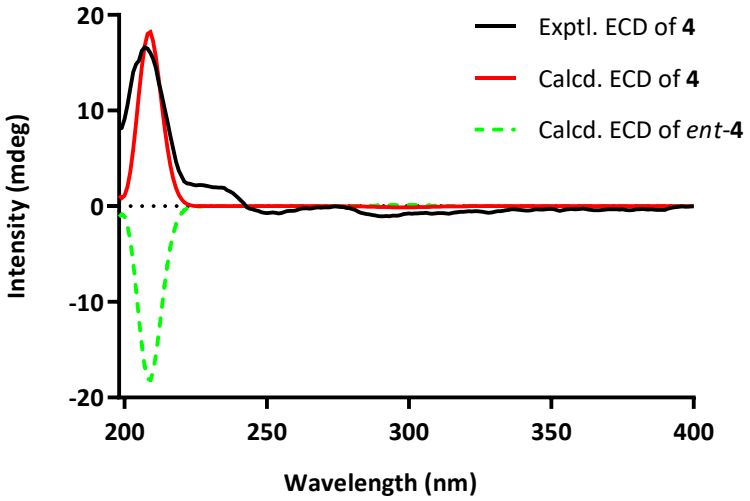

Figure 92. Experimental ECD spectrum (200-400 nm) of **4** in MeOH and the calculated ECD spectra of the model molecules of **4** at the DSD-PBEP86/def2-TZVP level.

ECD calculation details

1. Methods

In general, conformational analyses were carried out via random searching in the Sybyl-X 2.0 using the MMFF94S force field with an energy cutoff of 2.5 kcal/mol.[1] The results showed four lowest energy conformers for compound **4**. Subsequently, the conformers were re-optimized using DFT at the PBE0-D3(BJ)/def2-SVP level

in MeOH using the polarizable conductor calculation model (SMD) by the ORCA4.2.1 program.[2-3] The energies, oscillator strengths, and rotational strengths (velocity) of the first 60 electronic excitations were calculated using the TDDFT methodology at the DSD-PBEP86/def2-TZVP level in MeOH. The ECD spectra were simulated by the overlapping Gaussian function (half the bandwidth at 1/e peak height, sigma = 0.30 for all).[4] To get the final spectra, the simulated spectra of the conformers were averaged according to the Boltzmann distribution theory and their relative Gibbs free energy (ΔG). By comparing the experiment spectra with the calculated model molecules, the absolute configuration was determined.

(1). Sybyl Software, version X 2.0. Tripos Associates Inc.: St. Louis, MO, **2013**.
(2). Neese, F. The ORCA program system. WIREs Comput. Mol. Sci., **2012**, *2*, 73–78.
(3). Neese, F. Software update: the ORCA program system, version 4.0. WIREs Comput. Mol. Sci., **2017**, *8*, e1327.
(4). Stephens, P. J.; Harada, N. ECD cotton effect approximated by the Gaussian curve and other methods. Chirality **2010**, *22*, 229–233.

2. Results

Table S1. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **4**.

Conformers	ΔG (a.u.)	P(%)/100	Single point energy (a.u.)
000001_tddft_	0.00209	7.44	-1469.6101457046
000002_tddft_	0.00102	22.96	-1469.6112084795
000003_tddft_	0.0	68.02	-1469.6122333637
000004_tddft_	0.00355	1.58	-1469.6086816826

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15 K.

Table S2. Cartesian coordinates for the low-energy reoptimized random research conformers of **4** at PBE0-D3(BJ)/def2-SVP level of theory in methanol.

000001_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.773135	-8.573996	2.379122
1	6	0	-6.513339	-7.73243	2.21434
2	8	0	-6.886184	-5.971643	0.204569
3	6	0	-5.347115	-3.792442	0.495494
4	6	0	-2.518841	-4.438695	0.302833
5	6	0	-2.005048	-6.30383	2.469295
6	6	0	-6.170183	-1.774314	-1.34414
7	6	0	-4.729824	0.653224	-0.799495
8	6	0	-1.875895	0.299095	-0.911229
9	6	0	-1.052776	-1.960315	0.737738
10	8	0	-0.854241	2.562303	0.279654

11	6	0	1.6653	2.542613	0.824621
12	6	0	3.045633	0.306994	1.003474
13	6	0	1.805357	-2.215674	0.681919
14	6	0	2.789458	4.884187	1.247744
15	6	0	5.330858	5.052562	1.857462
16	6	0	6.759826	2.844927	1.96525
17	6	0	5.616458	0.52423	1.558652
18	8	0	6.947045	-1.695995	1.709307
19	6	0	-8.452585	-9.865098	1.854819
20	6	0	-8.121784	-11.234839	-0.652084
21	6	0	-11.114508	-8.798772	2.078659
22	8	0	-7.958581	-11.554809	3.928378
23	6	0	-0.953717	0.318245	-3.637317
24	6	0	-1.905775	-5.730299	-2.20561
25	6	0	6.493365	7.608518	2.331232
26	6	0	7.581097	8.025334	4.98556
27	6	0	5.775869	7.66217	7.237506
28	6	0	5.06813	4.920113	7.804503
29	6	0	3.471281	9.368523	7.003443
30	6	0	4.023122	4.531051	10.451628
31	6	0	8.447858	8.264375	0.30805
32	8	0	9.812227	6.516009	5.244521
33	1	0	-6.995378	-6.79011	4.003904
34	1	0	-5.6585	-3.044531	2.413043
35	1	0	-1.552333	-1.353452	2.652328
36	1	0	-3.301479	-9.765	0.770513

