Supporting Information

Decalin-Containing Tetramic acids and 4-hydroxy-2-pyridones with Antimicrobial and Cytotoxic Activity from the Fungus *Coniochaeta cephalothecoides* Collected in Tibetan Plateau (Medog)

Junjie Han,[†, ‡, #] Congcong Liu,[†, §, #] Li Li,[⊥, #] Hui Zhou,[†] Li Liu,[†, ‡] Li Bao,[†] Qian Chen,[†] Fuhang Song,[∥] Lixin Zhang,[∥] Erwei Li,[†] Ling Liu,[†] Yunfei Pei,[Ψ] Cheng Jin,[†] Yanfen Xue,[ǂ] Wenbing Yin,[†] Yanhe Ma,[ǂ] and Hongwei Liu[*, †, ‡]

[†]State Key Laboratory of Mycology, Institute of Microbiology, Chinese Academy of Sciences, Beijing, 100101, People's Republic of China

[‡]Savaid Medical School, University of Chinese Academy of Sciences, Beijing, 100049, People's Republic of China

[§]College of Life Sciences, Hebei University, Baoding 071002, People's Republic of China

[⊥]Institute of Materia Medica, CAMS & PUMC, Beijing, 100050, People's Republic of China

[∥]CAS Key Laboratory of Pathogenic Microbiology and Immunology, Institute of Microbiology, Chinese Academy of Sciences, Beijing, 100101, China

[Ψ]National Institutes for Food and Drug Control, Beijing, 100050, China

[ǂ] State Key Laboratory of Microbial Resources, Institute of Microbiology, Chinese Academy of Sciences, Beijing 100101, China

[#] authors contributed equally to this work.

* Corresponding Author Tel: +86 10 64806074; E-mail: liuhw@im.ac.cn (H-W, Liu)

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Table S1. Cartesian coordinates of low-energy optimized conformers of compounds **1**-**4**, and **7**.

Cartesian coordinate of low-energy optimized conformers of **1** optimized: [method: B3LYP/6-31+G (d,p)]
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.115759	-0.186914	0.521910
2	6	0	1.209013	-0.020688	0.887736
3	8	0	1.596481	-0.413880	2.091659
4	1	0	0.788180	-0.792915	2.564465
5	6	0	2.258733	0.609694	0.020444
6	1	0	1.893212	0.523467	-1.008328
7	6	0	-1.080300	-0.788806	1.447977
8	7	0	-2.286436	-0.842441	0.842275
9	1	0	-3.097585	-1.254609	1.283627
10	6	0	-2.280233	-0.325596	-0.525908
11	1	0	-2.489312	-1.134952	-1.237270
12	6	0	-0.811337	0.117794	-0.715859
13	8	0	-0.813103	-1.186780	2.608684
14	8	0	-0.397817	0.631289	-1.754489
15	6	0	3.639836	-0.083387	0.102806
16	6	0	4.579415	0.515589	-0.961552
17	6	0	4.508008	2.019693	-1.013858
18	1	0	5.305068	2.531763	-1.552780
19	6	0	3.526978	2.736652	-0.452956
20	1	0	3.546505	3.823810	-0.521540
21	6	0	2.361334	2.150435	0.310089
22	1	0	1.443479	2.603744	-0.088296
23	6	0	3.585773	-1.609103	-0.090201
24	1	0	2.954258	-1.851601	-0.960313
25	1	0	3.101687	-2.083445	0.771201
26	6	0	4.961796	-2.206702	-0.273862
27	1	0	5.039814	-3.288215	-0.163503
28	6	0	6.070749	-1.497589	-0.542021
29	6	0	6.013808	0.004079	-0.736182
30	1	0	6.459300	0.507048	0.136588
31	1	0	6.642643	0.285640	-1.592400
32	6	0	2.445038	2.542846	1.800153
33	1	0	3.293135	2.062091	2.297487
34	1	0	1.532930	2.278158	2.342850
35	1	0	2.579372	3.626408	1.884989
36	1	0	4.078353	0.118859	1.089229
37	1	0	4.257368	0.128045	-1.943597
38	6	0	7.431544	-2.134958	-0.667077

39	1	0	7.855091	-1.968287	-1.666474
40	1	0	7.392980	-3.213383	-0.485943
41	1	0	8.138500	-1.693559	0.048339
42	6	0	-3.275191	0.832097	-0.757900
43	1	0	-3.036194	1.642506	-0.060783
44	1	0	-3.093403	1.206345	-1.770967
45	6	0	-4.723618	0.419410	-0.599480
46	6	0	-5.432310	0.691508	0.578637
47	1	0	-4.944717	1.228793	1.387970
48	6	0	-6.763800	0.294483	0.737560
49	1	0	-7.294650	0.520174	1.658955
50	6	0	-7.409521	-0.389766	-0.296548
51	6	0	-6.722848	-0.668756	-1.484588
52	1	0	-7.234991	-1.192921	-2.285471
53	6	0	-5.396266	-0.264669	-1.626383
54	1	0	-4.877909	-0.481451	-2.557249
55	8	0	-8.713939	-0.807603	-0.207835
56	1	0	-9.086079	-0.562701	0.651512

Cartesian coordinate of low-energy optimized conformers of **2** optimized: [method: B3LYP/6-31+G (d,p)]
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.136105	-0.472077	0.695811
2	6	0	-1.217785	-0.407797	0.963309
3	8	0	-1.625407	-0.090697	2.183211
4	1	0	-0.797870	0.057951	2.746609
5	6	0	-2.291371	-0.717820	-0.040019
6	1	0	-1.846698	-0.538503	-1.025190
7	6	0	1.124884	-0.189318	1.742426
8	7	0	2.360591	-0.312966	1.202794
9	1	0	3.204657	-0.173682	1.742352
10	6	0	2.356388	-0.680504	-0.210108
11	1	0	2.810969	-1.670401	-0.348815
12	6	0	0.845872	-0.786529	-0.530978
13	8	0	0.861696	0.113675	2.926837
14	8	0	0.419944	-1.078961	-1.644404
15	6	0	-3.556025	0.161428	0.092354
16	6	0	-4.505399	-0.118538	-1.089211
17	6	0	-4.651829	-1.590506	-1.374624
18	1	0	-5.481141	-1.884011	-2.018766
19	6	0	-3.825615	-2.525232	-0.897358

20	1	0	-3.999678	-3.574311	-1.136556
21	6	0	-2.637887	-2.247828	-0.005102
22	1	0	-1.769042	-2.769402	-0.430302
23	6	0	-3.266465	1.671517	0.145226
24	1	0	-2.549739	1.942260	-0.648111
25	1	0	-2.773074	1.928549	1.090215
26	6	0	-4.525633	2.493658	0.003718
27	1	0	-4.449423	3.545481	0.280862
28	6	0	-5.706506	2.014190	-0.412358
29	6	0	-5.860597	0.568546	-0.838940
30	1	0	-6.427678	0.012911	-0.074723
31	1	0	-6.472075	0.517441	-1.751742
32	6	0	-2.877447	-2.838566	1.399814
33	1	0	-3.167526	-3.891575	1.310124
34	1	0	-3.683679	-2.315968	1.925226
35	1	0	-1.976784	-2.793858	2.020398
36	1	0	-4.081210	-0.114529	1.016853
37	1	0	-4.070405	0.360945	-1.983558
38	6	0	-6.946509	2.868126	-0.483113
39	1	0	-7.335345	2.920976	-1.509683
40	1	0	-6.757041	3.889274	-0.136293
41	1	0	-7.753373	2.444573	0.131696
42	6	0	3.073759	0.337297	-1.123384
43	1	0	2.891609	0.015979	-2.155159
44	1	0	2.596098	1.315637	-0.996181
45	6	0	4.558751	0.436749	-0.847619
46	6	0	5.458651	-0.487408	-1.402425
47	1	0	5.087069	-1.265154	-2.065980
48	6	0	6.822137	-0.428683	-1.129031
49	1	0	7.512628	-1.143490	-1.566555
50	6	0	7.319320	0.569920	-0.281829
51	6	0	6.441686	1.502715	0.279437
52	1	0	6.822743	2.285112	0.931951
53	6	0	5.076787	1.429521	-0.005953
54	1	0	4.407390	2.166770	0.430961
55	8	0	8.666671	0.584178	-0.046977
56	1	0	8.879624	1.319062	0.551217

Cartesian coordinate of low-energy optimized conformers of **3-1** optimized: [method: B3LYP/6-31+G (d,p)]

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	1.279305	0.769656	0.738670
2	8	0	1.748396	1.168537	1.913325
3	1	0	0.974098	1.259716	2.544127
4	6	0	2.544034	1.947725	-1.103888
5	1	0	1.627778	2.167619	-1.668361
6	6	0	2.289949	0.590130	-0.354710
7	6	0	3.613298	-0.064045	0.109510
8	6	0	3.421957	-1.350928	0.931648
9	1	0	2.684860	-2.003383	0.435734
10	1	0	2.997294	-1.114641	1.914071
11	6	0	3.665027	1.773752	-2.102750
12	1	0	3.762764	2.565056	-2.845246
13	6	0	4.521266	0.745226	-2.113442
14	1	0	5.294716	0.700686	-2.880126
15	6	0	4.480456	-0.388625	-1.121864
16	6	0	5.886592	-0.822008	-0.669787
17	1	0	6.457665	0.055349	-0.327223
18	1	0	6.442526	-1.219378	-1.530443
19	6	0	5.846394	-1.864382	0.429093
20	6	0	4.720445	-2.100364	1.122732
21	1	0	4.725179	-2.874448	1.890014
22	6	0	7.131682	-2.608320	0.690284
23	1	0	7.458611	-3.157060	-0.202984
24	1	0	7.027312	-3.322351	1.512811
25	1	0	7.943418	-1.912744	0.942836
26	1	0	4.164800	0.656184	0.728712
27	1	0	4.028107	-1.260976	-1.624324
28	1	0	1.820778	-0.071167	-1.090777
29	6	0	2.817550	3.166739	-0.197857
30	1	0	3.676161	2.996694	0.459174
31	1	0	1.952213	3.415401	0.423397
32	1	0	3.041924	4.039852	-0.819632
33	6	0	-2.286245	0.071511	-0.076818
34	6	0	-0.863530	0.108927	-0.557693
35	6	0	-0.080009	0.570225	0.586187
36	6	0	-1.000962	0.783703	1.699572
37	7	0	-2.269489	0.510551	1.261739
38	1	0	-3.051204	0.471784	1.900963
39	8	0	-0.493851	-0.191762	-1.697042
40	8	0	-0.693721	1.147029	2.855524
41	6	0	-3.320239	-0.331789	-0.848174
42	1	0	-3.008969	-0.680253	-1.830583
43	6	0	-4.750175	-0.403939	-0.572533
44	6	0	-5.405747	0.327559	0.440400
45	1	0	-4.859640	1.034907	1.054186

46	6	0	-6.778375	0.212987	0.645654
47	1	0	-7.260232	0.795718	1.425970
48	6	0	-7.537927	-0.641063	-0.165050
49	6	0	-6.916217	-1.365014	-1.191229
50	1	0	-7.513737	-2.014618	-1.822627
51	6	0	-5.547199	-1.236913	-1.390526
52	1	0	-5.075139	-1.798444	-2.191807
53	8	0	-8.885918	-0.798975	-0.010489
54	1	0	-9.212092	-0.246491	0.714842

Cartesian coordinate of low-energy optimized conformers of **3-2** optimized: [method: B3LYP/6-31+G (d,p)]
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.270629	-0.300247	0.952951
2	8	0	1.741047	-1.100356	1.899821
3	1	0	0.966120	-1.587816	2.310393
4	6	0	2.440841	1.928282	1.029353
5	1	0	1.506648	2.485875	0.879705
6	6	0	2.275445	0.569812	0.256934
7	6	0	3.638809	-0.113823	-0.000178
8	6	0	3.534206	-1.488829	-0.682697
9	1	0	2.841680	-1.427555	-1.537963
10	1	0	3.096516	-2.222299	0.003939
11	6	0	3.558611	2.734711	0.409619
12	1	0	3.598076	3.784827	0.697120
13	6	0	4.477128	2.241854	-0.429483
14	1	0	5.243505	2.903046	-0.833693
15	6	0	4.516722	0.803319	-0.875259
16	6	0	5.950831	0.247104	-0.933325
17	1	0	6.466044	0.435777	0.021737
18	1	0	6.526565	0.794541	-1.692793
19	6	0	5.985950	-1.235195	-1.246310
20	6	0	4.880946	-1.992820	-1.148356
21	1	0	4.941205	-3.050833	-1.403267
22	6	0	7.320481	-1.796759	-1.667276
23	1	0	8.083043	-1.614734	-0.897934
24	1	0	7.681467	-1.312076	-2.584175
25	1	0	7.268722	-2.874943	-1.846574
26	1	0	4.151320	-0.250190	0.961618
27	1	0	4.119588	0.757536	-1.903961
28	1	0	1.831689	0.830397	-0.709955

29	6	0	2.653557	1.802827	2.552874
30	1	0	3.527370	1.187301	2.788213
31	1	0	1.781897	1.370267	3.052972
32	1	0	2.821483	2.796849	2.980603
33	6	0	-2.301021	0.053844	-0.039755
34	6	0	-0.878799	0.484104	-0.261773
35	6	0	-0.087852	-0.283708	0.696840
36	6	0	-1.006437	-1.123243	1.461059
37	7	0	-2.272373	-0.914979	0.982628
38	1	0	-3.082543	-1.298977	1.448586
39	8	0	-0.513350	1.317207	-1.097018
40	8	0	-0.700151	-1.898807	2.392538
41	6	0	-3.349878	0.570234	-0.717933
42	1	0	-3.065363	1.361958	-1.407587
43	6	0	-4.775037	0.270412	-0.645303
44	6	0	-5.313131	-0.930448	-0.136004
45	1	0	-4.662807	-1.734642	0.189458
46	6	0	-6.687944	-1.148066	-0.090425
47	1	0	-7.075129	-2.085936	0.298420
48	6	0	-7.567757	-0.163208	-0.558845
49	6	0	-7.060273	1.029810	-1.090817
50	1	0	-7.748038	1.781637	-1.464217
51	6	0	-5.686538	1.232234	-1.137391
52	1	0	-5.302760	2.158959	-1.554660
53	8	0	-8.925160	-0.313753	-0.534154
54	1	0	-9.165696	-1.171645	-0.154881

Cartesian coordinate of low-energy optimized conformers of **4-1** optimized: [method: B3LYP/6-31+G (d,p)]
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.673916	-1.471102	-0.390141
2	8	0	2.042268	-2.526883	-1.106653
3	1	0	1.215880	-2.956469	-1.478925
4	6	0	3.554040	-1.624311	1.265140
5	1	0	3.766602	-2.578083	0.760077
6	6	0	2.798362	-0.711455	0.247475
7	6	0	3.800660	-0.163984	-0.816767
8	6	0	3.164154	0.577733	-2.010185
9	1	0	2.259392	0.060208	-2.352192
10	1	0	3.859249	0.517458	-2.861382
11	6	0	4.877888	-1.013995	1.668489

12	1	0	5.371835	-1.483643	2.518703
13	6	0	5.453163	0.034229	1.066758
14	1	0	6.398287	0.421581	1.444937
15	6	0	4.836317	0.739978	-0.114497
16	6	0	4.243965	2.106771	0.313187
17	1	0	5.068845	2.795220	0.542815
18	1	0	3.692148	1.996312	1.258675
19	6	0	3.328698	2.736549	-0.712597
20	6	0	2.843741	2.027469	-1.742898
21	1	0	2.186581	2.518440	-2.460586
22	6	0	2.975845	4.184838	-0.485090
23	1	0	3.873797	4.816766	-0.500524
24	1	0	2.511955	4.325848	0.500496
25	1	0	2.281208	4.556361	-1.244576
26	1	0	4.336551	-1.033771	-1.215338
27	1	0	5.628153	0.946302	-0.848897
28	1	0	2.347799	0.124454	0.789255
29	6	0	2.700032	-1.939624	2.507436
30	1	0	3.248735	-2.596258	3.190775
31	1	0	1.767330	-2.445878	2.237649
32	1	0	2.445054	-1.022941	3.050723
33	6	0	-1.821559	-0.292002	0.125053
34	6	0	-0.364151	-0.091259	0.430043
35	6	0	0.332585	-1.158164	-0.289415
36	6	0	-0.677448	-1.967880	-0.968154
37	7	0	-1.904411	-1.412526	-0.724504
38	1	0	-2.758505	-1.879581	-0.995684
39	8	0	0.089497	0.806766	1.144805
40	8	0	-0.467383	-2.991573	-1.654234
41	6	0	-2.801569	0.493469	0.624310
42	1	0	-2.434206	1.248177	1.316213
43	6	0	-4.244013	0.469950	0.411422
44	6	0	-4.874181	-0.128687	-0.700153
45	1	0	-4.287369	-0.574572	-1.495426
46	6	0	-6.259160	-0.113420	-0.844258
47	1	0	-6.718977	-0.572884	-1.714892
48	6	0	-7.056543	0.507981	0.125858
49	6	0	-6.456489	1.127999	1.230010
50	1	0	-7.080406	1.618236	1.970315
51	6	0	-5.073013	1.112465	1.358960
52	1	0	-4.617058	1.600562	2.215731
53	8	0	-8.419293	0.551577	0.041777
54	1	0	-8.724136	0.105448	-0.761883

Cartesian coordinate of low-energy optimized conformers of **7-1** optimized: [method: B3LYP/6-31+G (d,p)]
Thermal correction to Gibbs Free Energy=0.390449 (Hartree/Particle)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.781367	1.191268	0.312122
2	6	0	5.684200	2.022770	0.052795
3	1	0	5.826711	3.099175	0.047428
4	6	0	4.435097	1.467849	-0.202122
5	1	0	3.598328	2.125943	-0.408982
6	6	0	4.241662	0.074074	-0.202735
7	6	0	5.352358	-0.741117	0.066666
8	1	0	5.231552	-1.820623	0.097252
9	6	0	6.611431	-0.196900	0.317181
10	1	0	7.455703	-0.849352	0.527712
11	6	0	2.926277	-0.537372	-0.522236
12	6	0	1.693221	-0.099936	0.069375
13	8	0	1.769379	0.904052	0.927959
14	1	0	0.812718	1.072730	1.237521
15	6	0	2.839299	-1.588459	-1.397613
16	1	0	3.709723	-1.984432	-1.907683
17	7	0	1.662467	-2.191633	-1.687812
18	1	0	1.641667	-2.968024	-2.339845
19	6	0	0.412227	-1.841418	-1.158376
20	6	0	0.444443	-0.711771	-0.237274
21	6	0	-0.769268	-0.169135	0.381823
22	8	0	-0.678904	0.780107	1.200177
23	8	0	-0.565137	-2.511896	-1.511730
24	6	0	-2.449430	-1.931046	1.041552
25	1	0	-1.820899	-2.759222	0.690084
26	6	0	-2.153787	-0.720250	0.090192
27	6	0	-3.264310	0.350500	0.170719
28	6	0	-2.993276	1.601897	-0.683733
29	1	0	-2.651835	1.299910	-1.688608
30	1	0	-2.167613	2.178941	-0.252236
31	6	0	-3.892607	-2.357130	0.903228
32	1	0	-4.141486	-3.329357	1.329599
33	6	0	-4.847667	-1.624296	0.324687
34	1	0	-5.864099	-2.014893	0.263061
35	6	0	-4.606771	-0.263806	-0.275649
36	6	0	-5.754357	0.718424	0.023463
37	1	0	-5.959375	0.736343	1.106184
38	1	0	-6.681569	0.354845	-0.443761

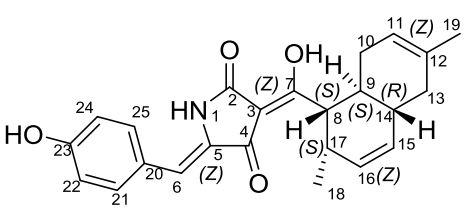
39	6	0	-5.456439	2.120711	-0.466272
40	6	0	-4.211165	2.487186	-0.801548
41	1	0	-4.040156	3.498365	-1.172772
42	8	0	7.983923	1.791897	0.555561
43	1	0	8.656221	1.110207	0.719192
44	6	0	-6.629226	3.063608	-0.552743
45	1	0	-6.326450	4.059215	-0.893595
46	1	0	-7.120846	3.173876	0.424379
47	1	0	-7.395915	2.683480	-1.242505
48	1	0	-3.373683	0.674155	1.214405
49	1	0	-4.569590	-0.377379	-1.373515
50	1	0	-2.143941	-1.136026	-0.920102
51	6	0	-2.109879	-1.693883	2.528652
52	1	0	-2.411681	-2.565674	3.120786
53	1	0	-2.638528	-0.821909	2.928130
54	1	0	-1.036709	-1.542741	2.683901

Cartesian coordinate of low-energy optimized conformers of **7-2** optimized: [method: B3LYP/6-31+G (d,p)]
Thermal correction to Gibbs Free Energy=0.390606 (Hartree/Particle)

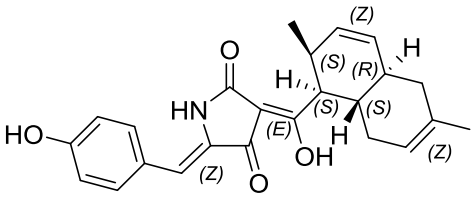
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	6.797471	1.141519	0.324482
2	6	0	6.405017	0.859044	-0.987779
3	1	0	7.078096	1.068331	-1.815955
4	6	0	5.141503	0.322410	-1.232070
5	1	0	4.842587	0.129800	-2.258905
6	6	0	4.247301	0.046198	-0.185791
7	6	0	4.661726	0.340199	1.126358
8	1	0	3.995636	0.136824	1.957686
9	6	0	5.916587	0.881539	1.382288
10	1	0	6.231435	1.101302	2.397950
11	6	0	2.932159	-0.580947	-0.473856
12	6	0	1.697575	-0.109619	0.087802
13	8	0	1.774485	0.930304	0.902618
14	1	0	0.815581	1.126454	1.187686
15	6	0	2.840165	-1.642934	-1.335388
16	1	0	3.714296	-2.079301	-1.804657
17	7	0	1.656015	-2.222159	-1.644013
18	1	0	1.634142	-3.022218	-2.266865
19	6	0	0.406449	-1.853113	-1.126212
20	6	0	0.444072	-0.710664	-0.221013
21	6	0	-0.770332	-0.133260	0.364946

22	8	0	-0.679004	0.847948	1.144286
23	8	0	-0.574739	-2.520698	-1.474652
24	6	0	-2.441652	-1.879580	1.074284
25	1	0	-1.808014	-2.712272	0.743397
26	6	0	-2.155122	-0.692091	0.091727
27	6	0	-3.269690	0.375081	0.149546
28	6	0	-3.007806	1.608691	-0.733521
29	1	0	-2.664122	1.286652	-1.731440
30	1	0	-2.185953	2.200983	-0.315637
31	6	0	-3.882156	-2.318519	0.947567
32	1	0	-4.124536	-3.281763	1.397414
33	6	0	-4.841713	-1.605295	0.352063
34	1	0	-5.855858	-2.003114	0.299883
35	6	0	-4.609468	-0.257225	-0.279799
36	6	0	-5.762742	0.723849	-0.001737
37	1	0	-5.966338	0.766233	1.080568
38	1	0	-6.688221	0.343310	-0.458783
39	6	0	-5.474462	2.116130	-0.524576
40	6	0	-4.232044	2.482871	-0.870207
41	1	0	-4.068165	3.486374	-1.264743
42	8	0	8.017341	1.671739	0.635810
43	1	0	8.530267	1.798793	-0.179257
44	6	0	-6.653689	3.049010	-0.630613
45	1	0	-7.418167	2.648633	-1.311279
46	1	0	-6.358103	4.039105	-0.993228
47	1	0	-7.145081	3.177089	0.344413
48	1	0	-3.378340	0.722249	1.185760
49	1	0	-4.573630	-0.395485	-1.374774
50	1	0	-2.147380	-1.133634	-0.907767
51	6	0	-2.103631	-1.604598	2.555211
52	1	0	-2.393848	-2.467271	3.166097
53	1	0	-2.643811	-0.731730	2.937043
54	1	0	-1.032353	-1.436747	2.706713

