

## Supporting Information

### Uncommon Polyketides from *Penicillium steckii* AS-324, a Marine Endozoic Fungus Isolated from Deep-Sea Coral in the Magellan Seamount

Xue-Yi Hu <sup>1,2,3</sup>, Xiao-Ming Li <sup>1,3</sup>, Bin-Gui Wang <sup>1,2,3,4,\*</sup> and Ling-Hong Meng <sup>1,2,4,\*</sup>

<sup>1</sup> CAS and Shandong Province Key Laboratory of Experimental Marine Biology, Institute of Oceanology, Chinese Academy of Sciences, Nanhai Road 7, Qingdao 266071, China; xueyihu61@163.com (X.-Y.H.); lixmqd@qdio.ac.cn (X.-M.L.)

<sup>2</sup> Laboratory of Marine Biology and Biotechnology, Qingdao National Laboratory for Marine Science and Technology, Wenhai Road 1, Qingdao 266237, China

<sup>3</sup> College of Marine Science, University of Chinese Academy of Sciences, Yuquan Road 19A, Beijing 100049, China

<sup>4</sup> Center for Ocean Mega-Science, Chinese Academy of Sciences, Nanhai Road 7, Qingdao 266071, China

\* Correspondence: wangbg@ms.qdio.ac.cn (B.-G.W.); menglh@ms.qdio.ac.cn (L.-H.M.); Tel.: +86-532-8289-8553 (B.-G.W.); +86-532-8289-8890 (L.-H.M.)

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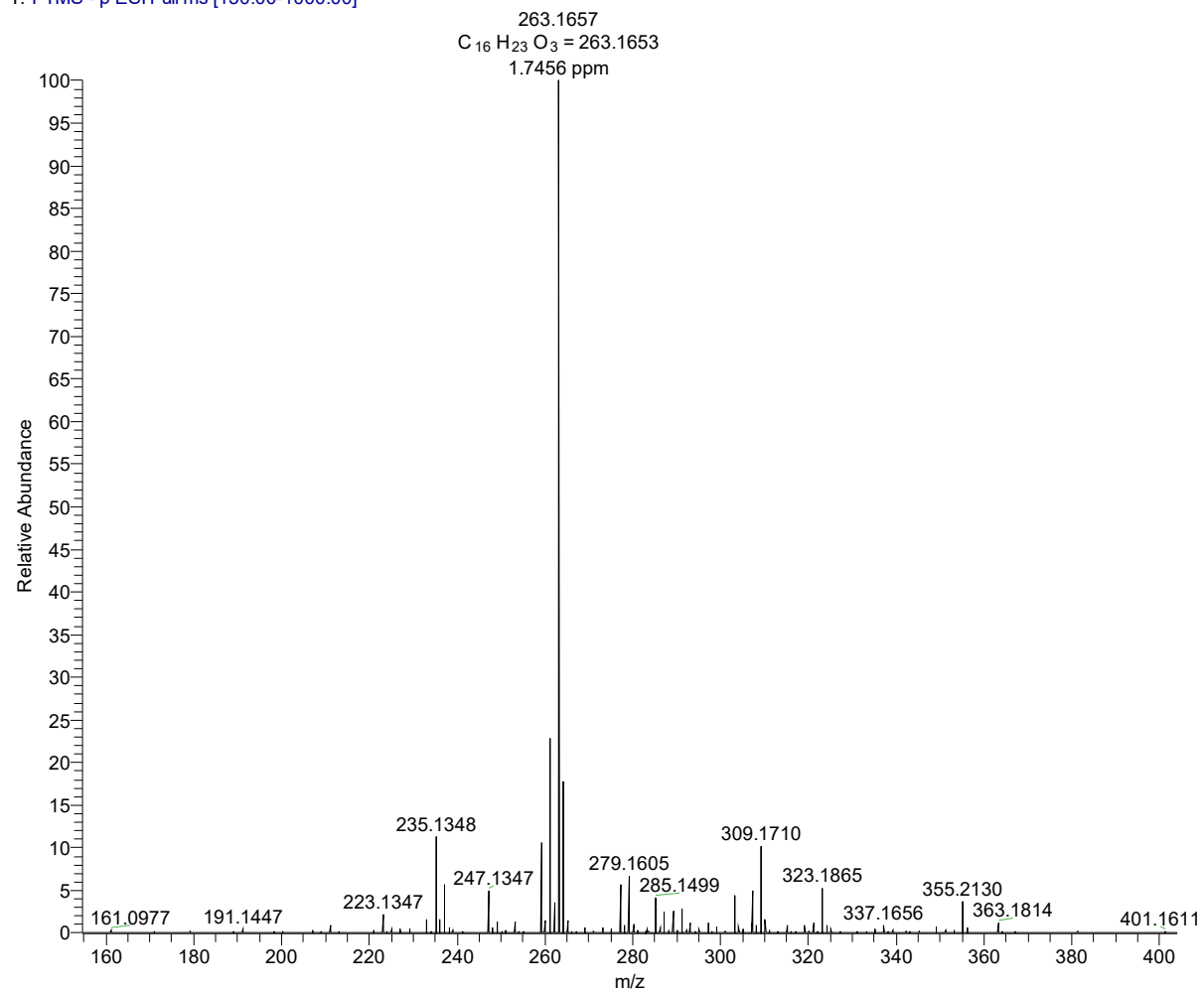
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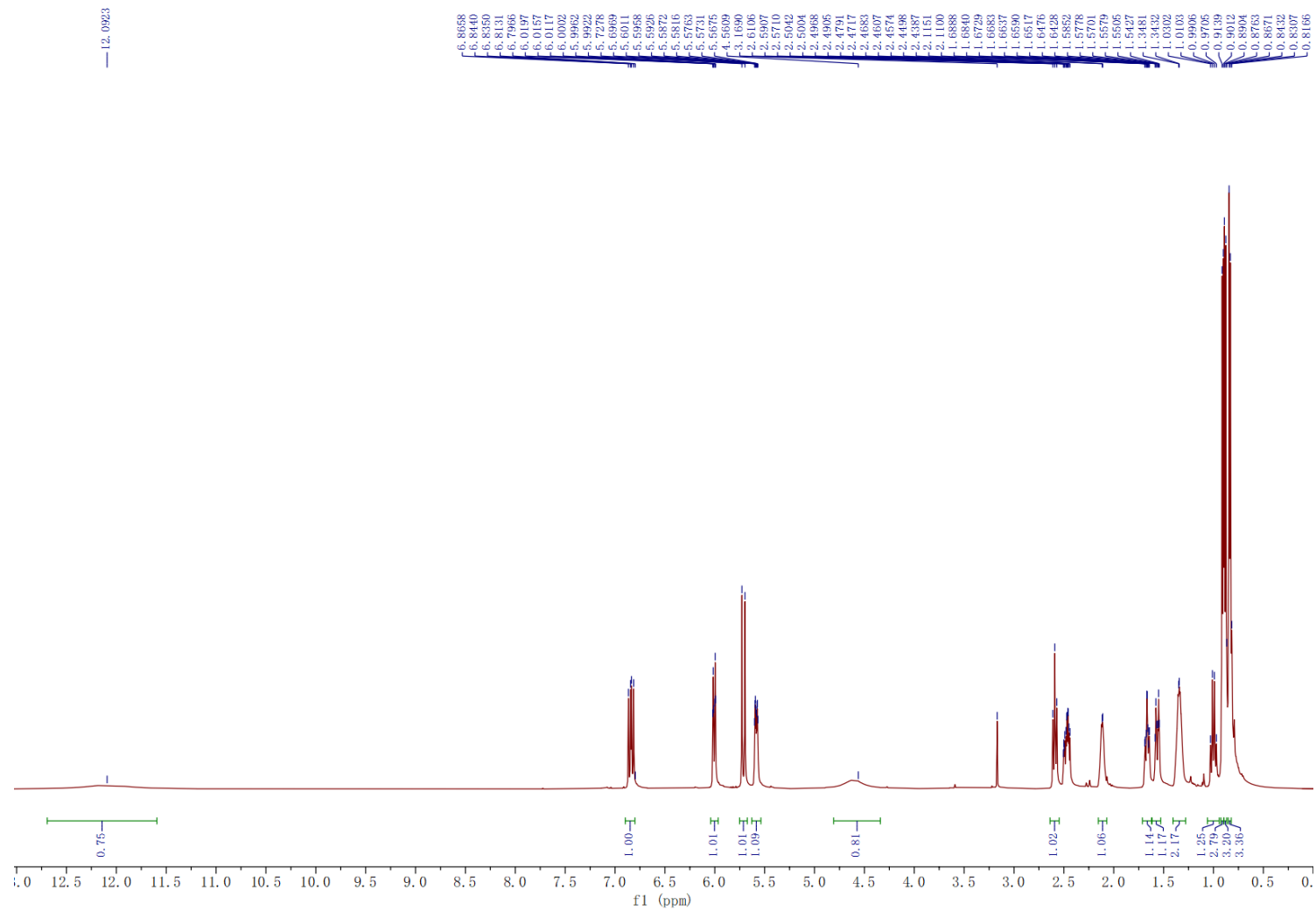
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**Figure S1.** HRESI mass spectrum of compound **1**;

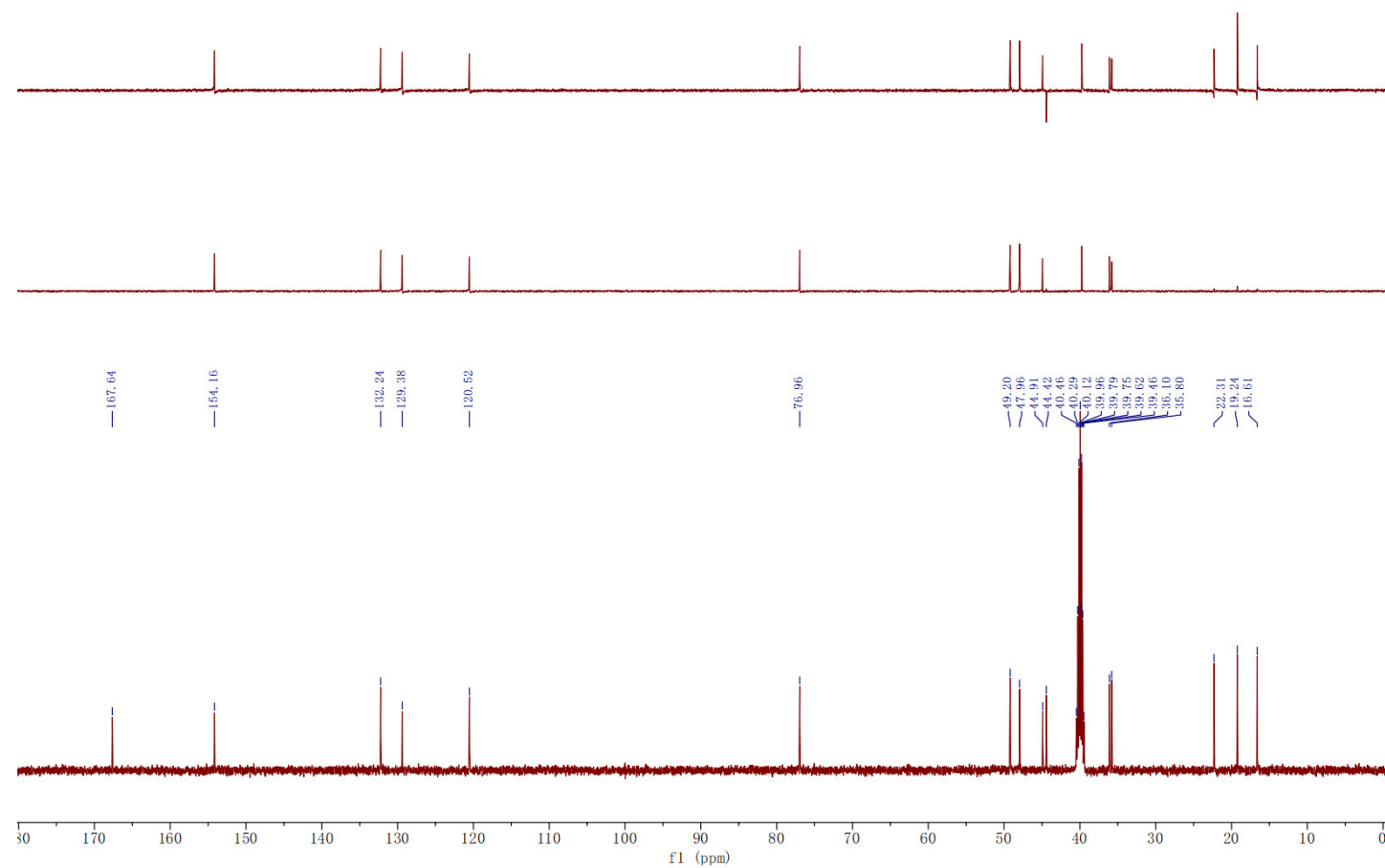
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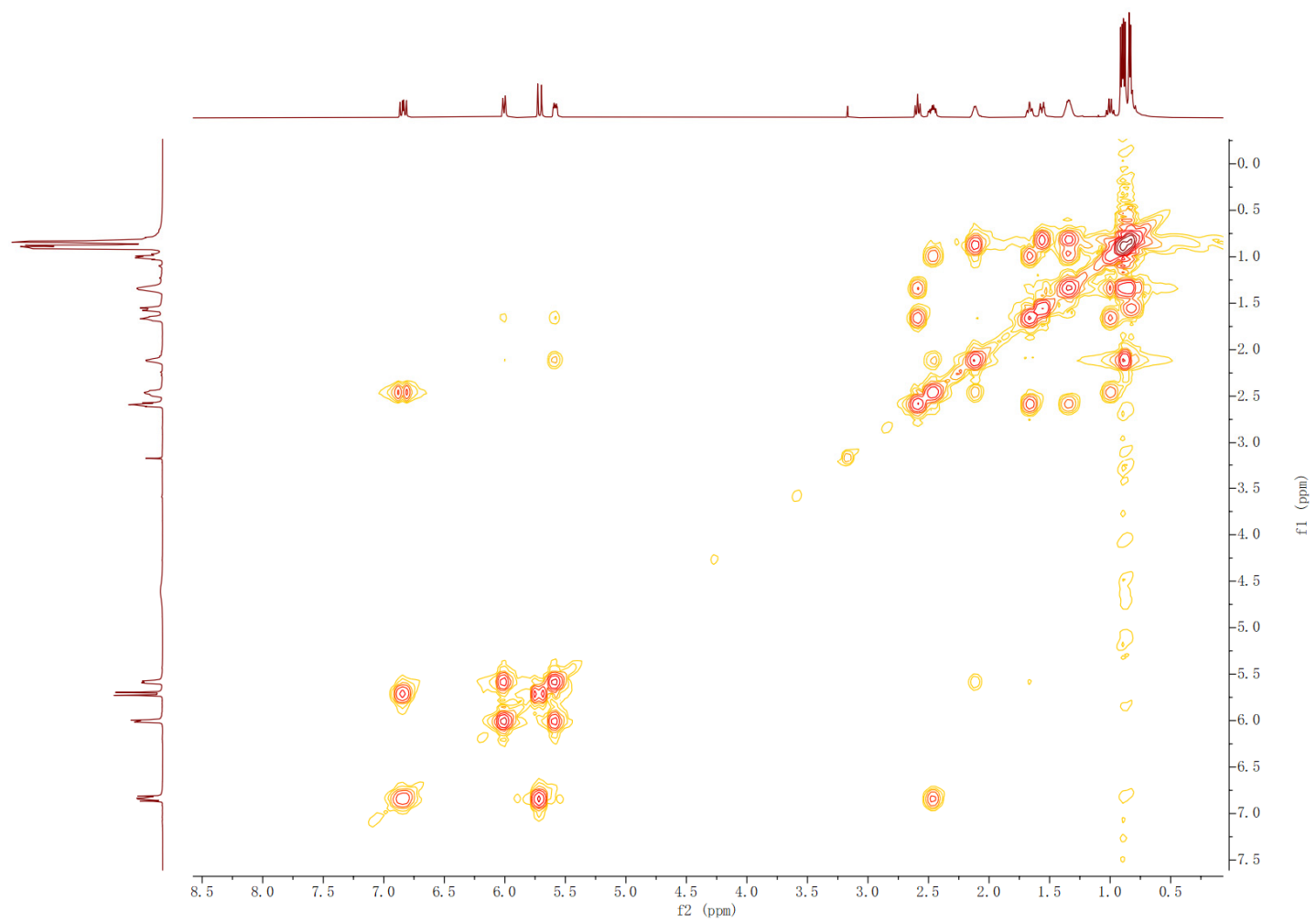
**Figure S2.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **1**;



**Figure S3.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **1**;

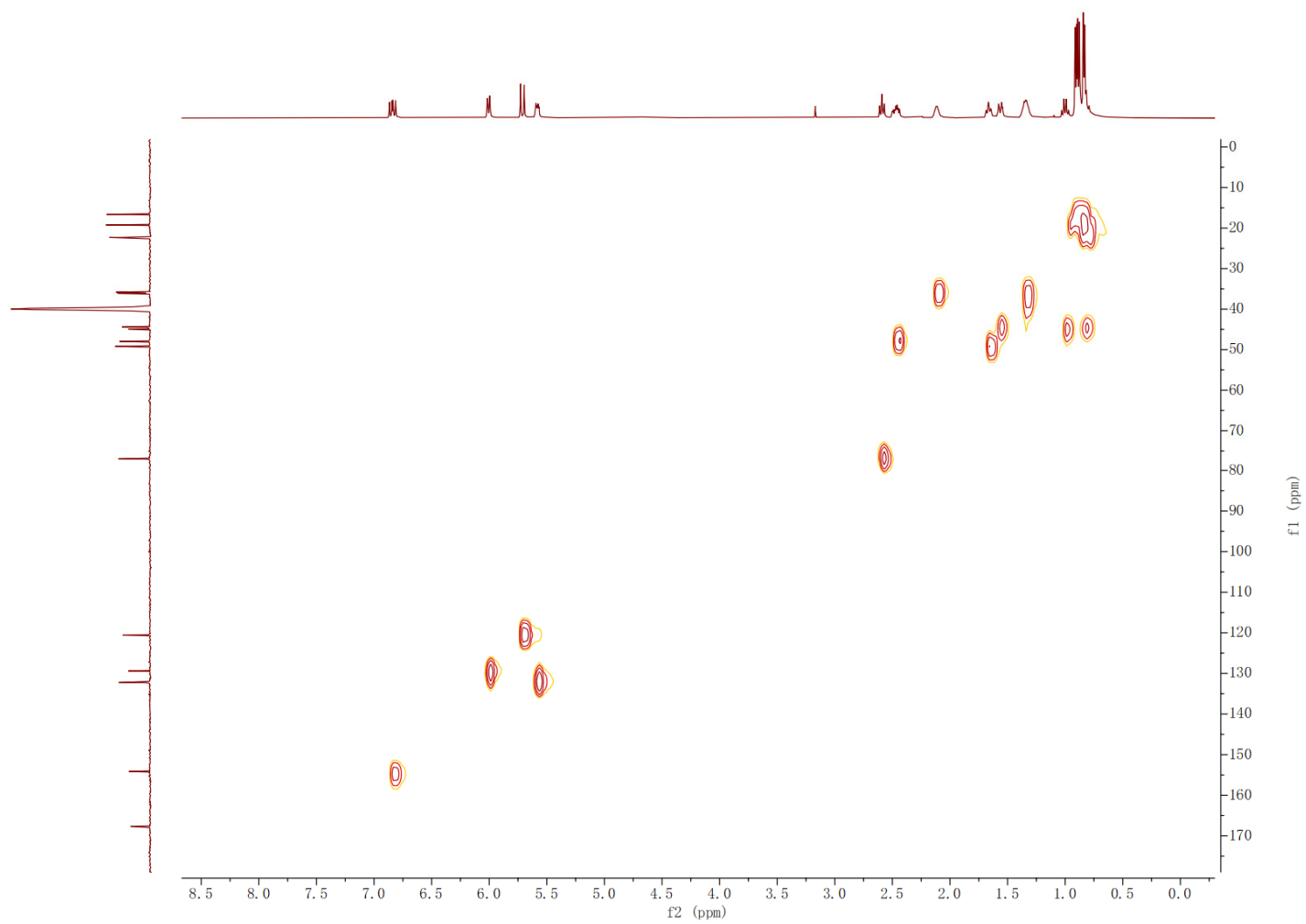


**Figure S4.** COSY spectrum of compound **1**;

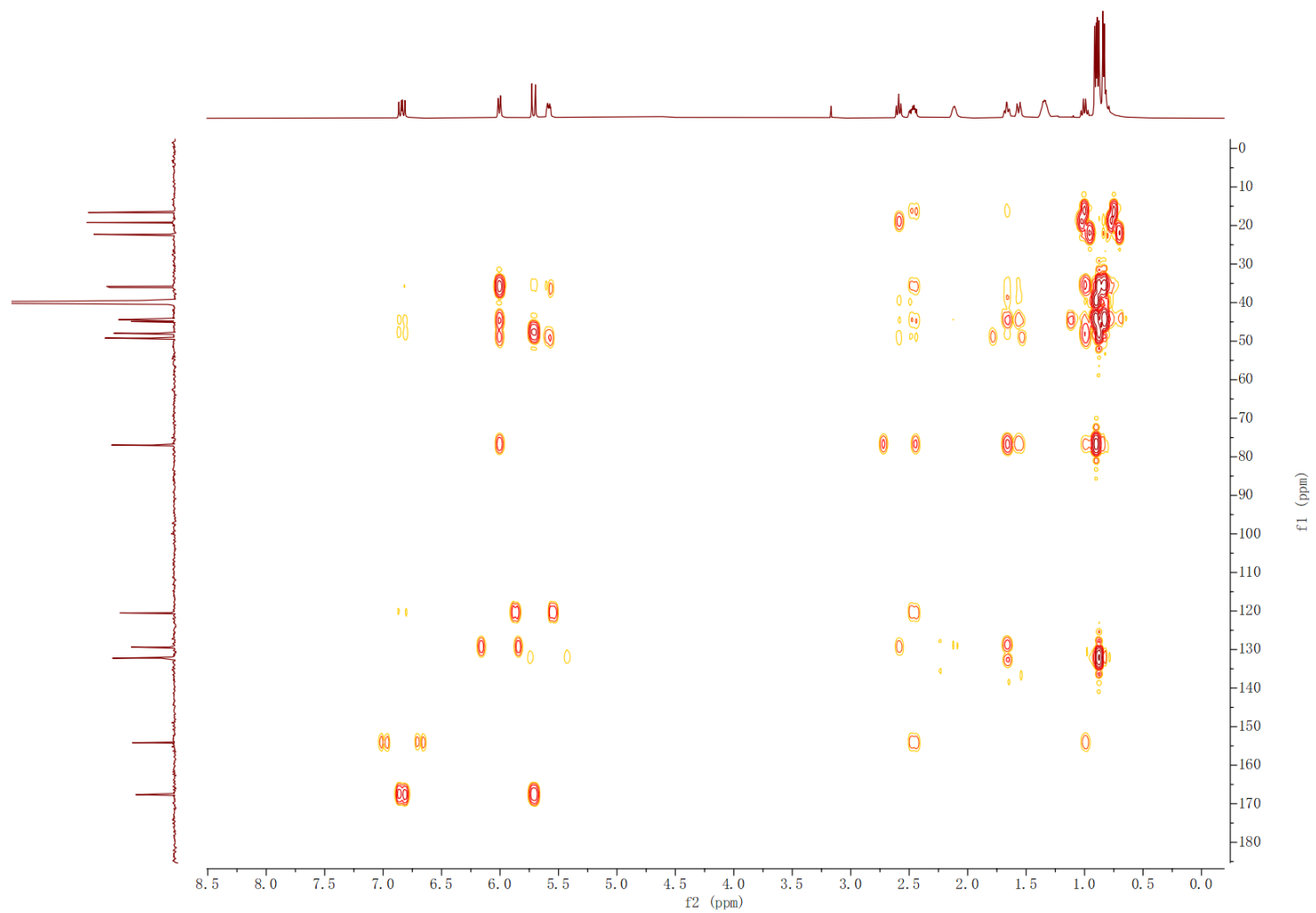




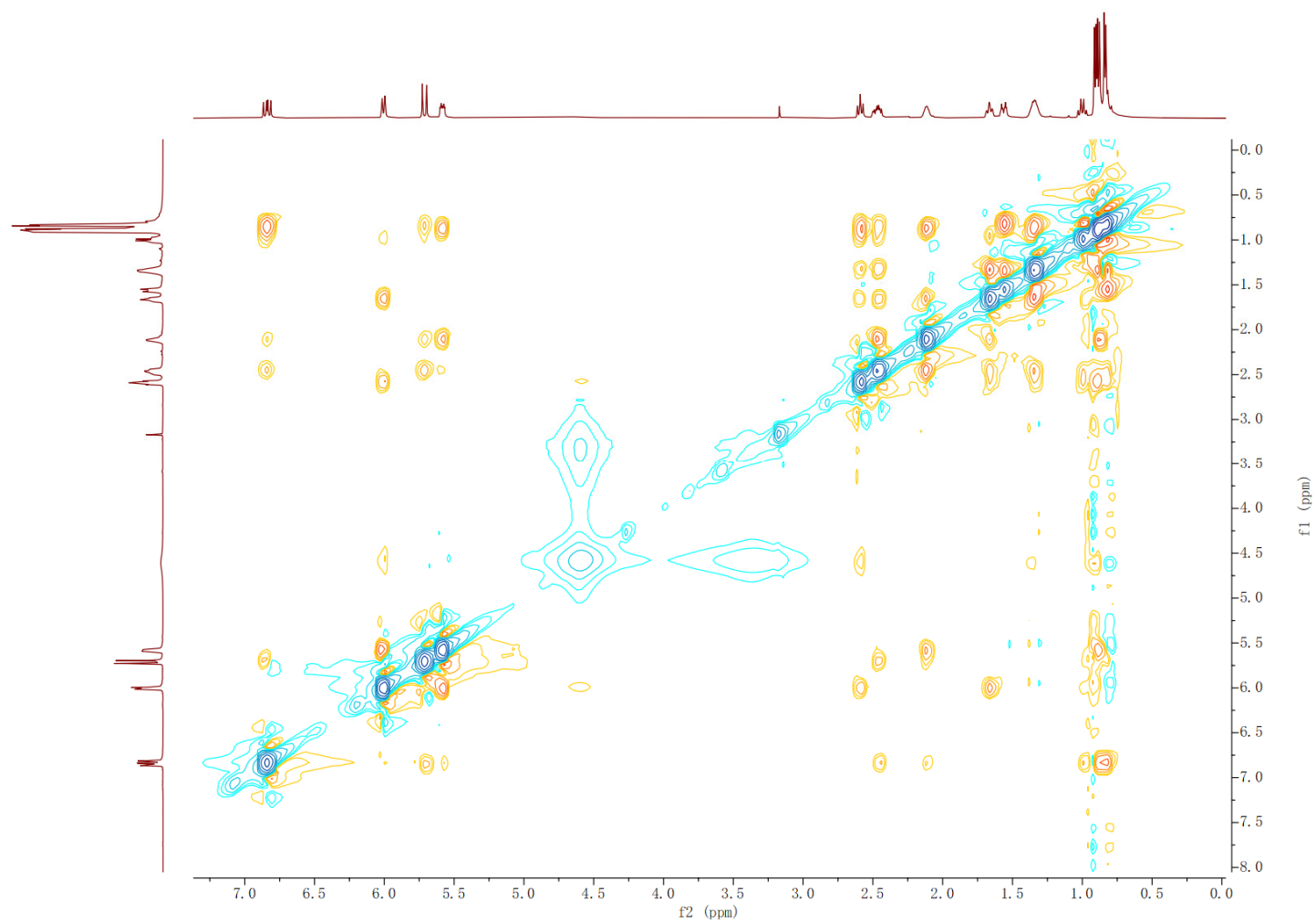
**Figure S5.** HSQC spectrum of compound **1**;