37	1	0	-3.53607	-9.734134	4.059324
38	1	0	-0.049125	-6.947117	2.423568
39	1	0	-2.258186	-5.312252	4.265386
40	1	0	-5.88063	-2.412816	-3.281253
41	1	0	-8.193308	-1.451752	-1.133362
42	1	0	-5.201902	1.312513	1.096192
43	1	0	-5.286023	2.150208	-2.10069
44	1	0	2.431822	-3.102752	-1.073421
45	1	0	2.439485	-3.473139	2.181816
46	1	0	1.6288	6.558565	1.090581
47	1	0	8.739707	2.938748	2.460232
48	1	0	8.671092	-1.299466	2.142516
49	1	0	-9.590492	-12.662752	-0.880604
50	1	0	-6.303869	-12.185933	-0.740923
51	1	0	-8.255957	-9.92178	-2.226627
52	1	0	-12.511946	-10.305209	1.89968
53	1	0	-11.368909	-7.893536	3.90857
54	1	0	-11.480521	-7.414199	0.606759
55	1	0	-9.286796	-12.800577	3.941963
56	1	0	1.022011	-0.207772	-3.814308
57	1	0	-2.057515	-0.928752	-4.833378
58	1	0	-1.164501	2.227756	-4.370772
59	1	0	-3.30678	-7.16771	-2.628768
60	1	0	-1.86649	-4.435486	-3.789067
61	1	0	-0.067415	-6.650132	-2.125952
62	1	0	4.971306	8.9884	2.164648

63	1	0	8.137496	10.028219	5.024396
64	1	0	6.864273	8.345152	8.872998
65	1	0	3.70153	4.258097	6.416993
66	1	0	6.738359	3.743636	7.551298
67	1	0	2.456233	9.504754	8.785884
68	1	0	4.000101	11.283225	6.453998
69	1	0	2.154337	8.644634	5.597944
70	1	0	3.661238	2.535985	10.810421
71	1	0	5.349714	5.187087	11.888785
72	1	0	2.248443	5.531243	10.745648
73	1	0	9.182749	10.169112	0.588468
74	1	0	7.59566	8.168803	-1.561504
75	1	0	10.038081	6.966656	0.352914
76	1	0	10.48676	6.821248	6.908441

000002_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.369545	-8.730242	1.936613
1	6	0	-6.055975	-7.846688	2.428384
2	8	0	-6.731616	-5.803831	0.800894
3	6	0	-5.085769	-3.707198	1.111575
4	6	0	-2.367259	-4.335027	0.294249
5	6	0	-1.524859	-6.52009	2.012667
6	6	0	-6.160084	-1.425126	-0.219435
7	6	0	-4.562211	0.882335	0.40321
8	6	0	-1.790192	0.531762	-0.290096
9	6	0	-0.764779	-1.959594	0.825696
10	8	0	-0.489396	2.579721	1.014452
11	6	0	2.087046	2.467349	1.051069
12	6	0	3.394806	0.21441	0.673141
13	6	0	2.031735	-2.225363	0.237821
14	6	0	3.353886	4.724687	1.528326
15	6	0	5.969868	4.791725	1.635625
16	6	0	7.311264	2.559878	1.237235
17	6	0	6.029204	0.324161	0.770418
18	8	0	7.284022	-1.913099	0.391317
19	6	0	-8.104095	-9.886084	2.14068
20	6	0	-8.294154	-10.872571	-0.554197
21	6	0	-10.637835	-8.845379	3.014778
22	8	0	-7.294829	-11.868592	3.818832

23	6	0	-1.382636	0.964979	-3.106023
24	6	0	-2.261432	-5.216586	-2.452353
25	6	0	7.306884	7.266683	2.105891
26	6	0	8.920333	7.29499	4.520162
27	6	0	7.531771	6.356107	6.890205
28	6	0	5.229051	8.002581	7.473054
29	6	0	9.320058	6.231153	9.144113
30	6	0	3.59221	7.055199	9.635884
31	6	0	8.83001	8.114684	-0.193561
32	8	0	11.158217	5.854691	4.017781
33	1	0	-6.1547	-7.174571	4.393012
34	1	0	-5.008662	-3.256559	3.141982
35	1	0	-0.907947	-1.654057	2.867948
36	1	0	-3.265079	-9.668956	0.110306
37	1	0	-2.862884	-10.134883	3.3494
38	1	0	0.355004	-7.17397	1.483322
39	1	0	-1.379503	-5.818758	3.951586
40	1	0	-6.24916	-1.762363	-2.249778
41	1	0	-8.098966	-1.127213	0.408167
42	1	0	-4.65516	1.249959	2.429811
43	1	0	-5.295413	2.563604	-0.534474
44	1	0	2.327615	-2.863566	-1.703102
45	1	0	2.869398	-3.686851	1.41987
46	1	0	2.244912	6.421421	1.785701
47	1	0	9.351059	2.566906	1.345234
48	1	0	9.071826	-1.596255	0.535509