Table S2. DP4 Analysis of the Carbon and Proton Data for (+)-conipyrrolidone C (**3a**)



3a



3ia

	^{13}C calcd		^{13}C expt	scaled shifts		Corrected error		Probability	
NO.	**3a**	**3ia**		**3a**	**3ia**	**3a**	**3ia**	**3a**	**3ia**
2	180.8	173.6	174.3	173.8	166.5	-0.50	-7.85	0.416	0.003
3	107.7	110.8	103.4	102.5	105.6	-0.91	2.18	0.350	0.182
4	189.9	197.4	183.9	182.7	190.0	-1.21	6.07	0.306	0.012
5	137.6	135.9	134.4	131.7	129.8	-2.73	-4.56	0.131	0.037
6	116.1	115.8	106.3	110.9	110.5	4.59	4.18	0.036	0.049
7	200.7	201.5	196.6	193.2	193.7	-3.41	-2.90	0.084	0.117
8	51.9	50.2	50.6	48.0	46.4	-2.57	-4.24	0.145	0.047
9	36.7	37.1	32.8	33.4	33.7	0.56	0.90	0.406	0.351
10	33.9	33.2	31.6	30.5	29.9	-1.07	-1.71	0.325	0.237
11	129.1	129.6	122.8	123.5	123.9	0.67	1.06	0.388	0.327
12	145.9	146.6	133.9	140.0	140.6	6.05	6.66	0.012	0.007
13	41.2	42.4	38.3	37.7	38.9	-0.62	0.58	0.396	0.403
15	43.3	42.9	39.0	39.7	39.3	0.72	0.34	0.381	0.443
16	141.0	140.1	133.7	135.1	134.1	1.35	0.37	0.284	0.437
17	40.9	41.6	33.2	37.6	38.3	4.35	5.08	0.043	0.025
18	19.0	19.1	18.7	16.0	16.1	-2.68	-2.62	0.135	0.140
19	25.3	25.6	24.1	22.2	22.5	-1.94	-1.60	0.209	0.251
20	133.2	132.5	127.6	127.4	126.6	-0.17	-0.97	0.471	0.342
14	140.0	139.5	130.4	134.2	133.5	3.75	3.13	0.066	0.101
21	141.4	141.6	131.8	135.5	135.6	3.67	3.80	0.070	0.064
22	121.3	121.4	117.4	115.8	115.8	-1.64	-1.63	0.246	0.247
23	165.7	166.0	159.2	159.1	159.2	-0.09	0.02	0.485	0.496
24	119.9	119.7	117.4	114.4	114.1	-3.00	-3.33	0.110	0.088
25	134.5	134.8	131.8	128.6	128.8	-3.17	-2.99	0.098	0.111
^{13}C, product of probabilties								3.33×10^{-16}	3.00×10^{-17}
^{13}C, Bayes's theorem probability (%)								91.7	8.3

	^{1}H calcd		^{1}H expt	scaled shifts		Corrected error		Probability	
NO.	**3a**	**3ia**		**3a**	**3ia**	**3a**	**3ia**	**3a**	**3ia**
6	6.86	6.89	7.03	6.80	6.84	-0.23	-0.19	0.113	0.165
8	4.19	4.01	4.62	4.15	3.98	-0.47	-0.64	0.012	0.002
9	2.12	2.08	2.16	2.10	2.06	-0.06	-0.10	0.378	0.295
10a	1.83	1.88	1.82	1.81	1.86	-0.01	0.04	0.481	0.415

10b	2.46	2.32	2.71	2.43	2.29	-0.28	-0.42	0.075	0.020
11	5.84	5.86	5.4	5.79	5.82	0.39	0.42	0.026	0.019
13a	1.97	1.97	1.77	1.95	1.95	0.18	0.18	0.177	0.171
13b	2.17	2.32	1.93	2.15	2.30	0.22	0.37	0.131	0.034
14	2.41	2.34	2.2	2.38	2.31	0.18	0.11	0.171	0.277
15	6.08	6.05	5.58	6.03	6.01	0.45	0.43	0.014	0.018
16	6.23	6.23	5.82	6.18	6.19	0.36	0.37	0.037	0.034
17	2.71	2.76	3.24	2.68	2.73	-0.56	-0.51	0.004	0.008
18	0.99	1.05	1.13	0.98	1.03	-0.15	-0.10	0.214	0.305
19	1.81	1.80	1.62	1.79	1.78	0.17	0.16	0.185	0.199
22	7.31	7.34	7.25	7.25	7.29	0.00	0.04	0.496	0.411
21	7.75	7.74	7.86	7.68	7.69	-0.18	-0.17	0.178	0.182
^{1}H, product of probabilties								1.51×10^{-17}	5.06×10^{-19}
^{1}H, Bayes's theorem probability (%)								96.8	3.2
^{13}C+^{1}H, Bayes's theorem probability (%)								99.7	0.3

Table S3. ^{1}H and ^{13}C NMR Data for Compound **9**

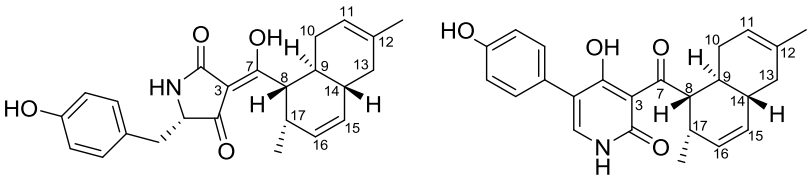
Pos.	**9** [a]		**9** [b]		
	δ_C	δ_H (J in Hz)	δ_C	δ_H (J in Hz)	HMBC
2	159.6		156.6		
3	108.6		106.5		
4	175.6		173.3		
4-OH				17.26 s	C-3, C-4, C-5, C-7
5	114.6		113.8		
6	140.0	8.03 s	133.5	8.01 s	C-2, C-3, C-4, C-5, C-20
7	211.7		211.1		
8	54.5	4.43 dd (5.2, 10.7)	53.6	4.32 dd (5.0, 10.0)	C-7, C-9, C-14, C-17, C-18
9	37.6	1.56 m	36.1	1.59 m	C-10, C-11, C-14
10	30.9	0.88 m 1.92 m	29.9	0.87 m 1.85 m	
11	36.6	0.88 m 1.92 m	35.4	1.05 m 1.72 m	
12	34.3	1.49 m	33.2	1.48 m	
13	43.1	0.77 m 1.73 m	41.8	0.81 m 1.72 m	
14	43.2	1.81 m	41.9	1.85 m	C-9, C-12, C-13, C-15
15	131.7	5.40 brd (9.6)	131.1	5.43 brd (9.0)	C-9, C-14, C-17
16	132.5	5.59 brd (8.7)	131.1	5.59 m	C-8, C-14, C-17
17	32.4	2.84 s	31.3	2.79 s	
18	18.4	0.81 d (6.6)	18.1	0.81 d (6.6)	C-8, C-16, C-17
19	22.9	0.92 d (6.3)	22.6	0.91 d (6.6)	C-11, C-12, C-13
20	70.4		70.7		
21	60.5	3.63 brs	58.8	3.56 brs	C-5, C-20, C-24, C-25
22	57.7	3.41 brs	56.2	3.56 brs	
23	67.1	4.12 m	63.9	4.21 m	
24	25.7	1.36 m 1.80 m	25.8	1.50 m 1.99 m	C-20, C-22, C-25
25	31.7	1.67 m 2.24 m	28.6	1.87 m	C-20, C-23, C-24

[a] NMR data were measured in CD_3OD

[b] NMR data were measured in $CDCl_3$

"m" means multiplet or overlapped with other signals

Table S4. Correlation of D (C3-C7-C8-C9) angles with absolute configurations of decalin rings



1a **7a**

Compounds	D(C3-C7-C8-C9)[#]	CE at around 210 nm	Absolute configuration
1a	–140.9	+	8*S*,9*S*,14*R*,17*S*
1b	+140.9	–	8*R*,9*R*,14*S*,17*R*
2a	–143.2	/	8*S*,9*S*,14*R*,17*S*
2b	+143.2	/	8*R*,9*R*,14*S*,17*R*
3a	–140.6	+	8*S*,9*S*,14*R*,17*S*
3b	+140.6	–	8*R*,9*R*,14*S*,17*R*
4a	–119.9	–	8*S*,9*S*,14*S*,17*R*
4b	+119.9	+	8*R*,9*R*,14*R*,17*S*
5	–137.4	+	8*S*,9*S*,14*R*,17*S*
6	+139.1	–	8*R*,9*R*,14*S*,17*R*
7a	–148.6	+	8*S*,9*S*,14*R*,17*S*
7b	+148.6	–	8*R*,9*R*,14*S*,17*R*
8	–142.1	+	8*S*,9*S*,14*R*,17*S*
9	–148.4	+	8*S*,9*S*,14*R*,17*S*
10	–148.3	+	8*S*,9*S*,14*R*,17*S*
11	–150.3	+	8*S*,9*S*,14*R*,17*S*

#: D(C3-C7-C8-C9) angles of the lowest-energy conformations.

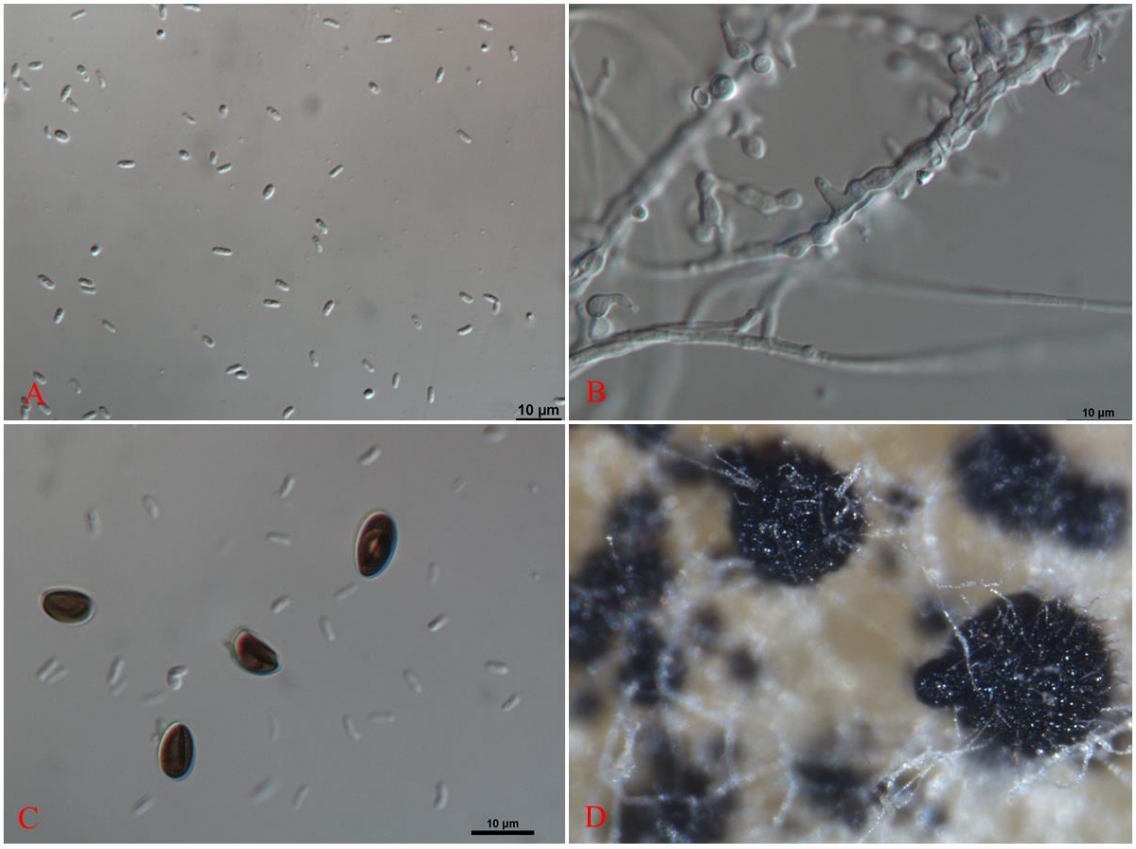


Figure S1. Morphological structures of *C. cephalothecoides* after 10 days on PDA.
A. Conidia B. Conidiogenous cells and conidia. C. Ascospores. D. Ascomata

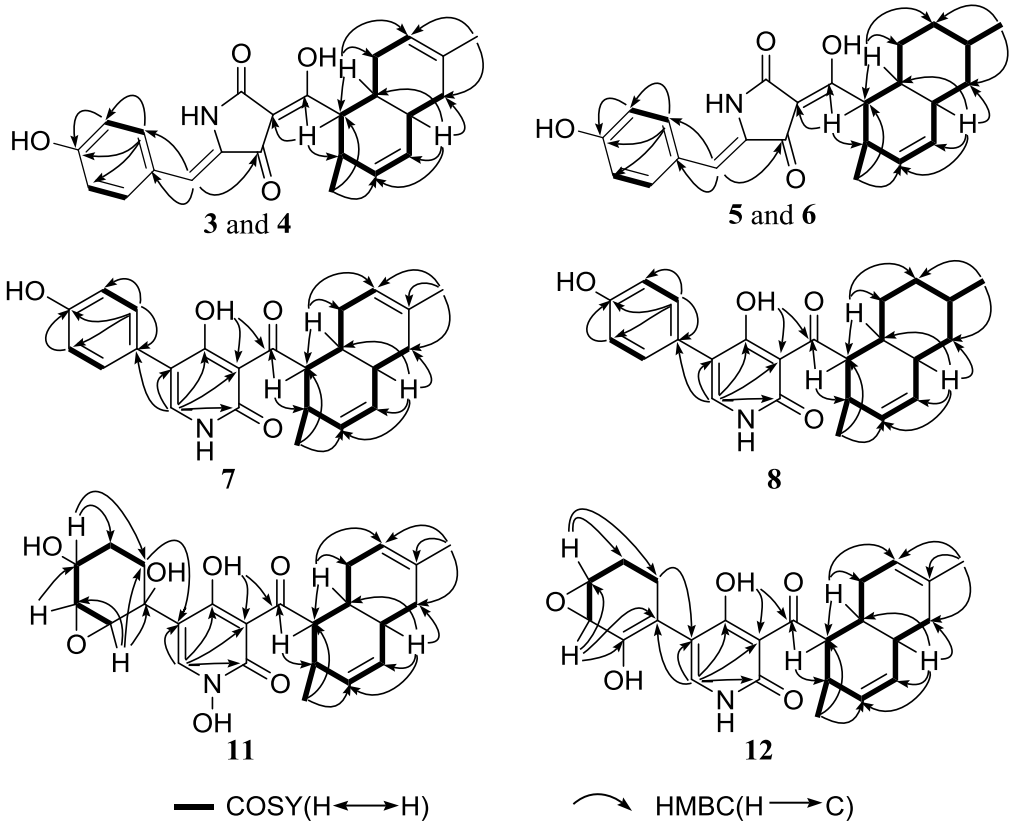


Figure S2. Selected key HMBC and ^{1}H-^{1}H COSY correlations of **3-6** and **8-12.**

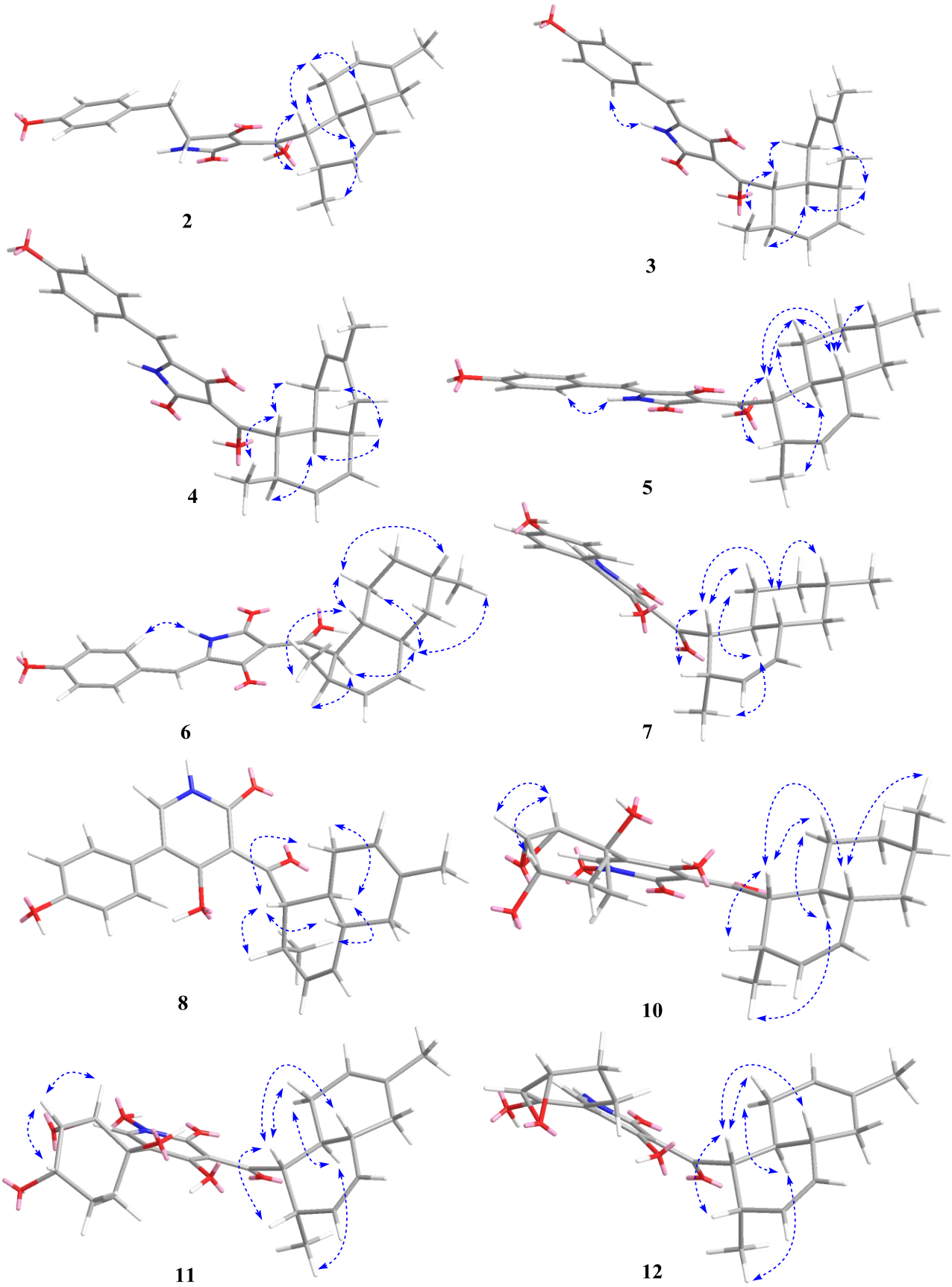


Figure S3. Selected key NOE correlations of **2-8** and **11-12**.

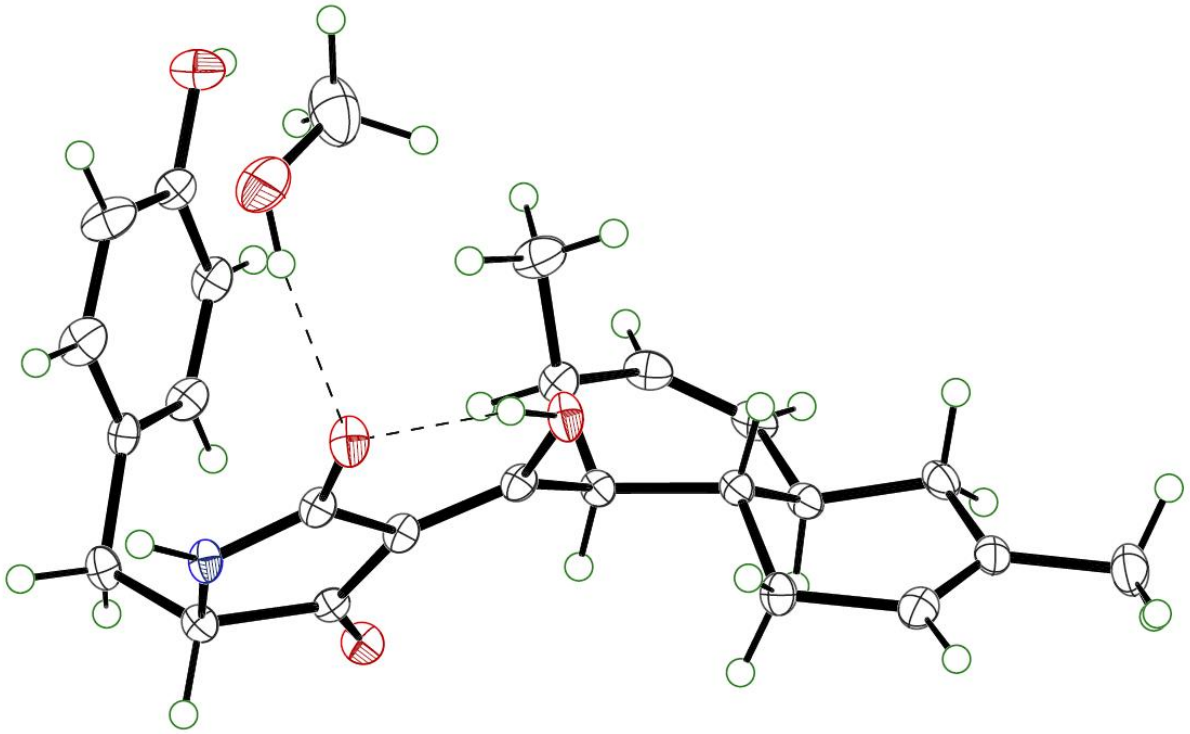


Figure S4. Thermal ellipsoid diagram of compound **1** (at the 50 % probability level), with hydrogen atoms omitted for clarity