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

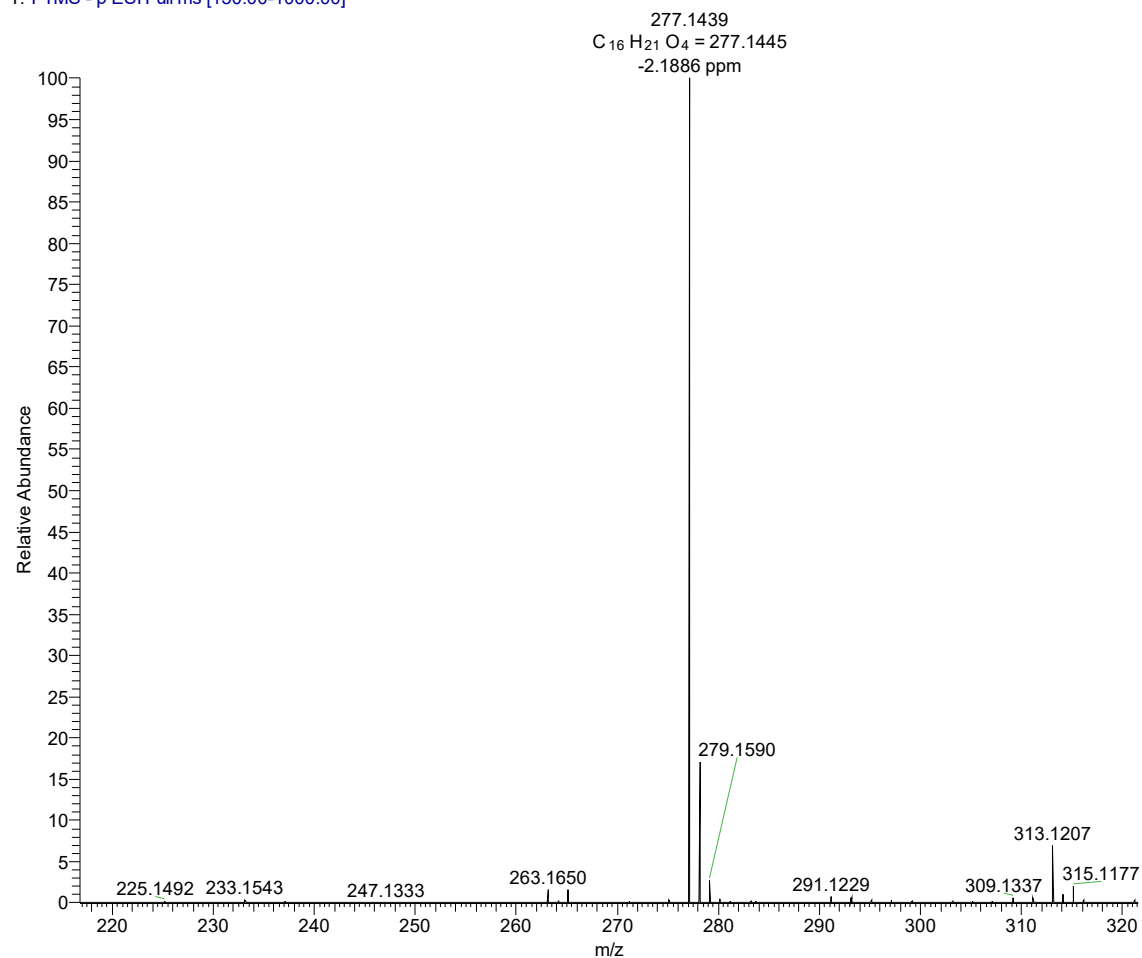


**Figure S7.** NOESY spectrum of compound **1**;

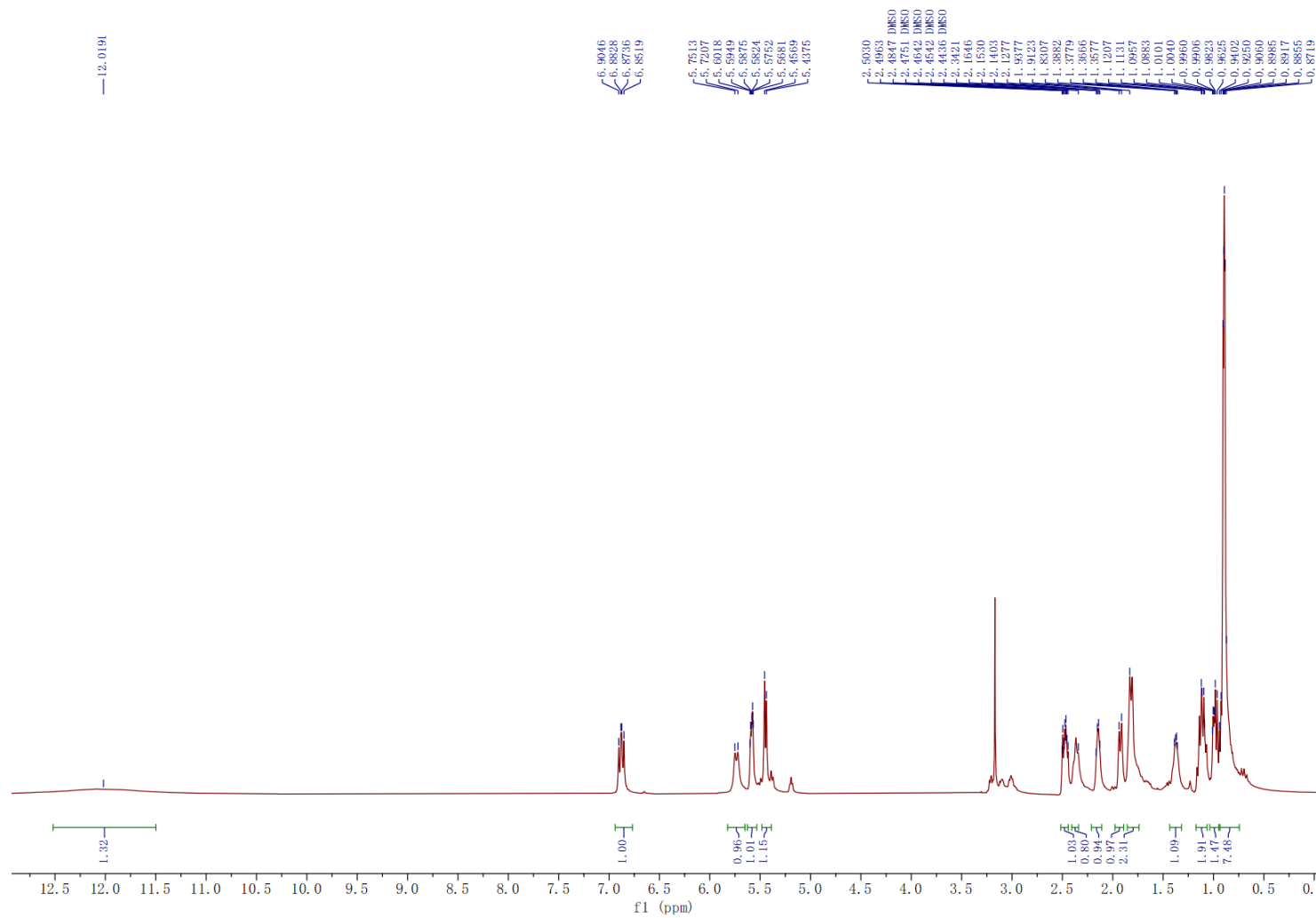


**Figure S8.** HRESI mass spectrum of compound **2**;

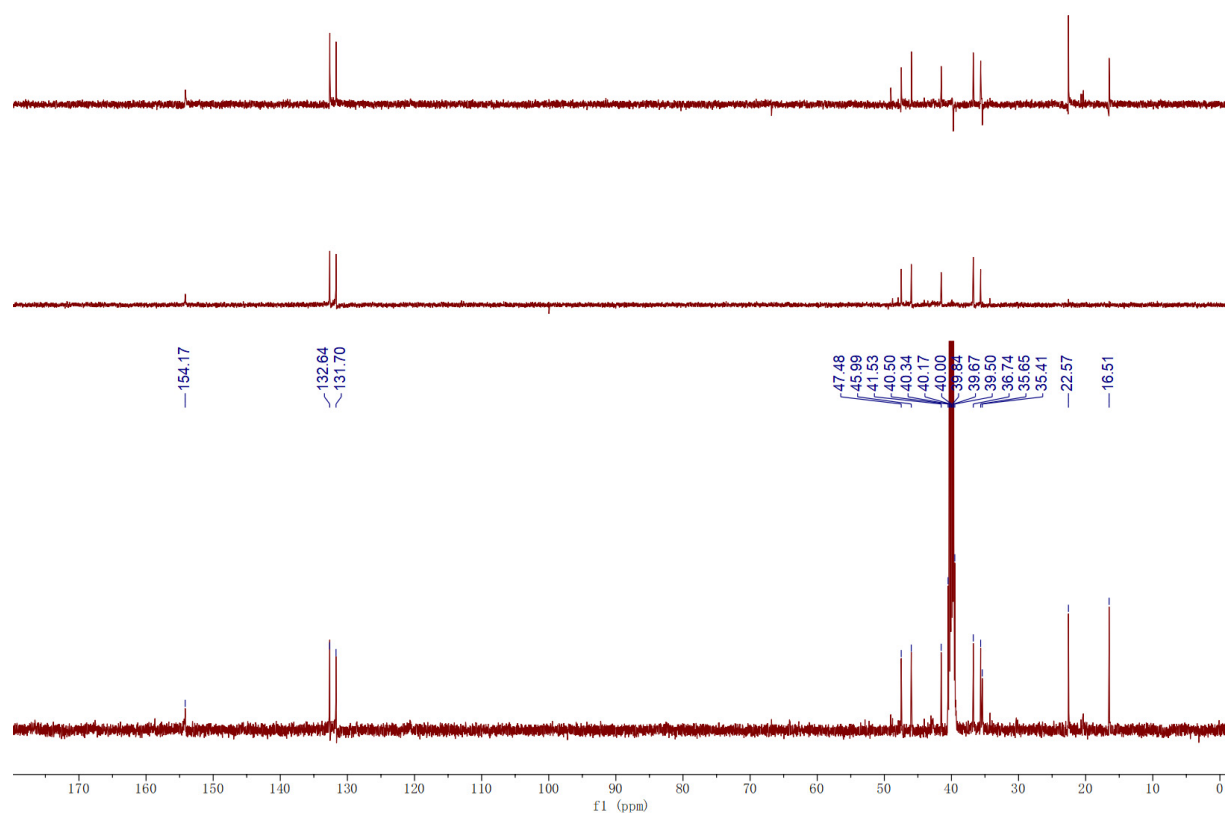
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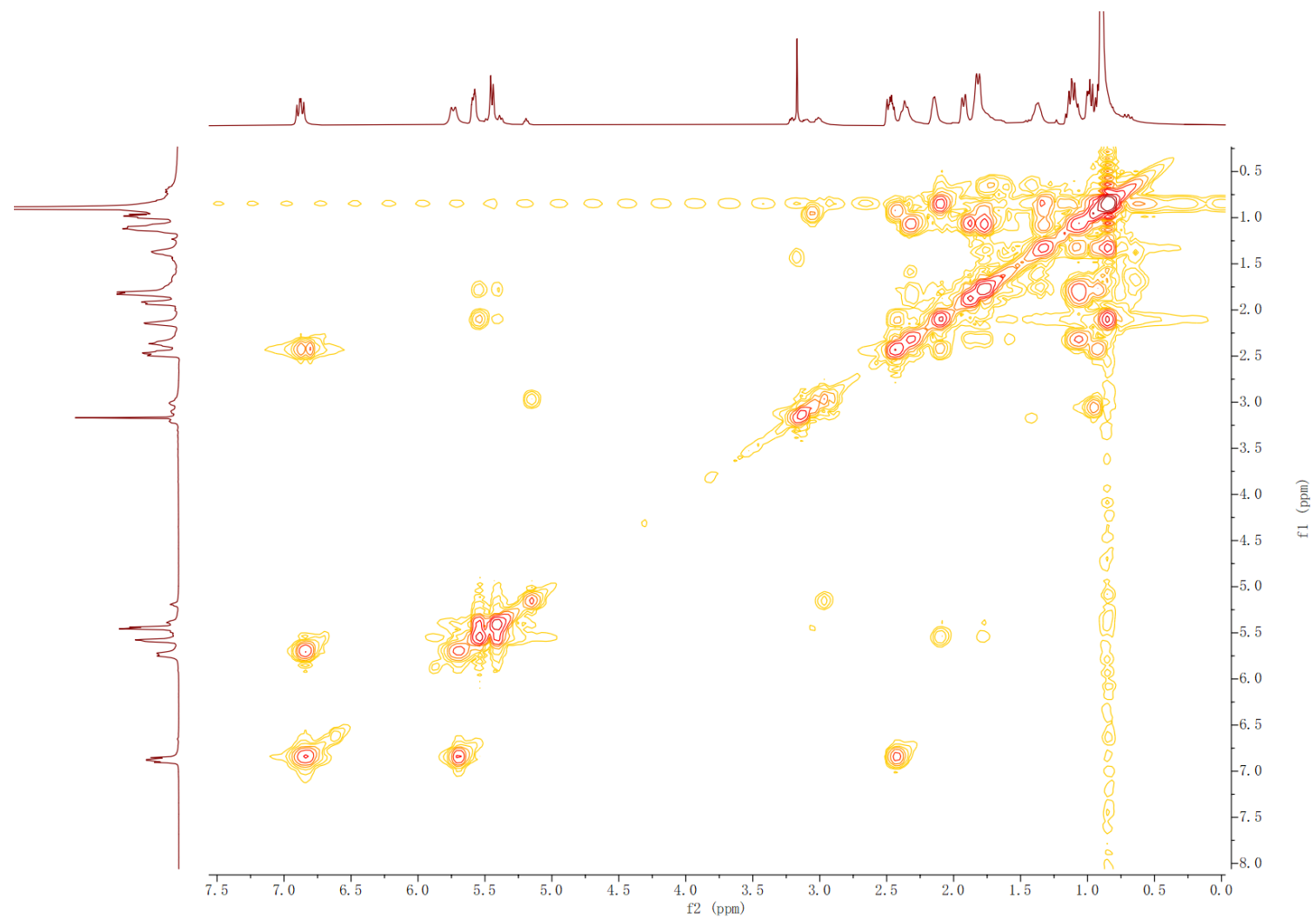
**Figure S9.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **2**;



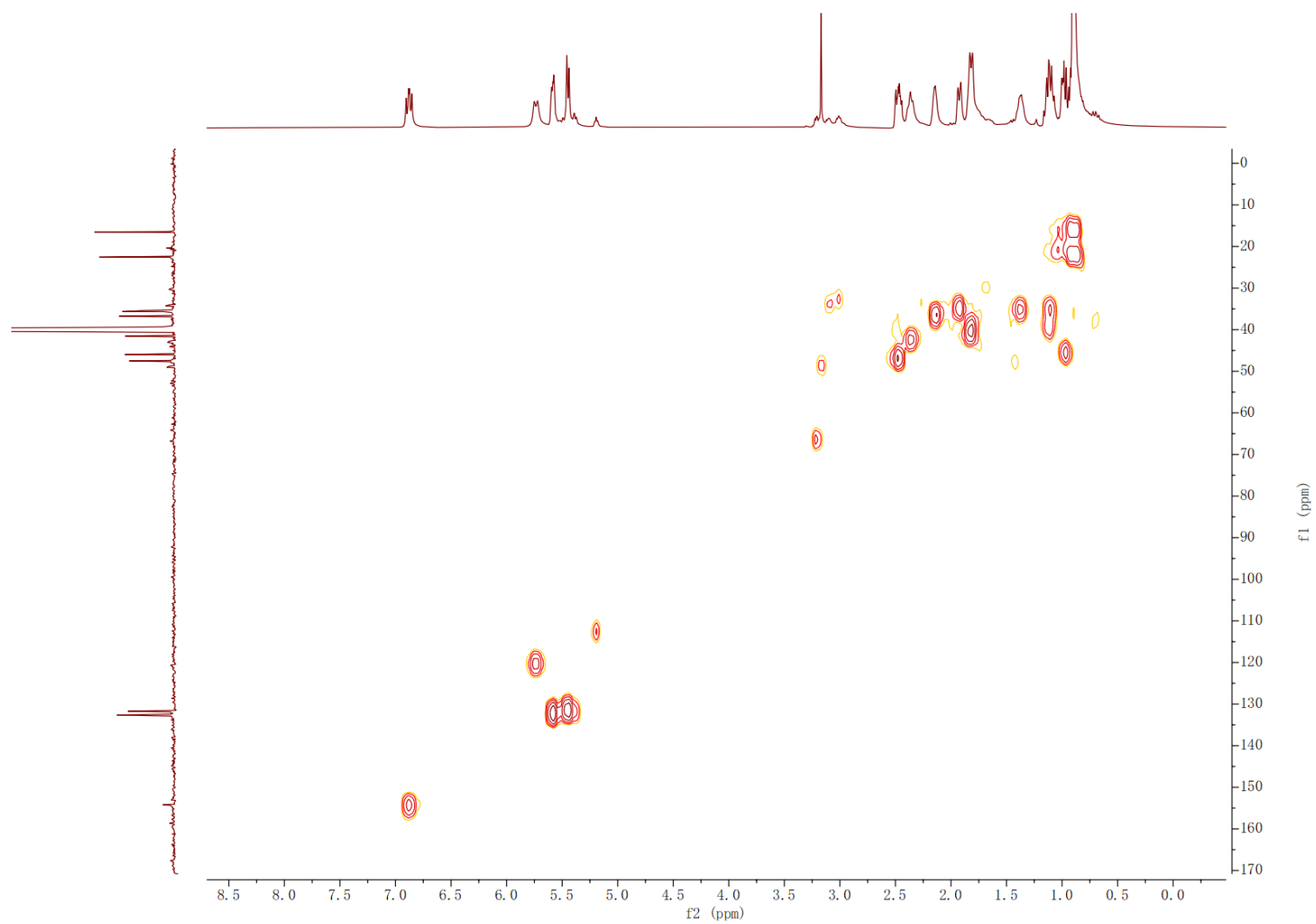
**Figure S10.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **2**;