49	1	0	-9.839965	-12.227188	-0.706391
50	1	0	-6.565566	-11.827493	-1.117298
51	1	0	-8.660579	-9.337114	-1.86953
52	1	0	-12.092727	-10.303173	2.903331
53	1	0	-10.512931	-8.205239	4.966028
54	1	0	-11.230927	-7.264923	1.84482
55	1	0	-8.643219	-13.089732	3.905365
56	1	0	0.501976	0.44583	-3.730546
57	1	0	-2.74303	-0.057951	-4.249435
58	1	0	-1.642268	2.968818	-3.487697
59	1	0	-3.710136	-6.621227	-2.822706
60	1	0	-2.538968	-3.699129	-3.795394
61	1	0	-0.439198	-6.074667	-2.870946
62	1	0	5.844121	8.685554	2.403566
63	1	0	9.465401	9.275438	4.846012
64	1	0	6.869678	4.443046	6.481001
65	1	0	5.85953	9.932661	7.869254
66	1	0	4.045884	8.121368	5.796288
67	1	0	8.354431	5.56783	10.831215
68	1	0	10.875758	4.920357	8.828141
69	1	0	10.110412	8.089373	9.577348
70	1	0	1.883813	8.19087	9.807898
71	1	0	3.00962	5.105036	9.315026
72	1	0	4.55621	7.131525	11.451587
73	1	0	9.714648	9.944103	0.150071
74	1	0	7.600662	8.28921	-1.833632

75	1	0	10.316549	6.775754	-0.645594
76	1	0	12.305168	6.106695	5.40488

000003_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-4.548746	-8.127971	2.821524
1	6	0	-7.002196	-7.02217	1.820766
2	8	0	-6.593332	-5.587945	-0.427754
3	6	0	-4.872256	-3.571533	-0.011058
4	6	0	-2.213749	-4.541376	0.655774
5	6	0	-2.544127	-6.079539	3.099687
6	6	0	-4.894523	-1.79622	-2.242988
7	6	0	-3.310764	0.523103	-1.626058
8	6	0	-0.60375	-0.145084	-0.909431
9	6	0	-0.559414	-2.196733	1.161846
10	8	0	0.394937	2.152976	0.230823
11	6	0	2.659623	1.954162	1.451544
12	6	0	3.609425	-0.364497	2.271852
13	6	0	2.152225	-2.761951	1.912136
14	6	0	3.953373	4.201369	1.883772
15	6	0	6.255555	4.185254	3.134082
16	6	0	7.248031	1.889139	3.934089
17	6	0	5.941859	-0.341756	3.497452
18	8	0	6.864822	-2.641658	4.261108
19	6	0	-9.097029	-8.949187	1.243259
20	6	0	-8.378468	-10.74839	-0.881285
21	6	0	-11.535827	-7.562706	0.607873
22	8	0	-9.391069	-10.314275	3.577795

23	6	0	0.97244	-0.655757	-3.262219
24	6	0	-1.175841	-6.281252	-1.401587
25	6	0	7.688971	6.608818	3.605927
26	6	0	8.741056	7.664733	1.123709
27	6	0	10.105229	10.217149	1.339402
28	6	0	10.923889	11.130143	-1.283298
29	6	0	12.31273	10.130777	3.17921
30	6	0	11.574678	13.92402	-1.423674
31	6	0	6.066962	8.528519	5.018819
32	8	0	10.373747	5.751033	0.129961
33	1	0	-7.756006	-5.744277	3.278131
34	1	0	-5.544304	-2.496853	1.640218
35	1	0	-1.432992	-1.252723	2.782682
36	1	0	-3.870252	-9.609726	1.566919
37	1	0	-4.916682	-9.019107	4.637125
38	1	0	-0.756956	-6.92935	3.670148
39	1	0	-3.095755	-4.79047	4.61901
40	1	0	-4.202603	-2.757751	-3.927975
41	1	0	-6.83579	-1.236894	-2.643836
42	1	0	-4.15344	1.518133	-0.029189
43	1	0	-3.294443	1.849133	-3.202558
44	1	0	3.076883	-3.953369	0.502835
45	1	0	2.195952	-3.852279	3.656752
46	1	0	3.114381	5.935826	1.206898
47	1	0	9.074829	1.839389	4.859973
48	1	0	8.465253	-2.372481	5.087075

49	1	0	-9.943658	-12.027003	-1.28687
50	1	0	-6.752903	-11.89343	-0.366955
51	1	0	-7.939563	-9.713307	-2.600963
52	1	0	-13.061009	-8.90584	0.256534
53	1	0	-12.09299	-6.344433	2.168889
54	1	0	-11.307535	-6.408427	-1.074973
55	1	0	-10.862144	-11.373924	3.405455
56	1	0	2.835081	-1.393885	-2.821475
57	1	0	0.045729	-1.96951	-4.535815
58	1	0	1.218261	1.119694	-4.269597
59	1	0	-2.589651	-7.664546	-1.945838
60	1	0	-0.617971	-5.285283	-3.099977
61	1	0	0.473946	-7.304535	-0.721743
62	1	0	9.311271	6.136609	4.787802
63	1	0	7.135065	7.934899	-0.162631
64	1	0	8.707574	11.57374	2.029537
65	1	0	12.552575	10.024482	-1.913408
66	1	0	9.400364	10.742259	-2.627408
67	1	0	13.335813	11.913661	3.214265
68	1	0	11.698652	9.752924	5.104969
69	1	0	13.634112	8.648545	2.641531
70	1	0	12.081446	14.471804	-3.342588
71	1	0	9.974692	15.087816	-0.848109
72	1	0	13.163966	14.410572	-0.211561
73	1	0	7.181459	10.109115	5.715689
74	1	0	5.159553	7.635297	6.632994