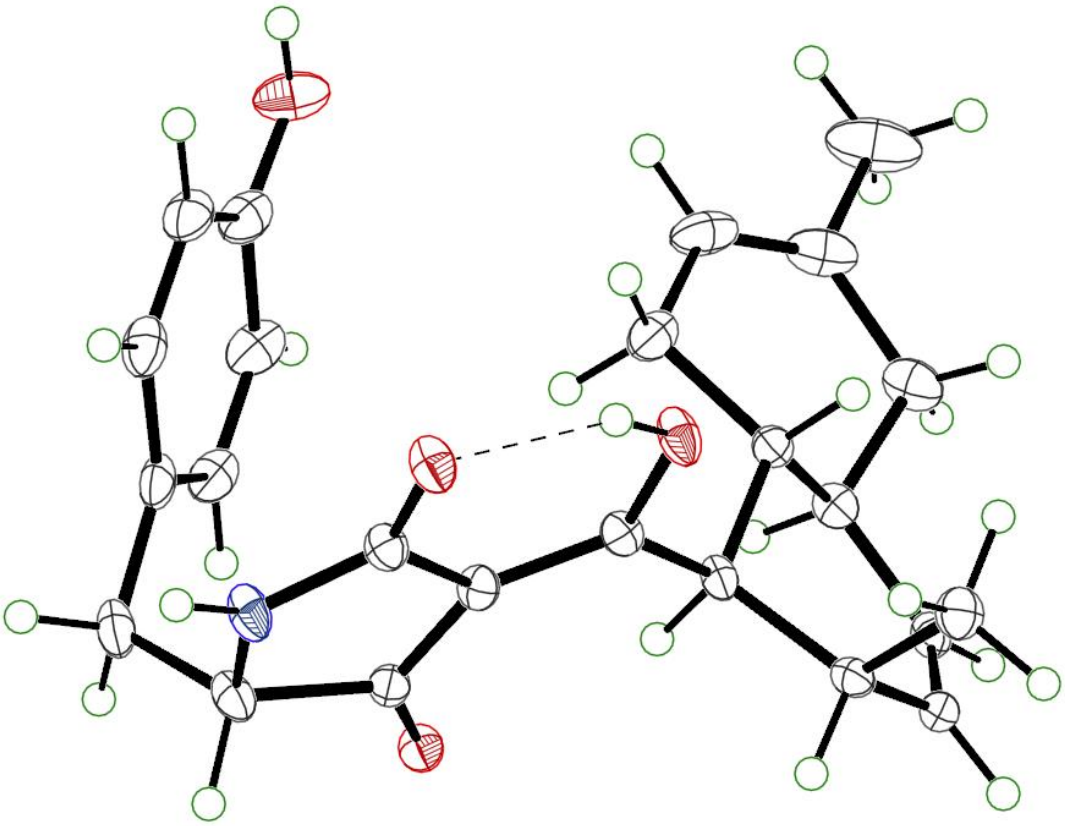
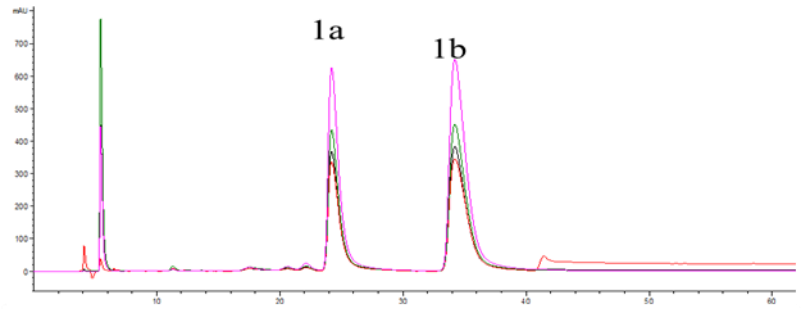
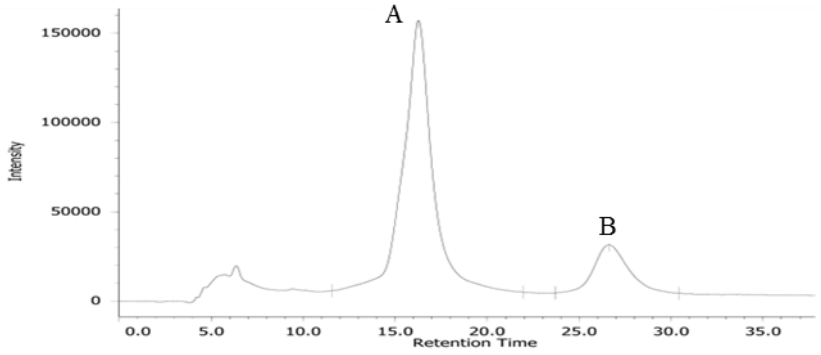


Figure S5. Thermal ellipsoid diagram of compound **2** (at the 50 % probability level), with hydrogen atoms omitted for clarity

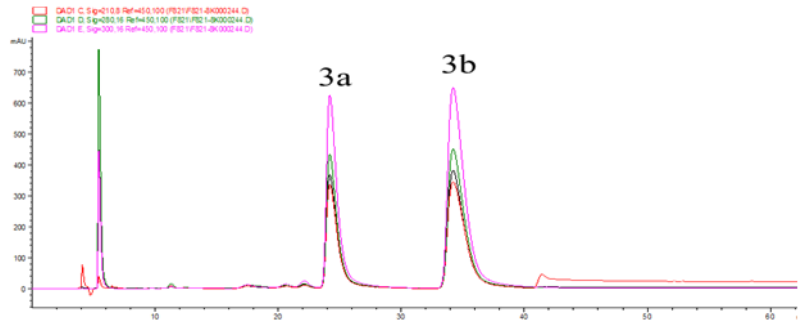
A:



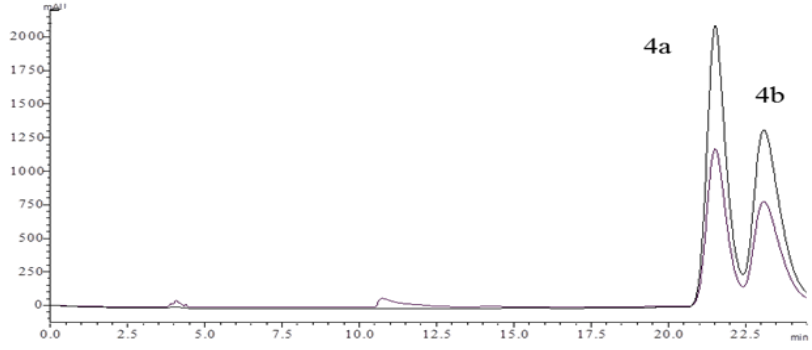
B:



C:



D:



E:

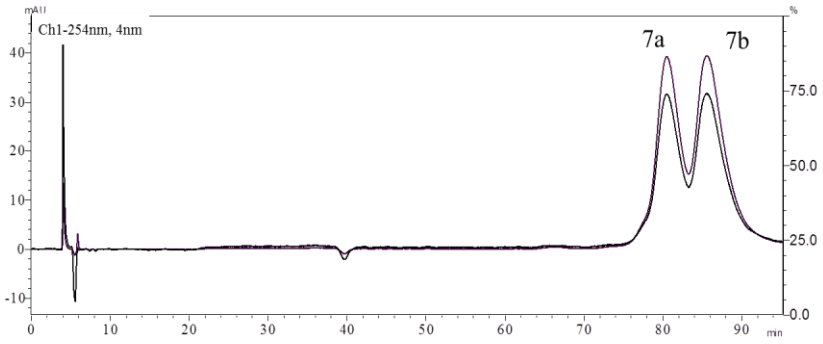
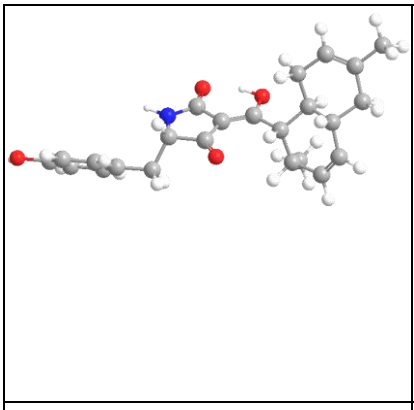
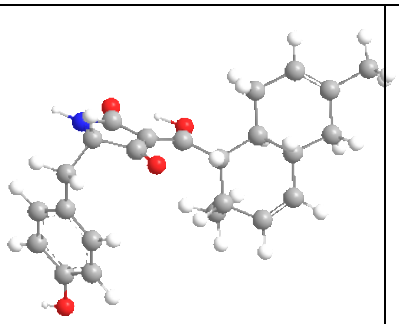
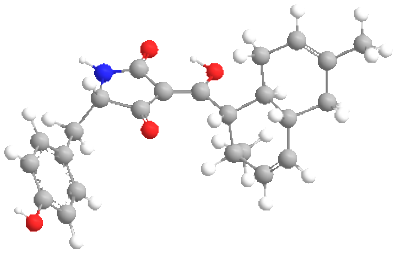
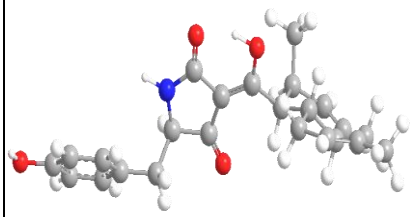
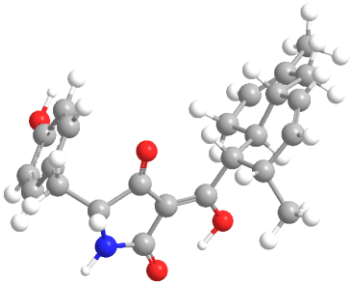
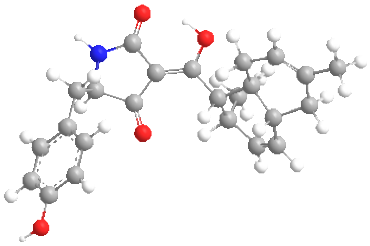
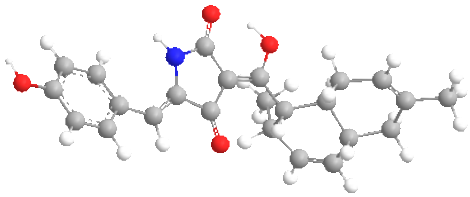
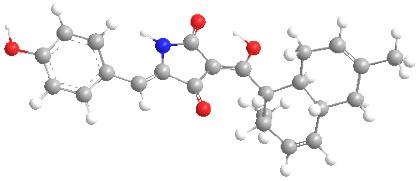
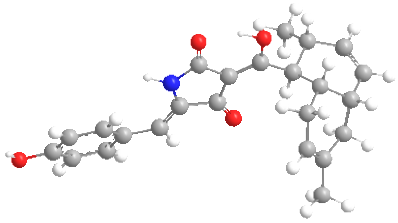
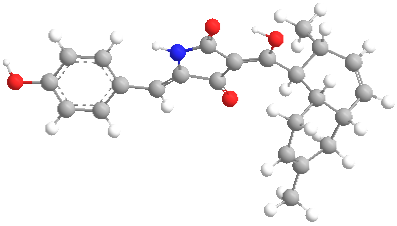


Figure S6. Chiral HPLC separation profiles of compounds **1**-**4** and **7**.

		
1-1 (87.18%)	1-2 (9.11%)	1-3 (3.71%)
A		
		
2-1 (88.35%)	2-2 (8.41%)	2-3 (3.24%)
B		
		
3-1 (52.06%)	3-2 (47.94%)	
C		
		
4-1 (64.87%)	4-2 (35.13%)	
D		

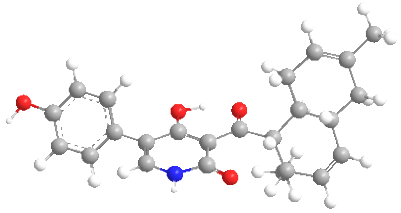
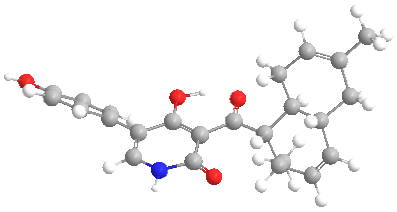
	
7-1 (52.41%)	7-2 (47.59%)
E	

Figure S7. (A) Most stable conformers of **1a**/**1b** in solvated model calculations at the B3LYP/6-31+G(d,p) level (d) (the relative populations are in parentheses). (B) Most stable conformers of **2a**/**2b** in solvated model calculations at the B3LYP/6-31+G(d,p) level (d) (the relative populations are in parentheses). (C)Most stable conformers of **3a**/**3b** in solvated model calculations at the B3LYP/6-31+G(d,p) level (d) (the relative populations are in parentheses). (D)Most stable conformers of **4a**/**4b** in solvated model calculations at the B3LYP/6-31+G(d,p) level (d) (the relative populations are in parentheses). (E) Most stable conformers of **7a**/**7b** in solvated model calculations at the B3LYP/6-31+G(d,p) level (d) (the relative populations are in parentheses).

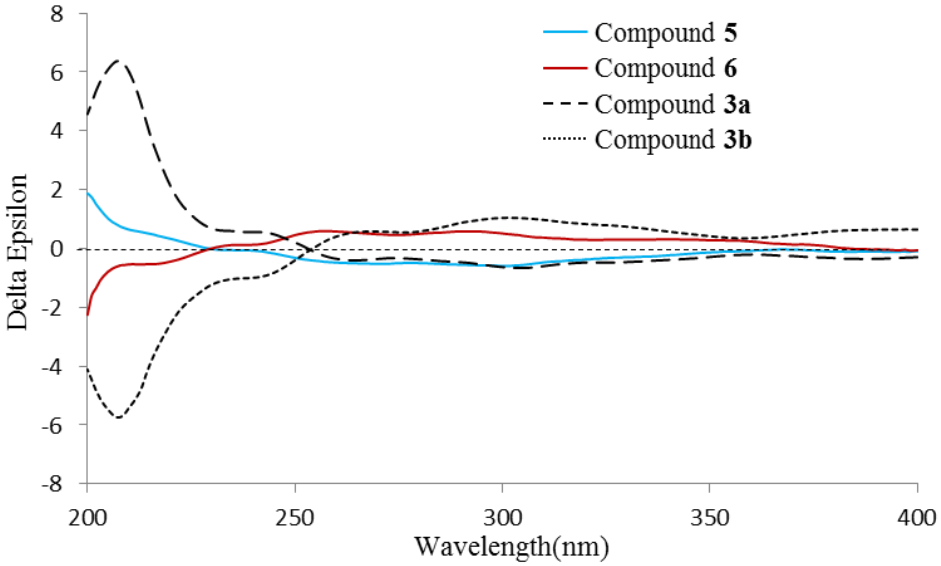


Figure S8. CD Spectra of conipyrrolidones E (**5**), F (**6**), (+)-conipyrrolidone C (**3a**) and (−)-conipyrrolidone C (**3b**) in MeOH.

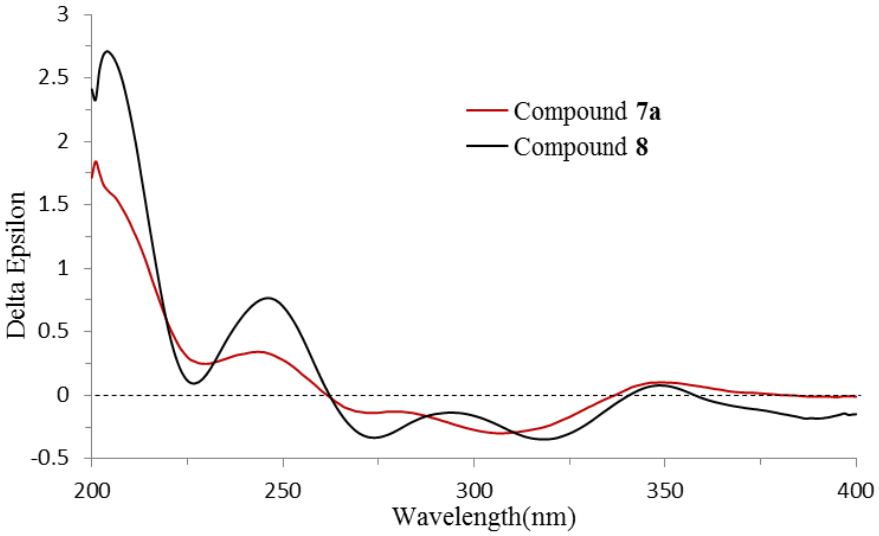


Figure S9. CD Spectra of (+)-didymellamides E (**7a**) and (+)-didymellamide B (**8**) in MeOH.

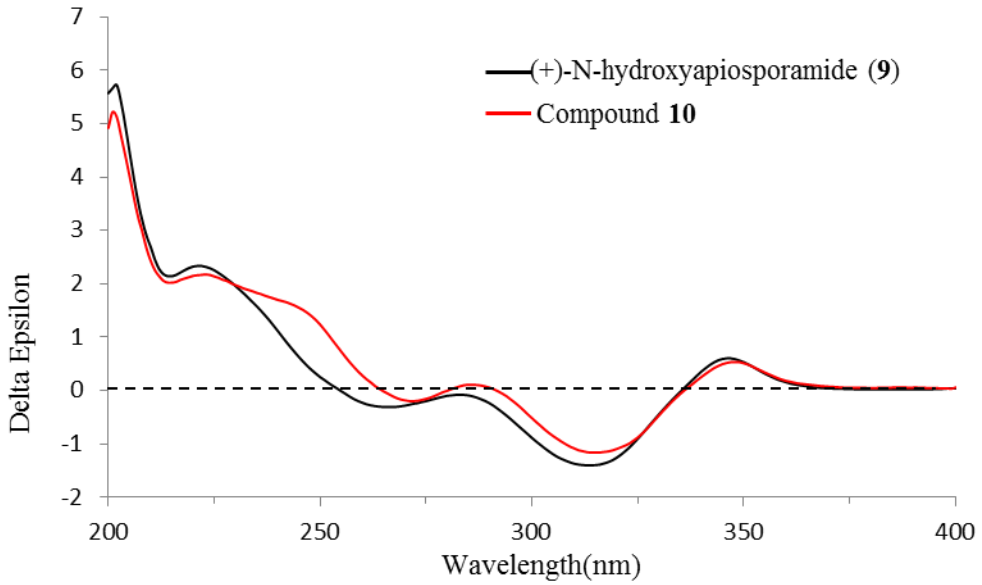


Figure S10. CD Spectra of didymellamide F (**10**) and (+)-*N*--hydroxyapiosporamide **(9)** in MeOH

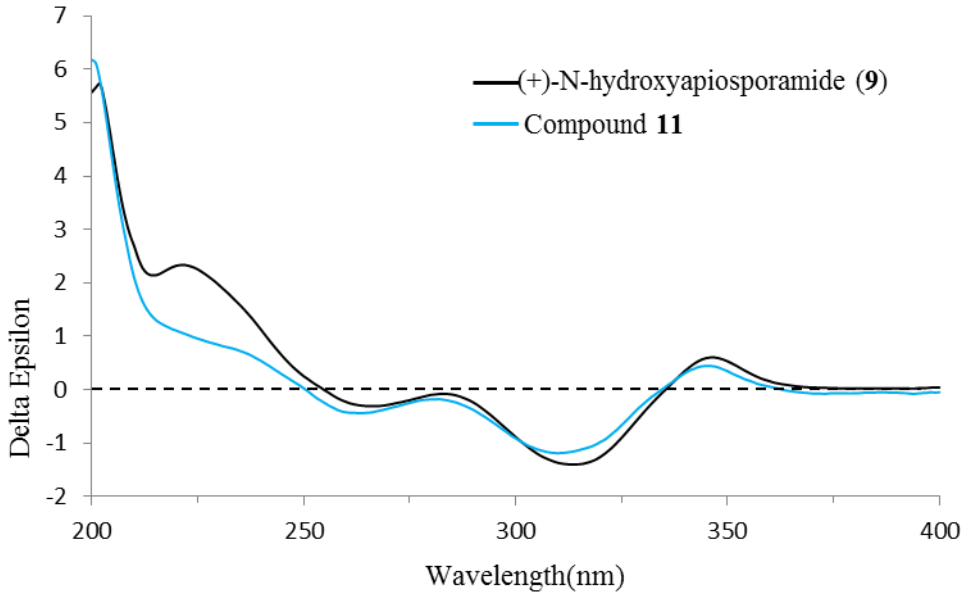


Figure S11. CD Spectra of didymellamide F (**11**) and (+)-*N*--hydroxyapiosporamide **(9)** in MeOH

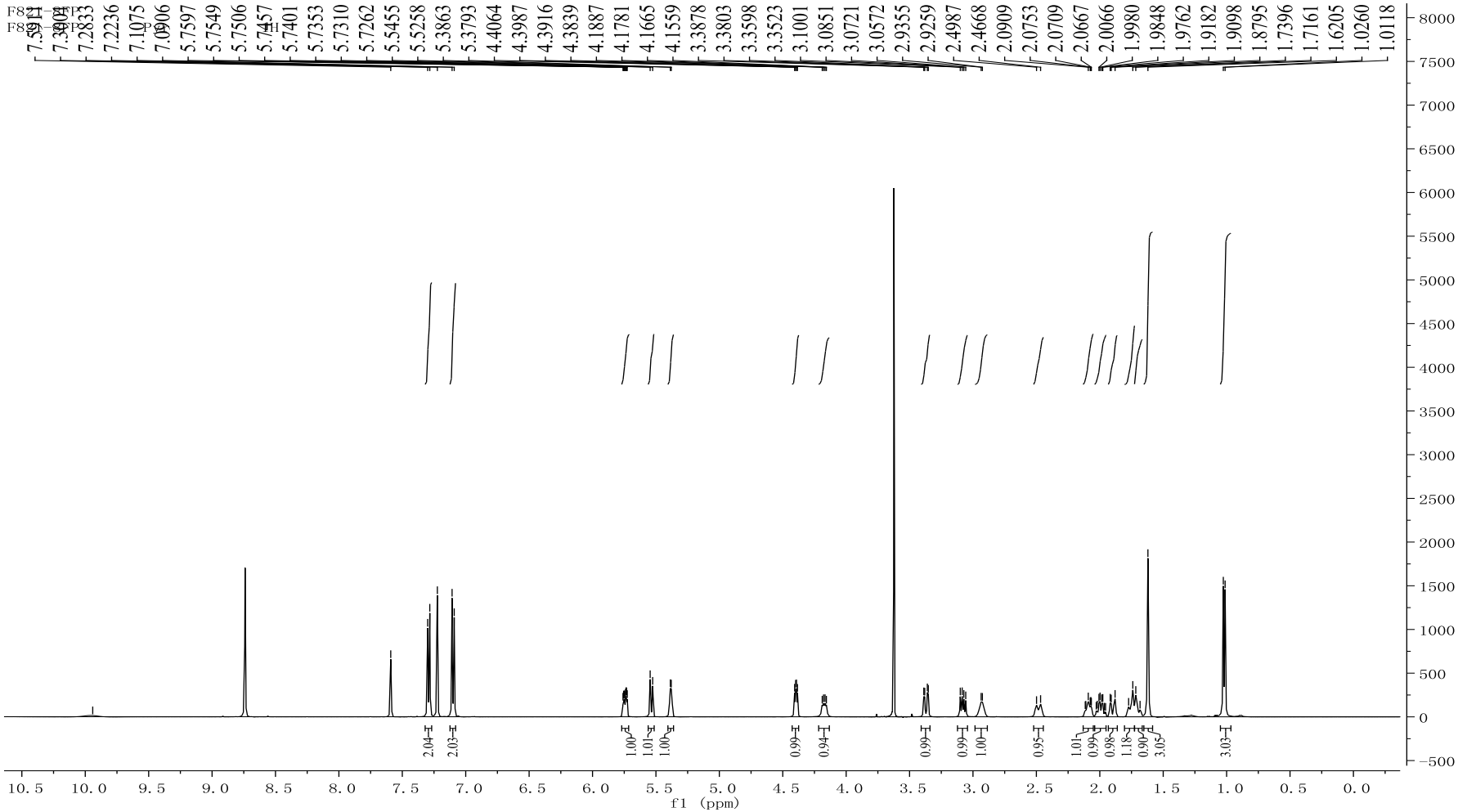


Figure S12. ^{1}H NMR spectrum of (±)-Conipyrrolidone A (**1**) in pyridine-d_5 (500 MHz)