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

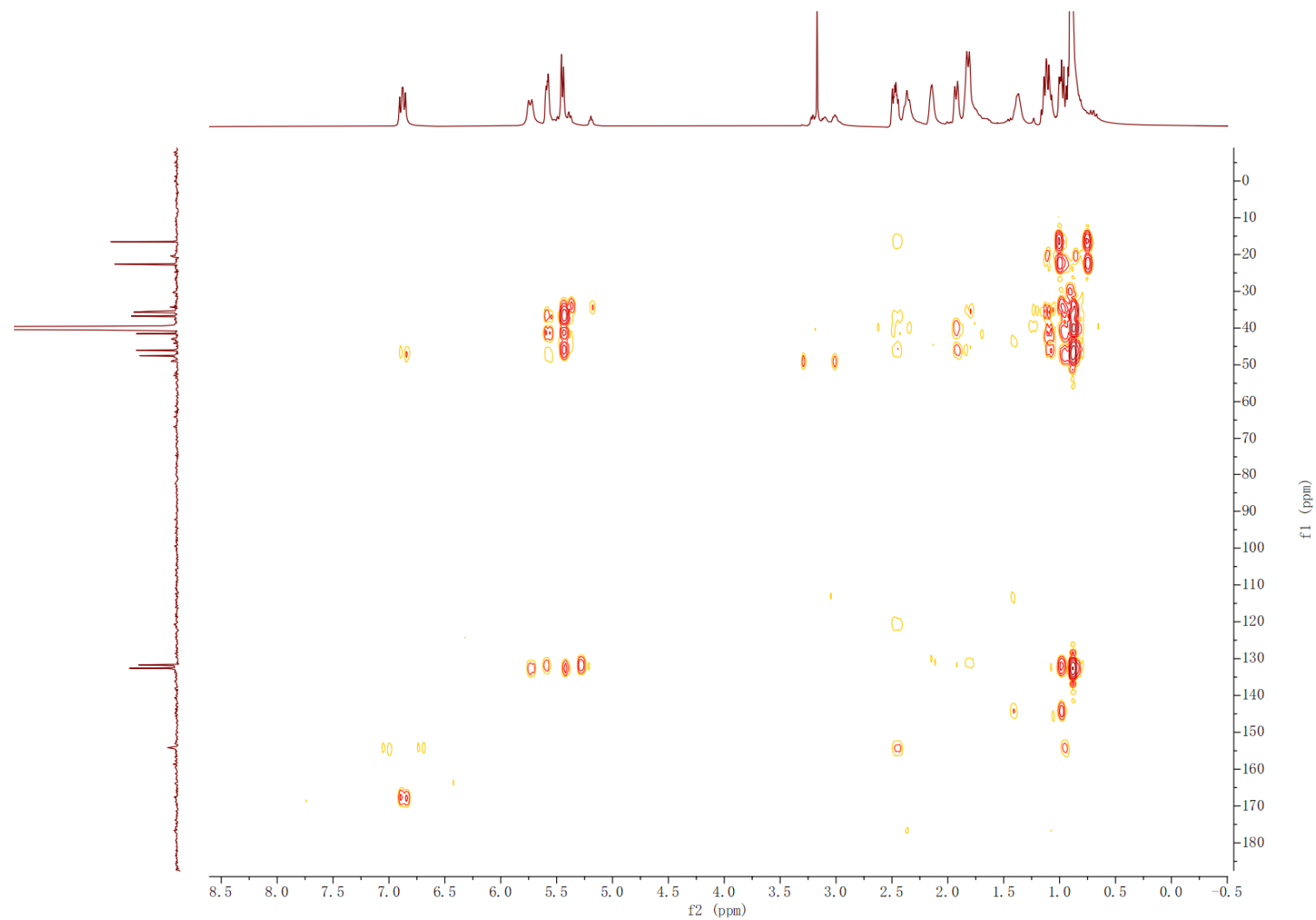


**Figure S12.** HSQC spectrum of compound **2**;

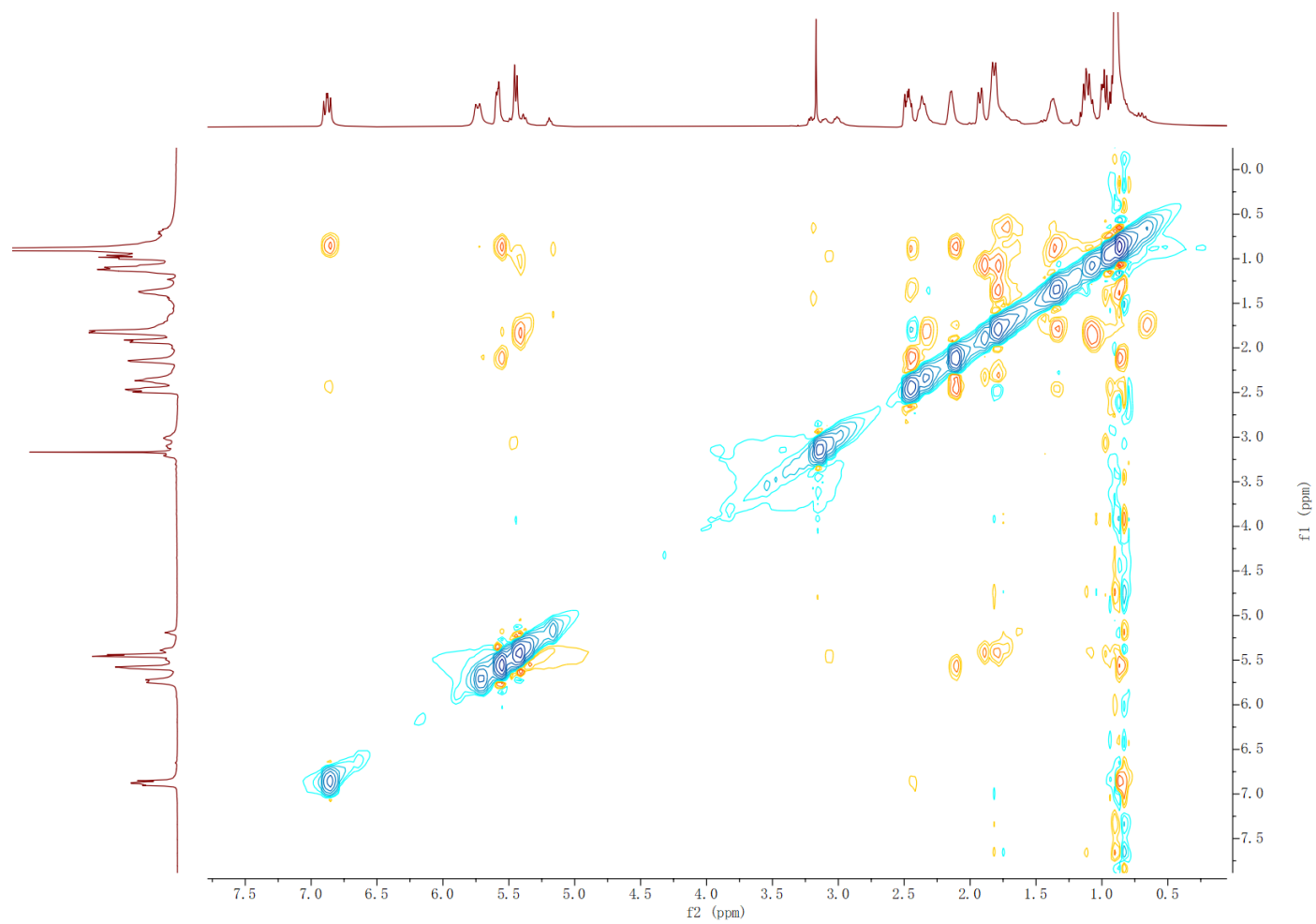




**Figure S13.** HMBC spectrum of compound **2**;

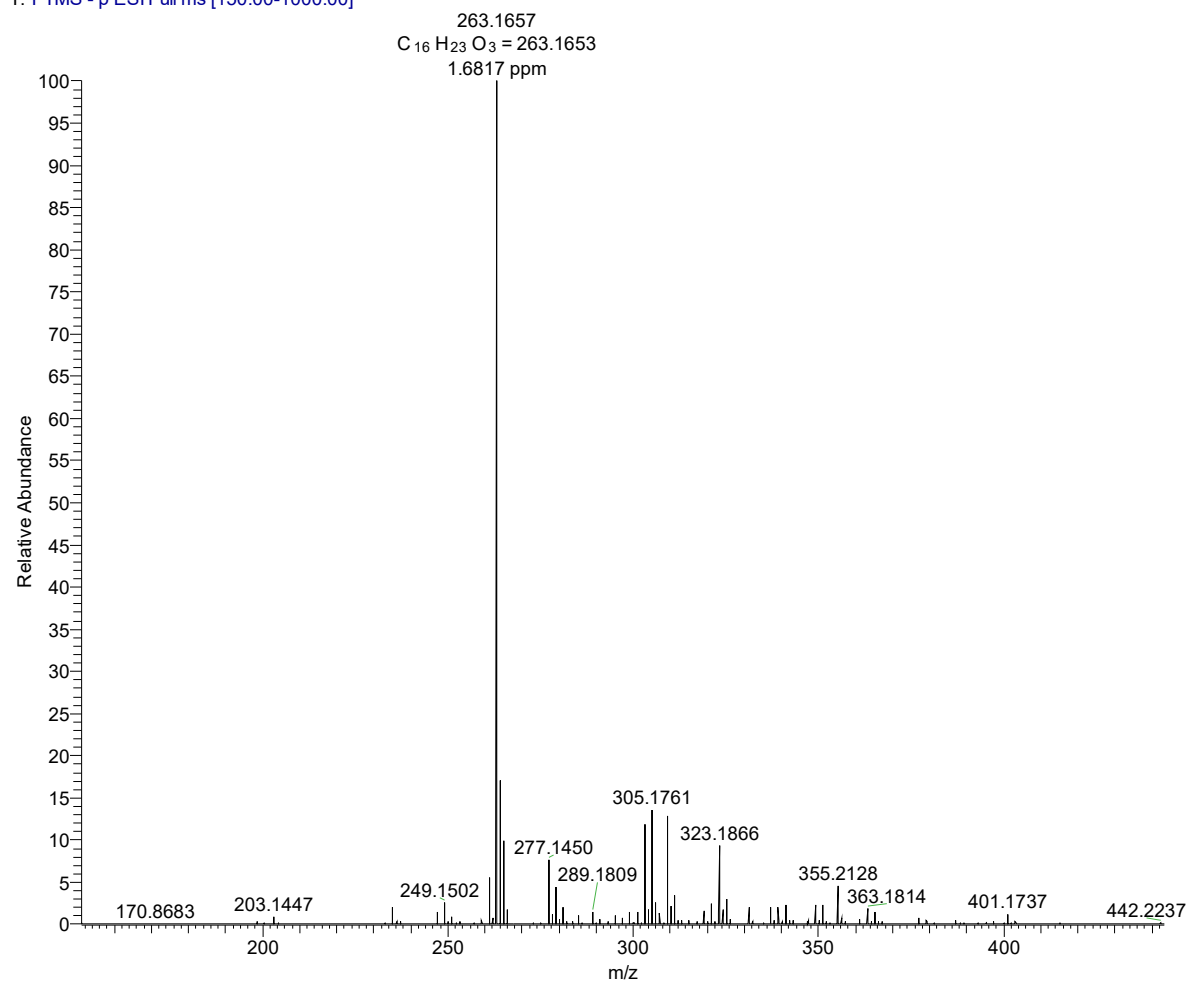


**Figure S14.** NOESY spectrum of compound **2**;

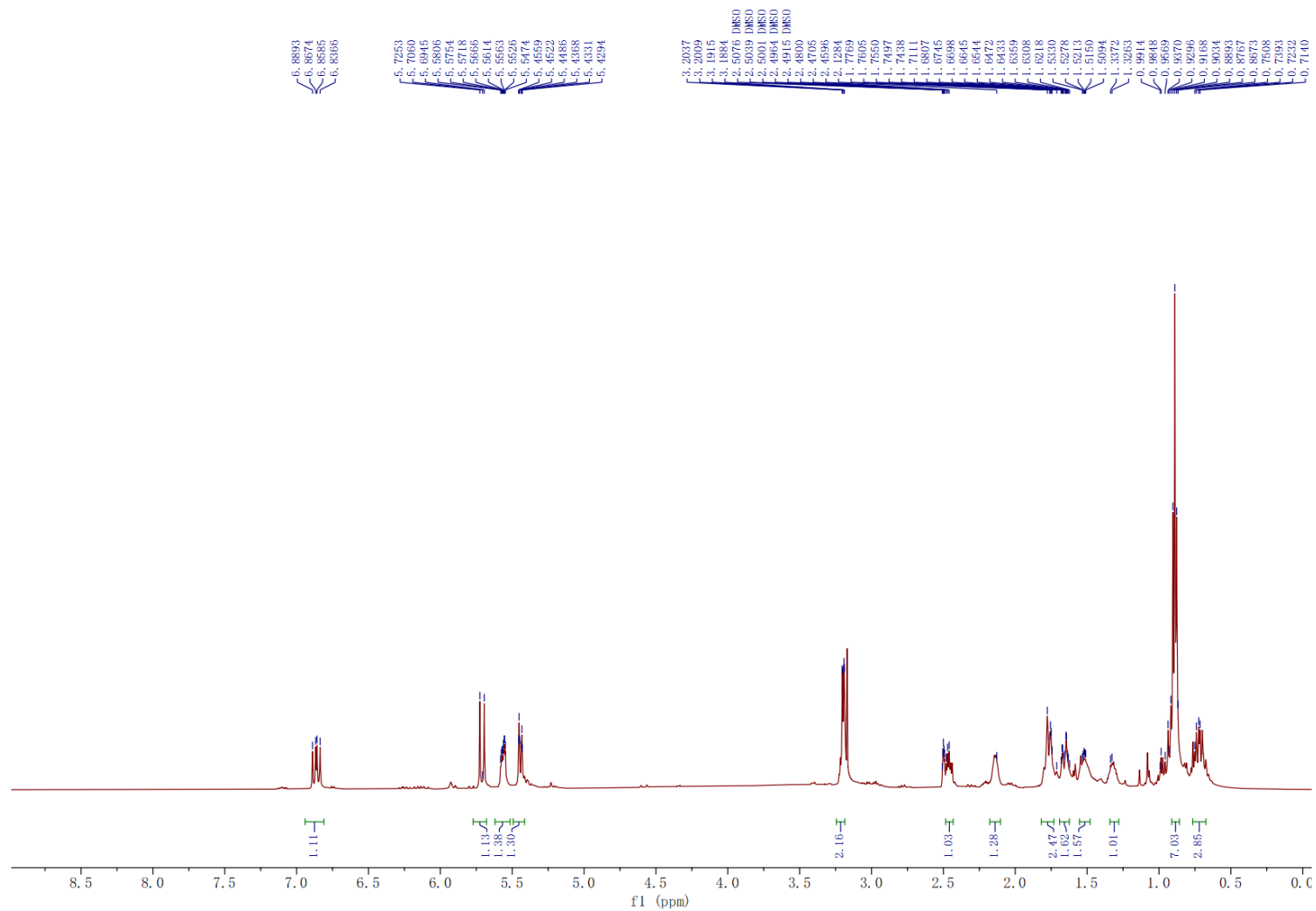


**Figure S15.** HRESI mass spectrum of compound **3**;

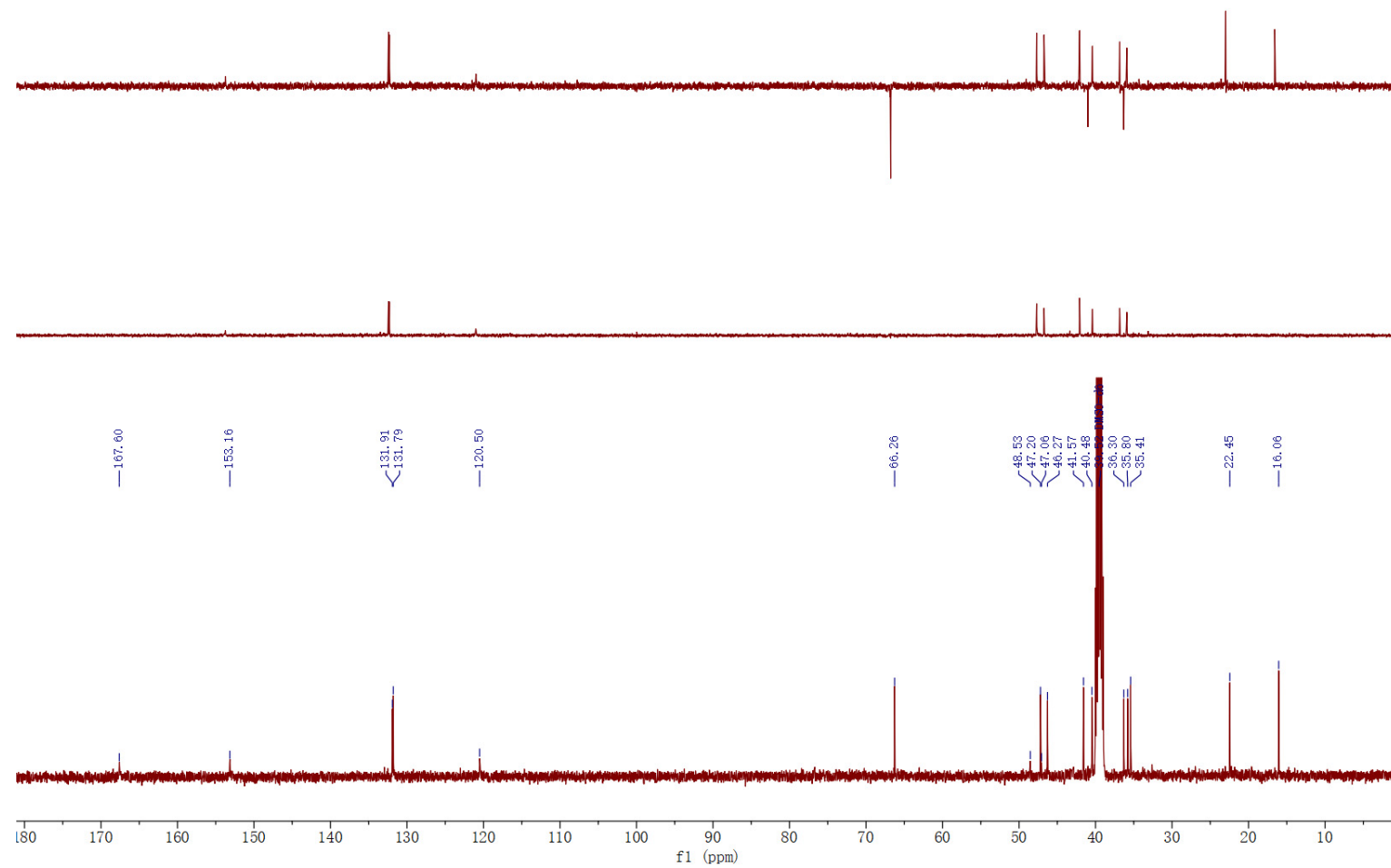
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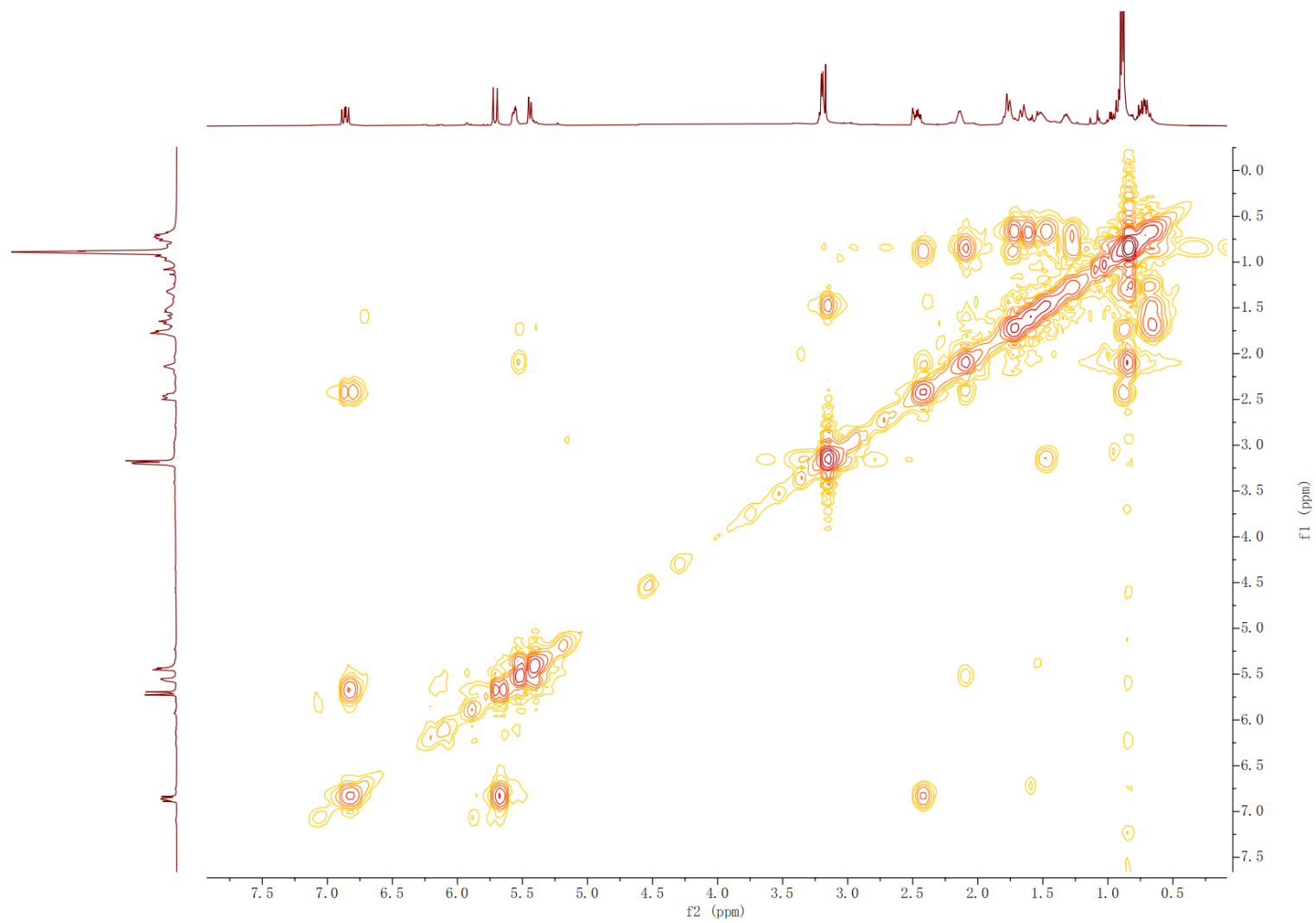
**Figure S16.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **3**;



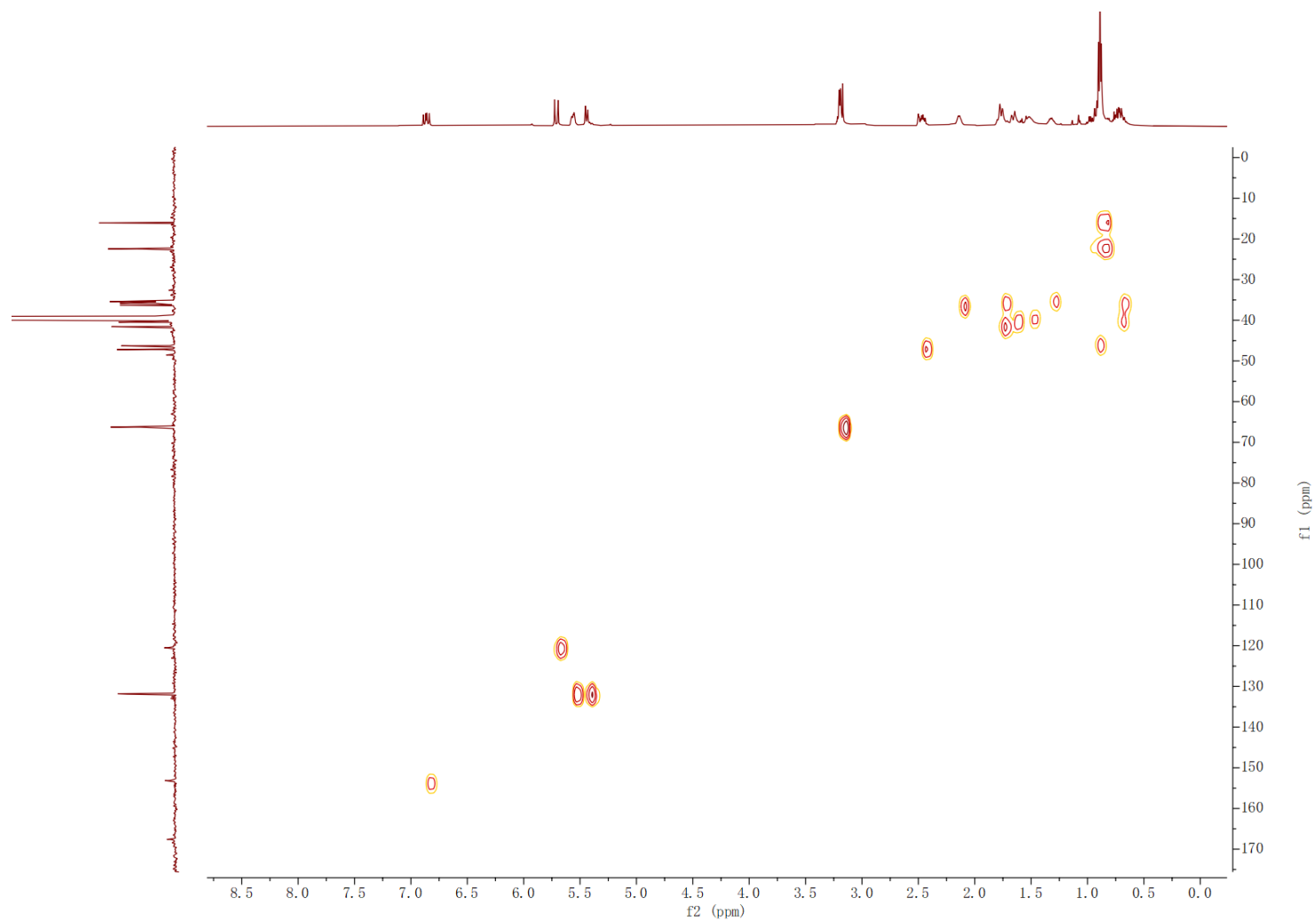
**Figure S17.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **3**;



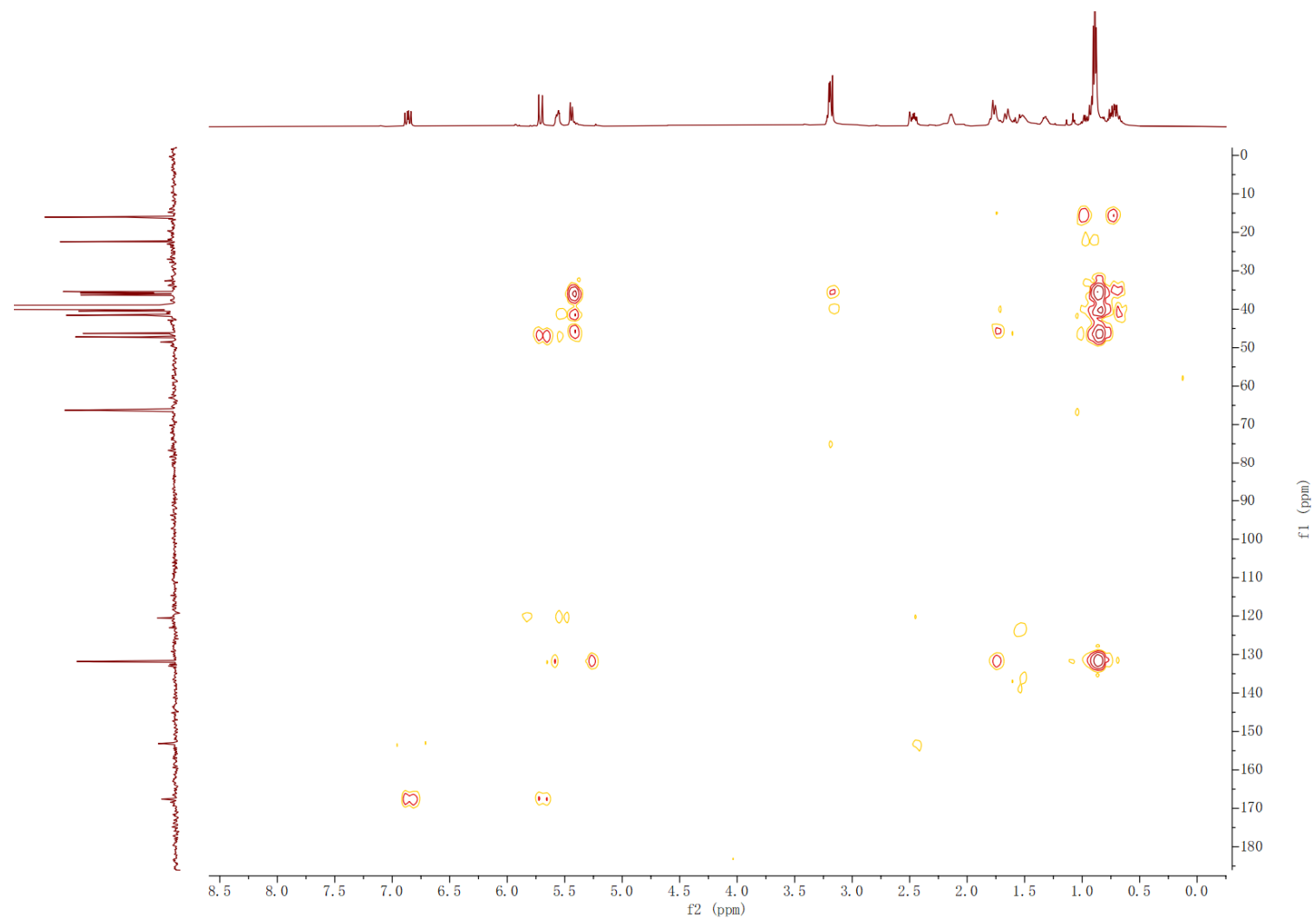
**Figure S18.** COSY spectrum of compound **3**;