75	1	0	4.577196	9.293521	3.821335
76	1	0	10.7482	6.178803	-1.597881

000004_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-3.754225	-8.718495	2.111987
1	6	0	-6.480544	-7.82047	2.185649
2	8	0	-6.937971	-5.904479	0.341885
3	6	0	-5.337873	-3.78006	0.703359
4	6	0	-2.543624	-4.4566	0.276826
5	6	0	-1.931244	-6.494536	2.255028
6	6	0	-6.229022	-1.611652	-0.919623
7	6	0	-4.70453	0.74313	-0.291356
8	6	0	-1.871111	0.349642	-0.607694
9	6	0	-0.997329	-2.046953	0.804999
10	8	0	-0.727749	2.491654	0.694849
11	6	0	1.823053	2.388842	1.0561
12	6	0	3.160125	0.122191	0.963855
13	6	0	1.845105	-2.346798	0.543458
14	6	0	3.030064	4.671774	1.567042
15	6	0	5.614876	4.748529	1.979882
16	6	0	6.994889	2.511415	1.822482
17	6	0	5.769237	0.248617	1.34008
18	8	0	7.05213	-2.00136	1.227064
19	6	0	-8.482332	-9.887407	1.786953
20	6	0	-8.301944	-11.10233	-0.813486
21	6	0	-11.105966	-8.785673	2.206802
22	8	0	-7.928888	-11.715129	3.724548

23	6	0	-1.111935	0.568625	-3.375489
24	6	0	-2.118968	-5.56102	-2.357681
25	6	0	6.882581	7.240368	2.522106
26	6	0	8.065351	7.516943	5.157083
27	6	0	6.224061	7.251608	7.391375
28	6	0	7.250822	8.588191	9.752072
29	6	0	5.537365	4.52938	8.026785
30	6	0	7.382822	11.452447	9.590242
31	6	0	8.795869	7.911219	0.466742
32	8	0	10.173592	5.830356	5.344792
33	1	0	-6.834433	-7.010428	4.067147
34	1	0	-5.512779	-3.183833	2.690181
35	1	0	-1.363158	-1.583345	2.788318
36	1	0	-3.412894	-9.791891	0.392015
37	1	0	-3.437124	-10.007983	3.681497
38	1	0	0.001253	-7.167408	2.020923
39	1	0	-2.036497	-5.64304	4.135954
40	1	0	-6.076114	-2.108399	-2.913481
41	1	0	-8.227693	-1.271006	-0.557626
42	1	0	-5.044061	1.273431	1.671821
43	1	0	-5.308241	2.341499	-1.443076
44	1	0	2.33885	-3.108878	-1.310301
45	1	0	2.545695	-3.72495	1.901386
46	1	0	1.903683	6.375325	1.633722
47	1	0	9.007295	2.528612	2.171932
48	1	0	8.811154	-1.673852	1.567556

49	1	0	-9.8328	-12.458063	-1.071554
50	1	0	-6.527448	-12.111466	-1.036906
51	1	0	-8.447325	-9.68575	-2.294787
52	1	0	-12.541928	-10.255592	2.028125
53	1	0	-11.245017	-7.97057	4.090536
54	1	0	-11.519896	-7.321573	0.827945
55	1	0	-9.273895	-12.942935	3.711606
56	1	0	0.824613	-0.017696	-3.714161
57	1	0	-2.337995	-0.527944	-4.599357
58	1	0	-1.283659	2.540492	-3.931259
59	1	0	-3.57044	-6.943711	-2.794521
60	1	0	-2.156033	-4.152914	-3.841742
61	1	0	-0.297671	-6.511195	-2.462814
62	1	0	5.405404	8.682145	2.476542
63	1	0	8.787026	9.459203	5.18961
64	1	0	4.493627	8.243679	6.83691
65	1	0	6.055252	8.069842	11.350966
66	1	0	9.119847	7.825965	10.222154
67	1	0	4.189859	4.489987	9.584104
68	1	0	4.697201	3.545983	6.438659
69	1	0	7.200169	3.464646	8.606338
70	1	0	8.005634	12.267028	11.37568
71	1	0	8.689073	12.104715	8.139407
72	1	0	5.532314	12.247755	9.155305
73	1	0	9.572139	9.795155	0.775766
74	1	0	7.89994	7.877823	-1.384319