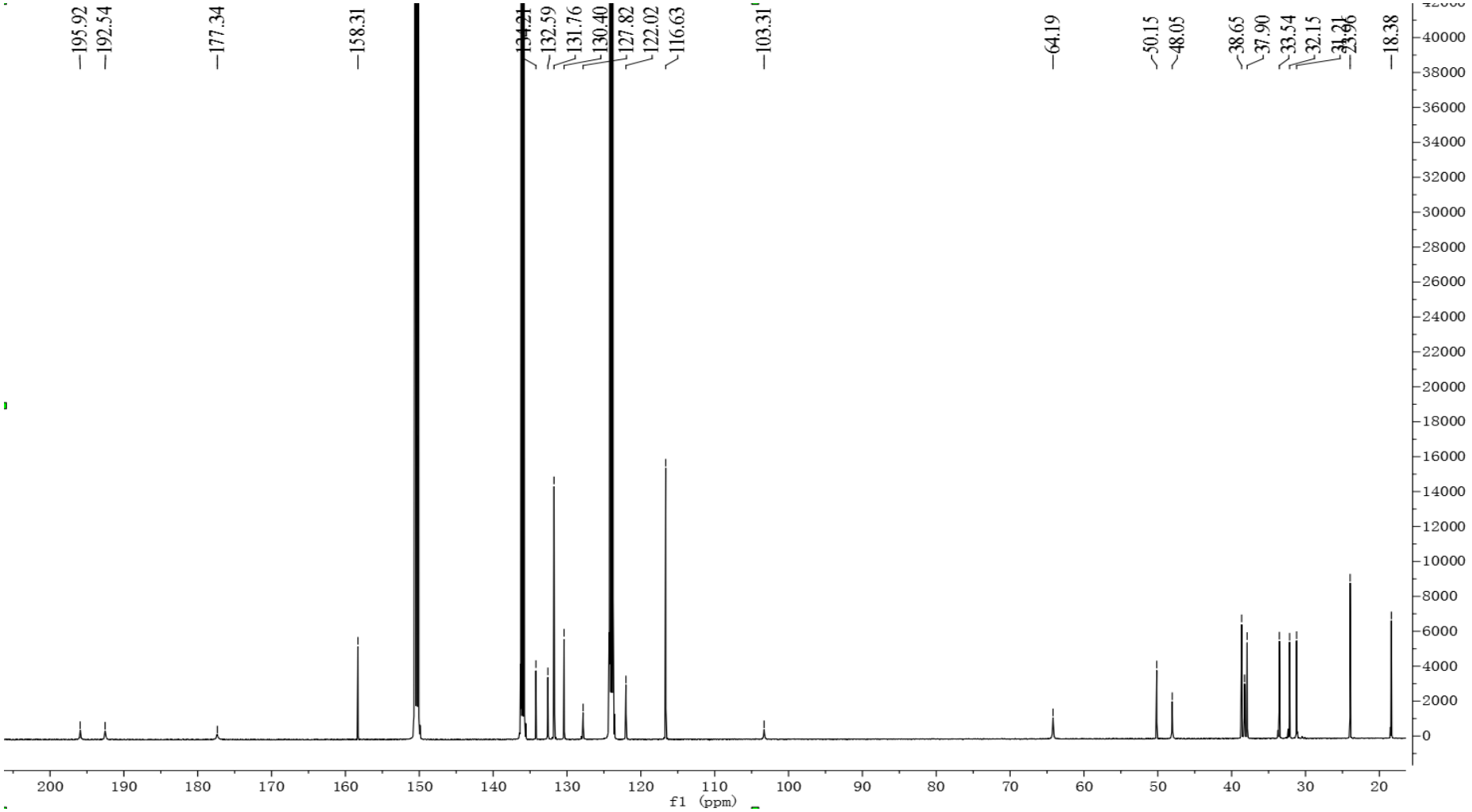


Figure S13. ^{13}C NMR spectrum of (±)-conipyrrolidone A (**1**) in pyridine-d_5 (125 MHz)

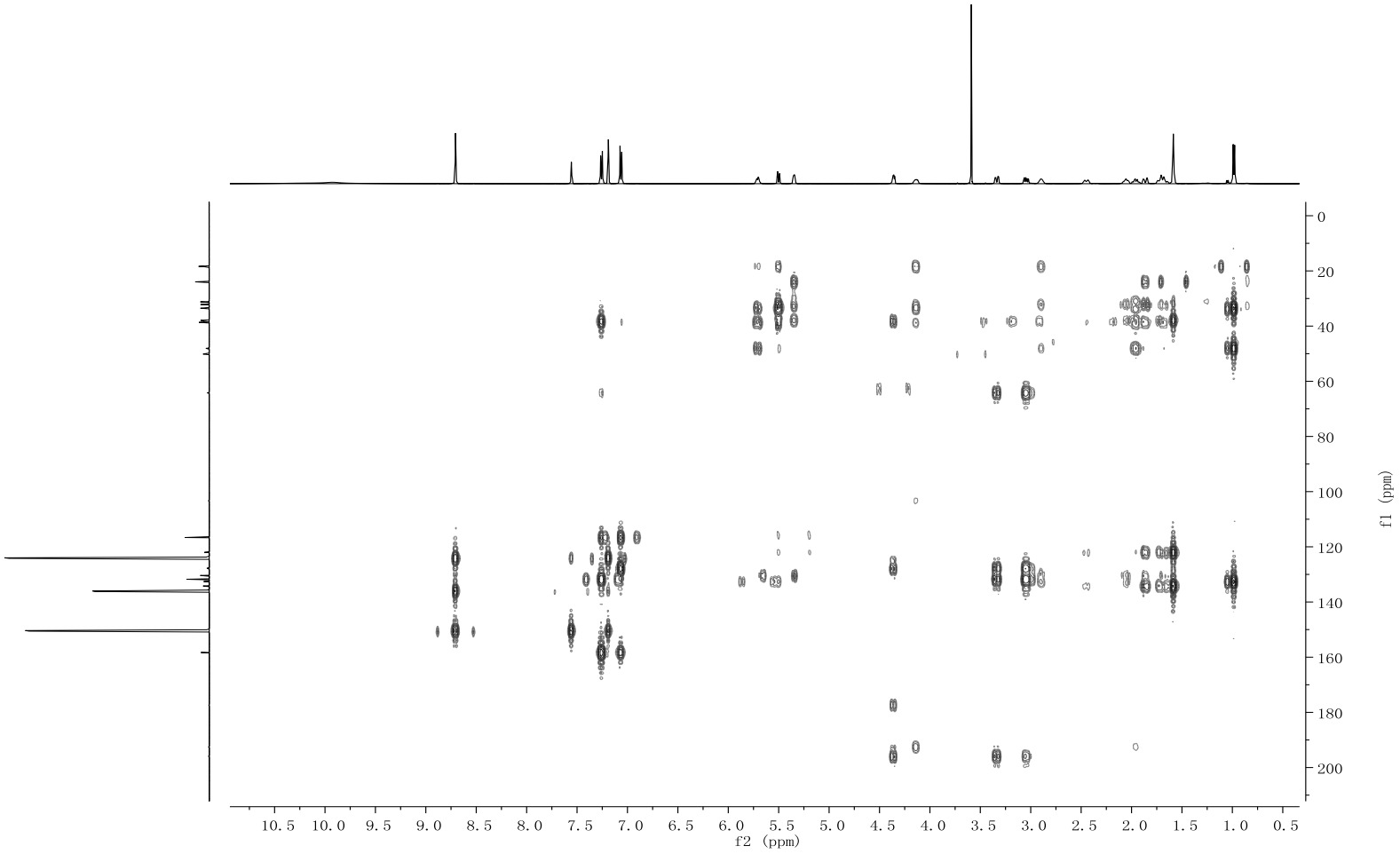


Figure S14. HMBC spectrum of (±)-conipyrrolidone A (**1**) in pyridine-d_5

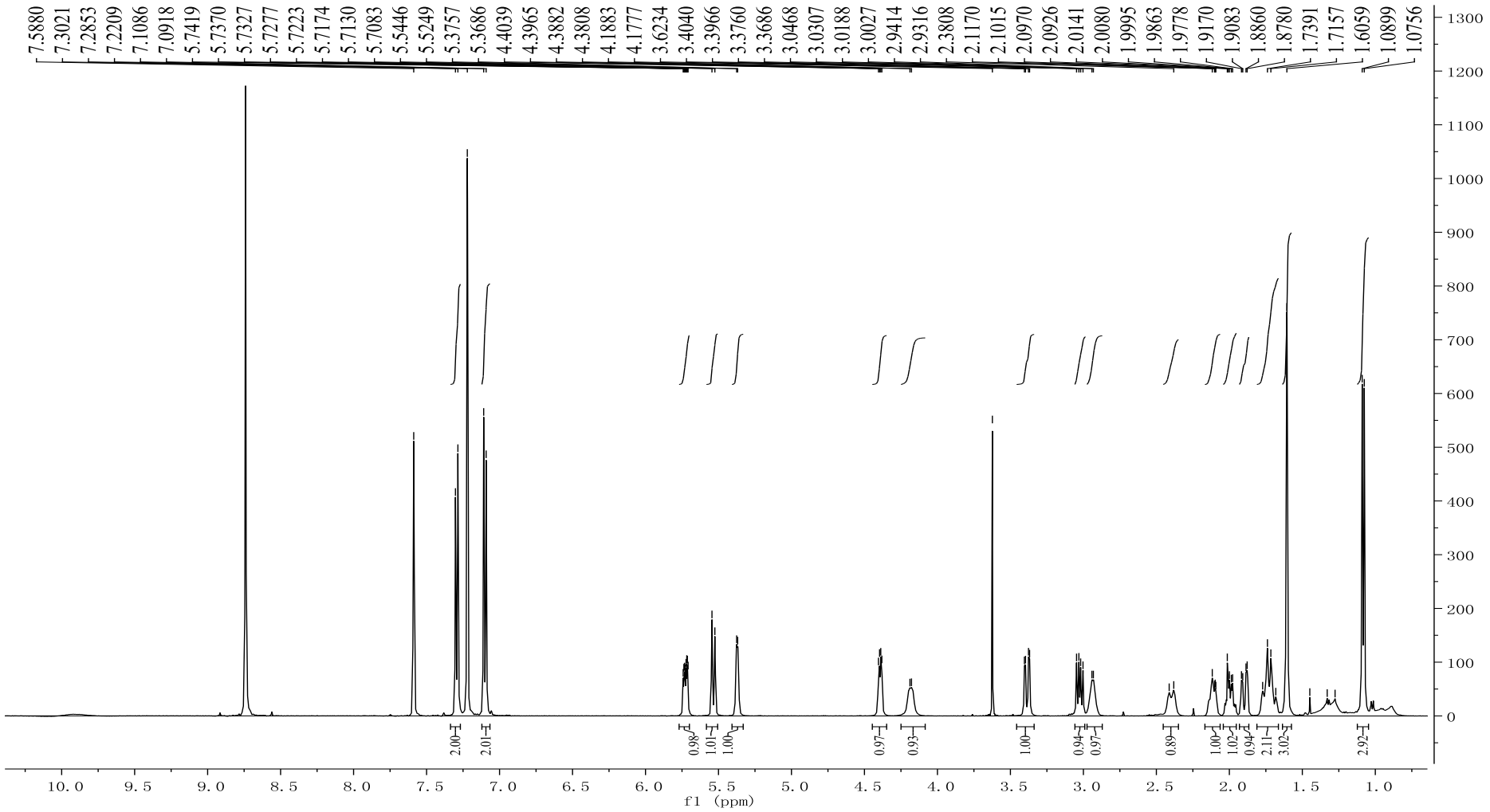


Figure S15. ^{1}H NMR spectrum of (±)-conipyrrolidone B (**2**) in pyridine-d_5 (500 MHz)

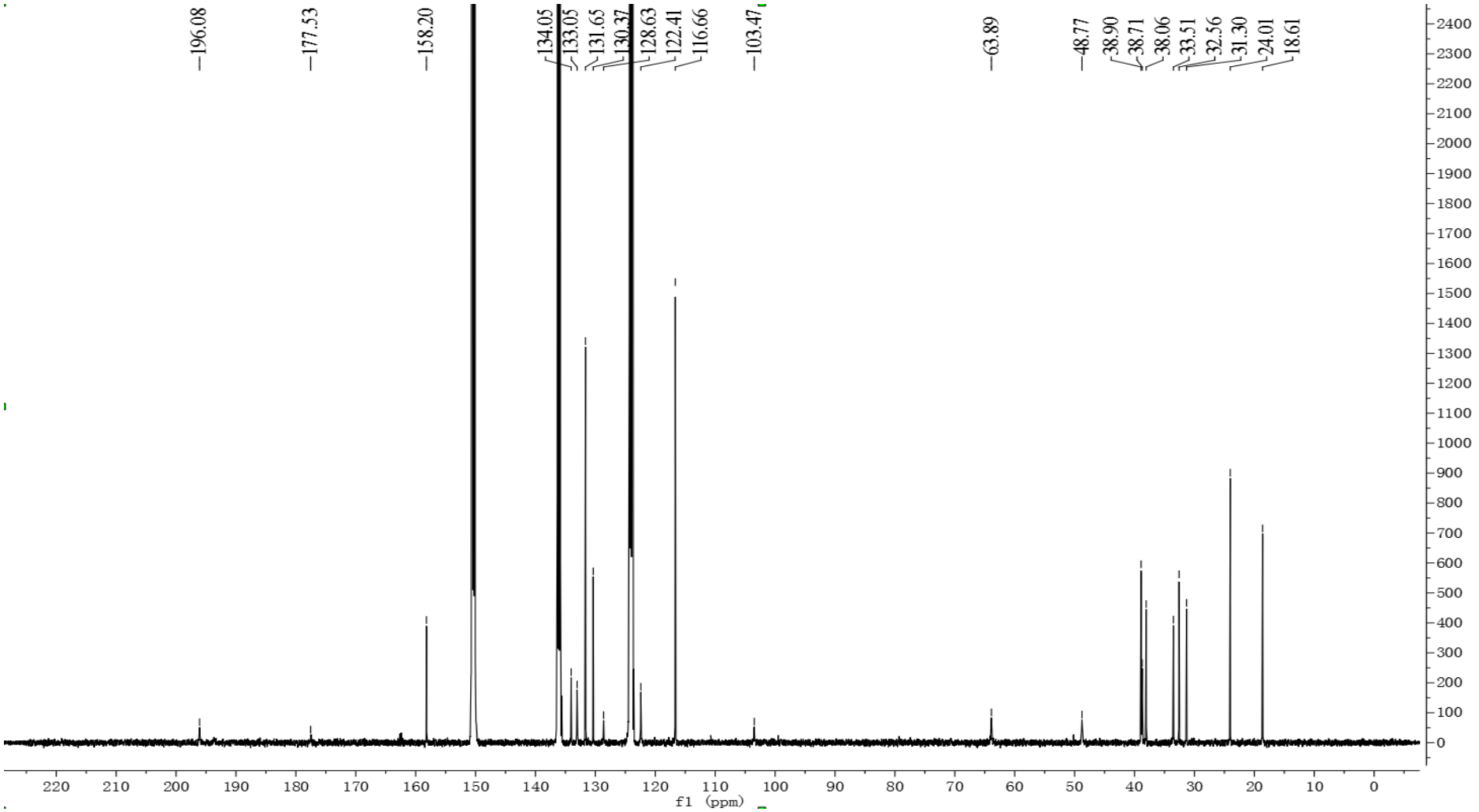


Figure S16. ^{13}C NMR spectrum of (±)-conipyrrolidone B (2) in pyridine-d_5 (125 MHz)

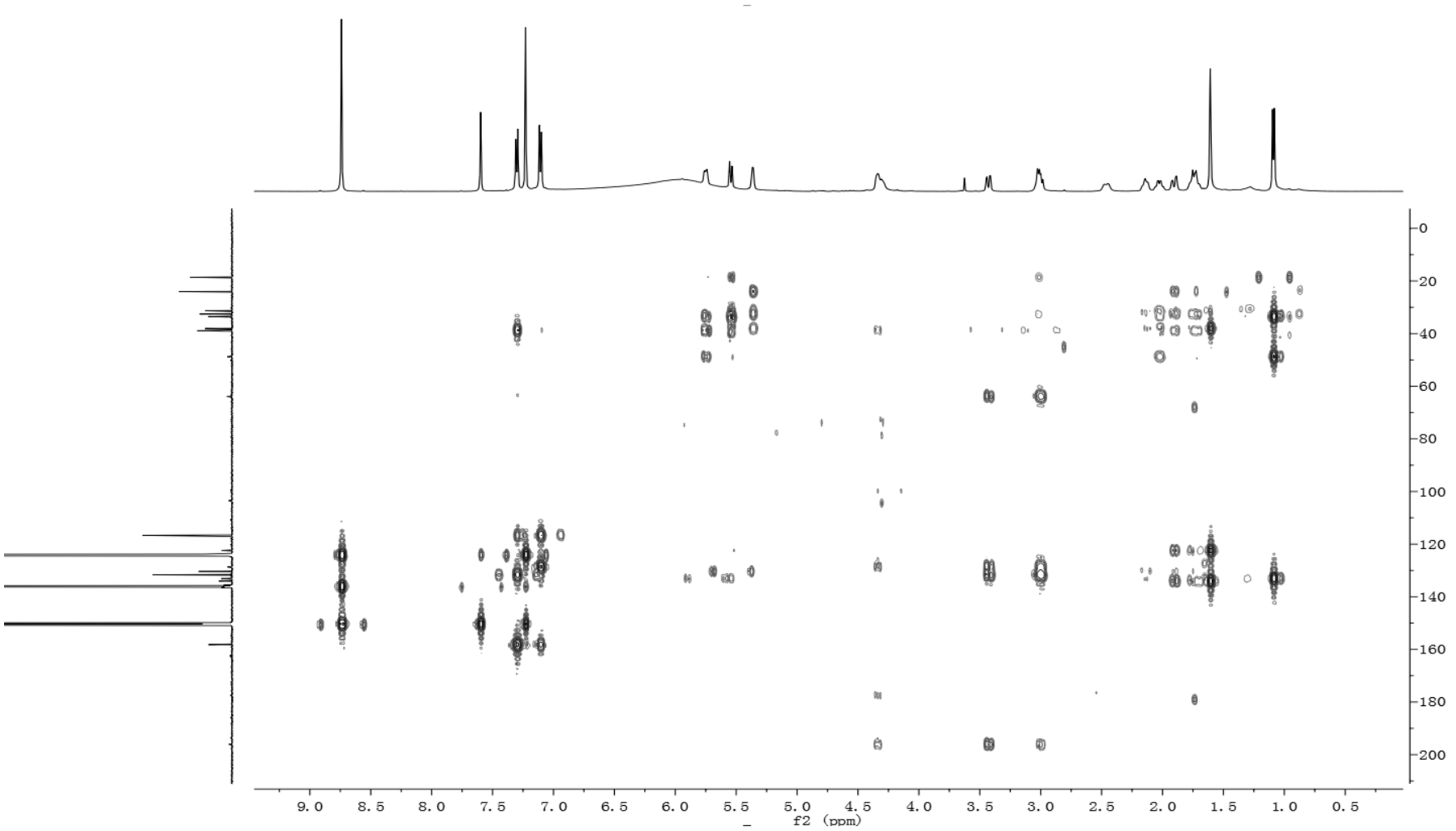


Figure S17. HMBC spectrum of (±)-conipyrrolidone B (**2**) in pyridine-d_5

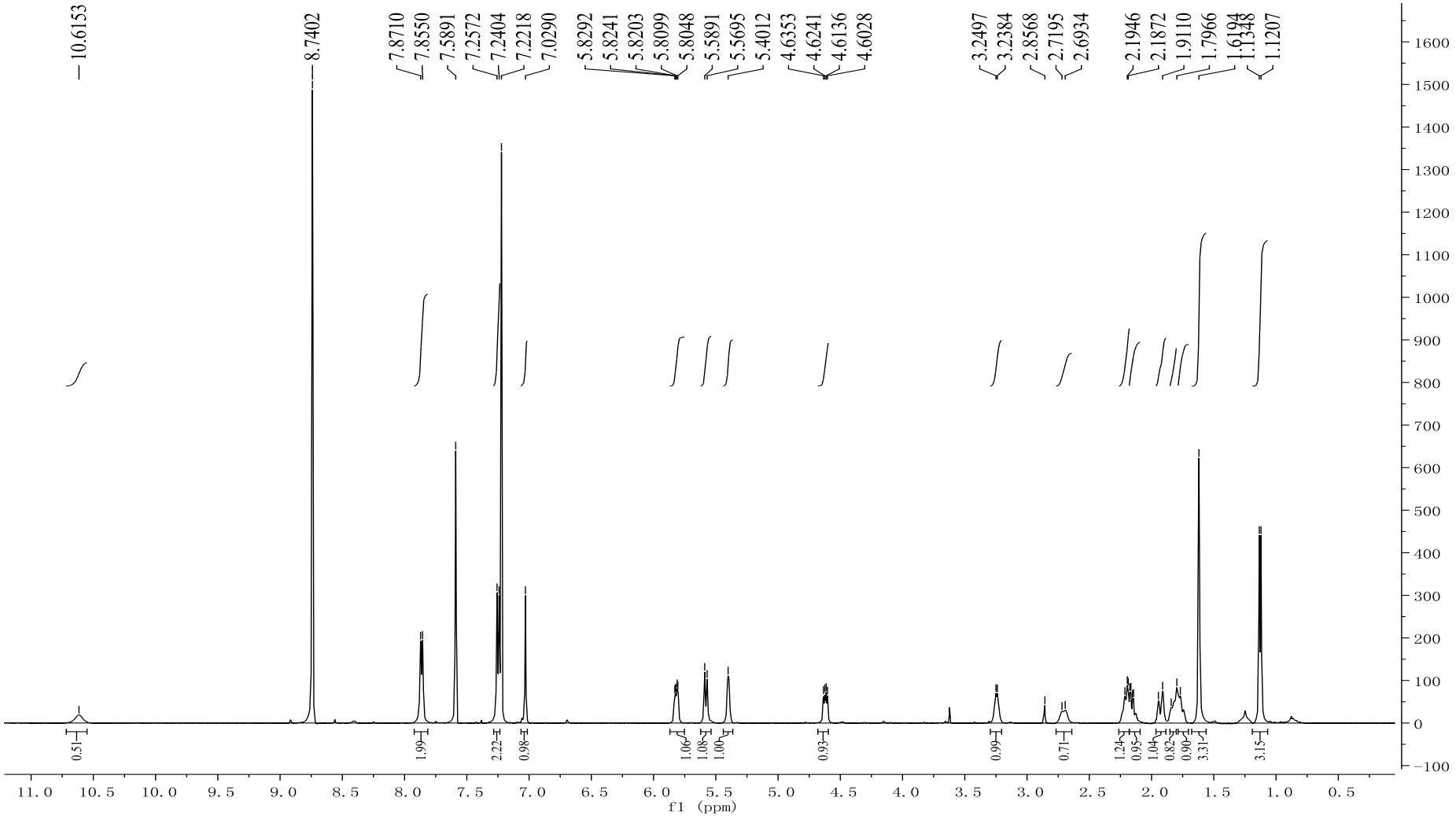


Figure S18. ^{1}H NMR spectrum of (±)-Conipyrrolidone C (3) in pyridine-d_5 (500 MHz)