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

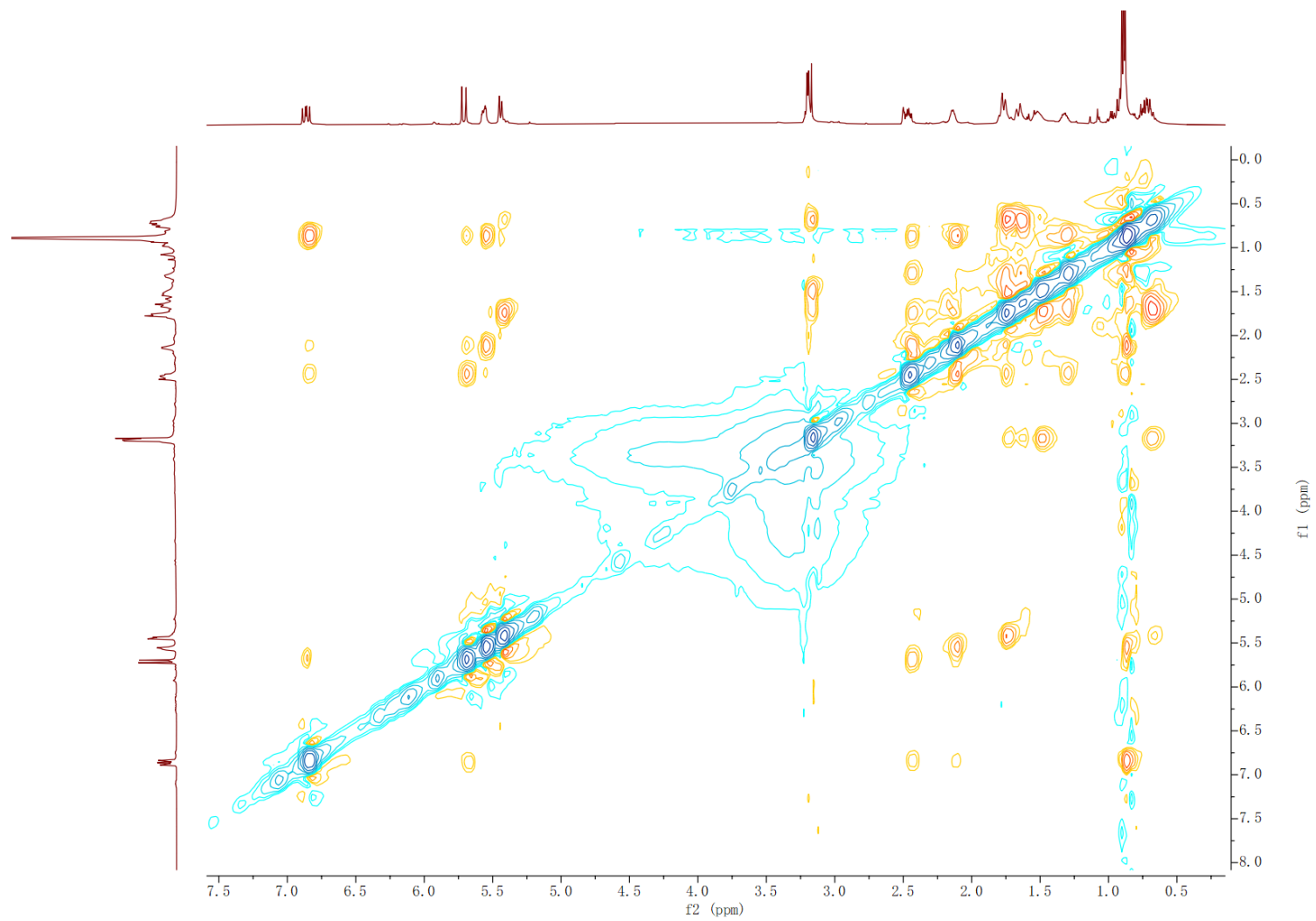


**Figure S20.** HMBC spectrum of compound **3**;



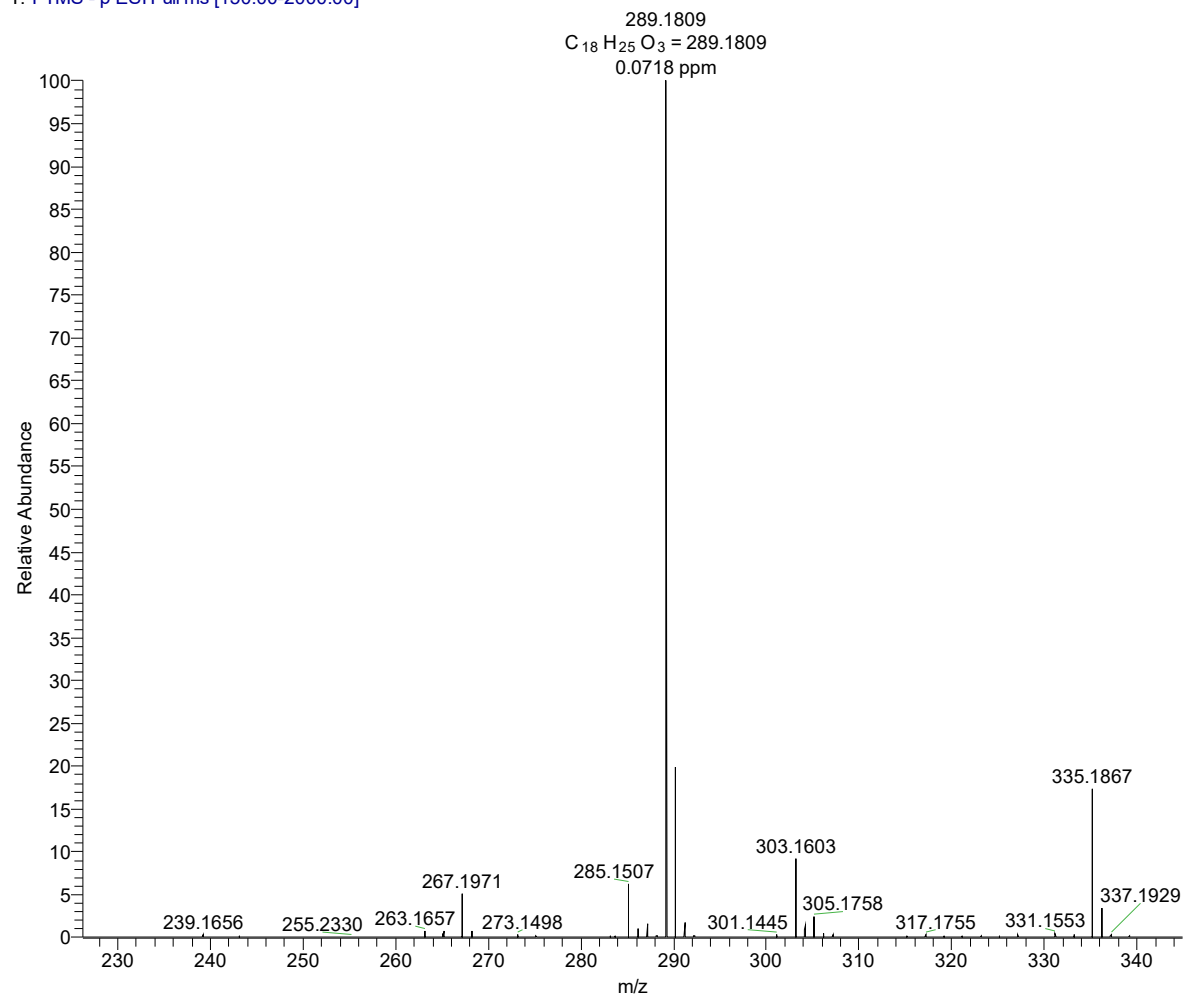


**Figure S21.** NOESY spectrum of compound **3**;

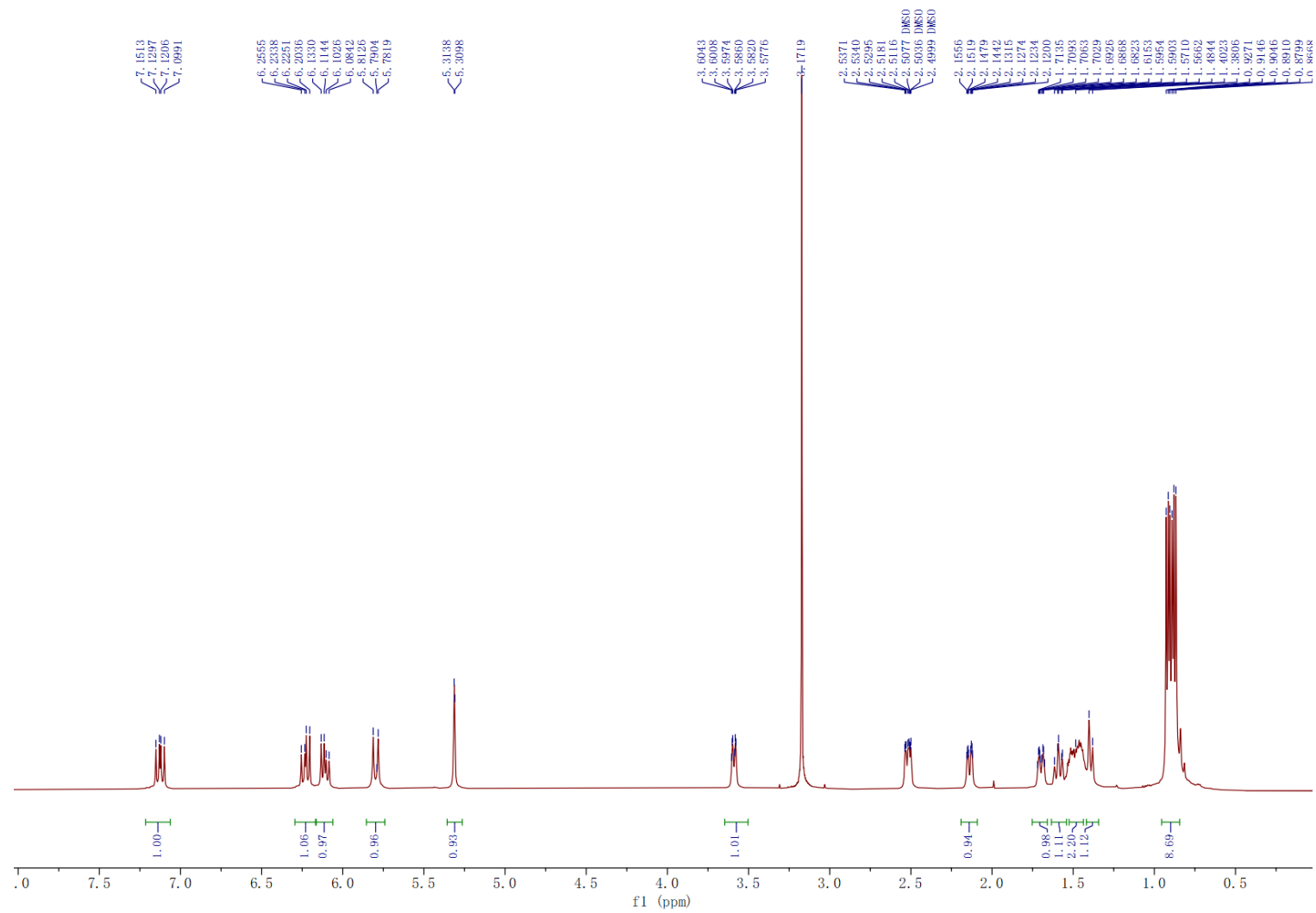


**Figure S22.** HRESI mass spectrum of compound **4**;

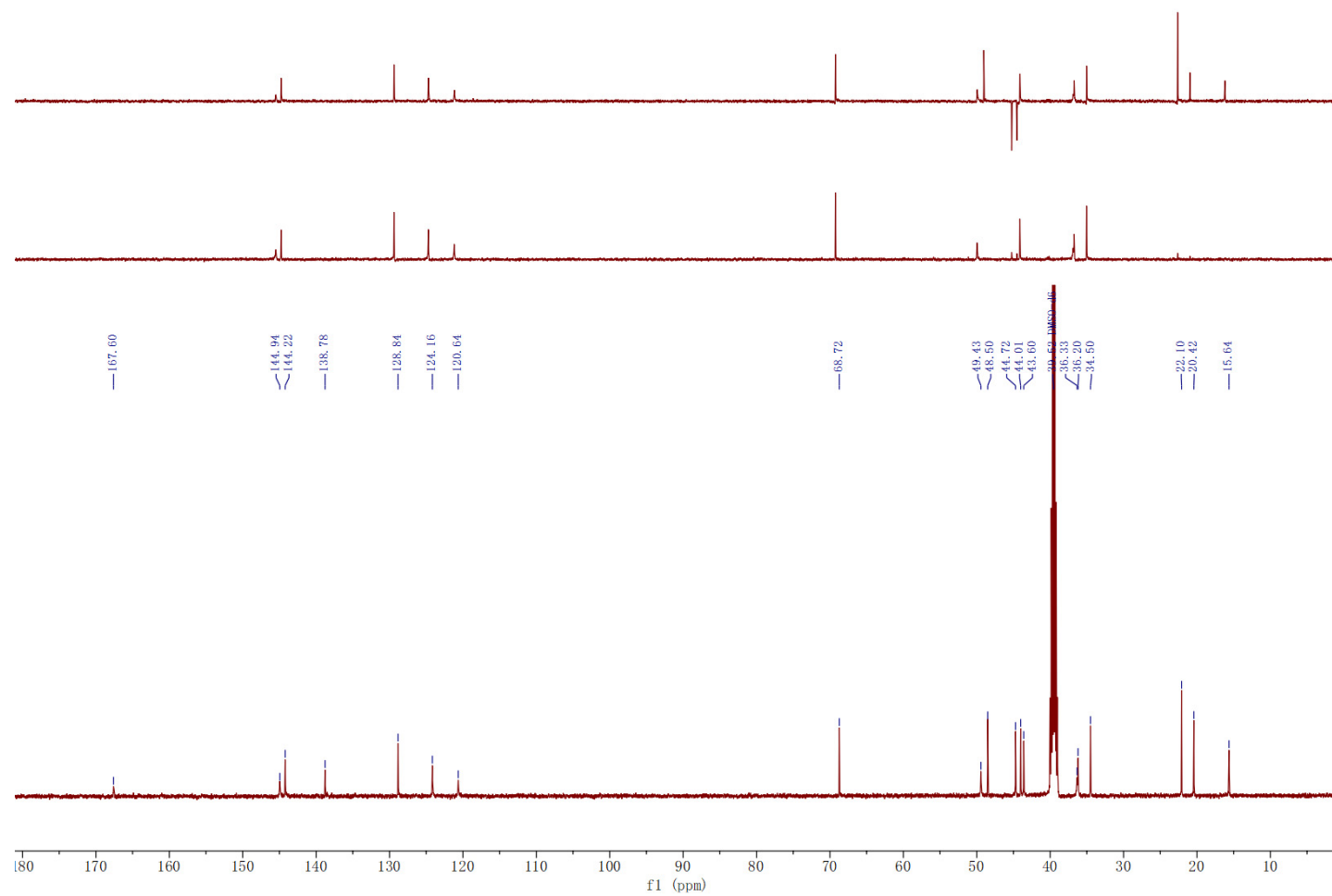
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T: FTMS - p ESI Full ms [150.00-2000.00]



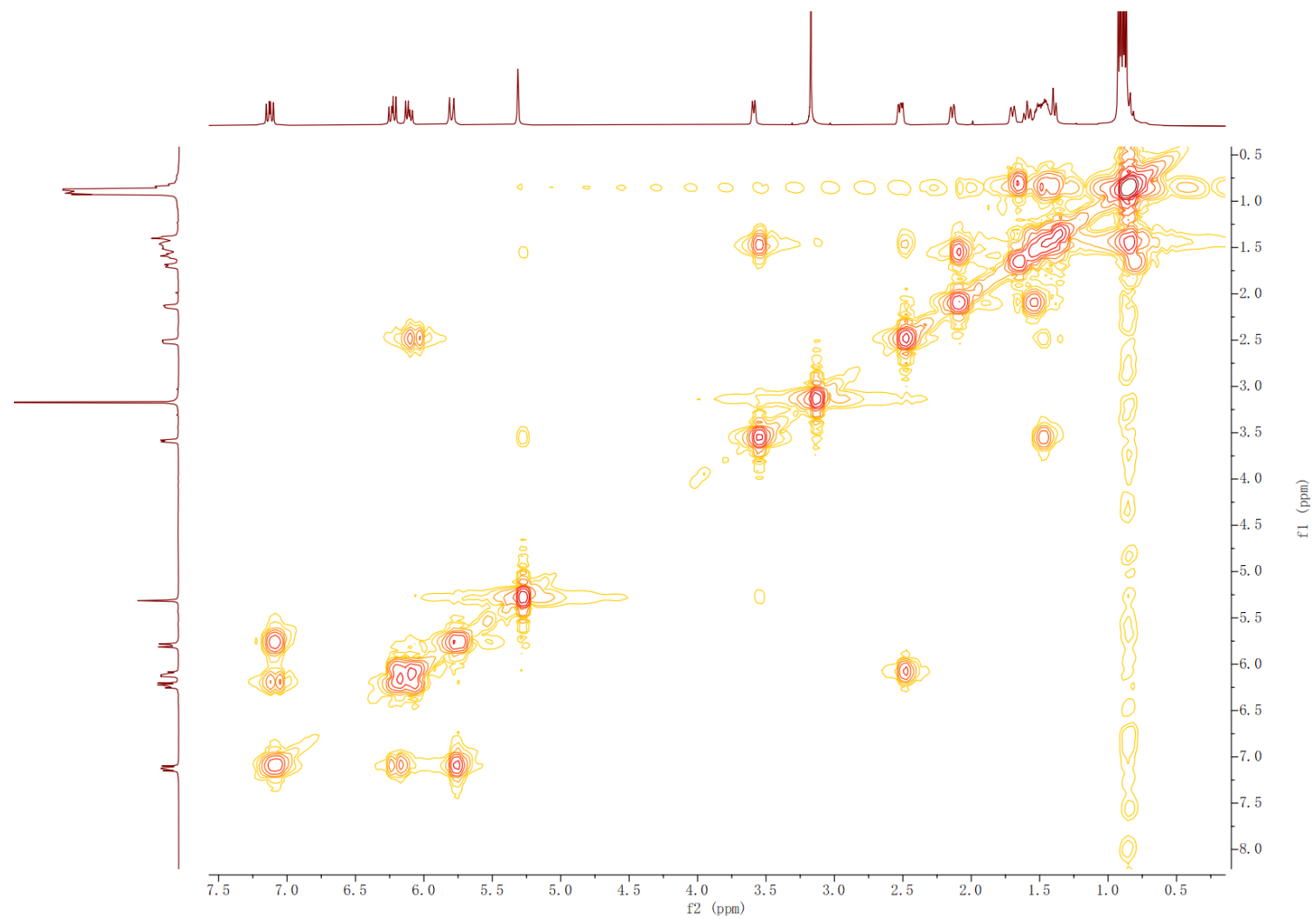
**Figure S23.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **4**;



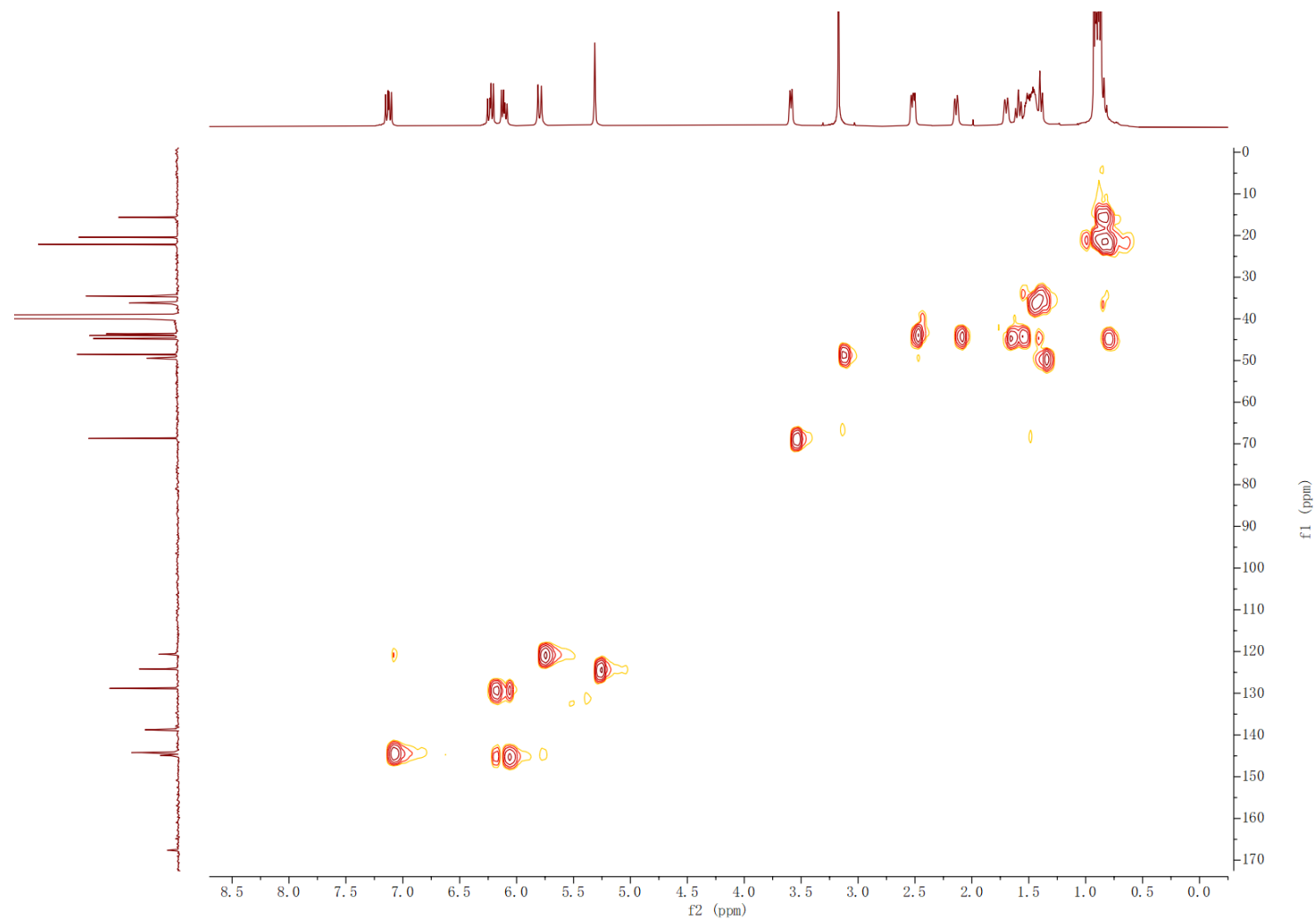
**Figure S24.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **4**;



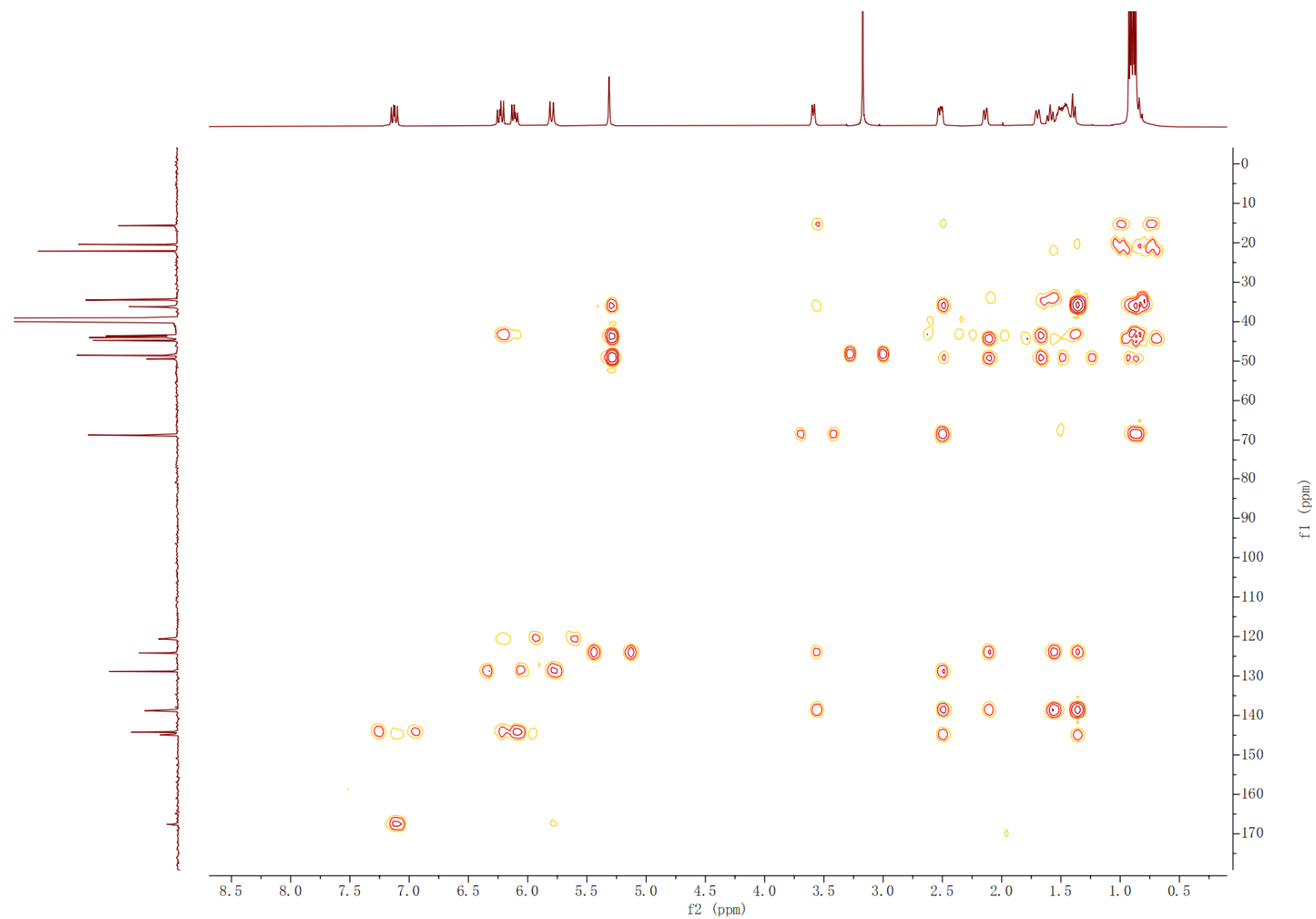
**Figure S25.** COSY spectrum of compound **4**;



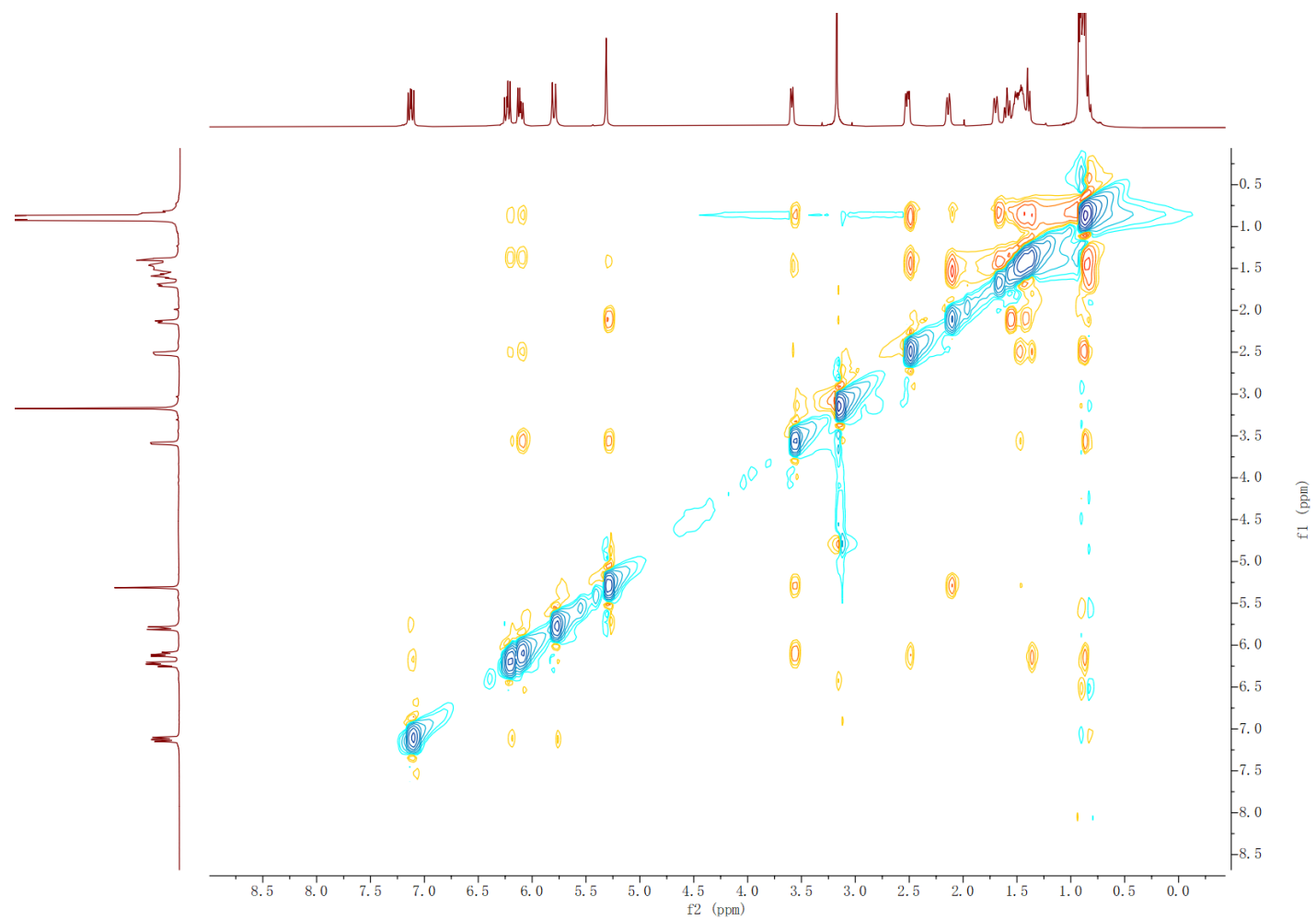
**Figure S26.** HSQC spectrum of compound **4**;



**Figure S27.** HMBC spectrum of compound **4**;



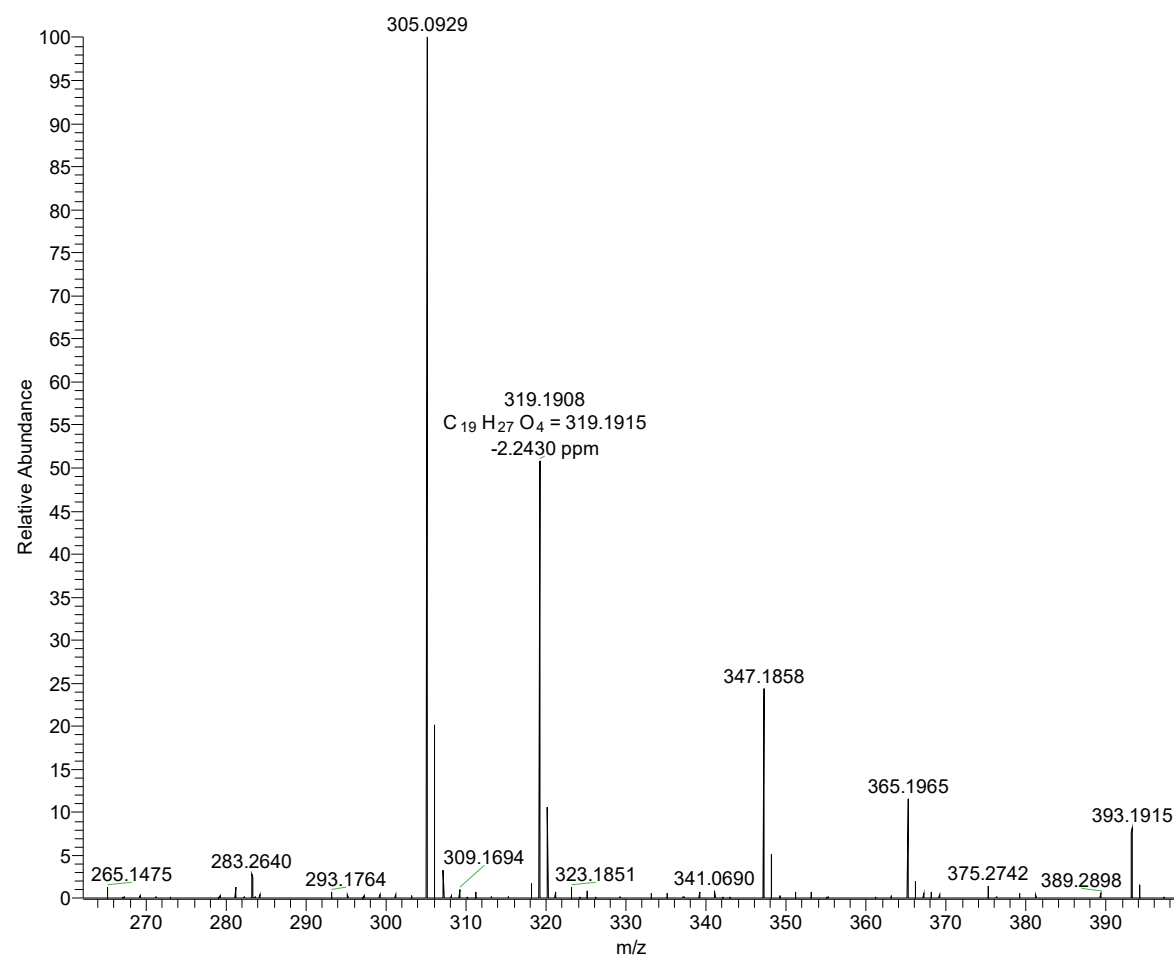
**Figure S28.** NOESY spectrum of compound **4**;