75	1	0	10.364624	6.586552	0.439422
76	1	0	11.018017	6.171223	6.92017

Calculated ECD data of 10

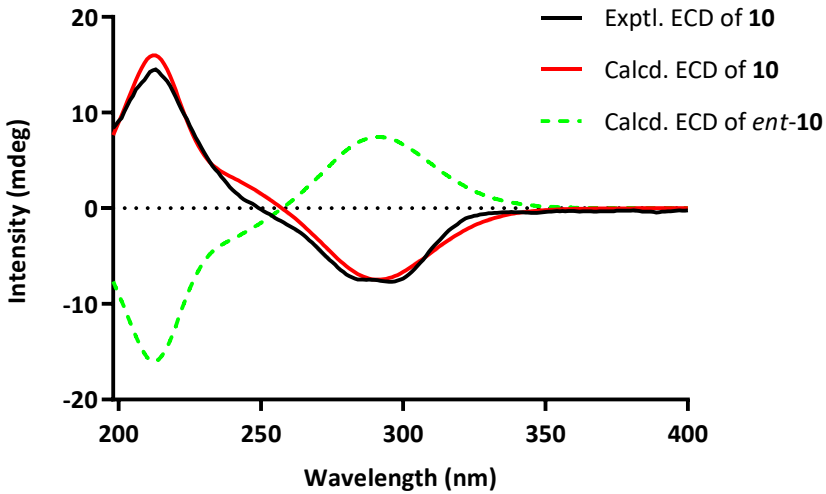

Figure S93. Experimental ECD spectrum (200-400 nm) of **10** in MeOH and the calculated ECD spectra of the model molecules of **10** at the PBE0/def2-TZVP level.

ECD calculation details

1. Methods

In general, conformational analyses were carried out via random searching in the Sybyl-X 2.0 using the MMFF94S force field with an energy cutoff of 2.5 kcal/mol.[1]

The results showed four lowest energy conformers for compound **10**. Subsequently, the conformers were re-optimized using DFT at the PBE0-D3(BJ)/def2-SVP level in MeOH using the polarizable conductor calculation model (SMD) by the ORCA4.2.1 program.[2-3] The energies, oscillator strengths, and rotational strengths (velocity) of the first 60 electronic excitations were calculated using the TDDFT methodology at the PBE0/def2-TZVP level in MeOH. The ECD spectra were simulated by the overlapping Gaussian function (half the bandwidth at 1/e peak height, sigma = 0.30 for all).[4] To get the final spectra, the simulated spectra of the conformers were averaged according to the Boltzmann distribution theory and their relative Gibbs free energy (ΔG). By comparing the experiment spectra with the calculated model molecules, the absolute configuration was determined.

(1). Sybyl Software, version X 2.0. Tripos Associates Inc.: St. Louis, MO, **2013**.
(2). Neese, F. The ORCA program system. WIREs Comput. Mol. Sci., **2012**, *2*, 73–78.
(3). Neese, F. Software update: the ORCA program system, version 4.0. WIREs Comput. Mol. Sci., **2017**, *8*, e1327.
(4). Stephens, P. J.; Harada, N. ECD cotton effect approximated by the Gaussian curve and other methods. Chirality **2010**, *22*, 229–233.

2. Results

Table S3. Gibbs free energies[a] and equilibrium populations[b] of low-energy conformers of **10**.

Conformers	ΔG (a.u.)	P(%)/100	Single point energy (a.u.)
000001000013_tddft_	0.00215	8.27	-1543.6588732475
000001000015_tddft_	0.0	80.72	-1543.6610230298
000001000018_tddft_	0.00234	6.76	-1543.6586828311
000001000019_tddft_	0.00278	4.25	-1543.6582444048

[a]wB97M-V/def2-TZVP, in a.u.

[b]From ΔG values at 298.15 K.

Table S4. Cartesian coordinates for the low-energy reoptimized random research conformers of **10** at PBE0-D3(BJ)/def2-SVP level of theory in methanol.

000001000013_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-4.913196	-8.940625	0.154167
1	6	0	-7.425991	-7.981399	1.142418
2	8	0	-7.817466	-5.406624	0.438106
3	6	0	-5.875784	-3.813141	1.37319
4	6	0	-3.302419	-4.406527	0.129082
5	6	0	-2.760219	-7.170343	0.877647
6	6	0	-6.695558	-1.097962	1.134117
7	6	0	-4.761348	0.574914	2.427815
8	6	0	-2.126385	0.254987	1.328408
9	6	0	-1.334679	-2.566295	1.283722
10	8	0	-0.487955	1.513195	3.140647
11	6	0	2.041068	1.299384	2.702724
12	6	0	3.027388	-0.712869	1.307129
13	6	0	1.345901	-2.733033	0.227759
14	6	0	3.575454	3.179459	3.694886
15	6	0	6.167502	3.087636	3.296426
16	6	0	7.195145	1.105268	1.914646
17	6	0	5.651539	-0.773274	0.925358
18	8	0	6.776736	-2.652685	-0.419658
19	6	0	-9.760512	-9.478317	0.279708
20	6	0	-10.146973	-9.361583	-2.567538
21	6	0	-12.094	-8.51933	1.658289
22	8	0	-9.215625	-12.030109	1.050332