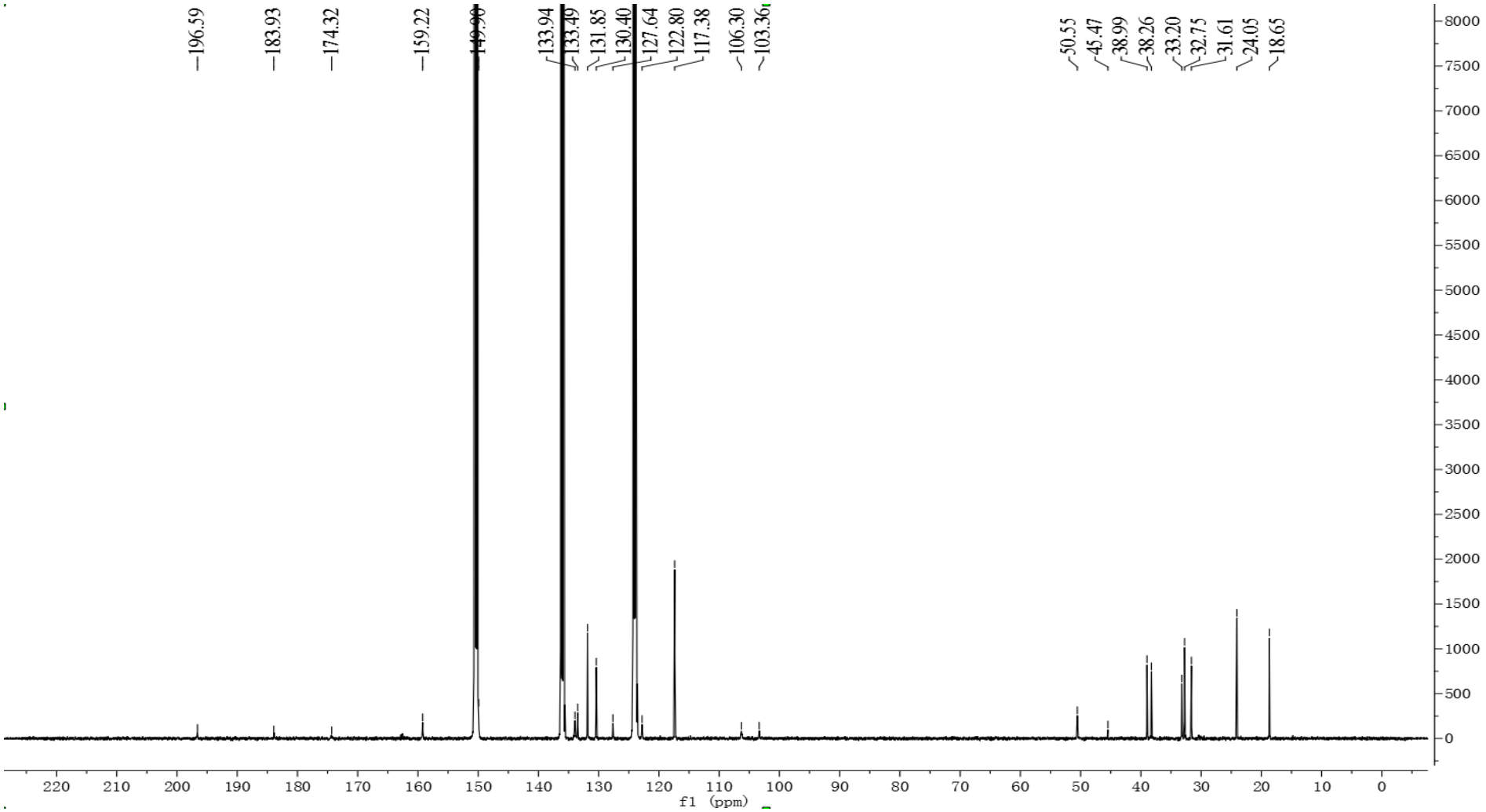


Figure S19. ^{13}C NMR spectrum of (±)-Conipyrrolidone C (3) in pyridine-d_5 (125 MHz)

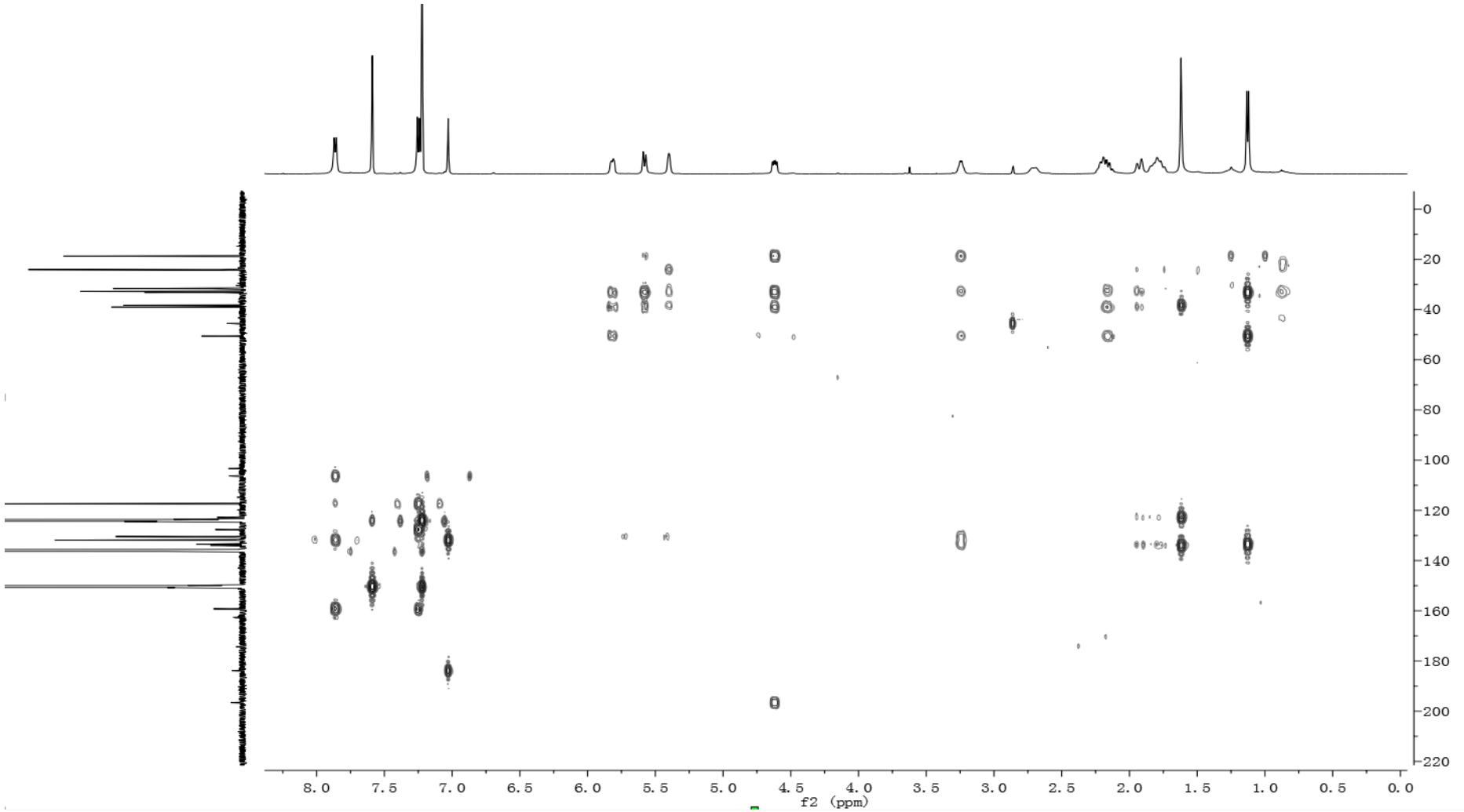


Figure S20. HMBC spectrum of (±)-Conipyrrolidone C (3) in pyridine-d_5

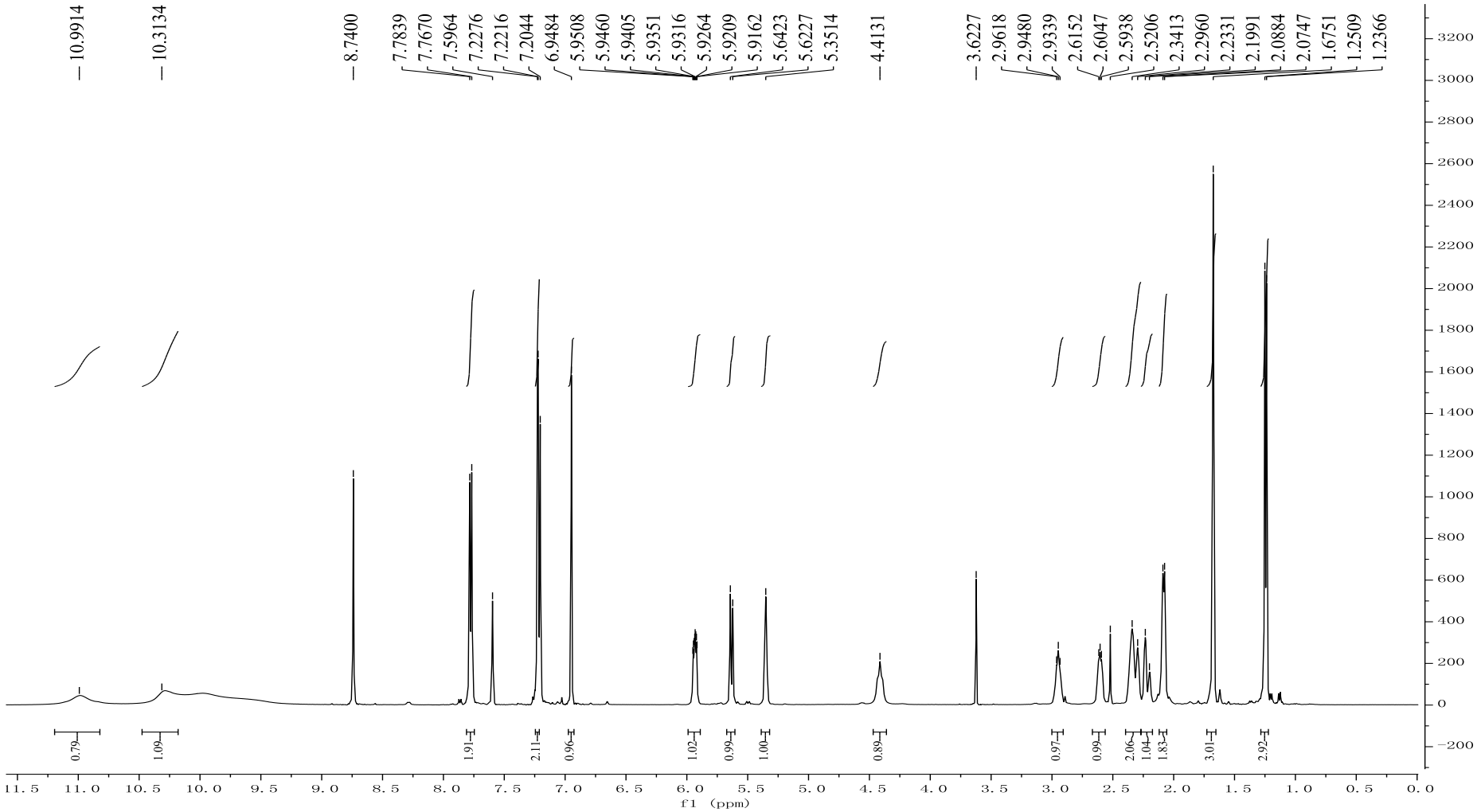


Figure S21. ^{1}H NMR spectrum of (±)-conipyrrolidone D (4) in pyridine-d_5 (500 MHz)

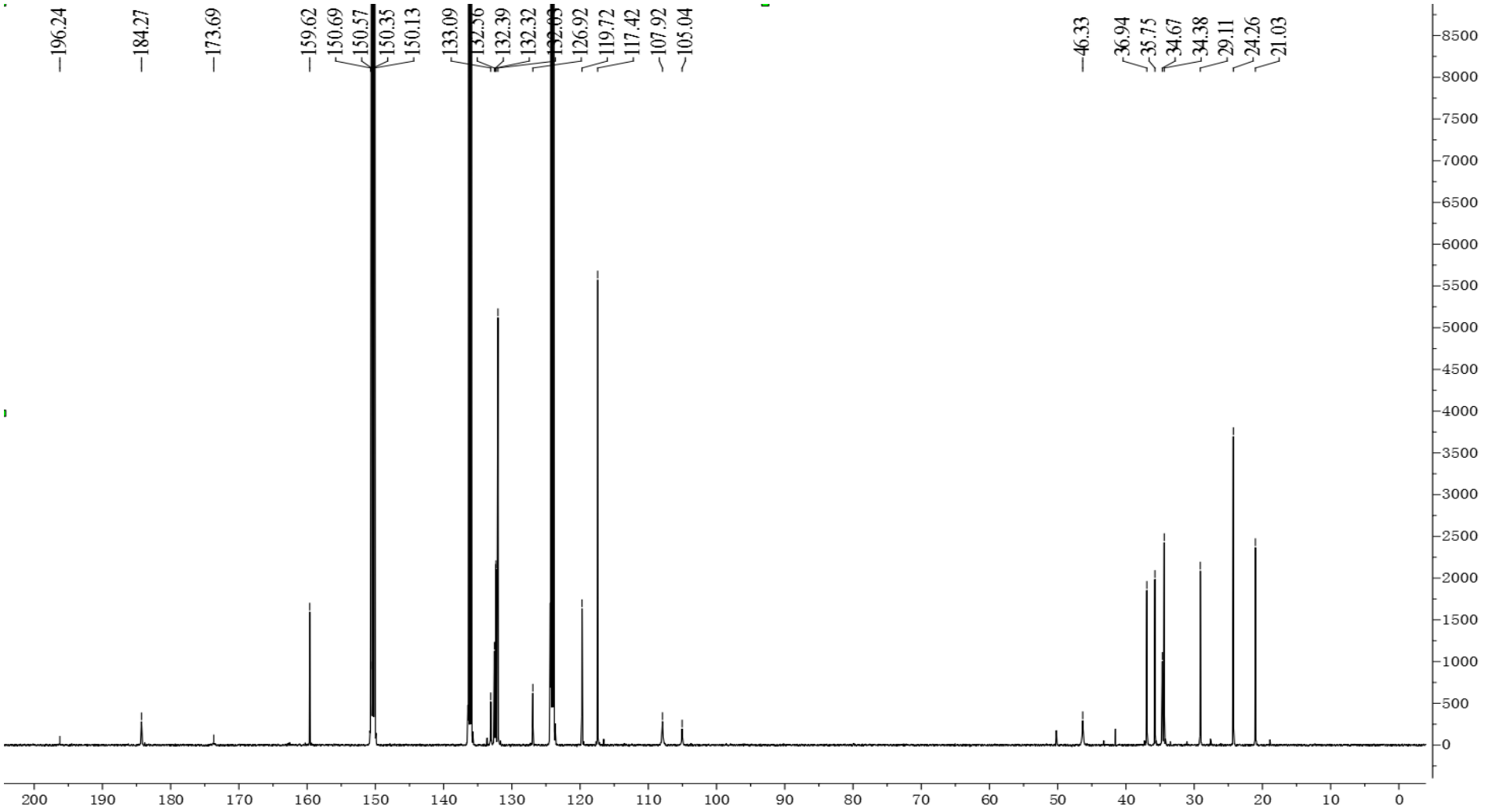


Figure S22. ^{13}C NMR spectrum of (±)-conipyrrolidone D (**4**) in pyridine-d_5 (125 MHz)

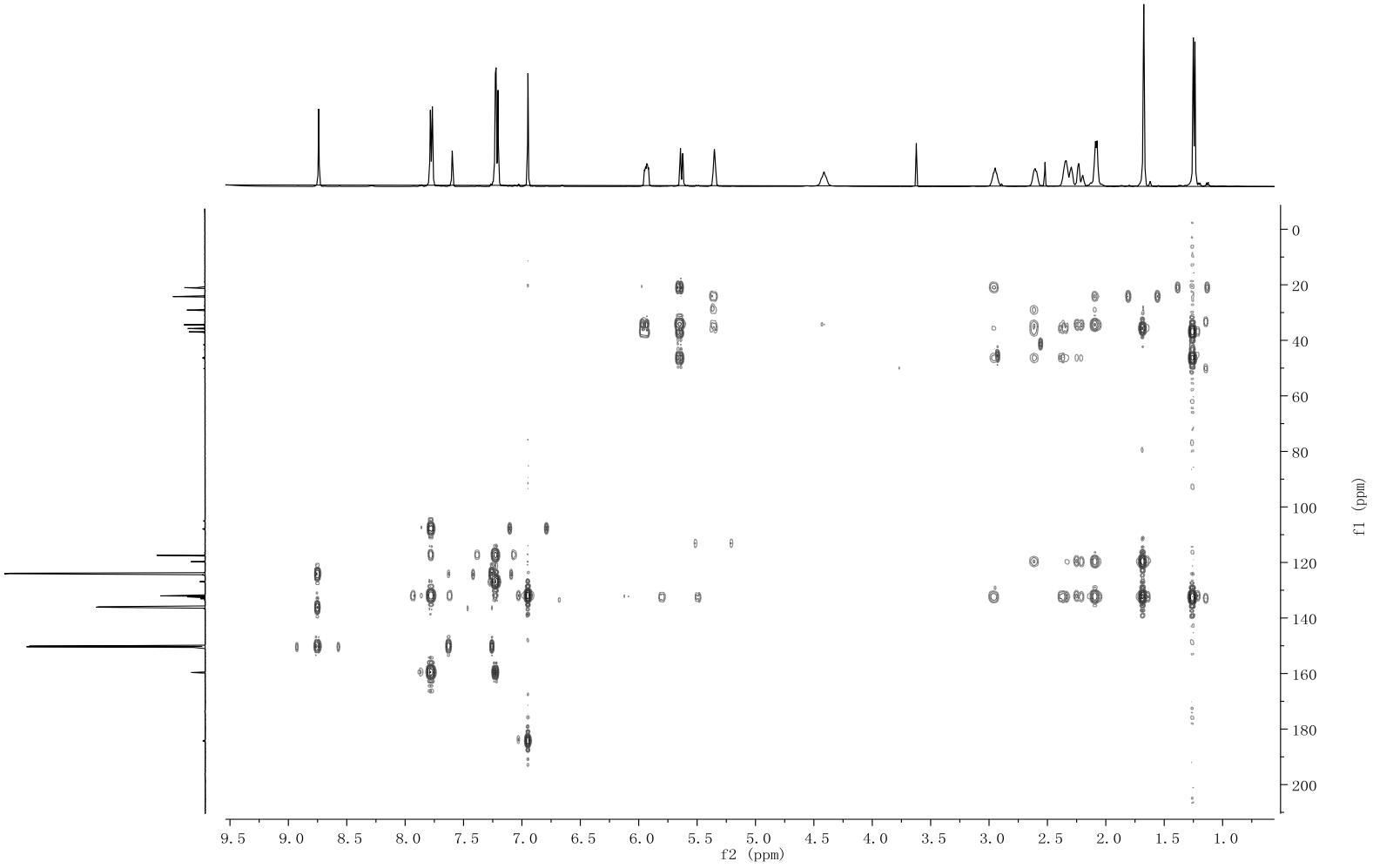


Figure S23. HMBC spectrum of (±)-conipyrrolidone D (**4**) in pyridine-d_5

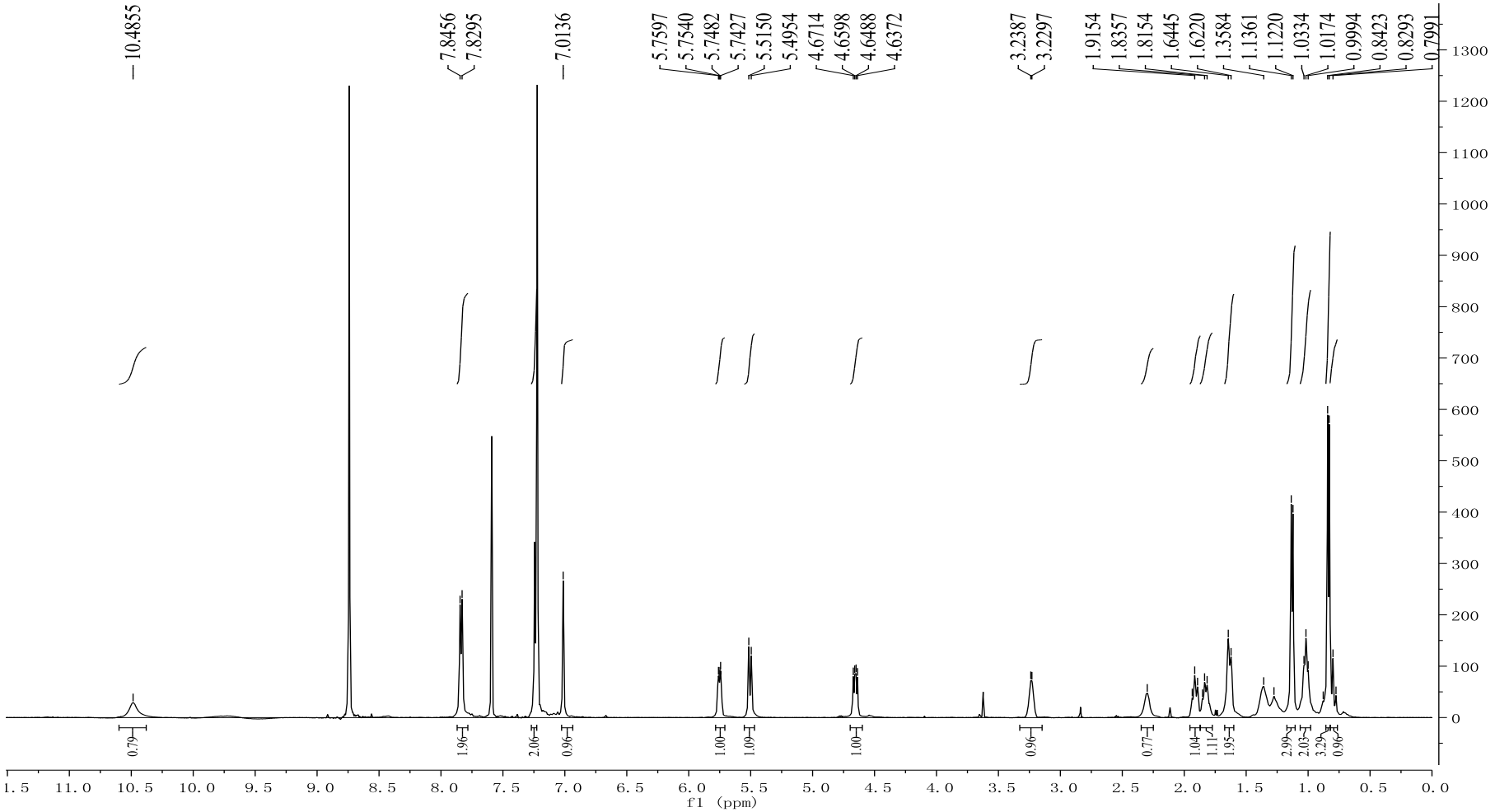


Figure S24. ^{1}H NMR spectrum of conipyrrolidone E (**5**) in pyridine-d_5 (500 MHz)