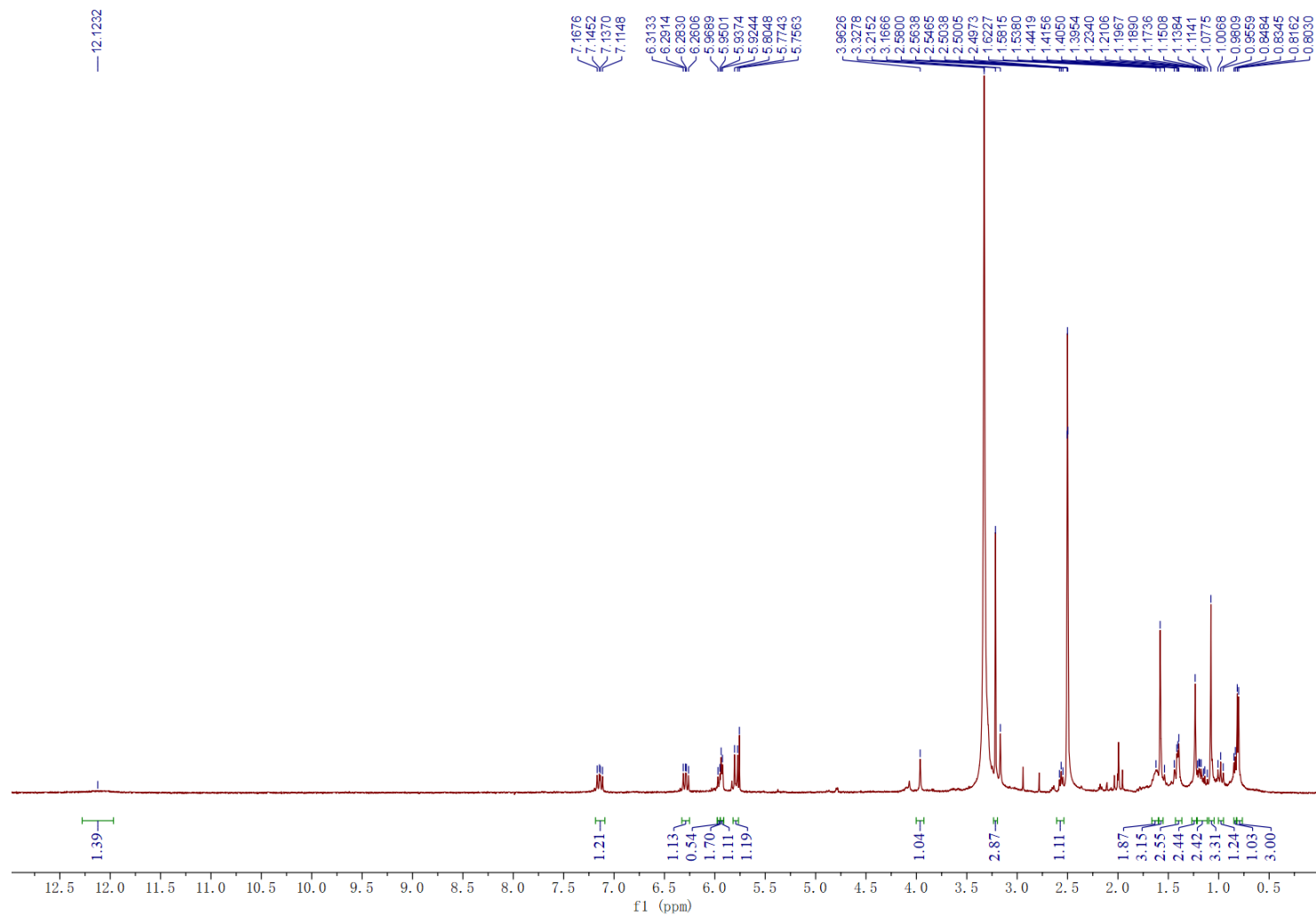


**Figure S29.** HRESI mass spectrum of compound **5**;

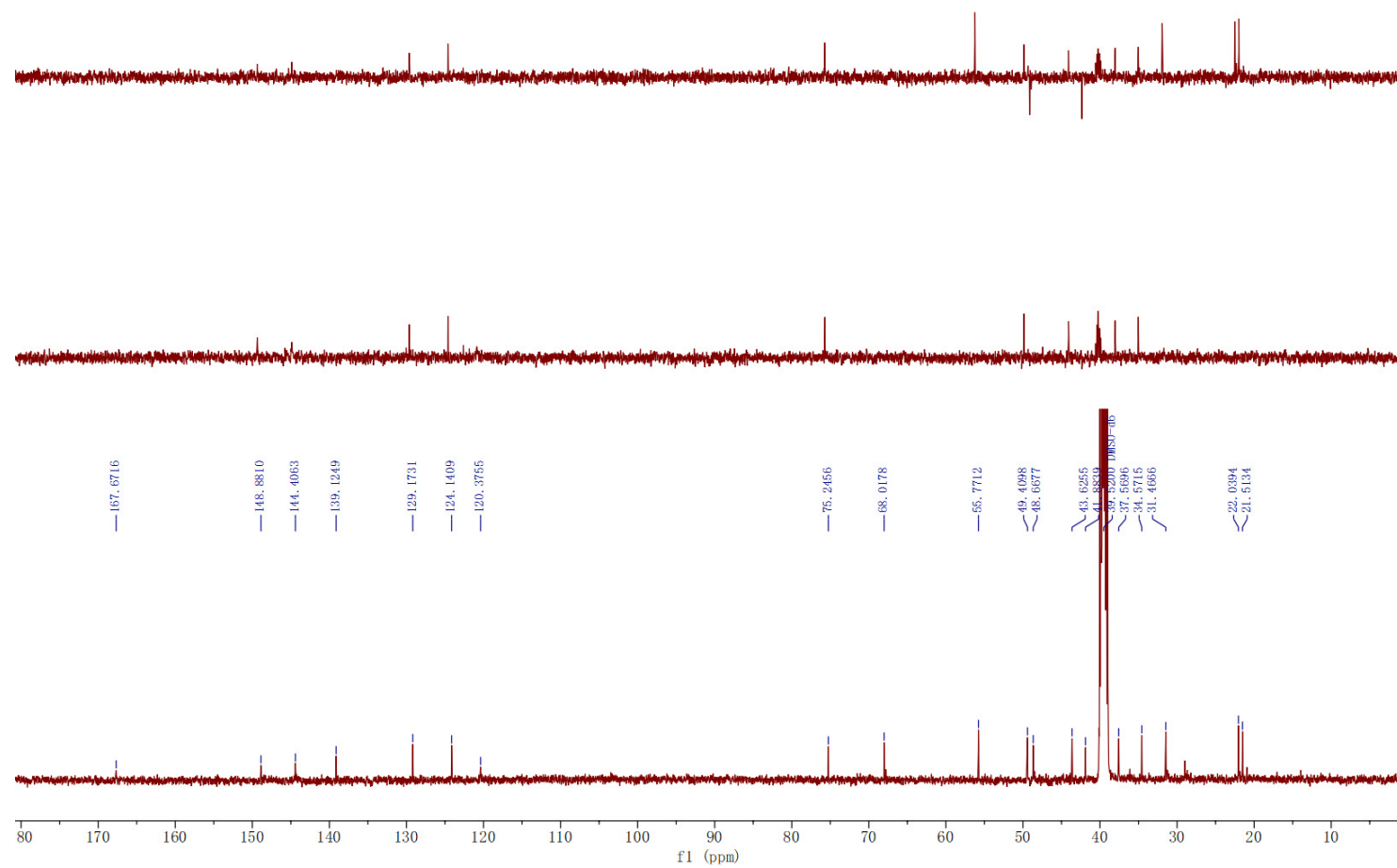
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T: FTMS - p ESI Full ms [150.00-1000.00]



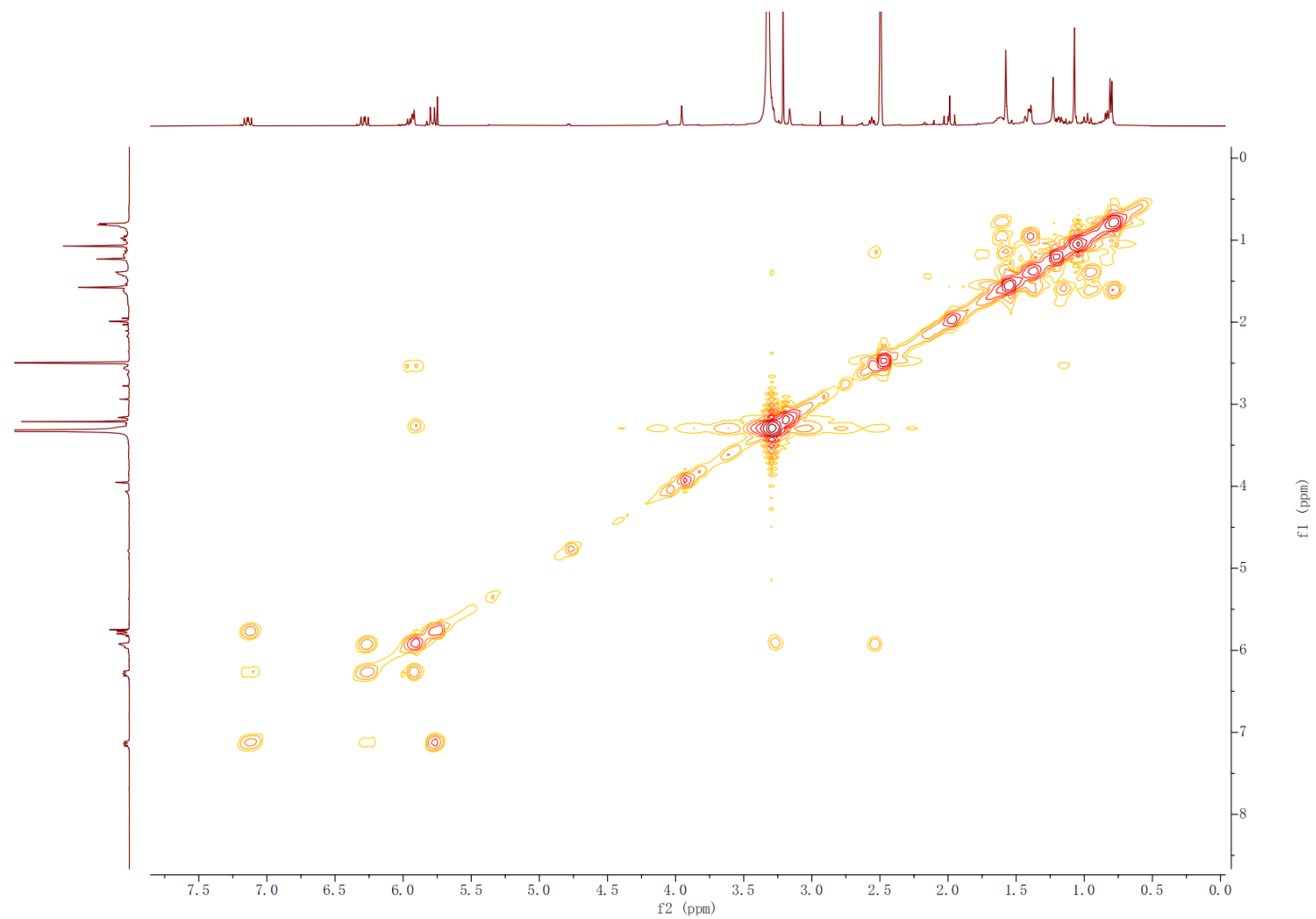
**Figure S30.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **5**;



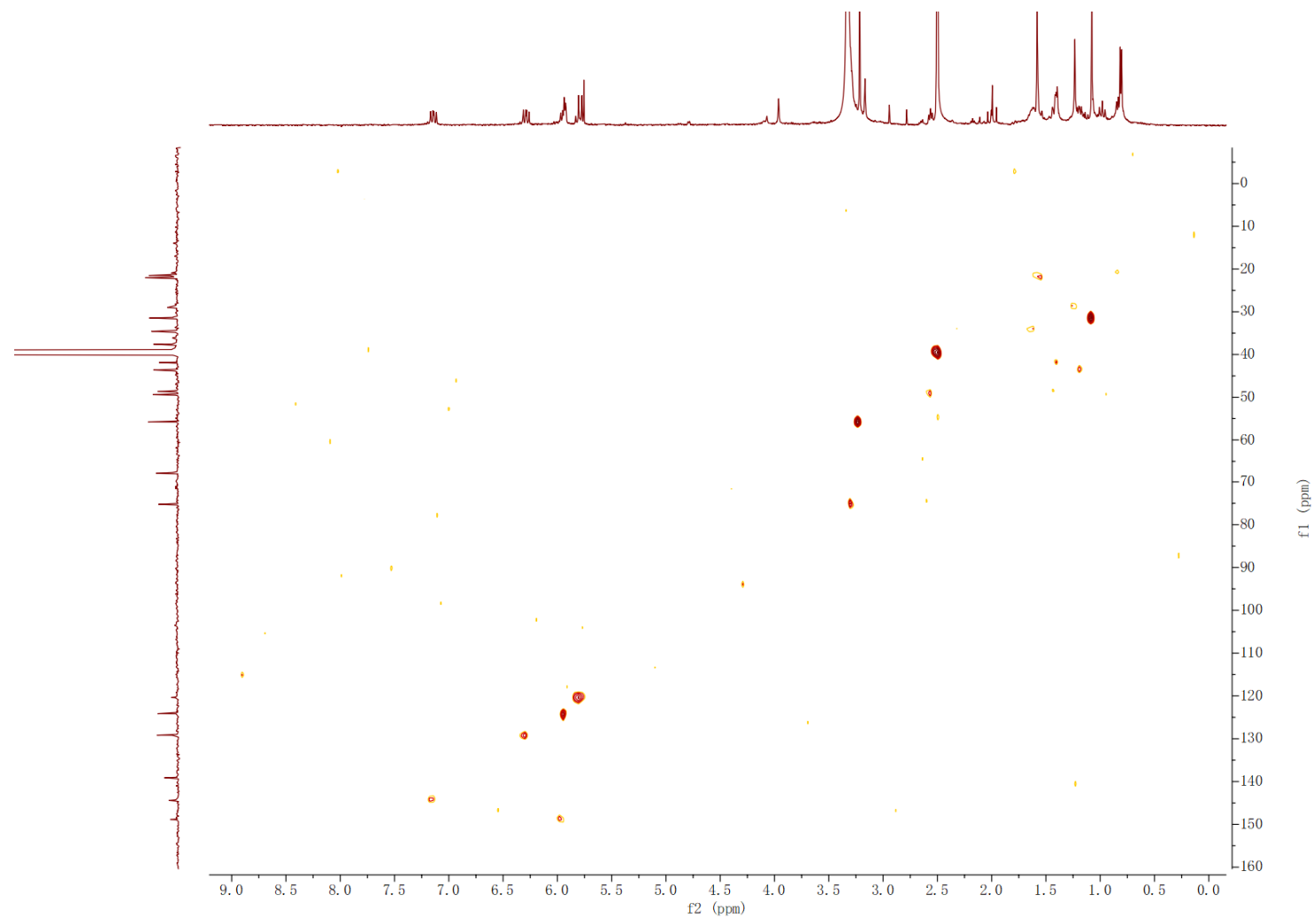
**Figure S31.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **5**;



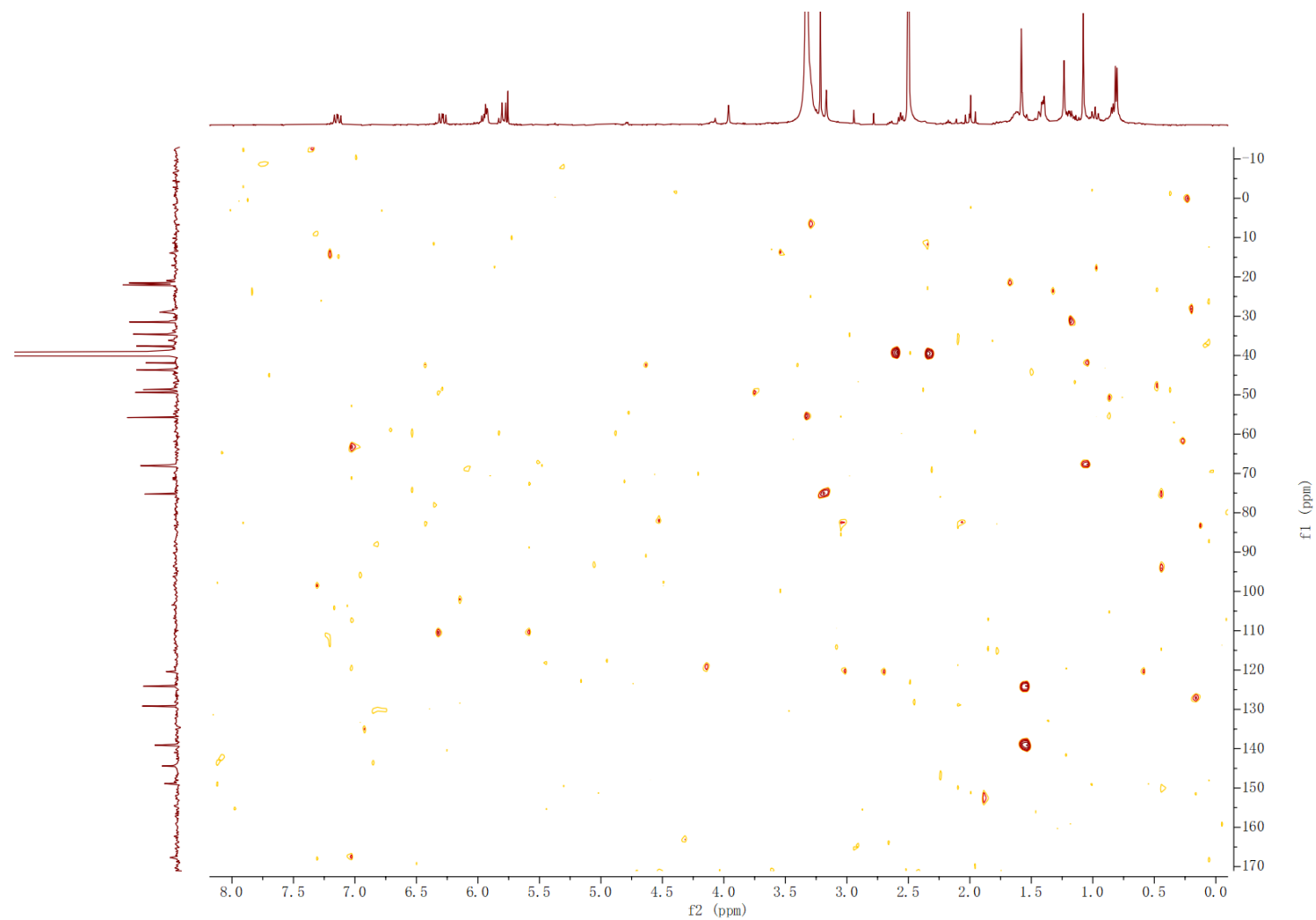
**Figure S32.** COSY spectrum of compound **5**;



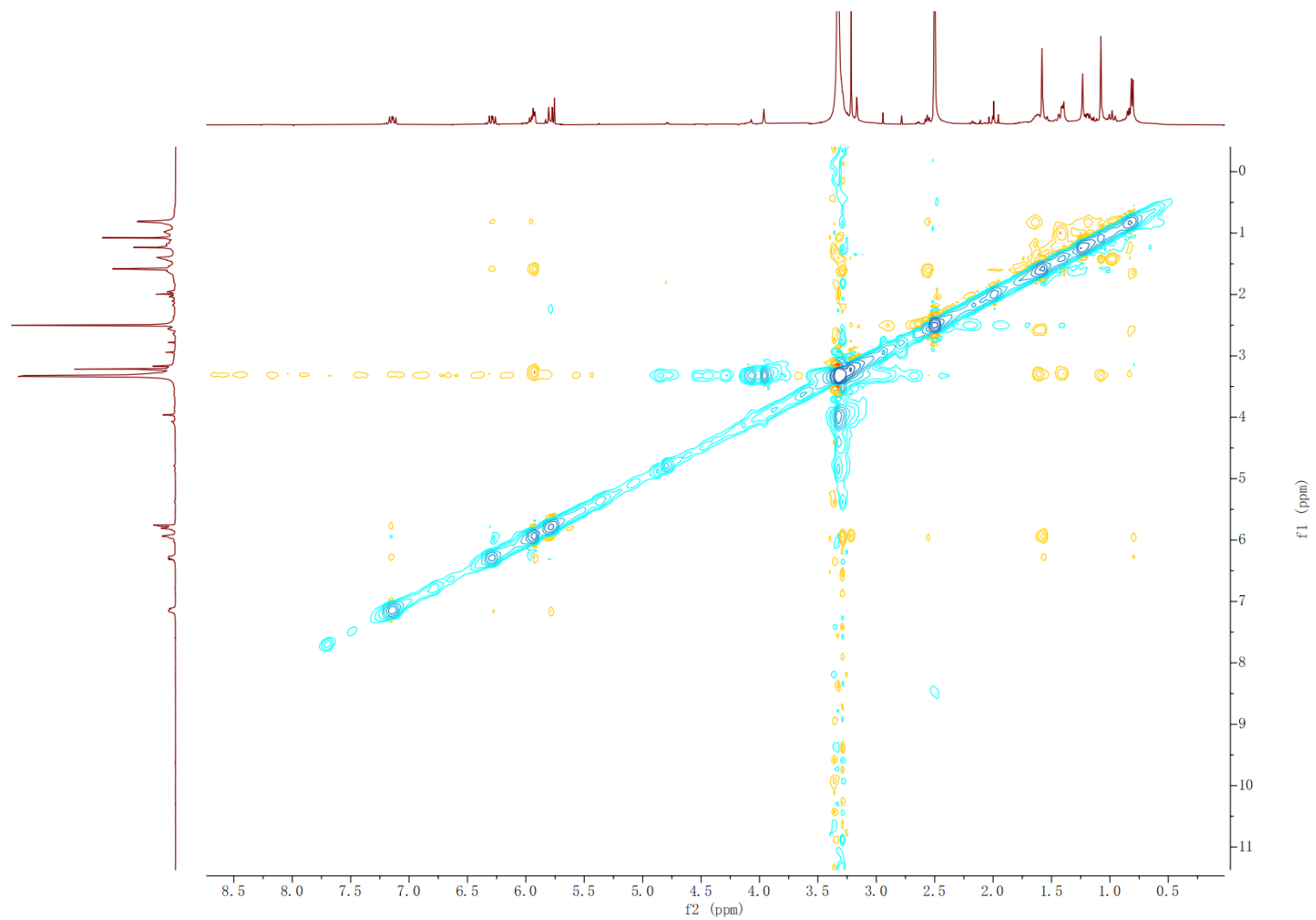
**Figure S33.** HSQC spectrum of compound **5**;



**Figure S34.** HMBC spectrum of compound **5**;

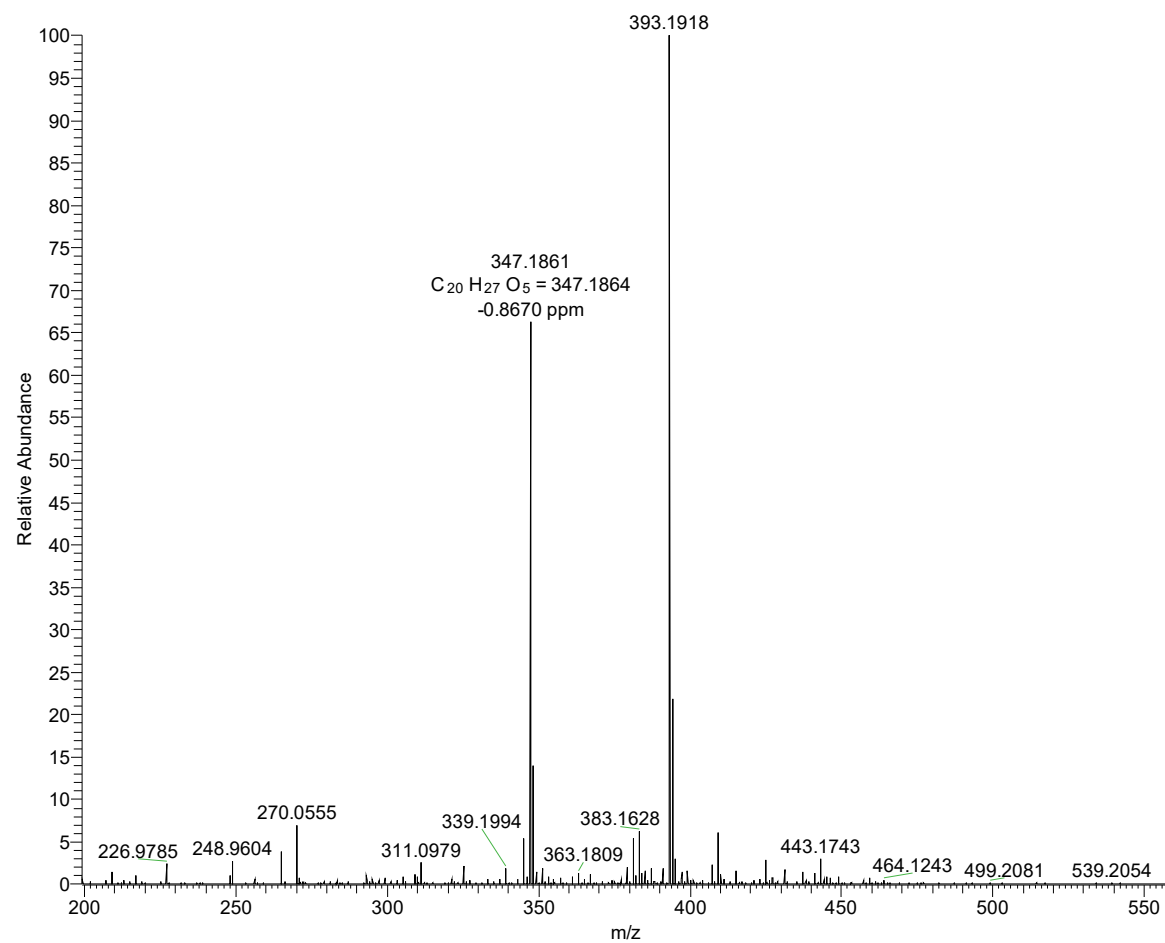


**Figure S35.** NOESY spectrum of compound **5**;



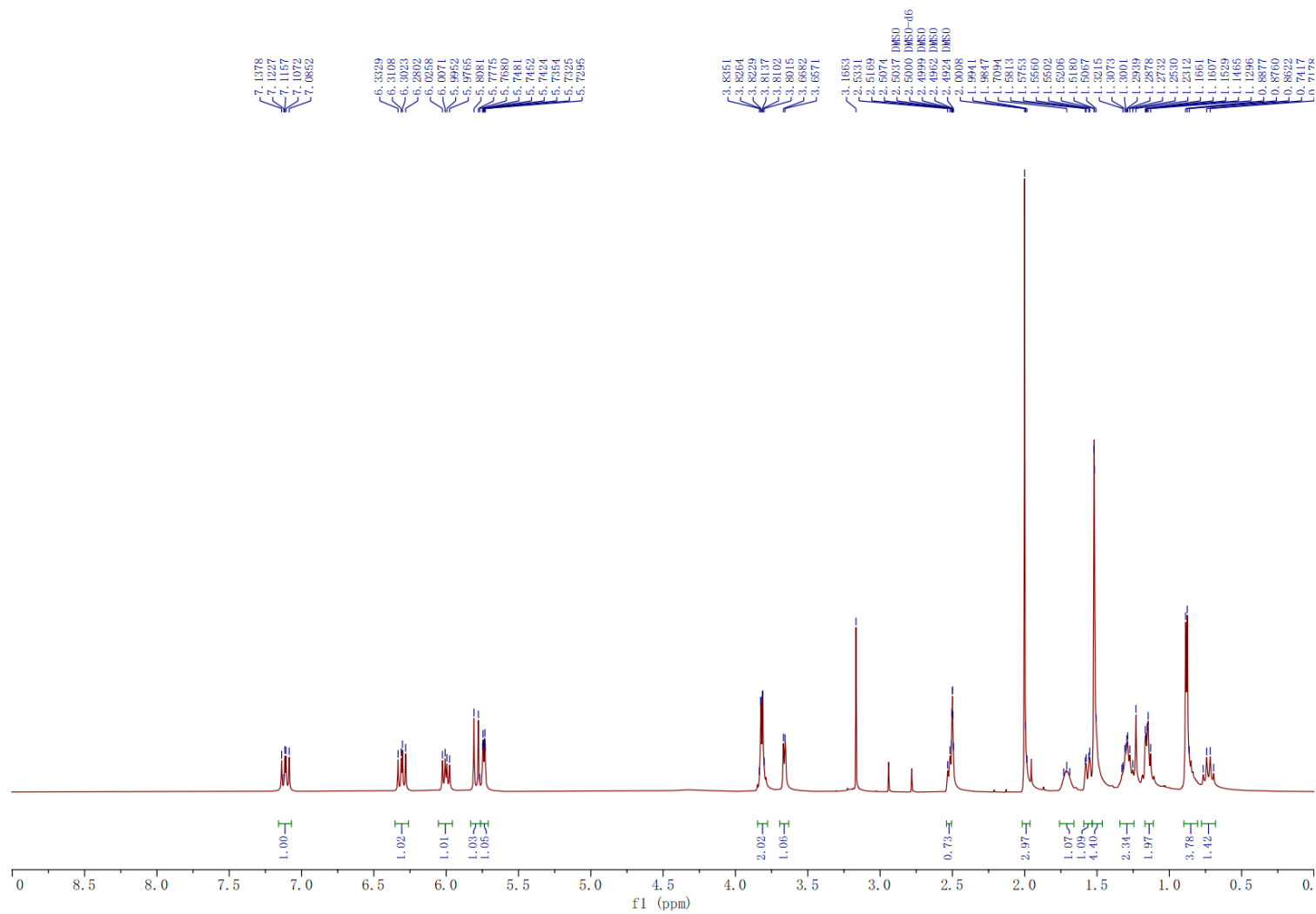
**Figure S36.** HRESI mass spectrum of compound **6**;