23	6	0	-1.908298	1.71342	-1.147481
24	6	0	-3.449089	-4.237774	-2.749343
25	6	0	7.886631	5.12224	4.315514
26	6	0	7.309823	7.67869	3.078075
27	6	0	9.308041	8.750462	1.32614
28	6	0	9.113845	11.601137	1.012058
29	6	0	9.09102	7.373873	-1.213449
30	6	0	9.663822	13.078299	3.409726
31	6	0	7.706337	5.411663	7.184
32	1	0	-7.384185	-8.087482	3.218284
33	1	0	-5.646948	-4.213084	3.403685
34	1	0	-1.201156	-3.057645	3.292617
35	8	0	2.487633	-5.195511	0.603204
36	8	0	5.328305	8.765151	3.484092
37	1	0	-4.991045	-9.145508	-1.890893
38	1	0	-4.568336	-10.819588	0.91468
39	1	0	-1.01412	-7.818245	0.020685
40	1	0	-2.479708	-7.251737	2.926009
41	1	0	-6.946993	-0.59356	-0.847335
42	1	0	-8.537374	-0.871164	2.026476
43	1	0	-4.669437	0.09917	4.43176
44	1	0	-5.294382	2.560937	2.31946
45	1	0	1.291446	-2.574776	-1.827494
46	1	0	2.709599	4.735058	4.685386
47	1	0	9.209749	0.964686	1.605275
48	1	0	5.579917	-4.056537	-0.489572

49	1	0	-8.59467	-10.26891	-3.55887
50	1	0	-10.29257	-7.414413	-3.208118
51	1	0	-11.884992	-10.33734	-3.090027
52	1	0	-12.454321	-6.547751	1.211754
53	1	0	-13.756177	-9.610372	1.110493
54	1	0	-11.845075	-8.694464	3.693008
55	1	0	-10.744134	-12.999119	0.847676
56	1	0	-3.421375	1.24553	-2.447858
57	1	0	-2.055048	3.717547	-0.713526
58	1	0	-0.1219	1.420781	-2.113074
59	1	0	-1.830785	-5.17027	-3.612571
60	1	0	-5.141326	-5.168251	-3.439272
61	1	0	-3.490228	-2.31335	-3.446368
62	1	0	9.820929	4.602528	3.834076
63	1	0	11.15406	8.281368	2.136906
64	1	0	10.434592	12.170291	-0.469283
65	1	0	7.228344	12.06593	0.323196
66	1	0	7.263733	7.755009	-2.079598
67	1	0	10.557886	8.036008	-2.495669
68	1	0	9.281763	5.336681	-1.023213
69	1	0	11.507579	12.586527	4.191843
70	1	0	9.676624	15.103836	3.041001
71	1	0	8.244458	12.725642	4.854412
72	1	0	9.086614	6.776109	7.874369
73	1	0	8.062942	3.607283	8.103338
74	1	0	5.840769	6.070919	7.729406

75	1	0	2.669737	-5.42305	2.406685

000001000015_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-4.376807	-8.771801	-0.504374
1	6	0	-6.953645	-7.95192	0.443445
2	8	0	-7.370258	-5.330602	-0.039288
3	6	0	-5.509964	-3.795476	1.125951
4	6	0	-2.869155	-4.226723	-0.039456
5	6	0	-2.297883	-7.037118	0.475508
6	6	0	-6.372679	-1.082181	1.091788
7	6	0	-4.541121	0.488856	2.639174
8	6	0	-1.851608	0.315705	1.644632
9	6	0	-1.001491	-2.474118	1.384409
10	8	0	-0.318842	1.435552	3.635531
11	6	0	2.22863	1.315116	3.274128
12	6	0	3.312841	-0.534211	1.742616
13	6	0	1.730043	-2.508686	0.453096
14	6	0	3.685127	3.139744	4.474101
15	6	0	6.286311	3.169701	4.134124
16	6	0	7.408099	1.345818	2.608401
17	6	0	5.95075	-0.489798	1.433932
18	8	0	7.157755	-2.215304	-0.03313
19	6	0	-9.214095	-9.403215	-0.66028
20	6	0	-9.459105	-9.058939	-3.505167
21	6	0	-11.631948	-8.585055	0.665614
22	8	0	-8.664543	-11.998845	-0.06515

23	6	0	-1.557018	1.987123	-0.684217
24	6	0	-2.876443	-3.791378	-2.894394
25	6	0	7.94253	5.223667	5.223655
26	6	0	8.472162	7.144788	3.118361
27	6	0	6.33816	8.862253	2.248982
28	6	0	6.072369	8.839163	-0.627293
29	6	0	6.870369	11.53249	3.219541
30	6	0	5.259179	6.310124	-1.710874
31	6	0	6.926981	6.469289	7.609616
32	1	0	-7.005923	-8.248262	2.500352
33	1	0	-5.365271	-4.36653	3.122853
34	1	0	-0.959688	-3.151051	3.342399
35	8	0	2.914349	-4.965143	0.719093
36	8	0	10.563636	7.291463	2.179655
37	1	0	-4.35746	-8.787291	-2.561285
38	1	0	-4.029097	-10.705562	0.100105
39	1	0	-0.502512	-7.566552	-0.36073
40	1	0	-2.096246	-7.29993	2.517324
41	1	0	-6.520658	-0.399566	-0.846397
42	1	0	-8.262956	-0.967577	1.899538
43	1	0	-4.538625	-0.180406	4.589576
44	1	0	-5.109548	2.467561	2.693441
45	1	0	1.769815	-2.209942	-1.586795
46	1	0	2.725529	4.520251	5.627328
47	1	0	9.426745	1.340724	2.29814
48	1	0	6.016057	-3.64946	-0.242008