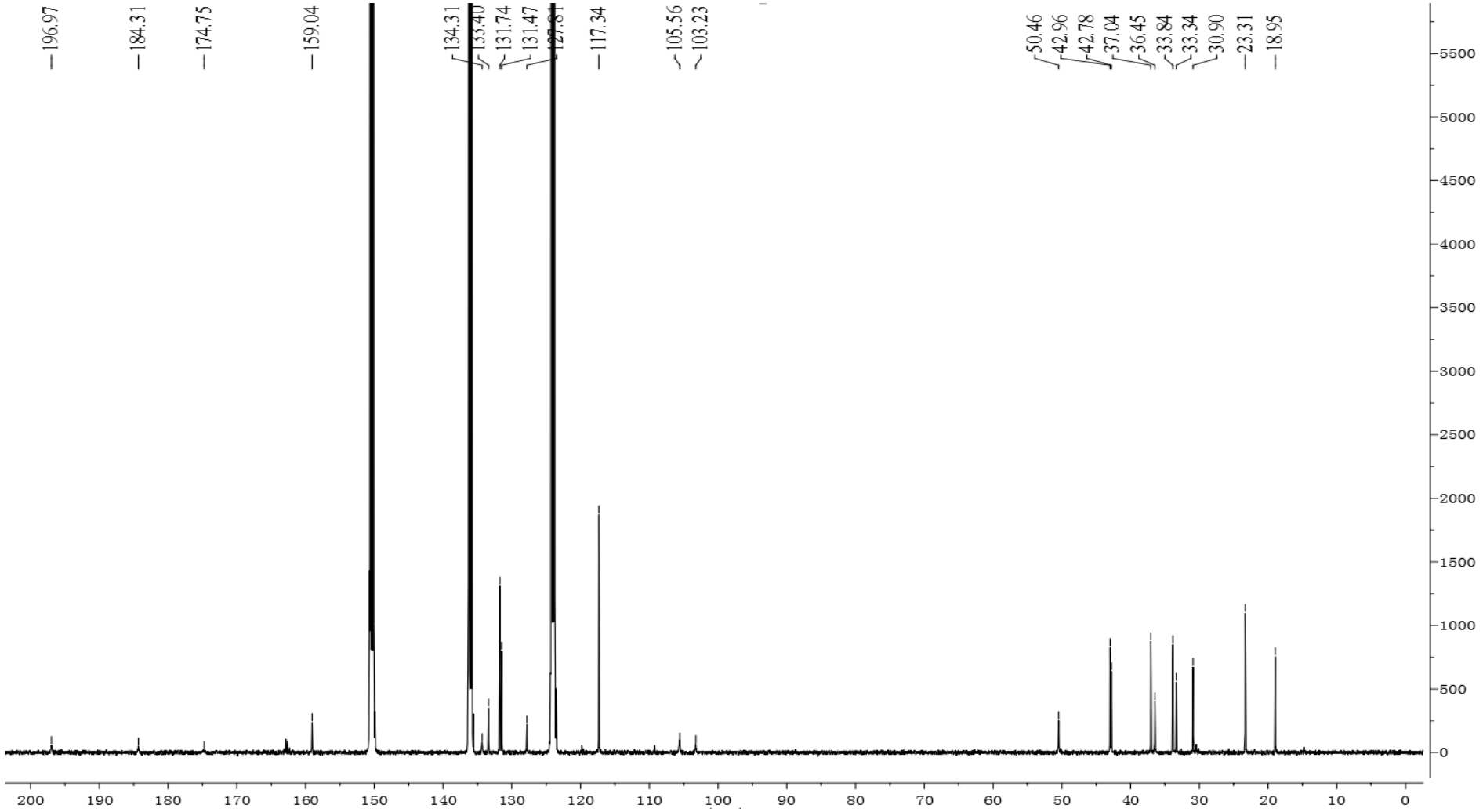


Figure S25. ^{13}C NMR spectrum of conipyrrolidone E (**5**) in pyridine-d_5 (125 MHz)

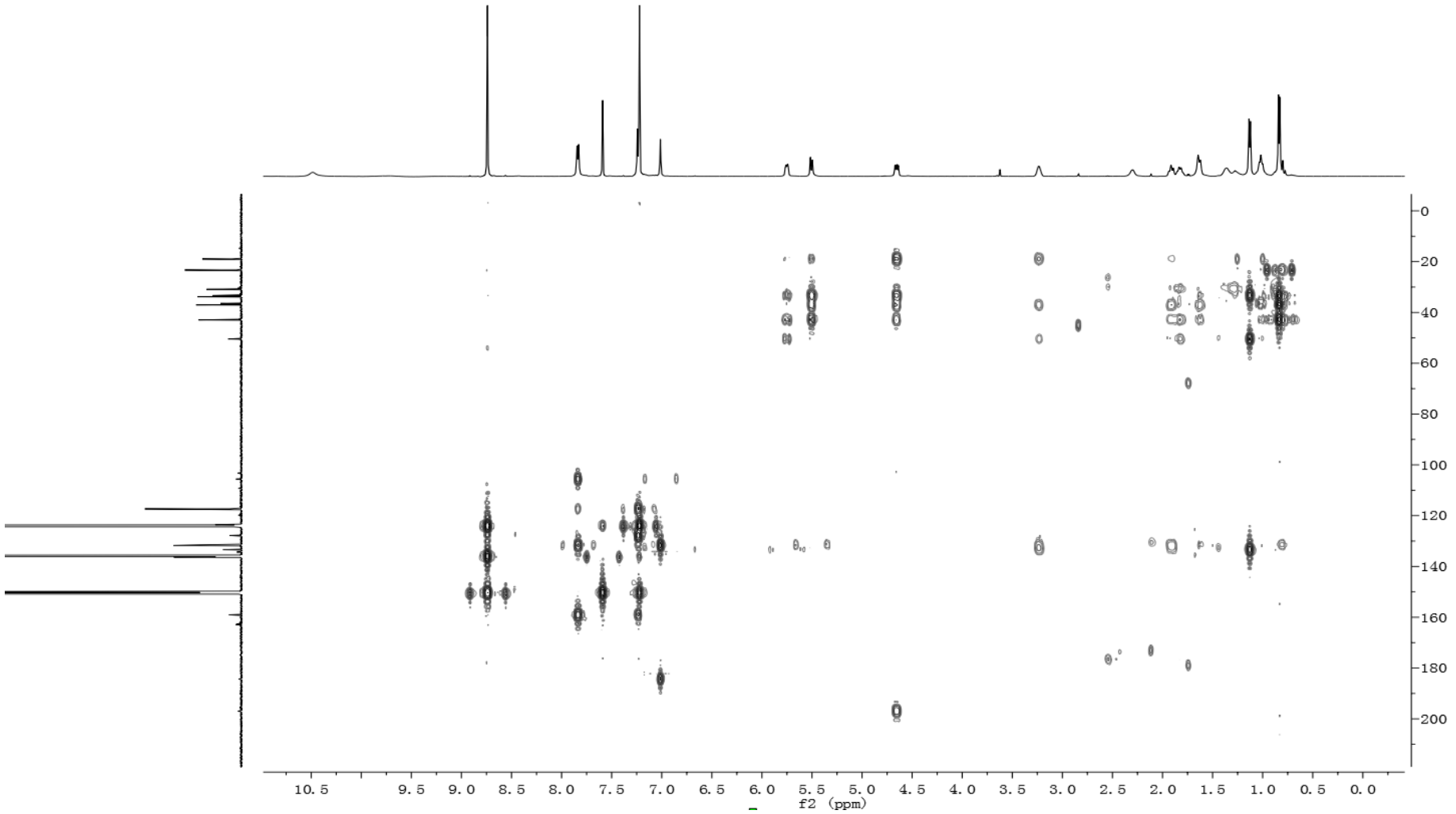


Figure S26. HMBC spectrum of conipyrrolidone E (**5**) in pyridine-d_5

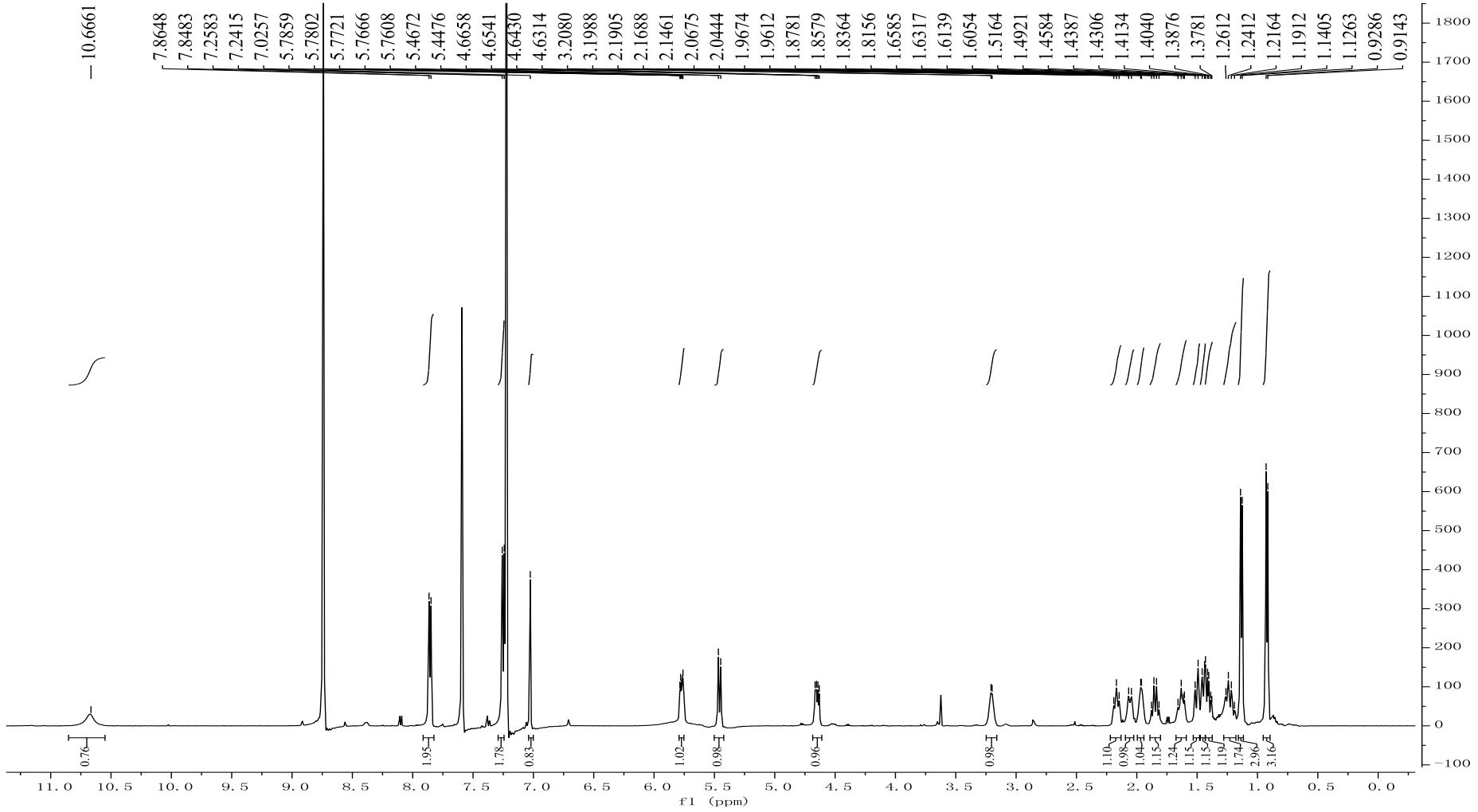


Figure S27. ^{1}H NMR spectrum of conipyrrolidone F (**6**) in pyridine-d_5 (500 MHz)

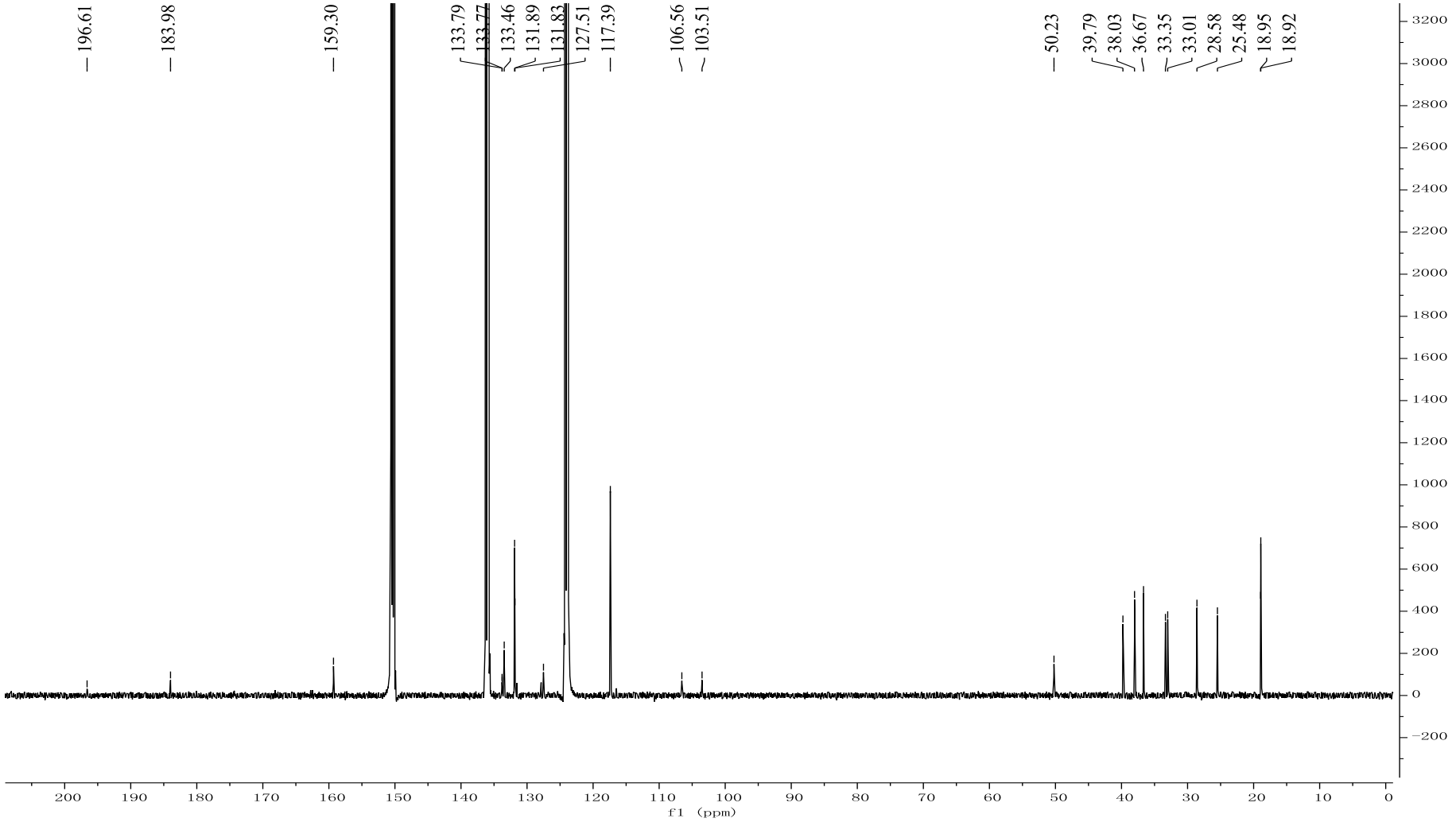


Figure S28. ^{13}C NMR spectrum of conipyrrolidone F (**6**) in pyridine-d_5 (125 MHz)

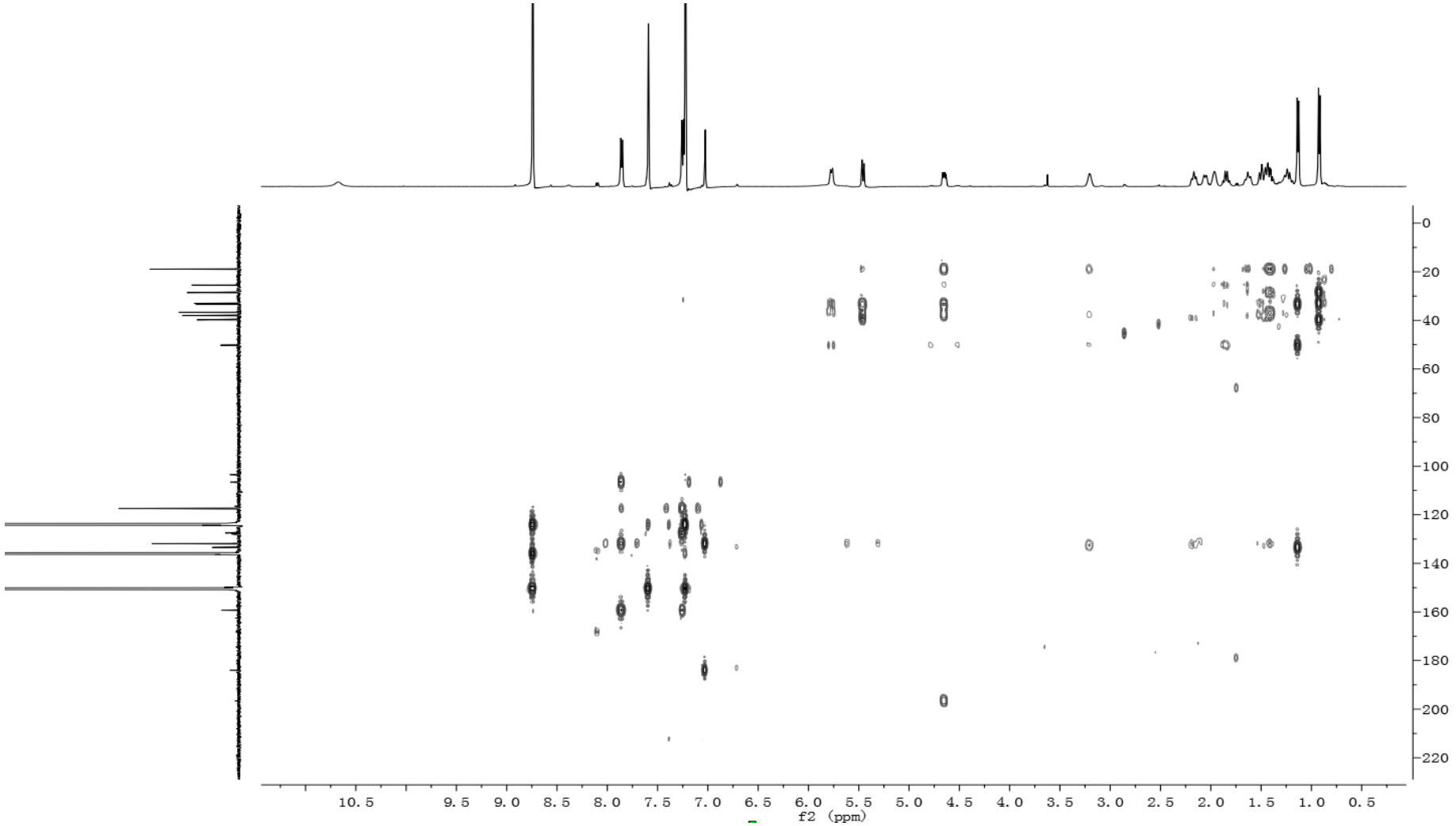


Figure S29. HMBC spectrum of conipyrrolidone F (**6**) in pyridine-d_5

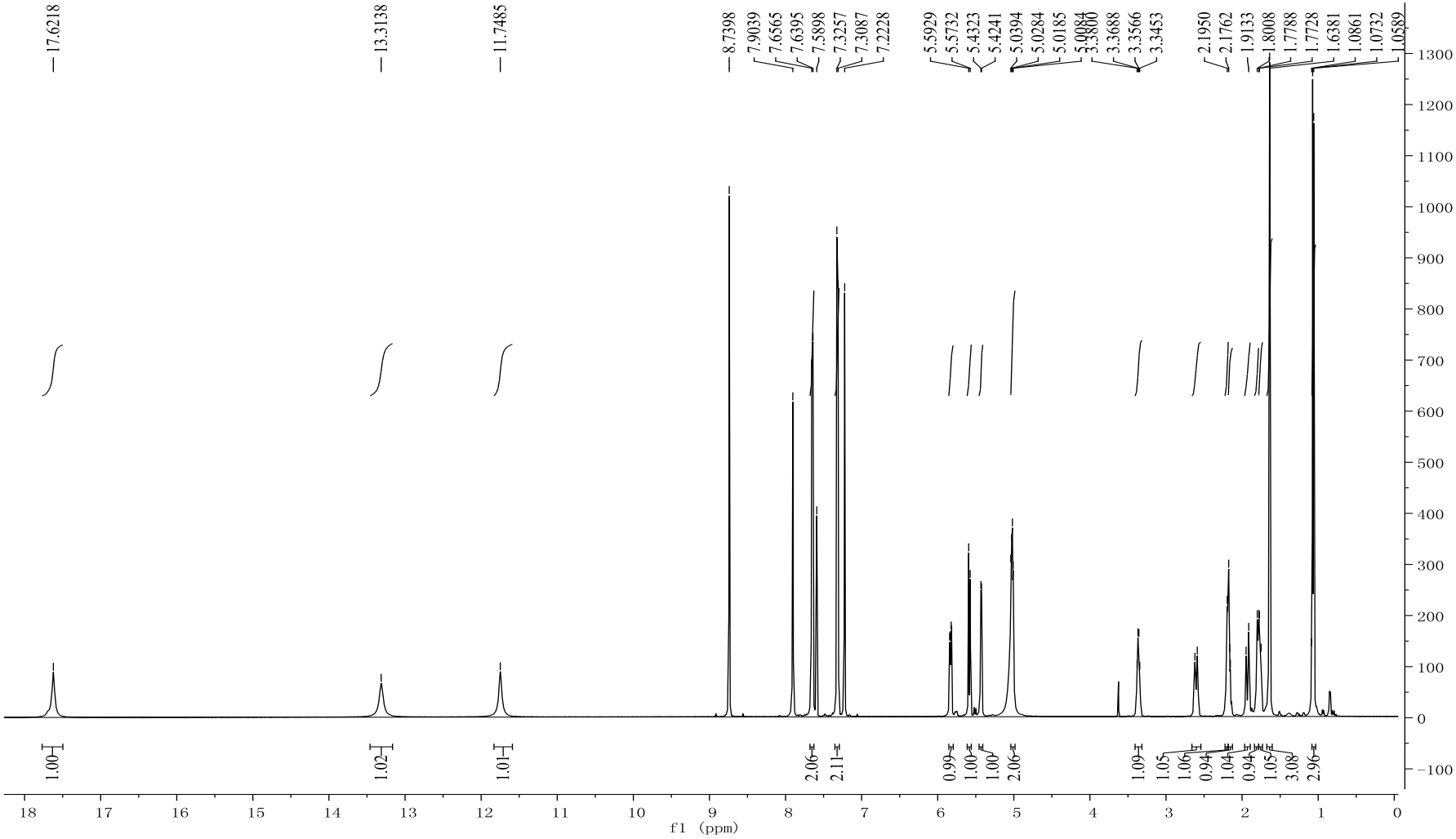


Figure S30. ^{1}H NMR spectrum of (±)-didymellamide E (**7**) in pyridine-d_5 (500 MHz)