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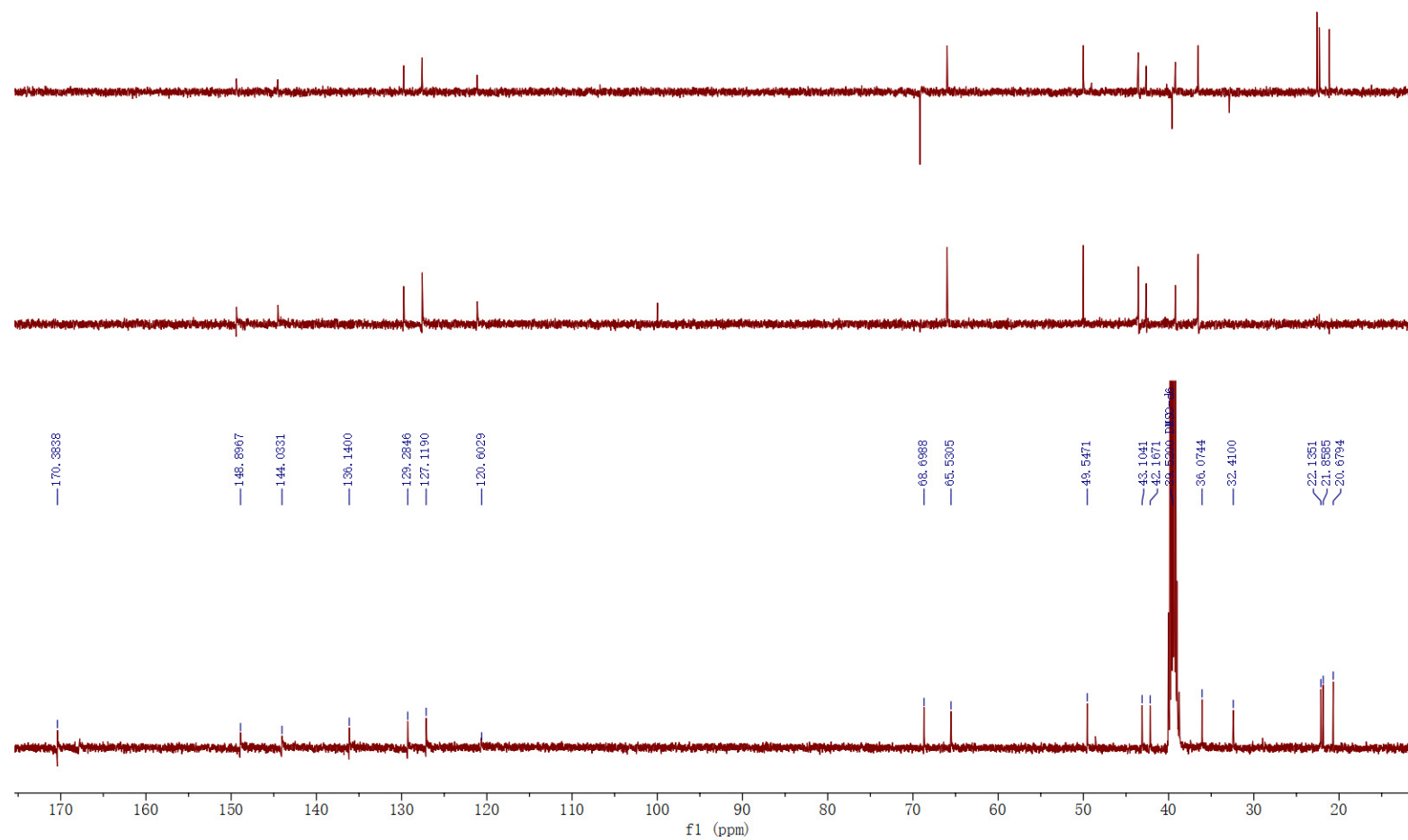




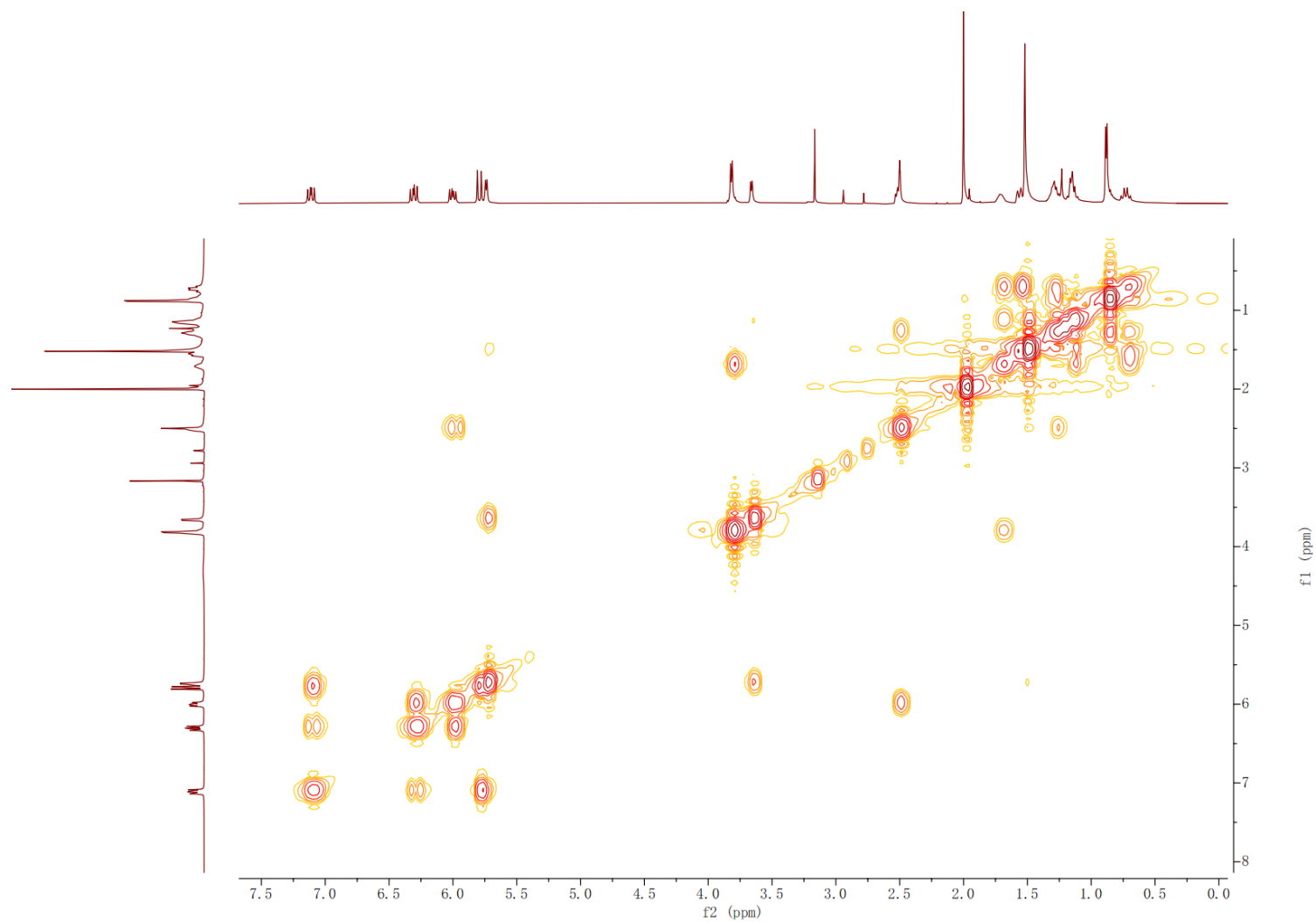
**Figure S37.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **6**;



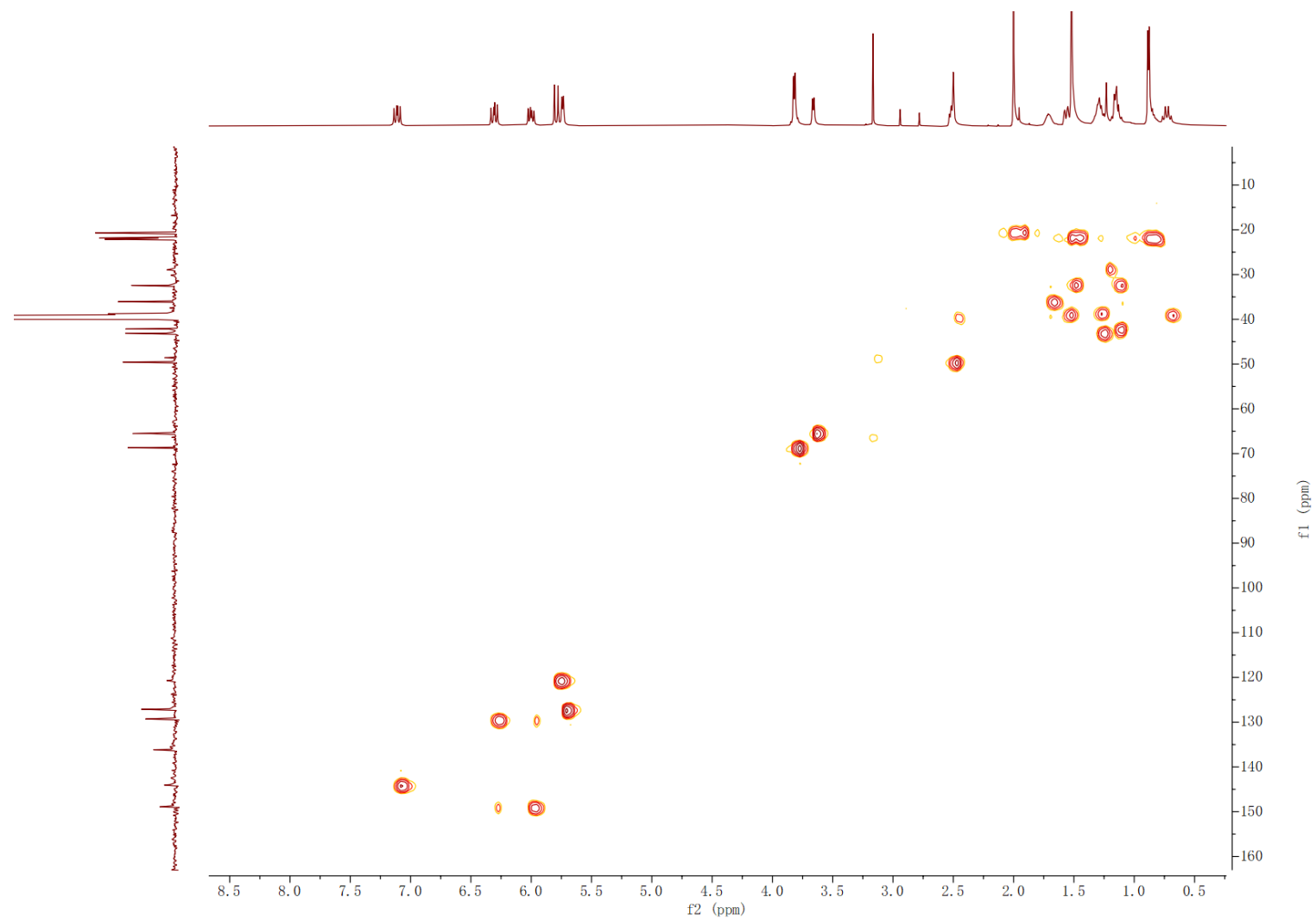
**Figure S38.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **6**;



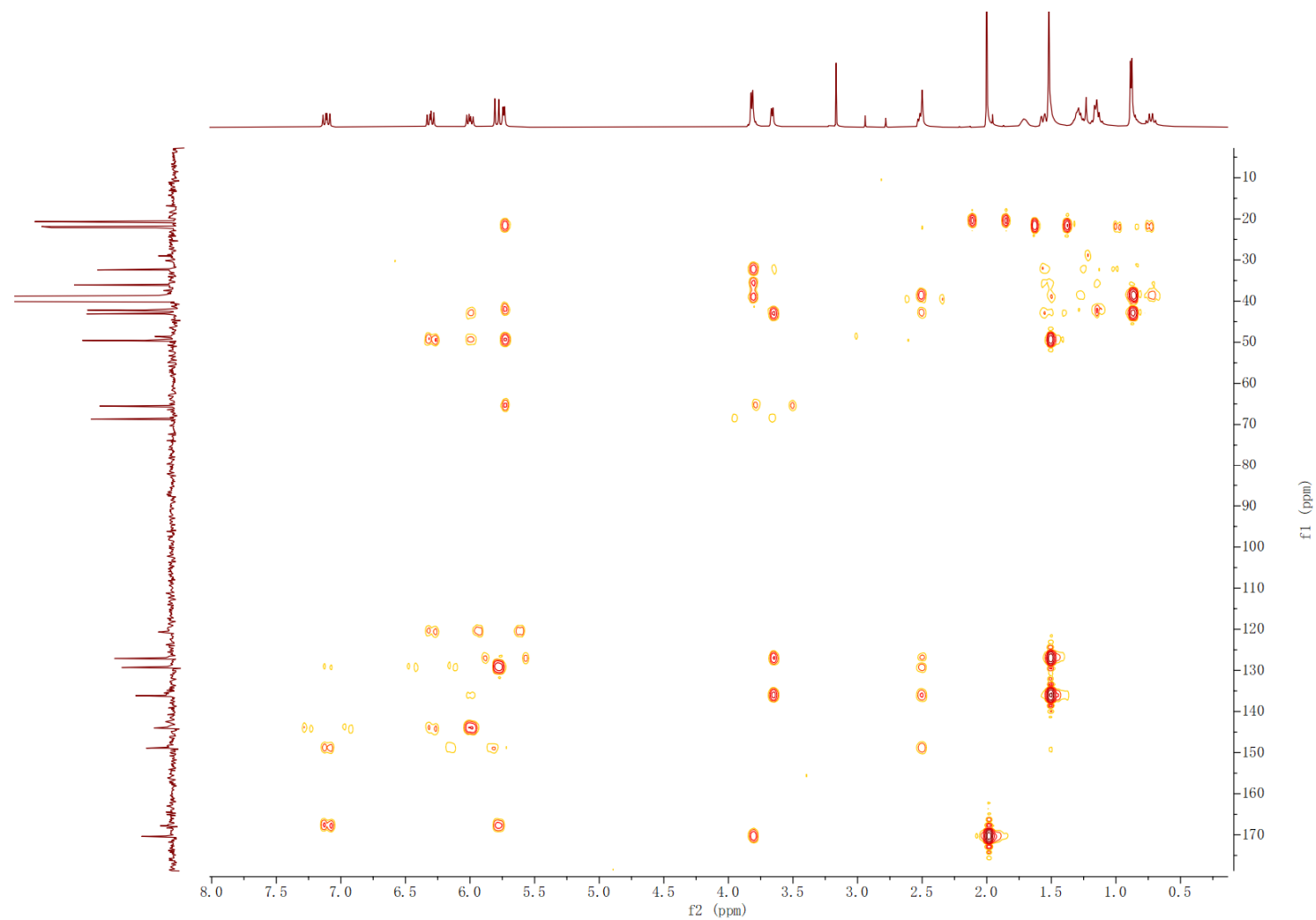
**Figure S39.** COSY spectrum of compound **6**;



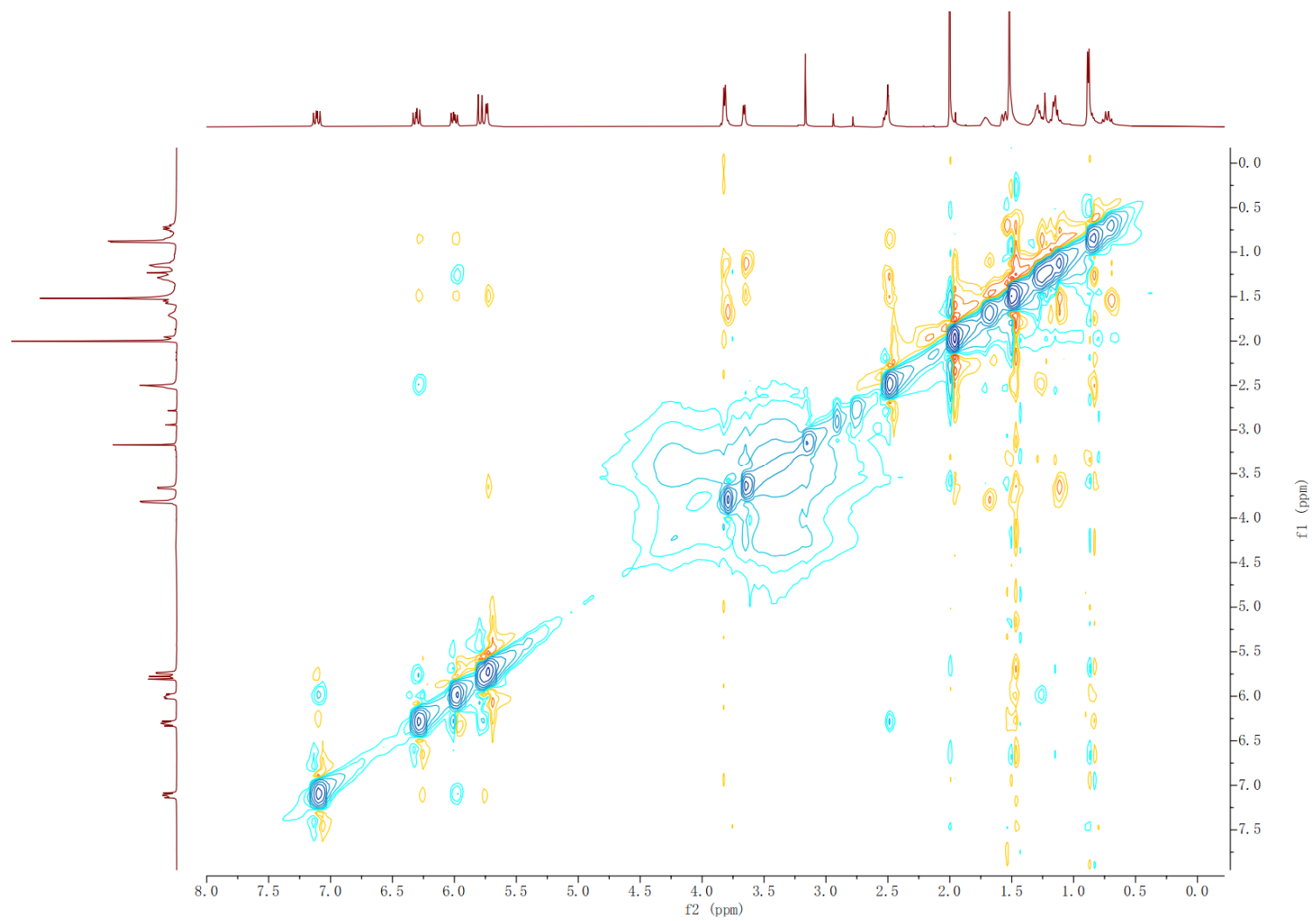
**Figure S40.** HSQC spectrum of compound **6**;



**Figure S41.** HMBC spectrum of compound **6**;

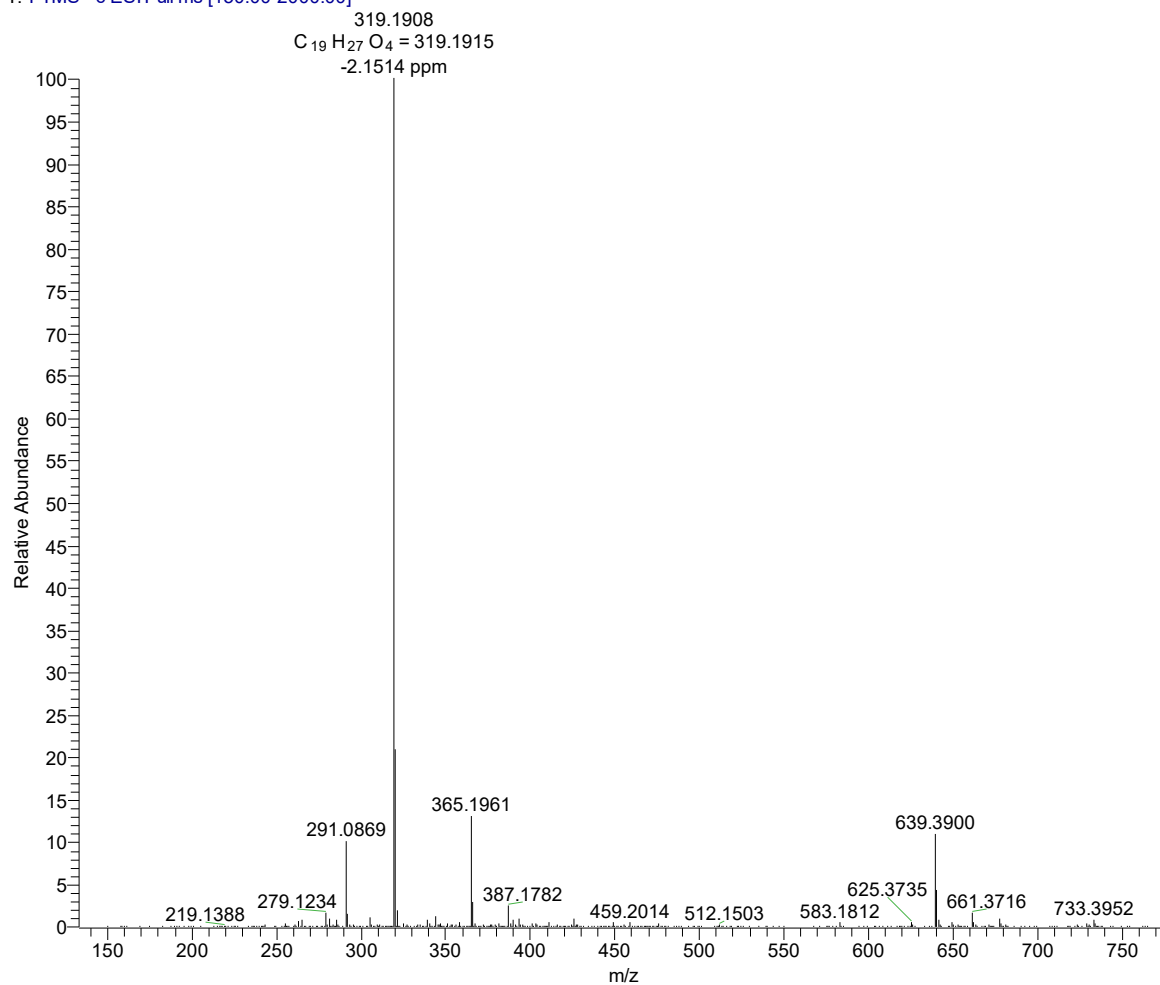


**Figure S42.** NOESY spectrum of compound **6**;



**Figure S43.** HRESI mass spectrum of compound **7**;

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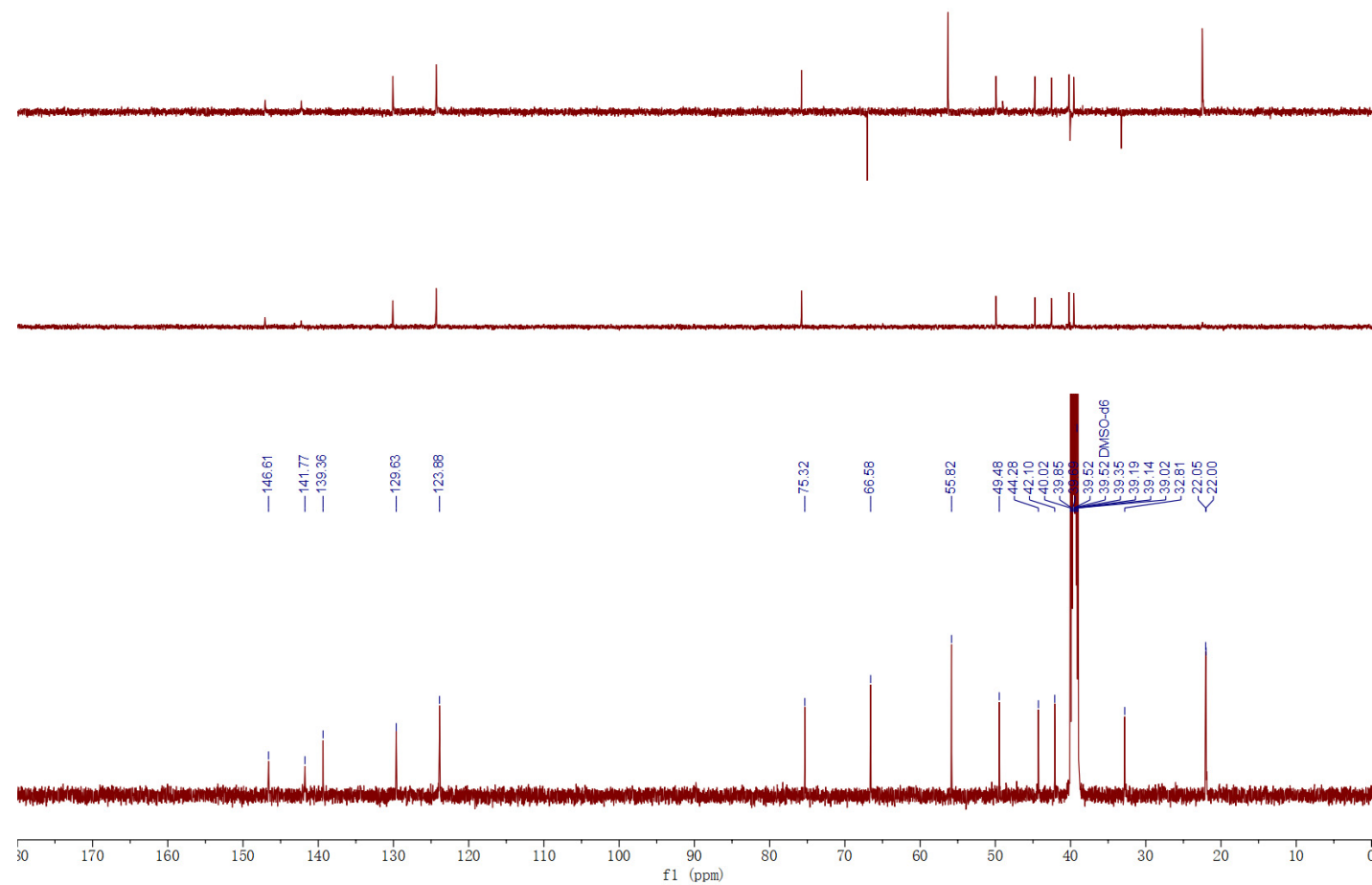