49	1	0	-7.833464	-9.838356	-4.488734
50	1	0	-9.635517	-7.070143	-3.992023
51	1	0	-11.138481	-10.035752	-4.193123
52	1	0	-12.02147	-6.597679	0.326002
53	1	0	-13.238343	-9.677569	-0.026012
54	1	0	-11.473191	-8.884686	2.69458
55	1	0	-10.121676	-12.985977	-0.533547
56	1	0	-1.705629	3.946478	-0.079639
57	1	0	0.248322	1.762639	-1.630387
58	1	0	-3.042121	1.650053	-2.054644
59	1	0	-1.253461	-4.705062	-3.768925
60	1	0	-4.566254	-4.589439	-3.740273
61	1	0	-2.812528	-1.812809	-3.418602
62	1	0	9.779476	4.395141	5.643416
63	1	0	4.5694	8.196185	3.073669
64	1	0	4.696562	10.290089	-1.141871
65	1	0	7.872809	9.413339	-1.448071
66	1	0	8.636937	12.236052	2.436756
67	1	0	5.357307	12.80877	2.654561
68	1	0	7.015	11.59737	5.27079
69	1	0	6.662037	4.849857	-1.35772
70	1	0	3.491356	5.672387	-0.869974
71	1	0	4.986322	6.43643	-3.747698
72	1	0	8.304755	7.7944	8.369034
73	1	0	6.54757	5.047	9.046719
74	1	0	5.183803	7.507744	7.283378

75	1	0	3.085503	-5.275064	2.511431

000001000018_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-4.373683	-9.168626	-0.486294
1	6	0	-6.878246	-8.464181	0.713129
2	8	0	-7.485188	-5.883257	0.216154
3	6	0	-5.609489	-4.21962	1.163003
4	6	0	-3.069735	-4.543228	-0.236974
5	6	0	-2.307	-7.309586	0.263732
6	6	0	-6.615067	-1.556251	1.145681
7	6	0	-4.741301	0.144178	2.492357
8	6	0	-2.137865	0.082564	1.279213
9	6	0	-1.172106	-2.667284	0.97522
10	8	0	-0.50446	1.298144	3.126149
11	6	0	2.011807	1.272921	2.586433
12	6	0	3.054225	-0.52907	0.963315
13	6	0	1.459371	-2.5694	-0.207026
14	6	0	3.480415	3.134263	3.708365
15	6	0	6.049543	3.249609	3.1934
16	6	0	7.128405	1.4969	1.563199
17	6	0	5.656291	-0.377825	0.464042
18	8	0	6.823779	-2.039976	-1.109273
19	6	0	-9.159049	-10.064139	-0.105685
20	6	0	-9.761492	-9.768954	-2.902096
21	6	0	-11.448514	-9.376796	1.493641
22	8	0	-8.385975	-12.615014	0.432301

23	6	0	-2.105993	1.734805	-1.082102
24	6	0	-3.369205	-4.162897	-3.084472
25	6	0	7.694851	5.238418	4.423156
26	6	0	6.540854	7.868867	4.064558
27	6	0	7.474791	9.424167	1.839736
28	6	0	6.721447	12.193454	2.088654
29	6	0	6.55091	8.22655	-0.627344
30	6	0	7.955569	13.918692	0.154054
31	6	0	8.093523	4.676433	7.223915
32	1	0	-6.693499	-8.70209	2.769871
33	1	0	-5.254141	-4.727701	3.151127
34	1	0	-0.906664	-3.303276	2.929725
35	8	0	2.778361	-4.966892	-0.077779
36	8	0	4.93021	8.651065	5.504761
37	1	0	-4.563247	-9.219797	-2.53358
38	1	0	-3.859679	-11.070242	0.101872
39	1	0	-0.567633	-7.767144	-0.719755
40	1	0	-1.913951	-7.519365	2.28389
41	1	0	-6.971272	-0.933176	-0.785177
42	1	0	-8.430255	-1.5164	2.116494
43	1	0	-4.541498	-0.474127	4.449531
44	1	0	-5.404173	2.092618	2.55556
45	1	0	1.295869	-2.259894	-2.238493
46	1	0	2.583031	4.498728	4.930138
47	1	0	9.125655	1.543745	1.134143
48	1	0	5.723812	-3.515363	-1.251782