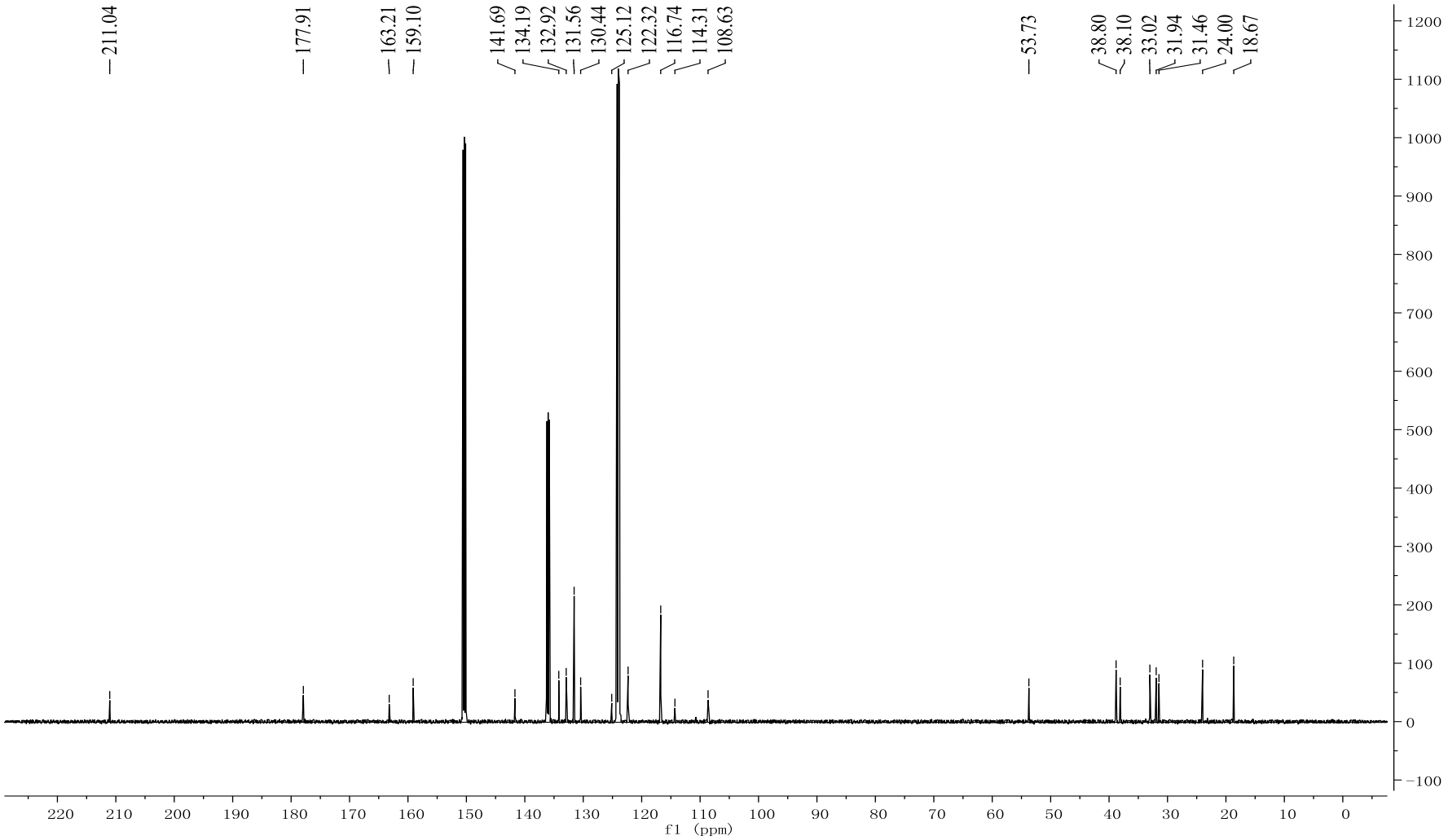


Figure S31. ^{1}H NMR spectrum of (±)-didymellamide E (**7**) in pyridine-d_5 (125 MHz)

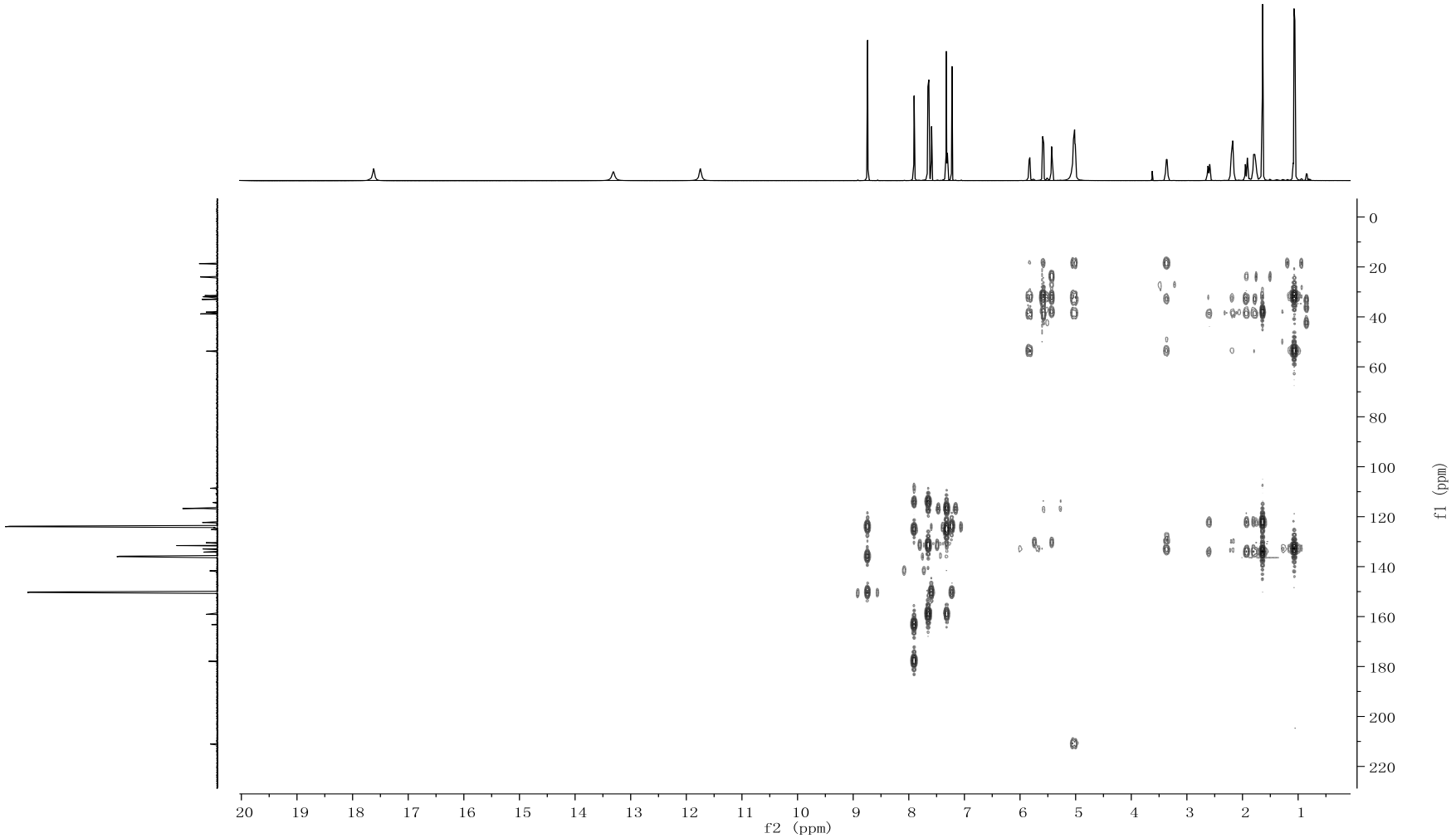


Figure S32. HMBC spectrum of (±)-didymellamide E (**7**) in pyridine-d_5

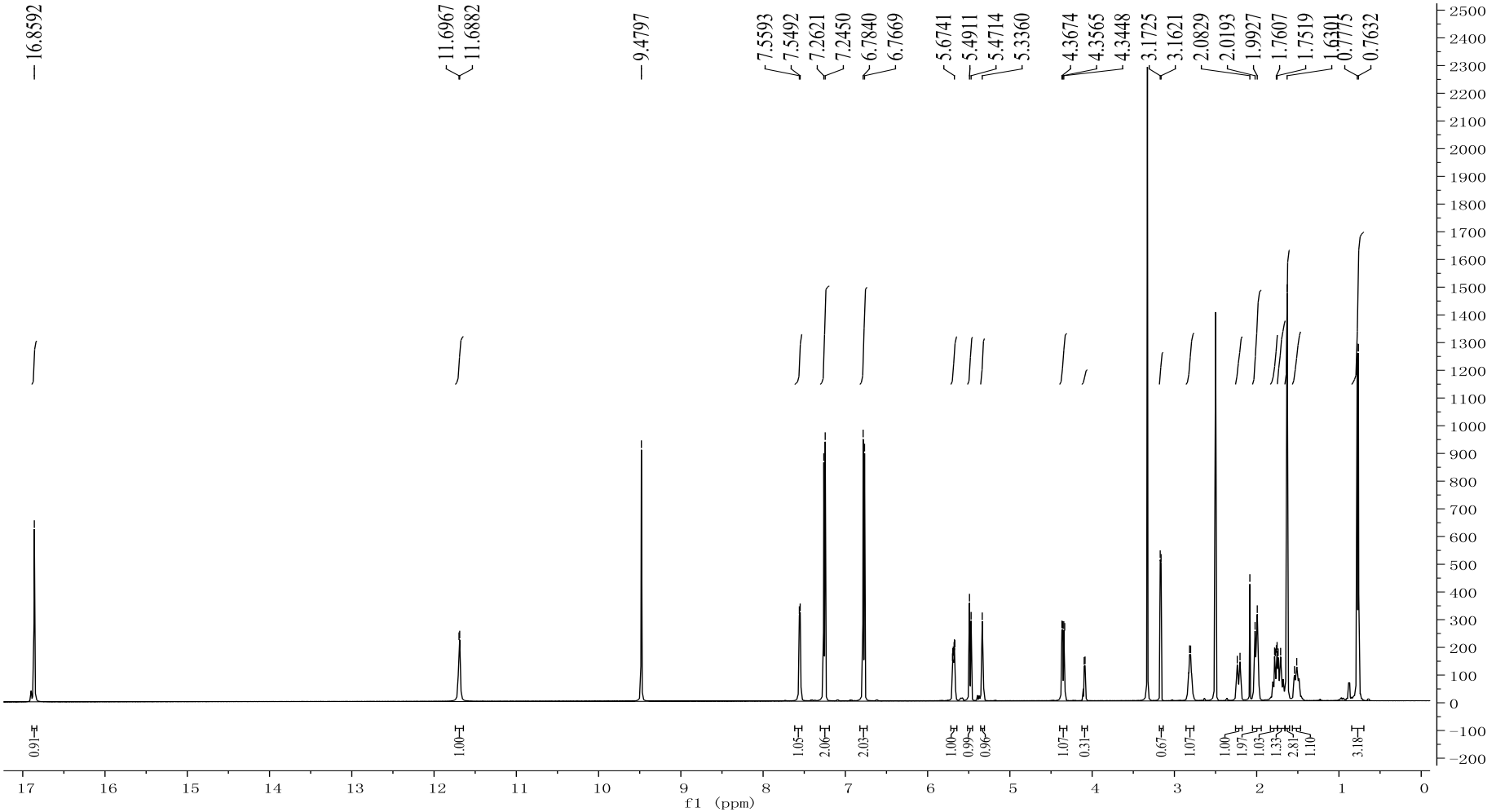


Figure S33. ^{1}H NMR spectrum of (±)-didymellamide E (**7**) in DMSO-d_6 (500 MHz)

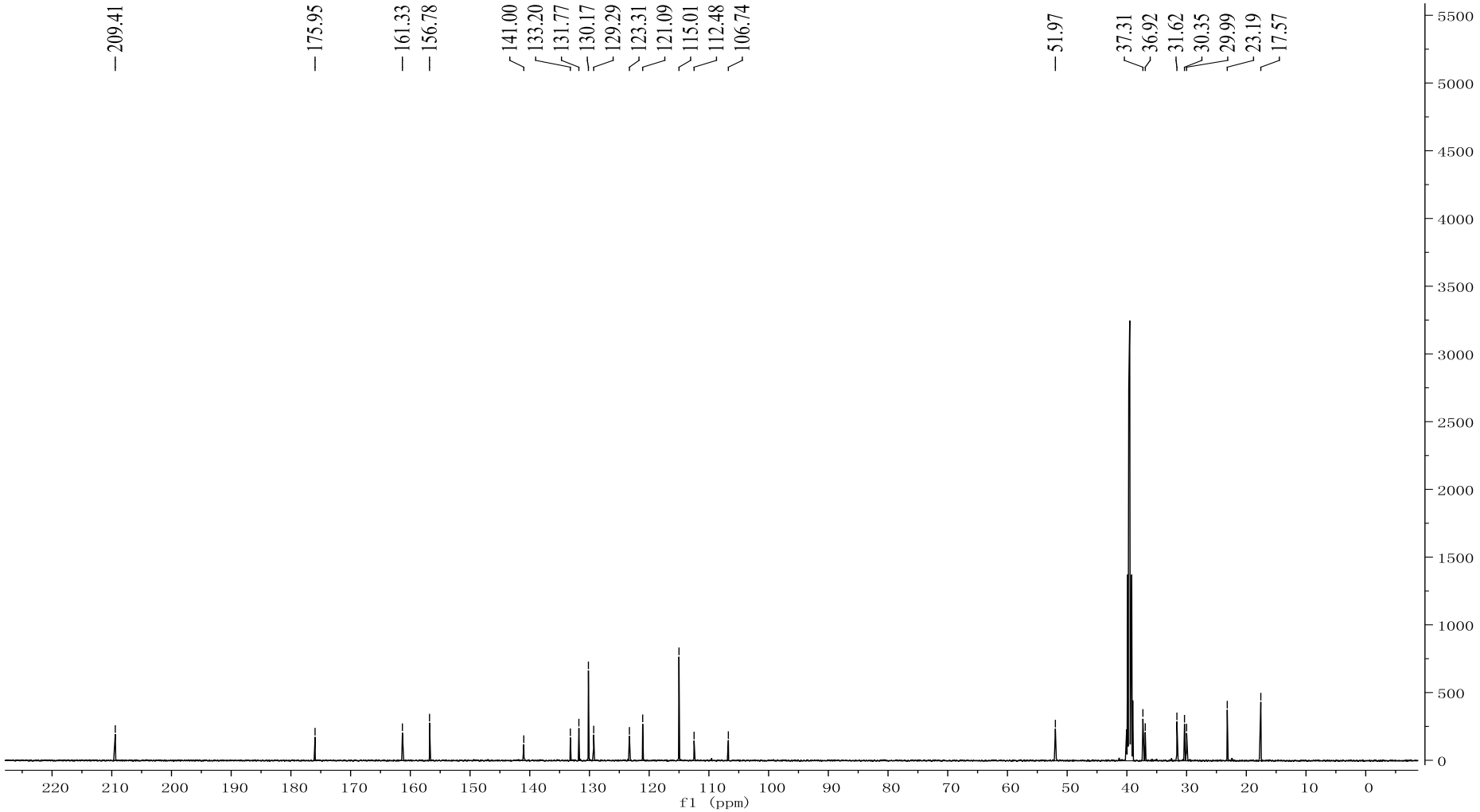


Figure S34 ^{13}C NMR spectrum of (±)-didymellamide E (**7**) in DMSO-d_6 (125 MHz)

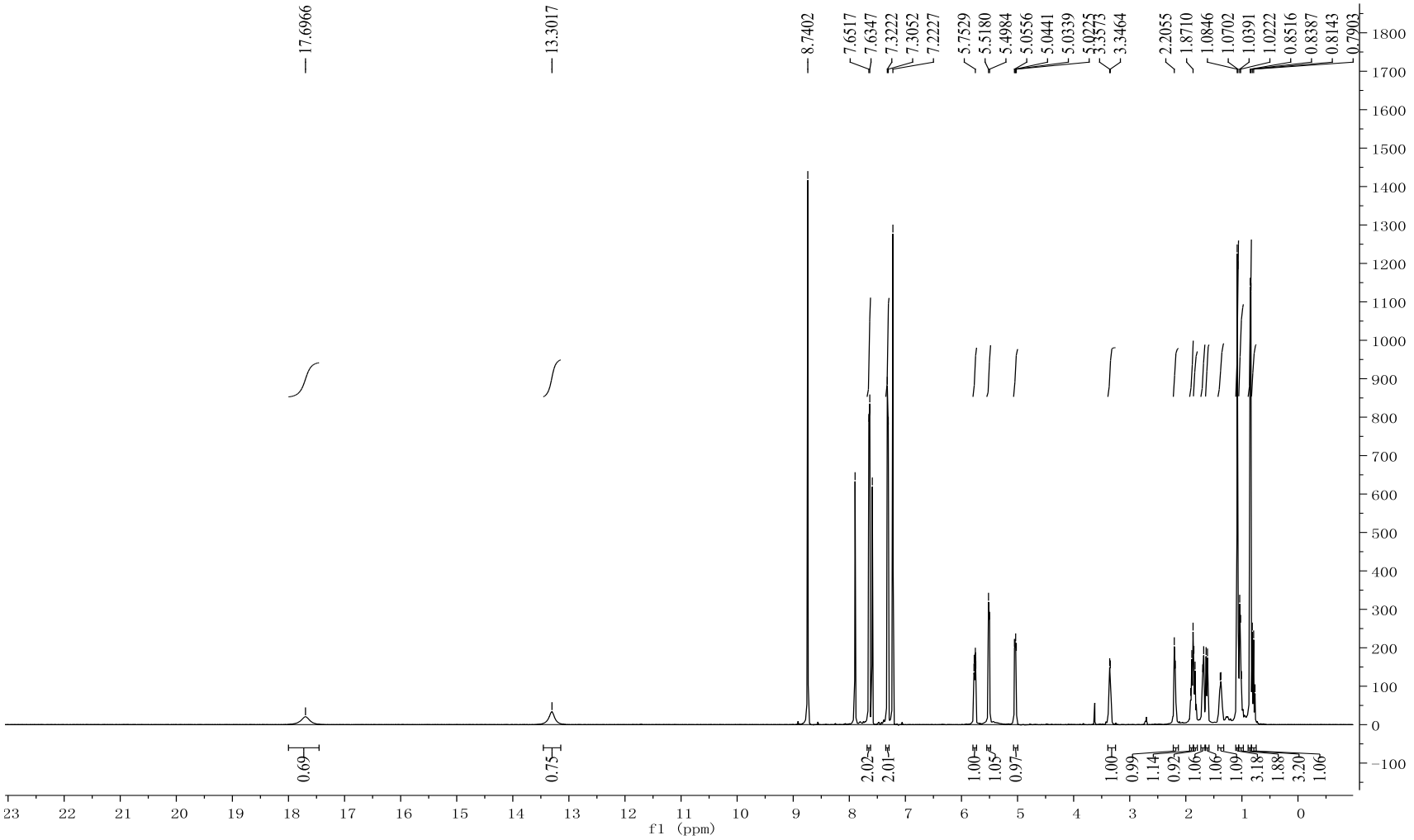


Figure S35. ^{1}H NMR spectrum of (+)-didymellamide B (**8**) in pyridine-d_5 (500 MHz)

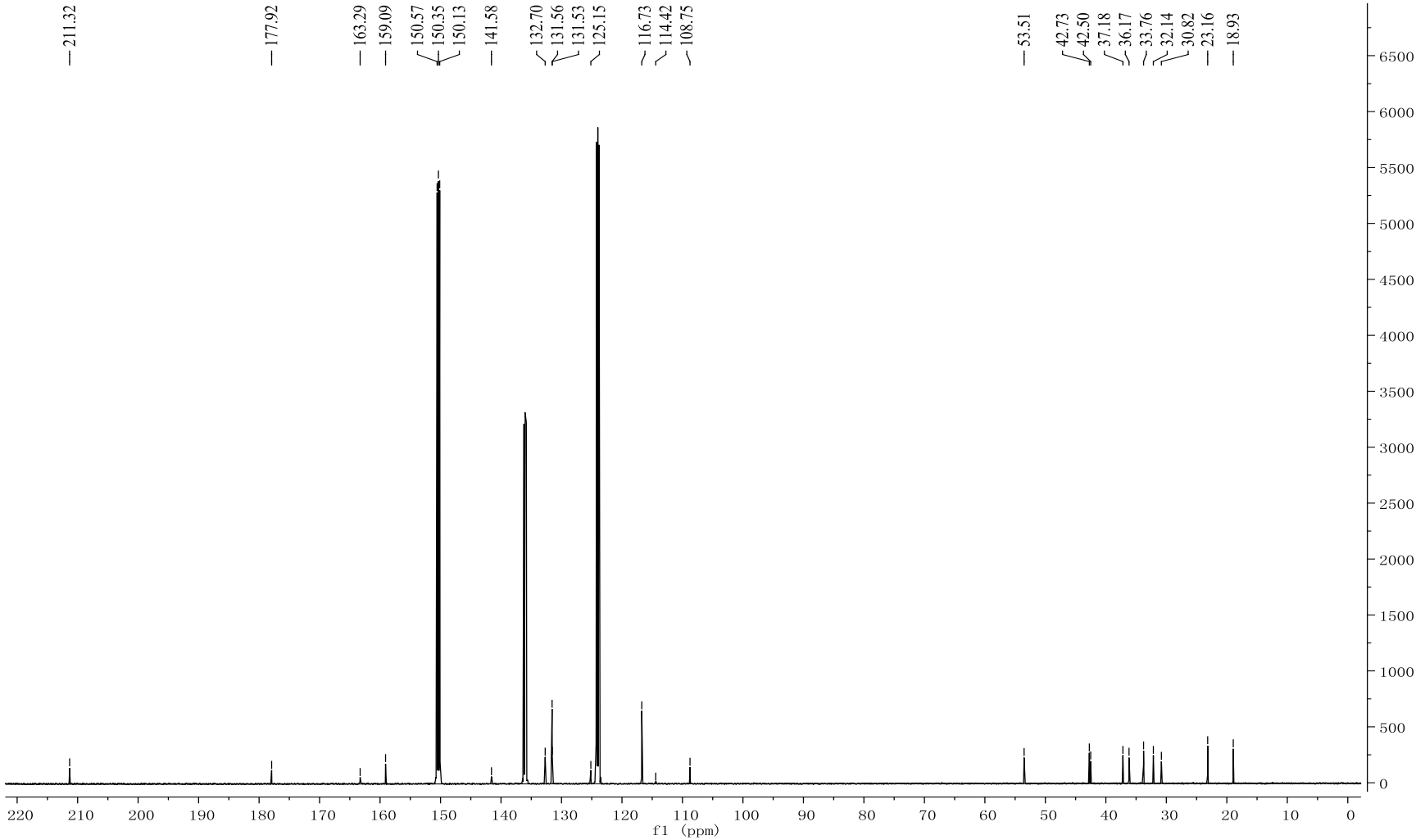


Figure S36. ^{13}C NMR spectrum of (+)-didymellamide B (**8**) in pyridine-d_5 (125 MHz)