**Figure S44.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **7**;

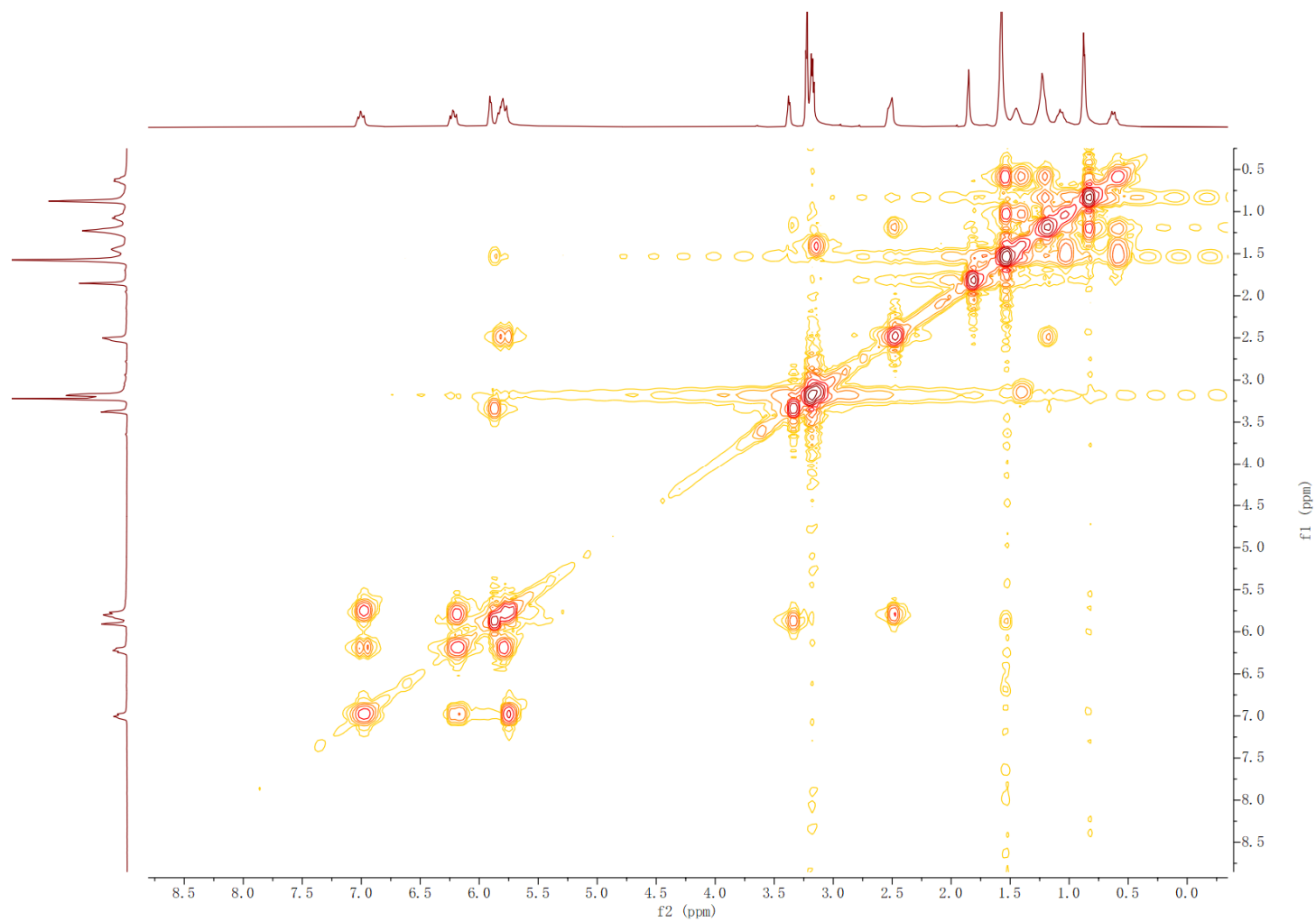




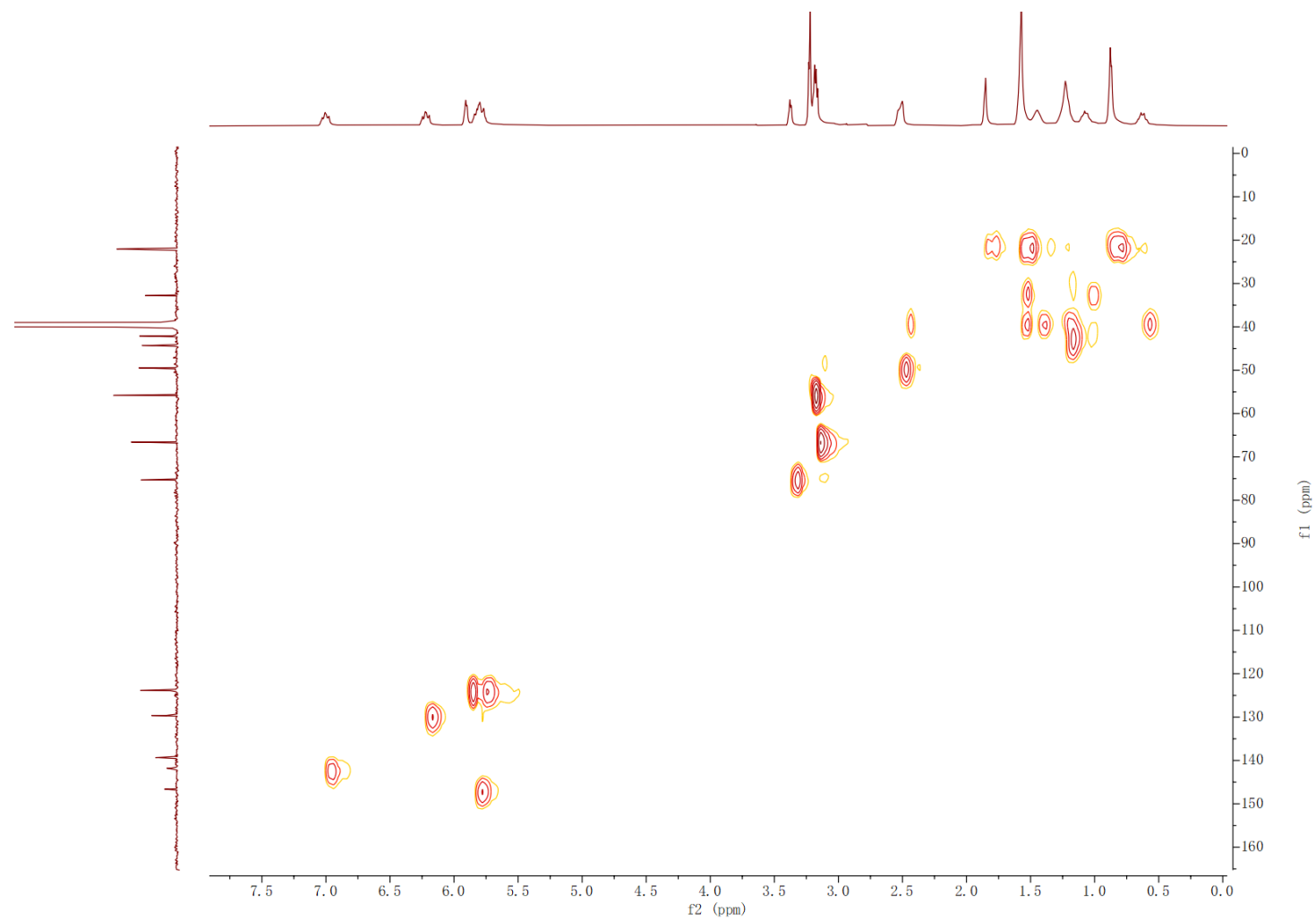
**Figure S45.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **7**;



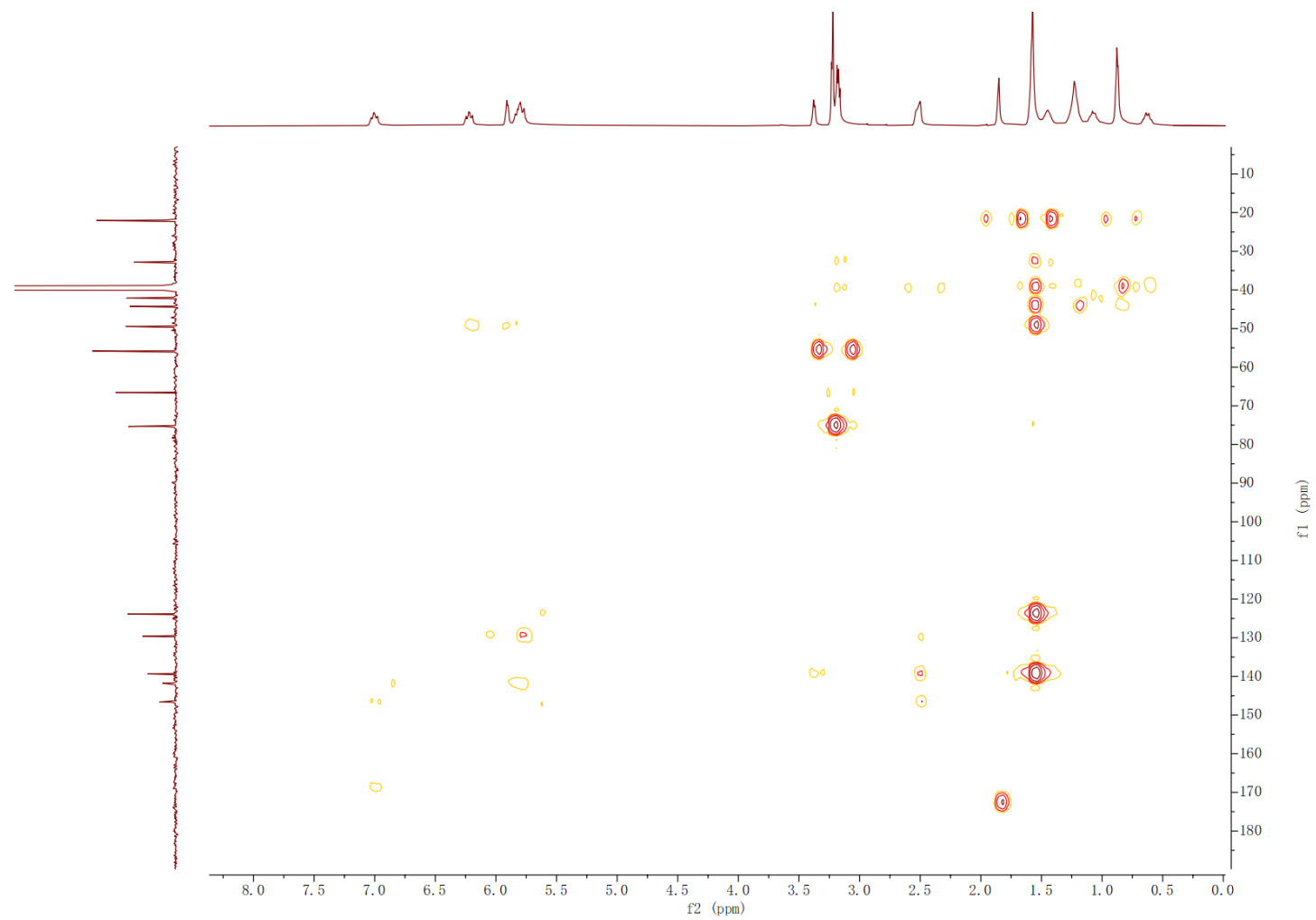
**Figure S46.** COSY spectrum of compound **7**;



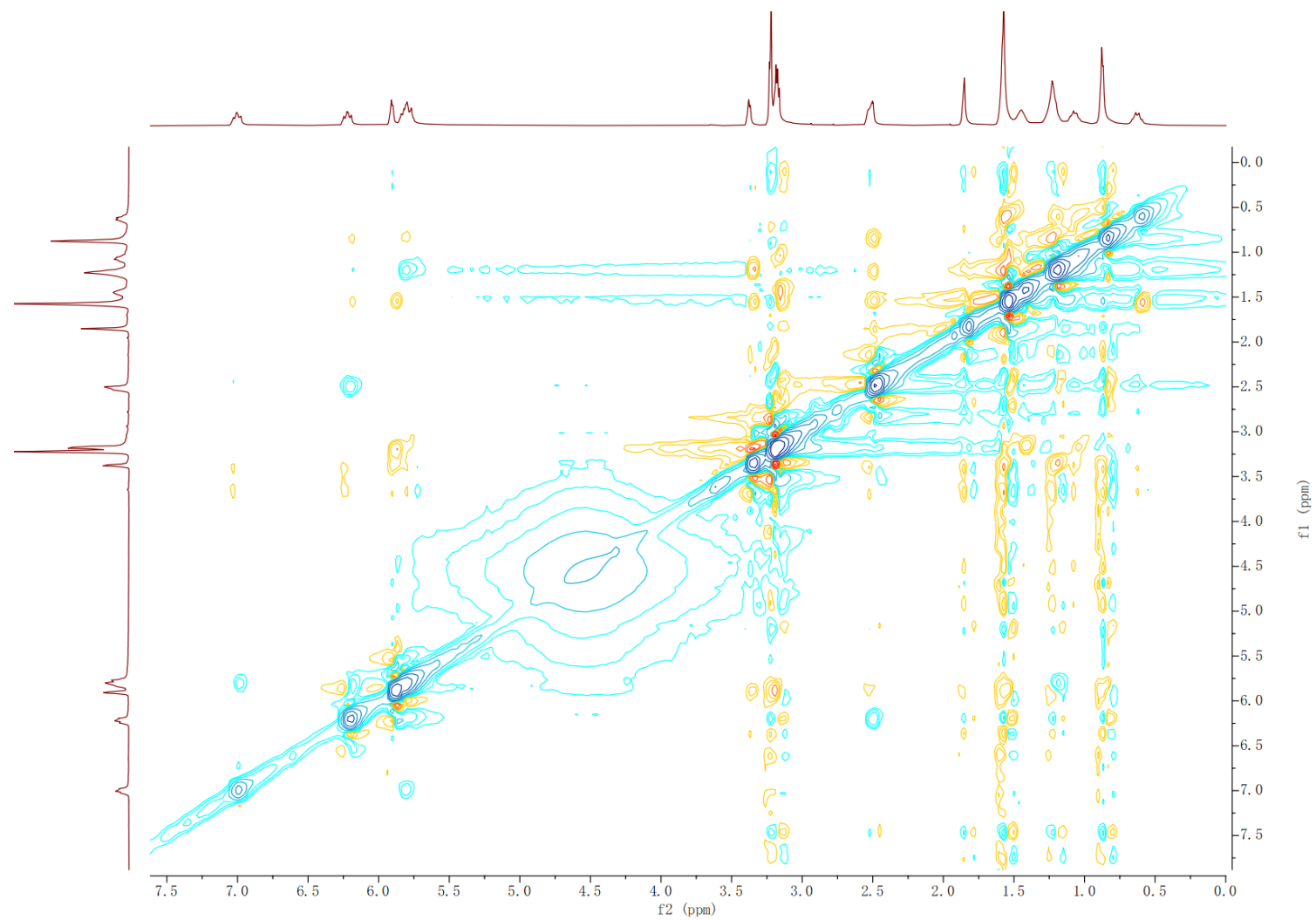
**Figure S47.** HSQC spectrum of compound 7;



**Figure S48.** HMBC spectrum of compound **7**;

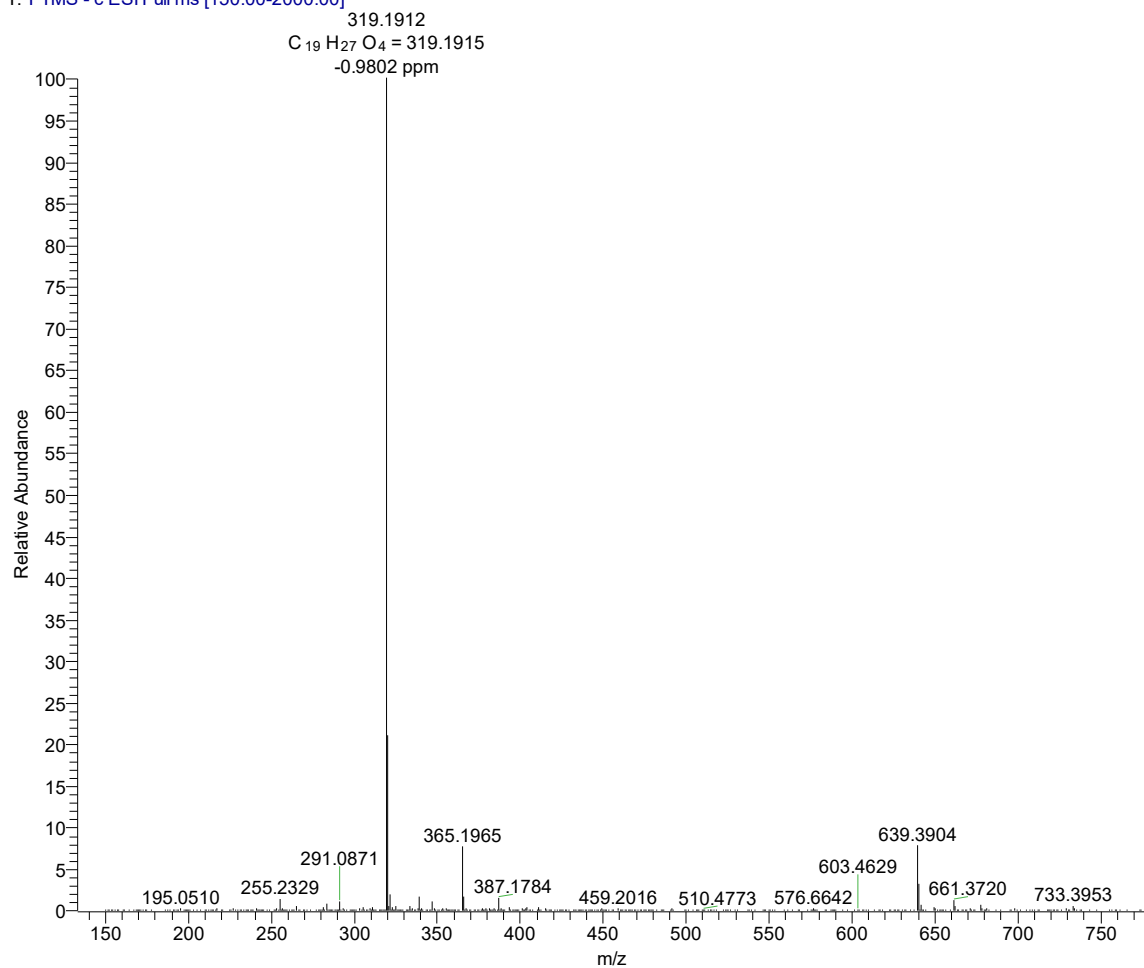


**Figure S49.** NOESY spectrum of compound **7**;

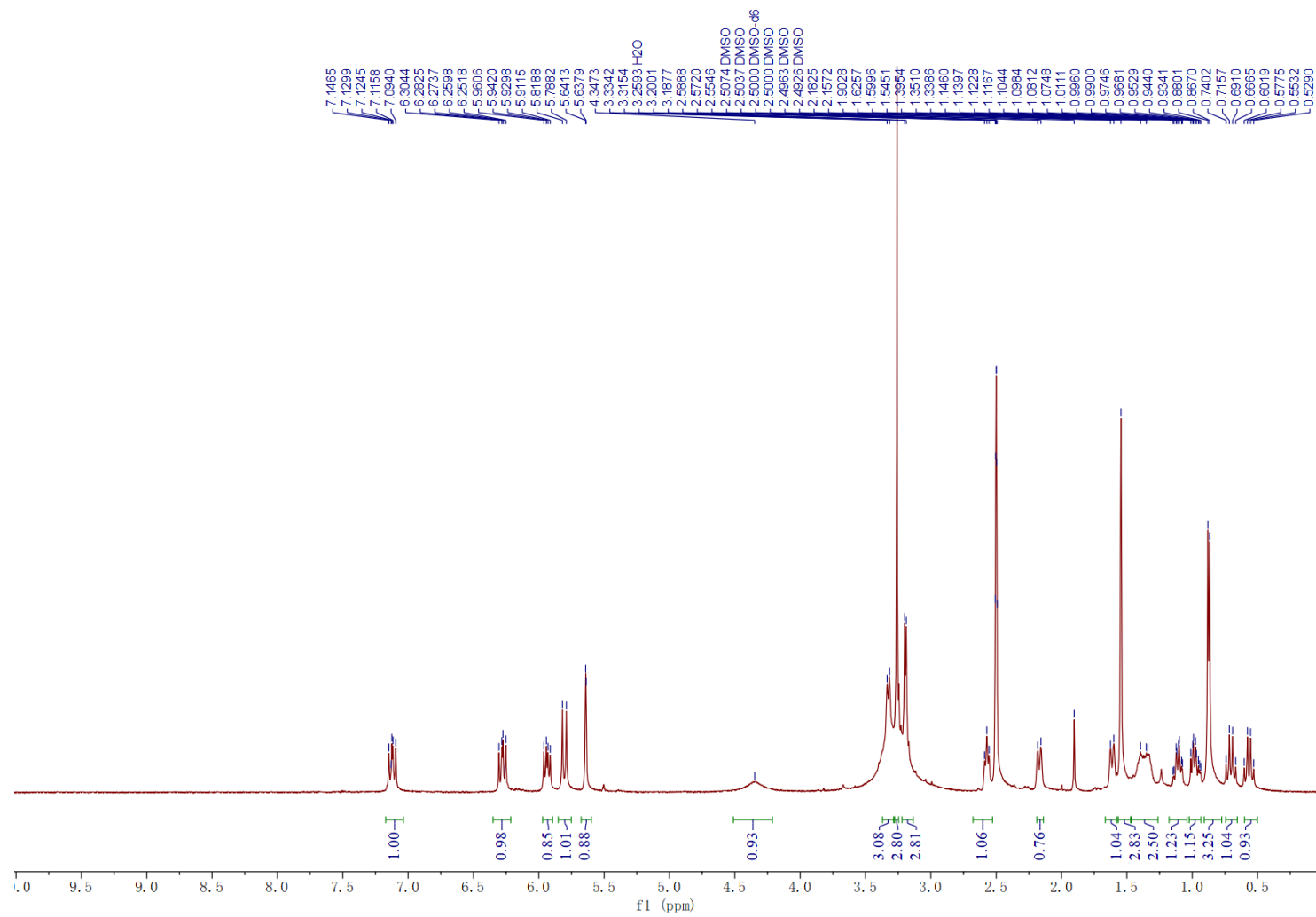


**Figure S50.** HRESI mass spectrum of compound **8**;

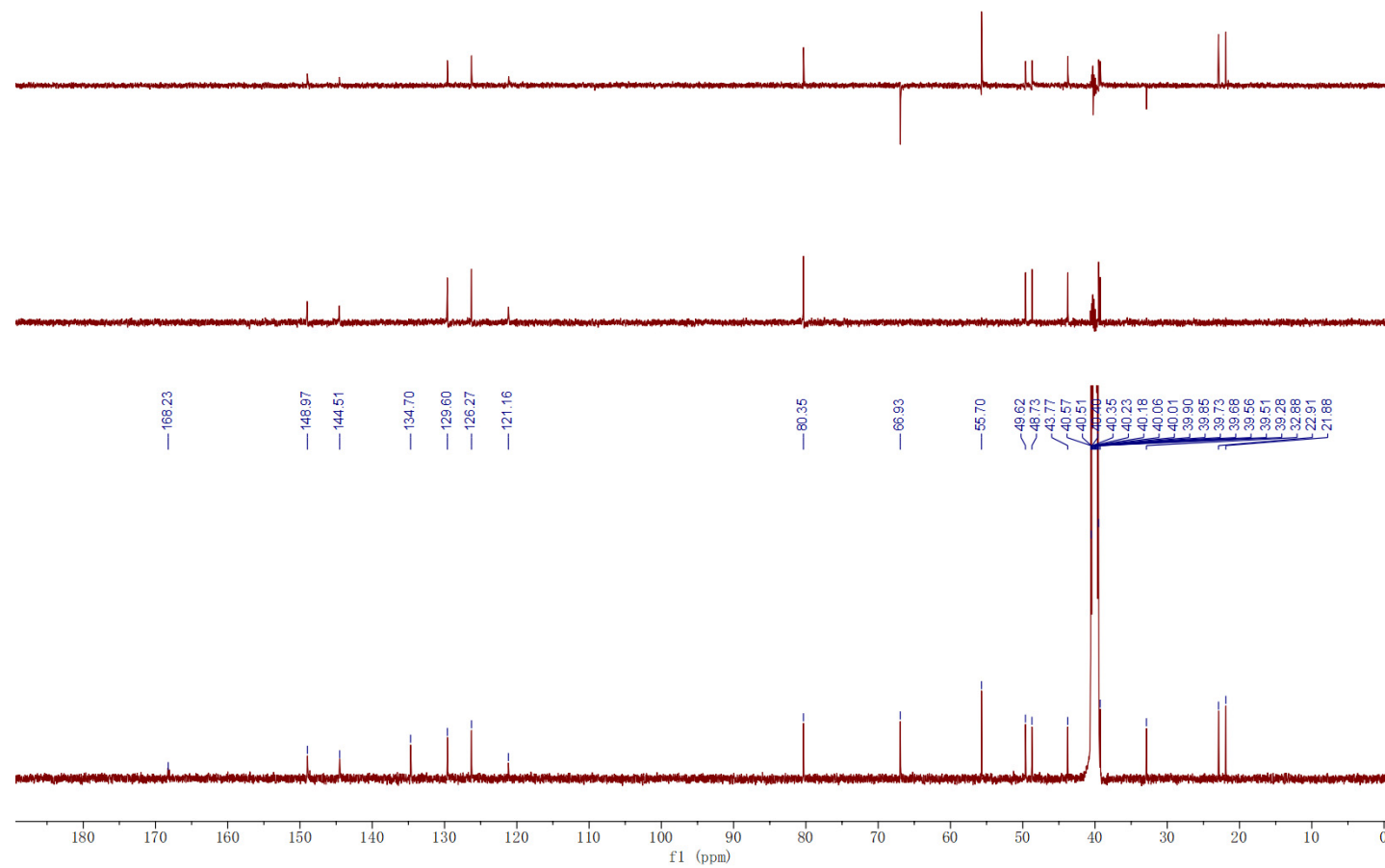
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**Figure S51.**  $^1\text{H}$  NMR (500 MHz,  $\text{DMSO}-d_6$ ) spectrum of compound **8**;