49	1	0	-11.44178	-10.861533	-3.382622
50	1	0	-8.216041	-10.44944	-4.070578
51	1	0	-10.128357	-7.801271	-3.366713
52	1	0	-13.059345	-10.562688	0.99216
53	1	0	-11.03831	-9.654897	3.49037
54	1	0	-11.988939	-7.417011	1.202751
55	1	0	-9.838566	-13.687238	0.193565
56	1	0	-0.341607	1.616728	-2.120633
57	1	0	-3.636385	1.269735	-2.362511
58	1	0	-2.356334	3.688177	-0.49194
59	1	0	-3.531104	-2.196144	-3.63226
60	1	0	-1.756672	-4.947988	-4.092296
61	1	0	-5.050571	-5.120979	-3.764949
62	1	0	9.517097	5.207707	3.460898
63	1	0	9.542559	9.289518	1.856329
64	1	0	4.669484	12.339392	1.966181
65	1	0	7.204195	12.835223	3.986629
66	1	0	4.497209	8.317443	-0.738493
67	1	0	7.324881	9.224973	-2.248443
68	1	0	7.096744	6.253993	-0.791116
69	1	0	7.463895	15.884884	0.514065
70	1	0	10.0117	13.776133	0.2205
71	1	0	7.364917	13.48994	-1.769976
72	1	0	8.876229	2.789569	7.460071
73	1	0	6.309398	4.779793	8.232159
74	1	0	9.385818	6.034269	8.075759

75	1	0	3.107992	-5.292037	1.689685

000001000019_tddft_		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-4.780942	-8.663385	-0.622423
1	6	0	-7.127242	-7.990098	0.876665
2	8	0	-7.665878	-5.353888	0.683652
3	6	0	-5.632897	-3.85918	1.585099
4	6	0	-3.267024	-4.122089	-0.103511
5	6	0	-2.570936	-6.94691	0.058552
6	6	0	-6.518522	-1.177548	1.940201
7	6	0	-4.440694	0.315287	3.232944
8	6	0	-1.994856	0.303774	1.724357
9	6	0	-1.177239	-2.430092	1.0622
10	8	0	-0.119434	1.297662	3.470064
11	6	0	2.318397	1.250682	2.647172
12	6	0	3.105783	-0.426086	0.767489
13	6	0	1.312735	-2.301362	-0.389858
14	6	0	3.975317	2.958047	3.752222
15	6	0	6.47913	3.03331	2.971251
16	6	0	7.304192	1.397658	1.092673
17	6	0	5.644907	-0.317997	0.002108
18	8	0	6.566868	-1.87022	-1.825865
19	6	0	-9.541236	-9.426114	0.138569
20	6	0	-10.348552	-8.900578	-2.571001
21	6	0	-11.661838	-8.762713	1.964696
22	8	0	-8.848854	-12.039091	0.432217

23	6	0	-2.18512	2.17658	-0.461365
24	6	0	-3.846673	-3.460563	-2.853327
25	6	0	8.324211	4.849874	4.187778
26	6	0	7.222378	7.519624	4.147372
27	6	0	7.781541	9.19833	1.888748
28	6	0	7.186414	7.936541	-0.644958
29	6	0	10.51503	10.124972	2.065639
30	6	0	7.267913	9.748469	-2.871754
31	6	0	8.996247	4.03219	6.867626
32	1	0	-6.76434	-8.432514	2.874959
33	1	0	-5.09517	-4.582127	3.461884
34	1	0	-0.732842	-3.259303	2.908092
35	8	0	2.541182	-4.741371	-0.612143
36	8	0	5.955693	8.29594	5.902769
37	1	0	-5.17251	-8.532146	-2.637292
38	1	0	-4.289788	-10.624992	-0.251289
39	1	0	-0.972687	-7.362327	-1.156012
40	1	0	-1.962277	-7.357091	1.992549
41	1	0	-7.042047	-0.349789	0.127719
42	1	0	-8.220962	-1.175853	3.09802
43	1	0	-4.049077	-0.508181	5.082307
44	1	0	-5.012046	2.265537	3.565885
45	1	0	0.944948	-1.808705	-2.35784
46	1	0	3.269959	4.234713	5.178547
47	1	0	9.246407	1.411329	0.459096
48	1	0	5.397317	-3.291397	-1.970239

49	1	0	-12.134729	-9.845932	-2.97559
50	1	0	-8.953351	-9.594351	-3.908334
51	1	0	-10.61321	-6.88551	-2.874559
52	1	0	-13.352459	-9.861739	1.532022
53	1	0	-11.099554	-9.178835	3.899686
54	1	0	-12.149058	-6.771832	1.837623
55	1	0	-10.359661	-13.032789	0.215811
56	1	0	-0.594354	2.096662	-1.754799
57	1	0	-3.905085	1.908259	-1.542407
58	1	0	-2.244795	4.069564	0.338449
59	1	0	-4.005569	-1.44562	-3.179215
60	1	0	-2.371575	-4.174279	-4.096966
61	1	0	-5.617083	-4.315031	-3.43794
62	1	0	10.033081	4.837533	3.035146
63	1	0	6.536078	10.826102	2.125546
64	1	0	8.497407	6.382499	-0.974331
65	1	0	5.316551	7.075335	-0.538131
66	1	0	11.854588	8.596599	1.734422
67	1	0	10.87925	11.583847	0.6646
68	1	0	10.908294	10.933397	3.916284
69	1	0	6.673702	8.802063	-4.600359
70	1	0	6.009007	11.352286	-2.573773
71	1	0	9.157384	10.492176	-3.20274
72	1	0	10.403916	5.290218	7.688291
73	1	0	9.752692	2.119785	6.851716
74	1	0	7.3369	4.071285	8.073589

75	1	0	3.044141	-5.232048	1.074531