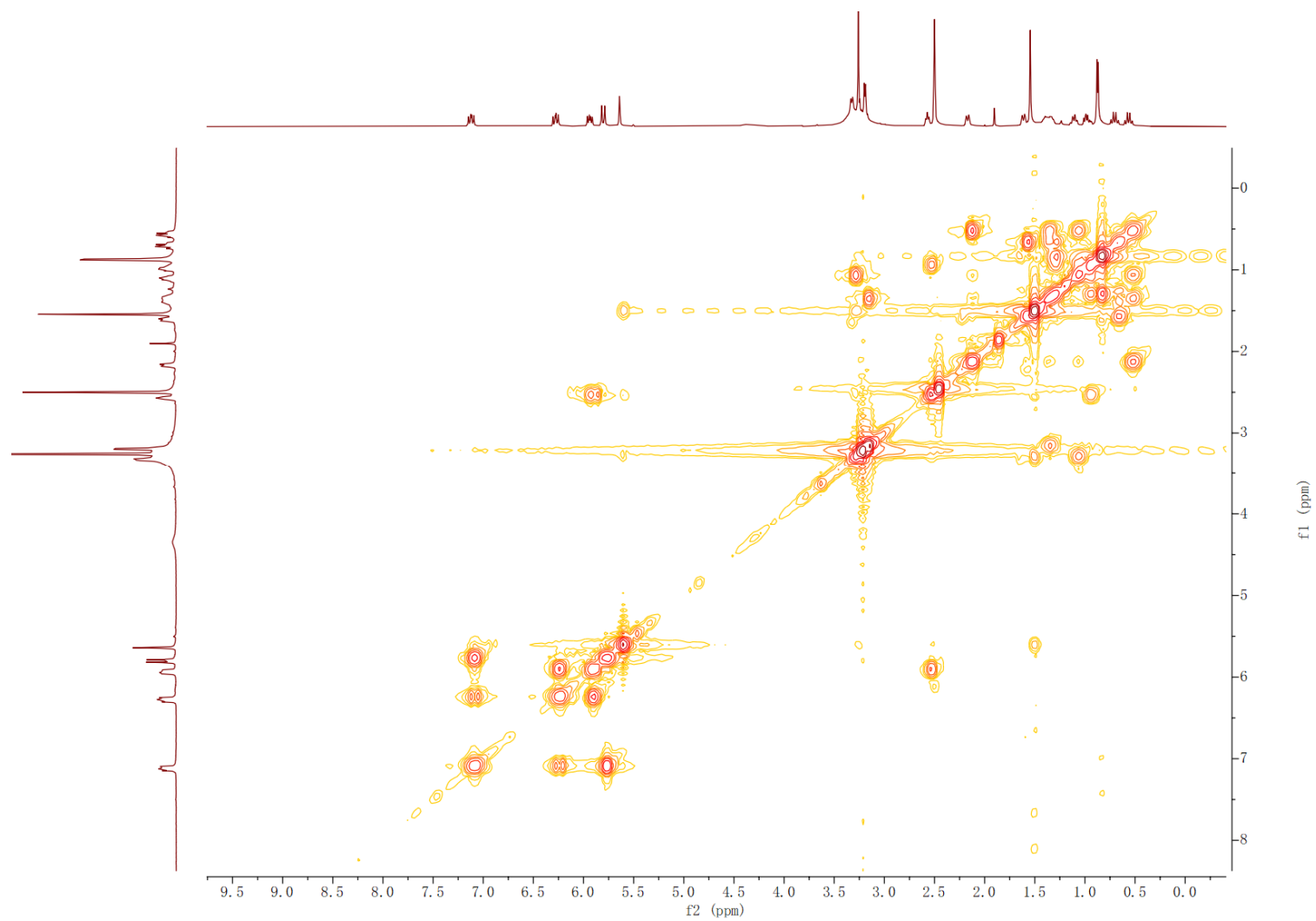


**Figure S52.**  $^{13}\text{C}$  NMR (125 MHz,  $\text{DMSO-}d_6$ ) and DEPT spectra of compound **8**;

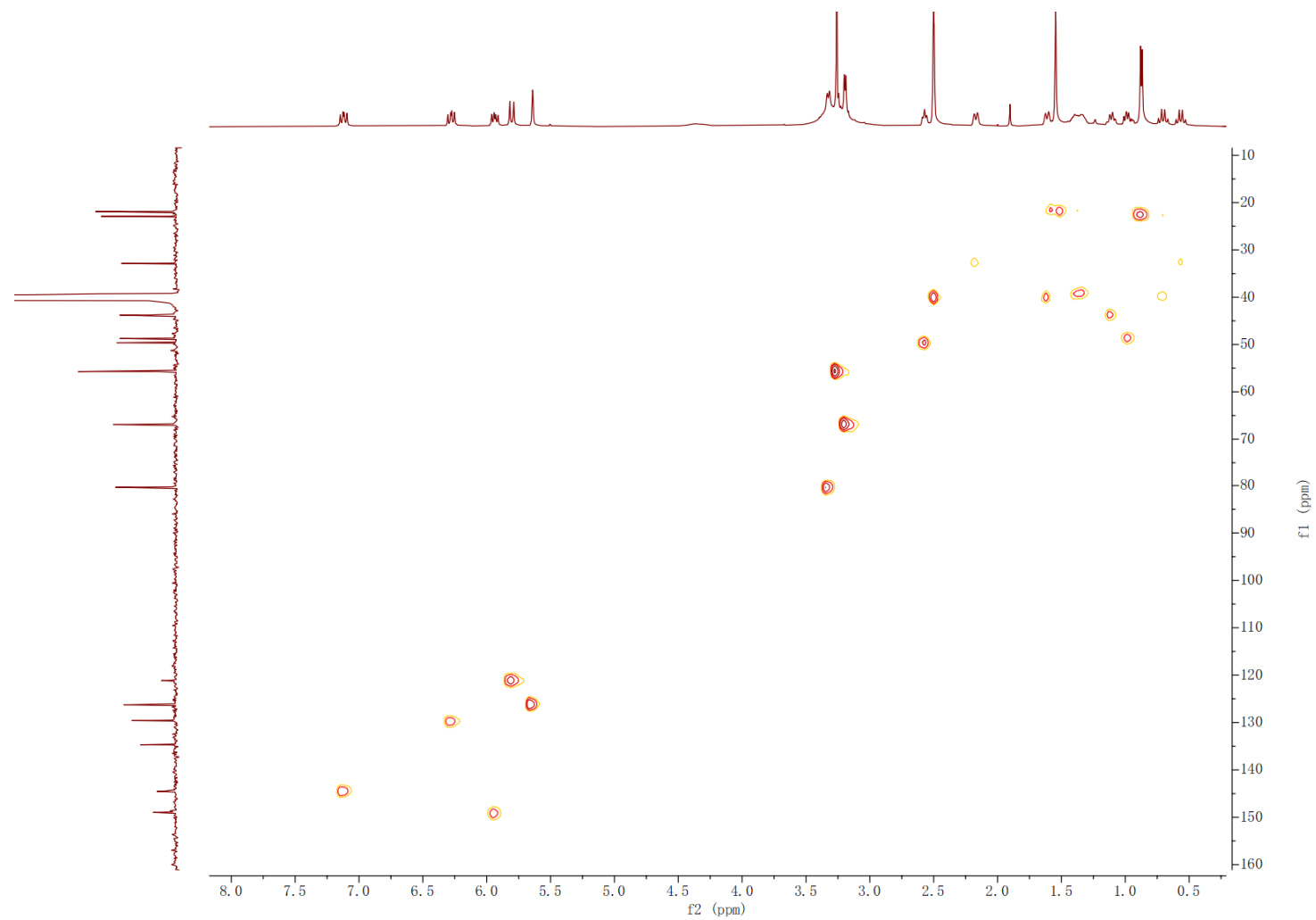




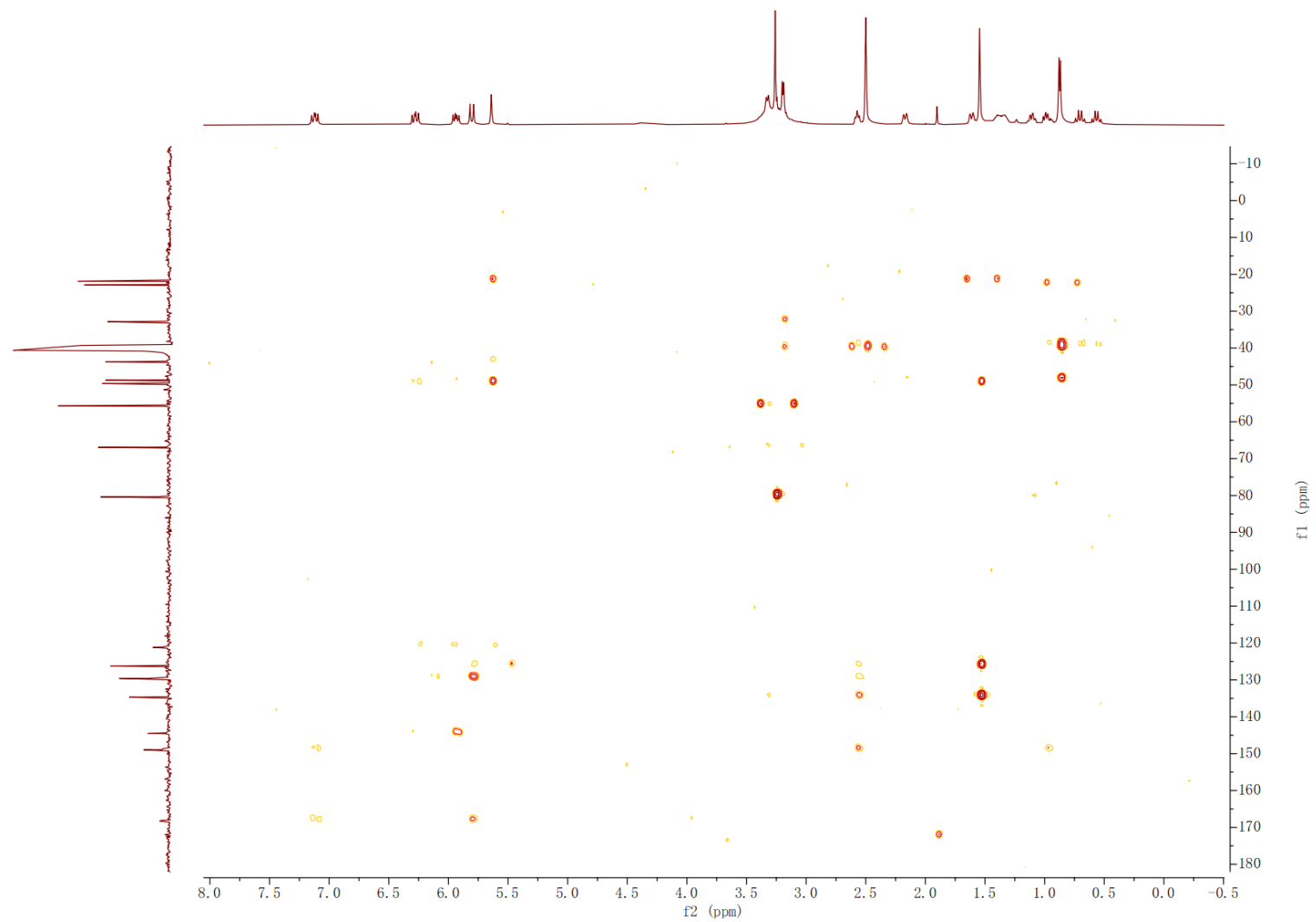
**Figure S53.** COSY spectrum of compound **8**;



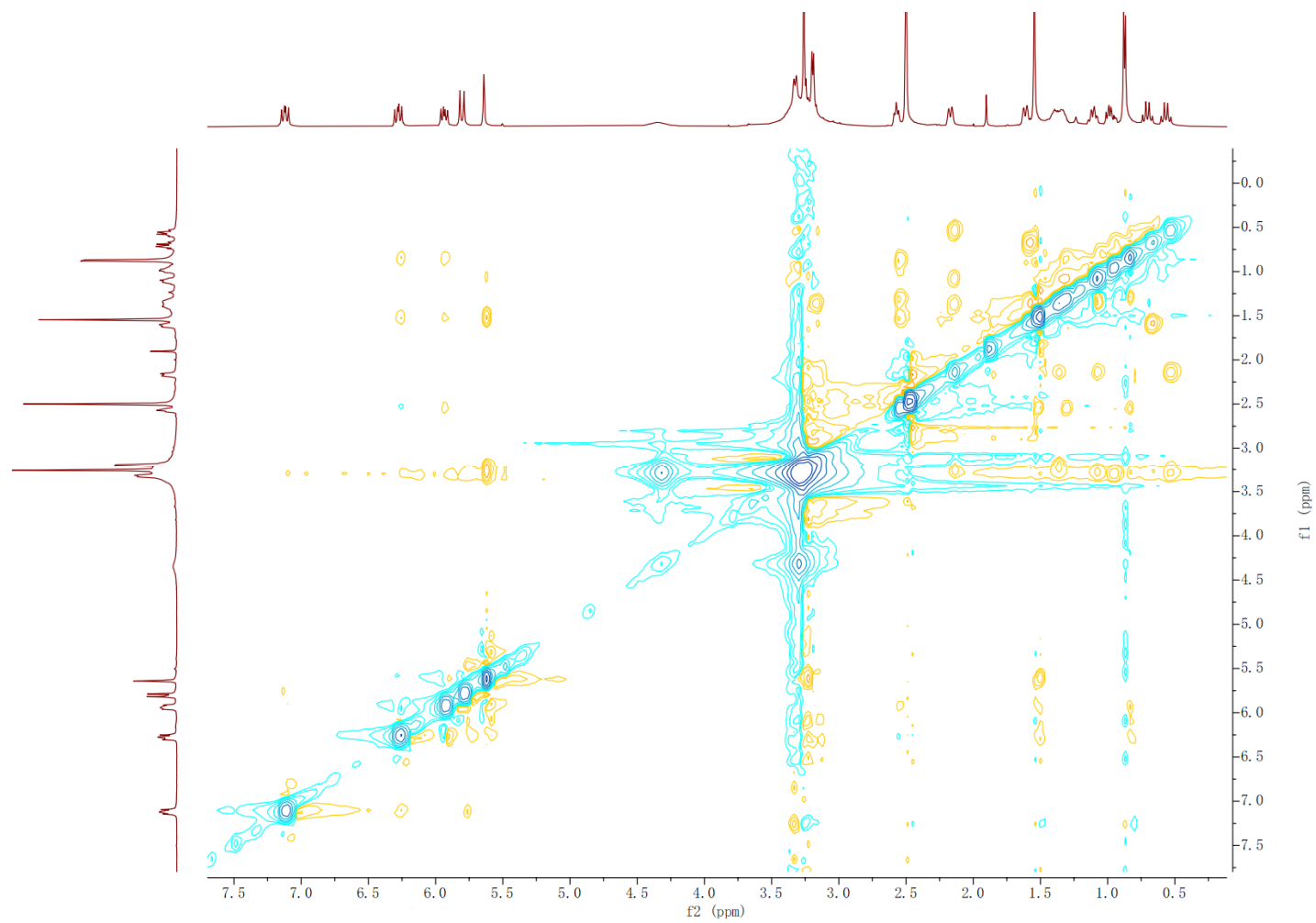
**Figure S54.** HSQC spectrum of compound **8**;



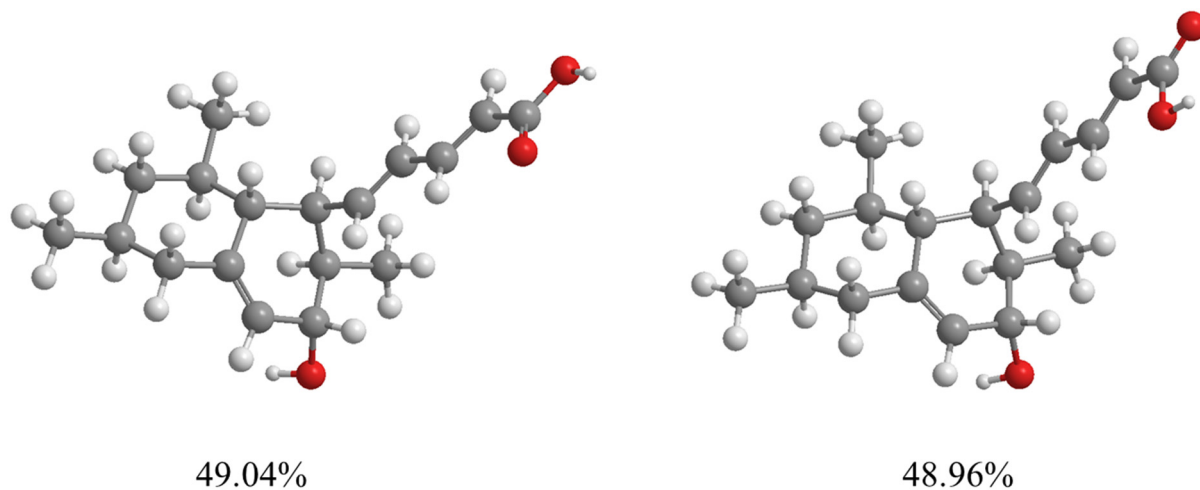
**Figure S55.** HMBC spectrum of compound **8**;



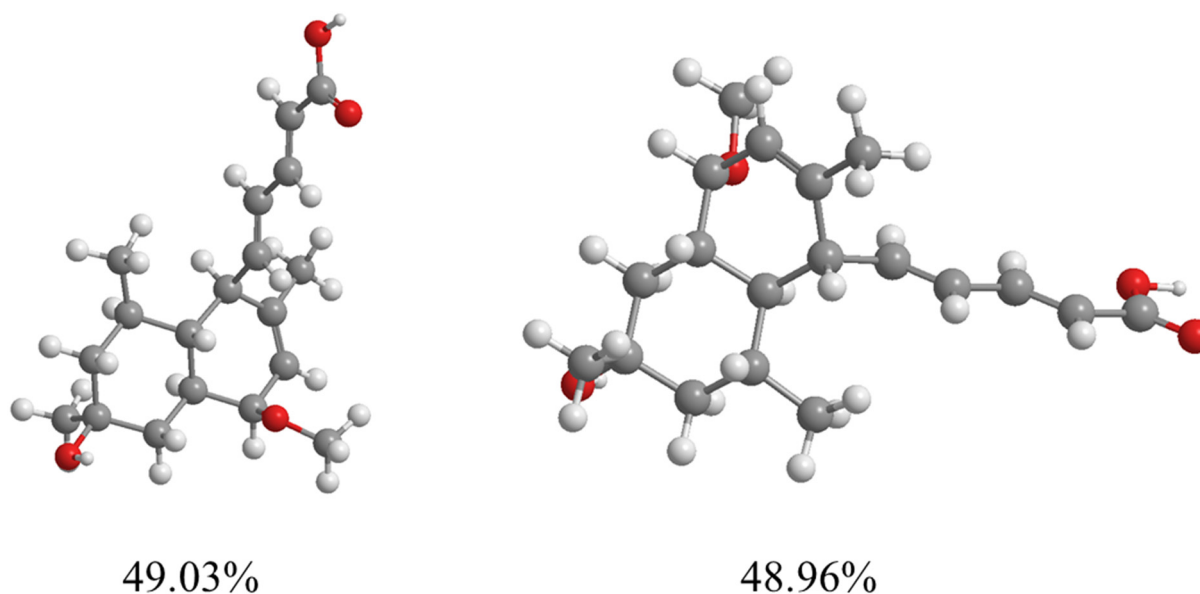
**Figure S56.** NOESY spectrum of compound **8**;



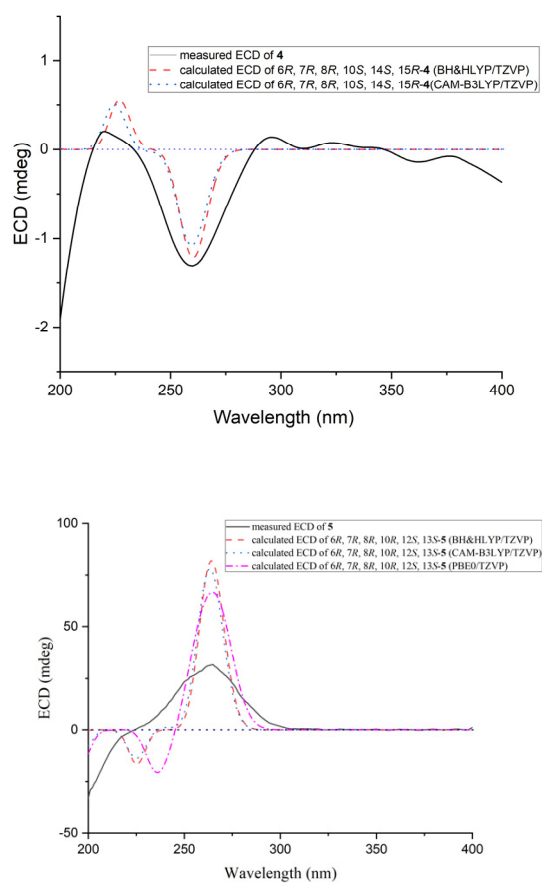
**Figure S57.** Structures and populations of conformers obtained by gas phase B3LYP/6-31G(d) reoptimization of the initial MMFF conformers of (6*R*, 7*R*, 8*R*, 10*S*, 14*S*, and 15*R*)-**4** above 2% population;



**Figure S58.** Structures and populations of conformers obtained by gas phase B3LYP/6-31G(d) reoptimization of the initial MMFF conformers of (6*R*, 7*R*, 8*R*, 10*R*, 12*S*, and 13*S*)-**5** above 2% population;



**Figure S59.** Experimental and calculated ECD at different levels of compound **4** and **5**;



**Table S1.** Cartesian coordinates for the low-energy reoptimized MMFF conformers of **4** calculated at B3LYP/6-31G(d) level of theory in vacuo;

Compound <b>4</b> Conformer A		Standard Orientation (Ångstroms)		
	Type	X	Y	Z
1	C	-3.430922	-1.837529	0.712851
2	C	-4.059837	-1.357744	-0.606239
3	C	-2.952493	-0.941961	-1.601788
4	C	-2.020619	0.05162	-0.955533
5	C	-1.347473	-0.451088	0.311031
6	C	-2.439744	-0.842037	1.356015
7	C	-1.866771	1.303371	-1.416432
8	C	-1.069721	2.383223	-0.73
9	C	-0.739164	2.007703	0.725231
10	C	-0.248961	0.533243	0.814727
11	C	1.029539	0.293616	0.053187
12	C	2.213847	-0.033953	0.60963
13	C	3.410356	-0.289913	-0.165473
14	C	4.610791	-0.617972	0.360385
15	C	5.773553	-0.863044	-0.505587
16	O	6.883488	-1.176705	0.223041
17	O	5.799353	-0.807608	-1.723458
18	C	-1.860688	-1.45082	2.643084
19	C	-4.993126	-2.415714	-1.207568
20	C	0.229723	3.001208	1.37557
21	O	-1.764761	3.641097	-0.805019
22	H	-0.841116	-1.397317	0.055109
23	H	-0.040815	0.325403	1.870414
24	H	-4.227312	-2.066325	1.434845
25	H	-2.90193	-2.787401	0.529343
26	H	-4.656574	-0.457787	-0.389301
27	H	-2.393826	-1.843969	-1.900694
28	H	-3.397438	-0.521658	-2.512304
29	H	-2.997709	0.068116	1.624841
30	H	-2.364009	1.608164	-2.338174
31	H	-0.139485	2.583923	-1.279196
32	H	-1.690382	2.049466	1.27908
33	H	0.97333	0.363427	-1.034784
34	H	2.294515	-0.11753	1.694588
35	H	3.334591	-0.212912	-1.250102
36	H	4.761884	-0.712071	1.432308
37	H	7.605445	-1.322876	-0.416178
38	H	-1.220087	-2.313845	2.417072
39	H	-1.267493	-0.734501	3.221202
40	H	-2.669538	-1.801253	3.295946
41	H	-4.442906	-3.335115	-1.448514
42	H	-5.460199	-2.054297	-2.132199
43	H	-5.796208	-2.68065	-0.508534

44	H	-0.165301	4.019704	1.30783
45	H	1.209711	2.984947	0.884052
46	H	0.38448	2.762651	2.43551
47	H	-2.666003	3.50618	-0.467216

B3LYP Energy = -926.904287.

Compound 4 Conformer B		Standard Orientation (Ångstroms)		
	Type	X	Y	Z
1	C	-3.438337	-1.817075	0.713268
2	C	-4.049904	-1.347314	-0.617575
3	C	-2.929109	-0.948922	-1.605235
4	C	-1.99836	0.045779	-0.959102
5	C	-1.342052	-0.447745	0.319849
6	C	-2.448254	-0.820701	1.356758
7	C	-1.832898	1.29224	-1.430364
8	C	-1.037528	2.374594	-0.745623
9	C	-0.725583	2.011468	0.71691
10	C	-0.243269	0.535565	0.824689
11	C	1.041059	0.284169	0.076582
12	C	2.218638	-0.045285	0.645434
13	C	3.42329	-0.310101	-0.116254
14	C	4.612486	-0.640691	0.435162
15	C	5.836165	-0.91104	-0.32913
16	O	5.685405	-0.799254	-1.681453
17	O	6.907297	-1.211453	0.170876
18	C	-1.887311	-1.418779	2.65675
19	C	-4.983199	-2.405852	-1.217891
20	C	0.240475	3.006348	1.36932
21	O	-1.723902	3.635625	-0.841732
22	H	-0.838781	-1.399761	0.079871
23	H	-0.045418	0.336155	1.883958
24	H	-4.24382	-2.033645	1.428869
25	H	-2.913118	-2.771895	0.545272
26	H	-4.643285	-0.44146	-0.416691
27	H	-2.372822	-1.857565	-1.888117
28	H	-3.36141	-0.535695	-2.52506
29	H	-3.003598	0.095665	1.609229
30	H	-2.319137	1.590898	-2.359972
31	H	-0.099705	2.564221	-1.285888
32	H	-1.682865	2.062812	1.259375
33	H	0.994664	0.347667	-1.012302
34	H	2.289702	-0.123274	1.731433
35	H	3.3511	-0.234671	-1.200145
36	H	4.734617	-0.728053	1.511276
37	H	6.55594	-0.999105	-2.07135
38	H	-2.705457	-1.756577	3.304652
39	H	-1.250126	-2.288542	2.447479
40	H	-1.29565	-0.699975	3.233329



41	H	-5.438671	-2.051215	-2.150903
42	H	-5.794929	-2.658962	-0.524516
43	H	-4.43598	-3.33088	-1.44368
44	H	1.22613	2.980898	0.889657
45	H	0.381668	2.776803	2.4331
46	H	-0.14868	4.026082	1.287698
47	H	-2.62863	3.510785	-0.5094

B3LYP Energy = -926.903351

**Table S2.** Cartesian coordinates for the low-energy reoptimized MMFF conformers of **5** calculated at B3LYP/6-31G(d) level of theory in vacuo.

Compound <b>5</b> Conformer A		Standard Orientation (Ångstroms)		
	Type	X	Y	Z
1	C	-2.525044	-2.343825	-0.304048
2	C	-3.839207	-1.541247	-0.291768
3	C	-3.536702	-0.074297	-0.645076
4	C	-2.435889	0.542965	0.231887
5	C	-1.124398	-0.269974	0.1488
6	C	-1.384496	-1.747887	0.54896
7	C	-2.18696	2.018805	-0.106032
8	C	-1.164282	2.588991	0.846472
9	C	-0.181039	1.8455	1.37401
10	C	0.041965	0.382508	0.971719
11	C	-0.147279	-2.653031	0.434109
12	O	-4.753537	-2.095299	-1.261258
13	C	1.338448	0.321689	0.19481
14	C	2.513397	-0.170044	0.637061
15	C	3.722494	-0.164458	-0.159089
16	C	4.915053	-0.649168	0.251946
17	C	6.09368	-0.600888	-0.625384
18	O	7.190265	-1.142664	-0.020964
19	O	6.142298	-0.146814	-1.756117
20	C	0.772671	2.402713	2.402085
21	O	-1.790601	2.097956	-1.485266
22	C	-4.58891	-1.682629	1.036614
23	C	-1.702285	3.418328	-1.991239
24	H	-0.824276	-0.268134	-0.909049
25	H	0.17723	-0.182061	1.90721
26	H	-2.781026	0.540332	1.27591
27	H	-2.173718	-2.407282	-1.346834
28	H	-2.732083	-3.373574	0.014679
29	H	-4.460179	0.51509	-0.567161
30	H	-3.216295	-0.022058	-1.694823
31	H	-1.702732	-1.752716	1.603967

32	H	-3.132976	2.576242	0.004996
33	H	-1.270904	3.628594	1.154595
34	H	-0.412761	-3.689292	0.677222
35	H	0.657964	-2.352733	1.110754
36	H	0.257926	-2.642961	-0.585918
37	H	-4.360453	-2.003648	-2.144874
38	H	1.292605	0.755932	-0.805681
39	H	2.576457	-0.603734	1.63633
40	H	3.664518	0.261476	-1.160724
41	H	5.047499	-1.088627	1.236873
42	H	7.923886	-1.075199	-0.66004
43	H	0.713732	1.828149	3.33774
44	H	0.541635	3.447706	2.632396
45	H	1.814529	2.348155	2.064071
46	H	-3.998391	-1.320355	1.883709
47	H	-4.834425	-2.735359	1.214256
48	H	-5.526255	-1.116653	1.000671
49	H	-1.482349	3.333268	-3.05868
50	H	-2.654275	3.958452	-1.863068
51	H	-0.899597	3.991253	-1.5047

B3LYP Energy = -1041.394654.

Compound <b>5</b> Conformer B		Standard Orientation (Ångstroms)		
	Type	X	Y	Z
1	C	-2.523748	-2.337095	-0.308258
2	C	-3.834307	-1.528663	-0.303353
3	C	-3.523085	-0.063135	-0.655028
4	C	-2.424419	0.549236	0.228095
5	C	-1.116178	-0.269638	0.152862
6	C	-1.385492	-1.746442	0.551445
7	C	-2.167136	2.023966	-0.108441
8	C	-1.146482	2.589802	0.848741
9	C	-0.169748	1.841941	1.382245
10	C	0.048099	0.377429	0.982909
11	C	-0.151959	-2.657466	0.444179
12	O	-4.745656	-2.078465	-1.278051
13	C	1.349663	0.307974	0.21499
14	C	2.518441	-0.19019	0.665516
15	C	3.734675	-0.195252	-0.121911
16	C	4.916597	-0.689647	0.310536
17	C	6.153054	-0.697785	-0.48001
18	O	6.022991	-0.152686	-1.725056
19	O	7.217833	-1.144477	-0.087094
20	C	0.7804	2.395154	2.415754
21	O	-1.7639	2.101972	-1.486061
22	C	-4.59225	-1.666566	1.020713
23	C	-1.670529	3.422161	-1.991315
24	H	-0.809652	-0.269221	-0.903211

25	H	0.173634	-0.186808	1.91993
26	H	-2.775507	0.548375	1.27012
27	H	-2.166707	-2.401861	-1.34905
28	H	-2.7372	-3.365959	0.009011
29	H	-4.444236	0.530545	-0.582533
30	H	-3.196387	-0.012615	-1.702941
31	H	-1.710157	-1.749728	1.60447
32	H	-3.111171	2.585576	-0.002022
33	H	-1.249676	3.630135	1.155587
34	H	-0.423953	-3.692505	0.685171
35	H	0.650385	-2.361462	1.126061
36	H	0.259755	-2.649051	-0.573271
37	H	-4.346783	-1.989506	-2.159335
38	H	1.312441	0.741083	-0.786467
39	H	2.572758	-0.622517	1.665844
40	H	3.678688	0.228979	-1.123175
41	H	5.022282	-1.12307	1.301297
42	H	6.90018	-0.217086	-2.144818
43	H	1.824341	2.332214	2.085783
44	H	0.710504	1.823427	3.352371
45	H	0.555069	3.442305	2.641862
46	H	-4.004951	-1.307155	1.871256
47	H	-4.843711	-2.718128	1.196868
48	H	-5.526735	-1.096246	0.979444
49	H	-2.621554	3.9647	-1.866374
50	H	-0.868205	3.993105	-1.501732
51	H	-1.447181	3.336998	-3.058091

B3LYP Energy = -1041.393827.