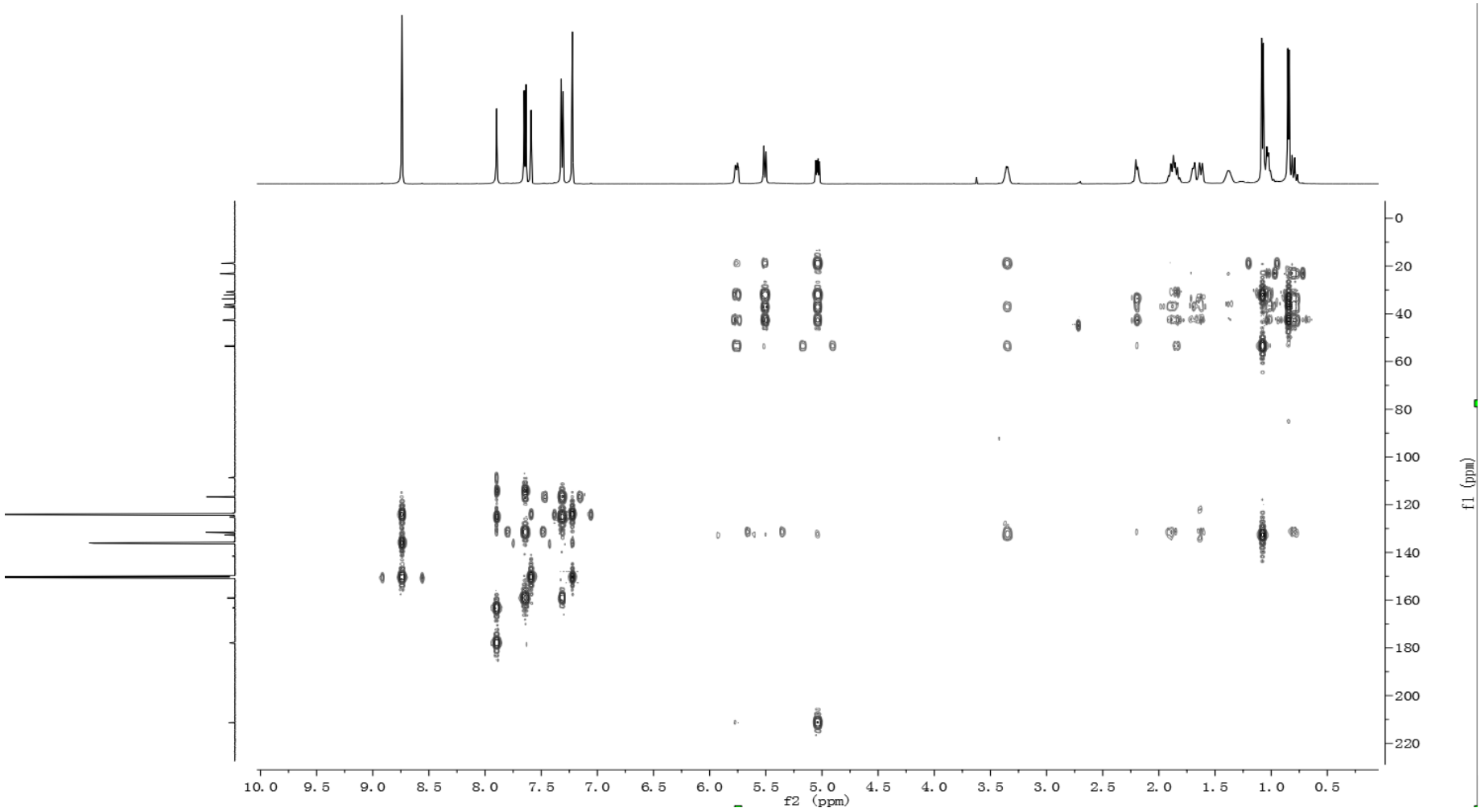


Figure S37. HMBC spectrum of (+)-didymellamide B (**8**) in pyridine-d_5 (125 MHz)

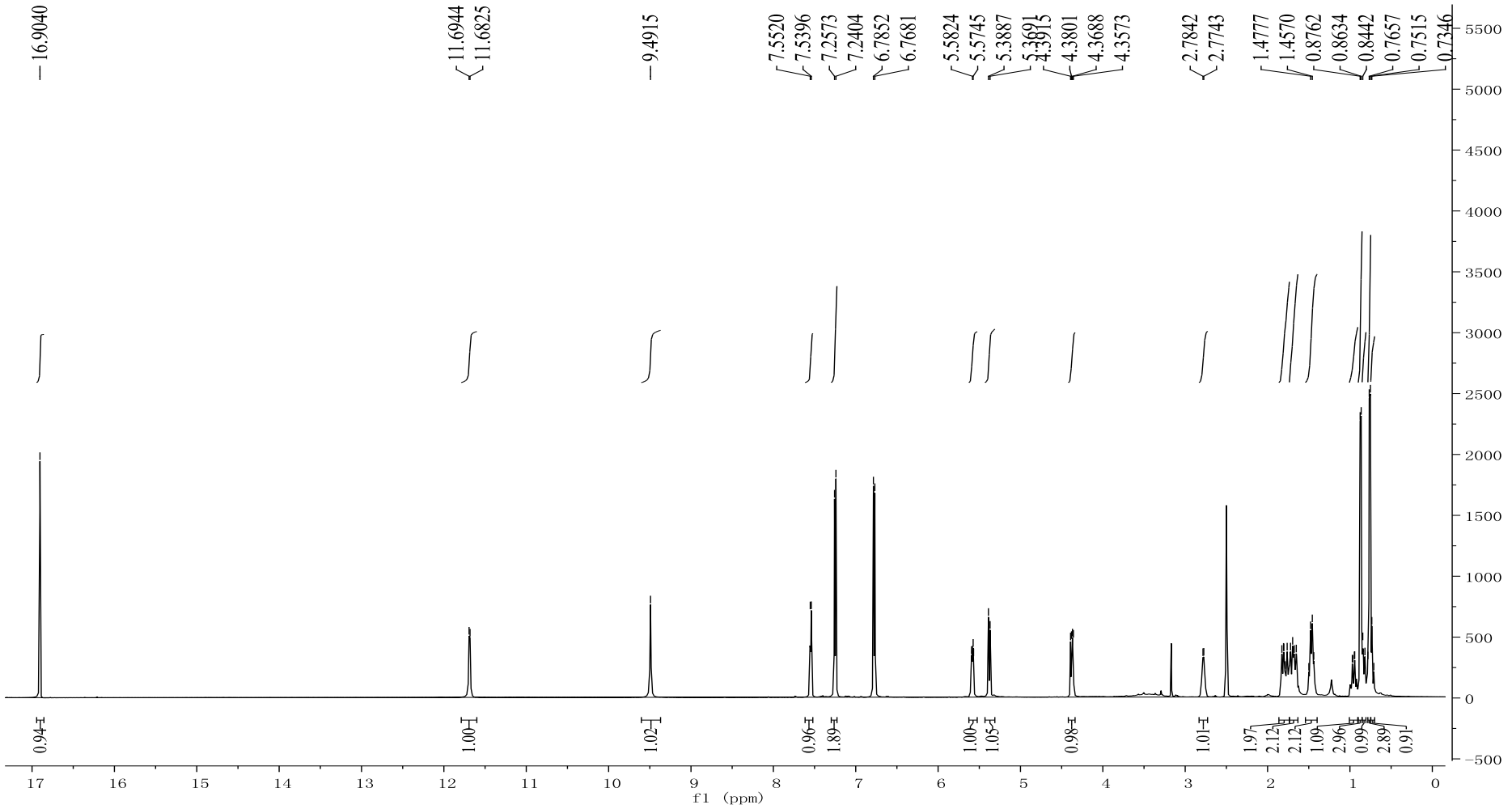


Figure S38. ^{1}H NMR spectrum of (+)-didymellamide B (**8**) in DMSO-d_6 (500 MHz)

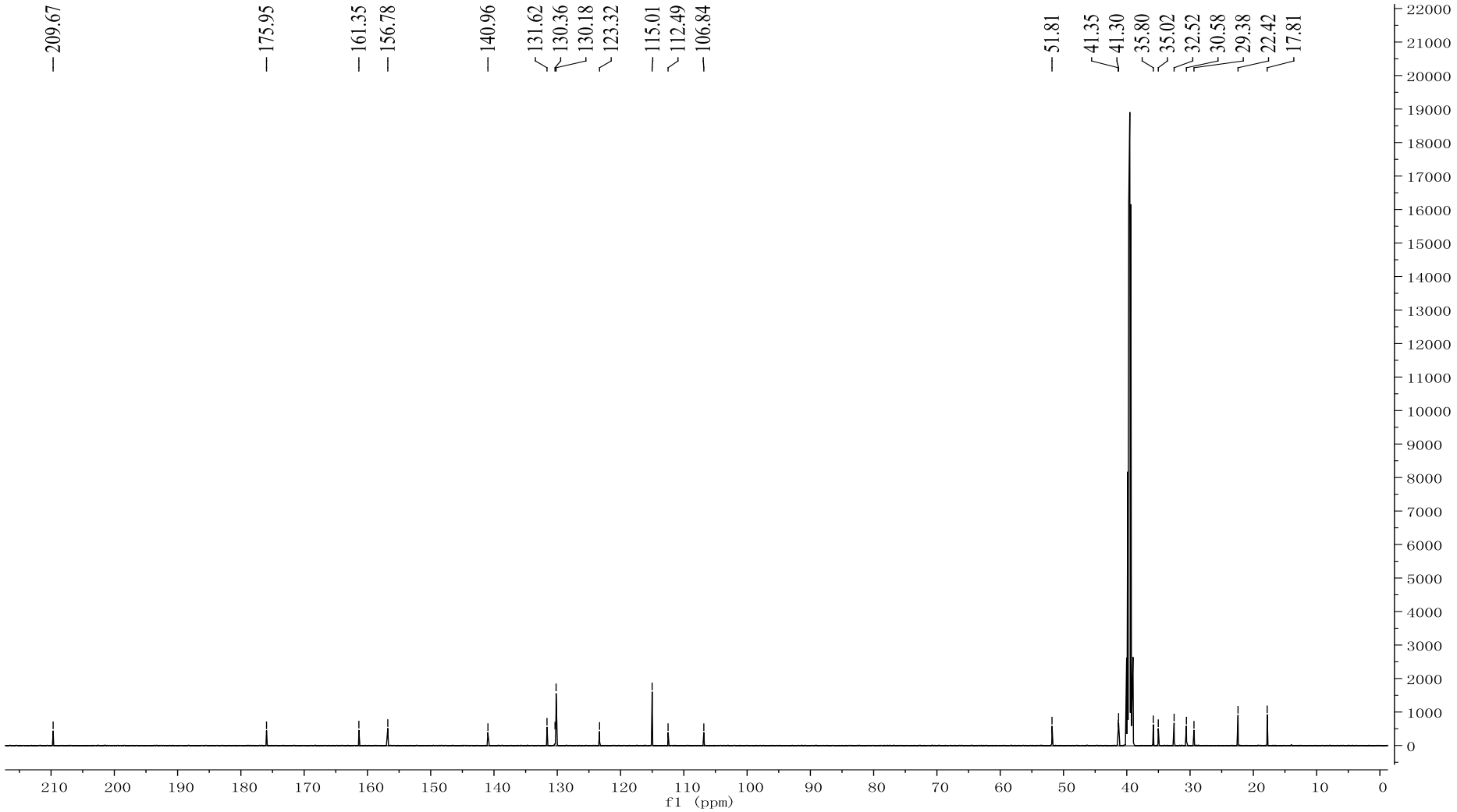


Figure S39. ^{13}C NMR spectrum of (+)-didymellamide B (**8**) in DMSO-d_6 (125 MHz)

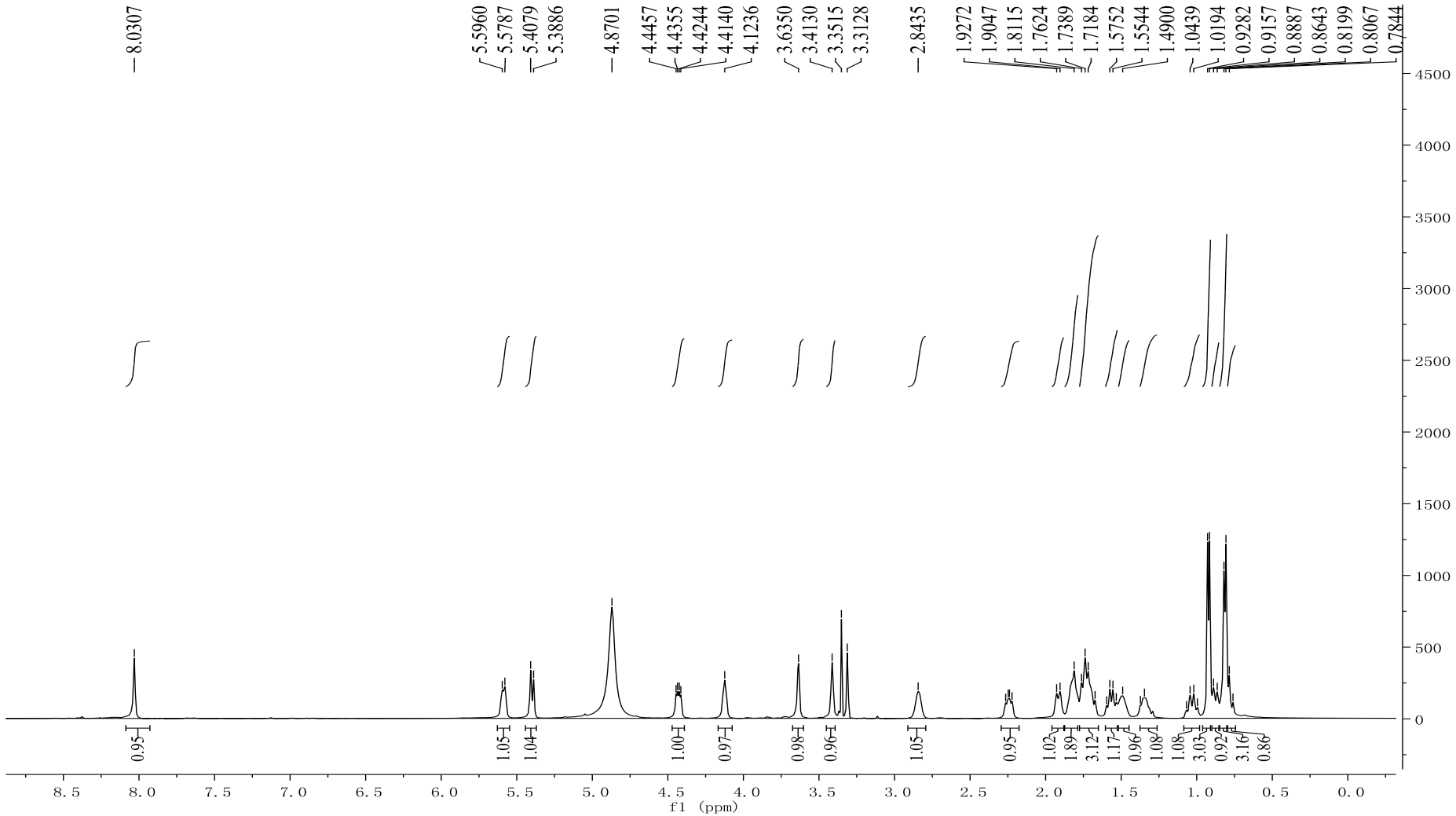


Figure S40. ^{1}H NMR spectrum of (+)-*N*-hydroxyapiosporamide (**9**) in CD_3OD (500 MHz)

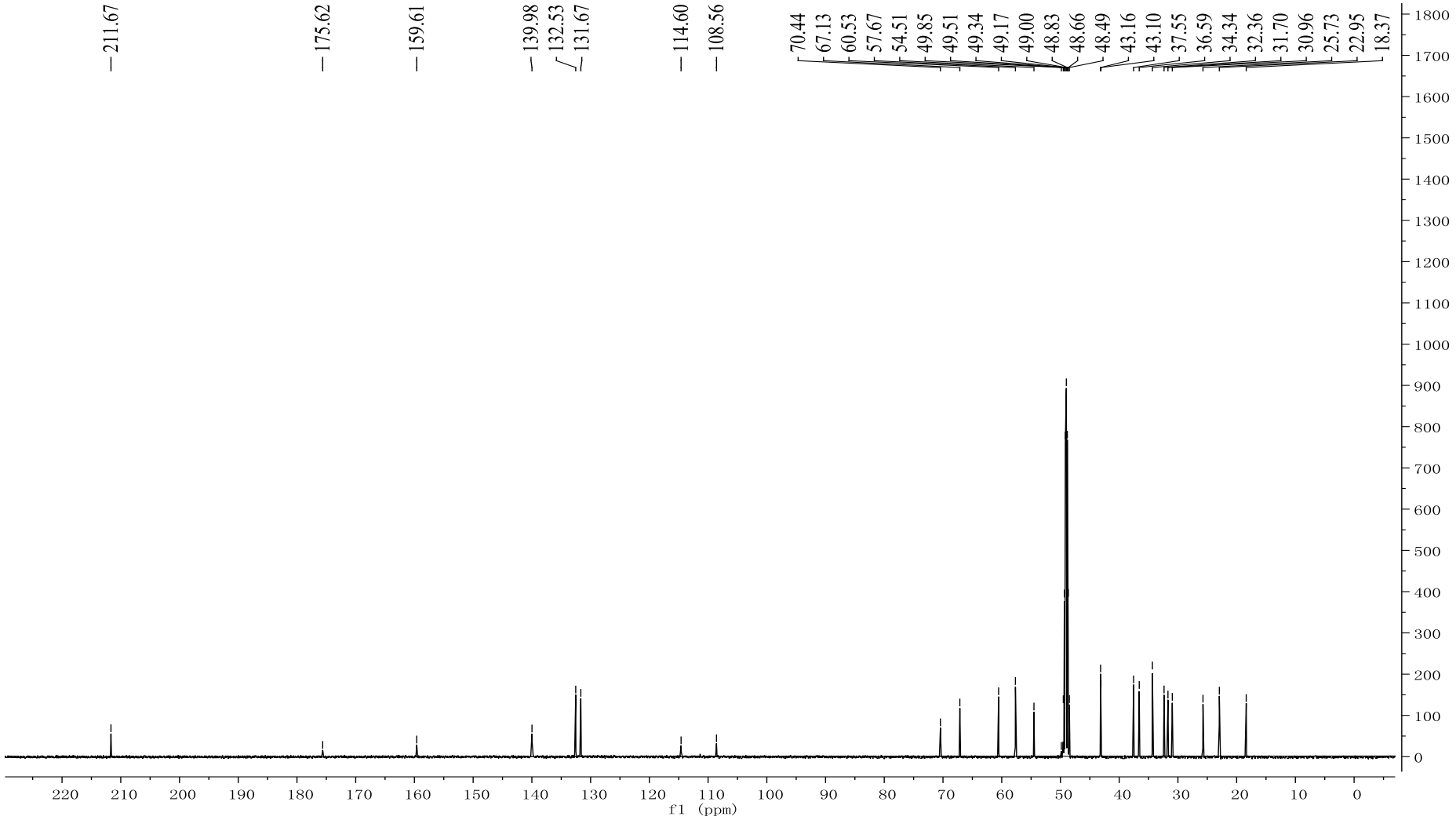


Figure S41. ^{13}C NMR spectrum of (+)-*N*-hydroxyapiosporamide (**9**) in CD_3OD (125 MHz)

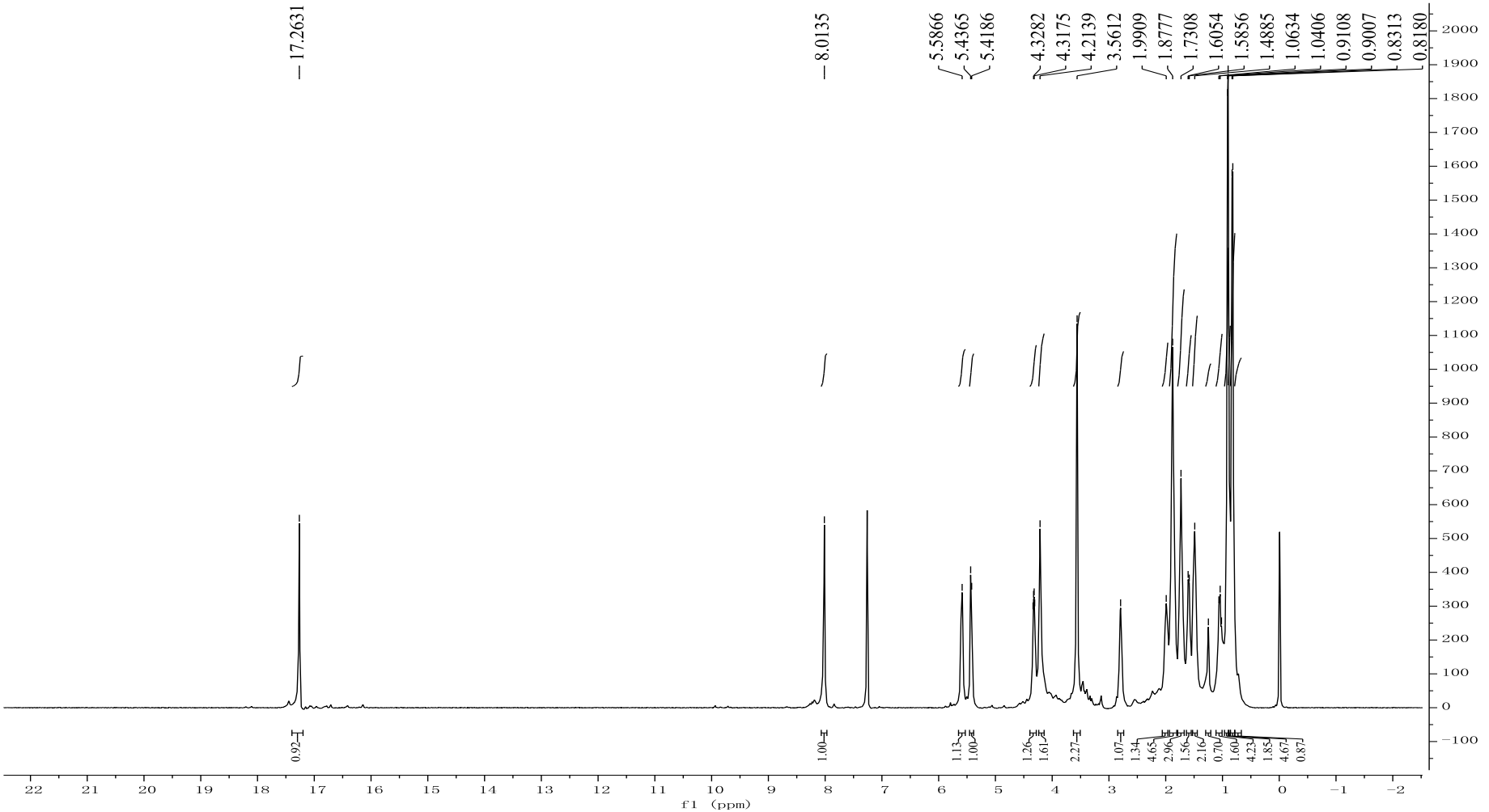


Figure S42. ^{1}H NMR spectrum of (+)-*N*-hydroxyapiosporamide (**9**) in $CDCl_3$ (500 MHz)

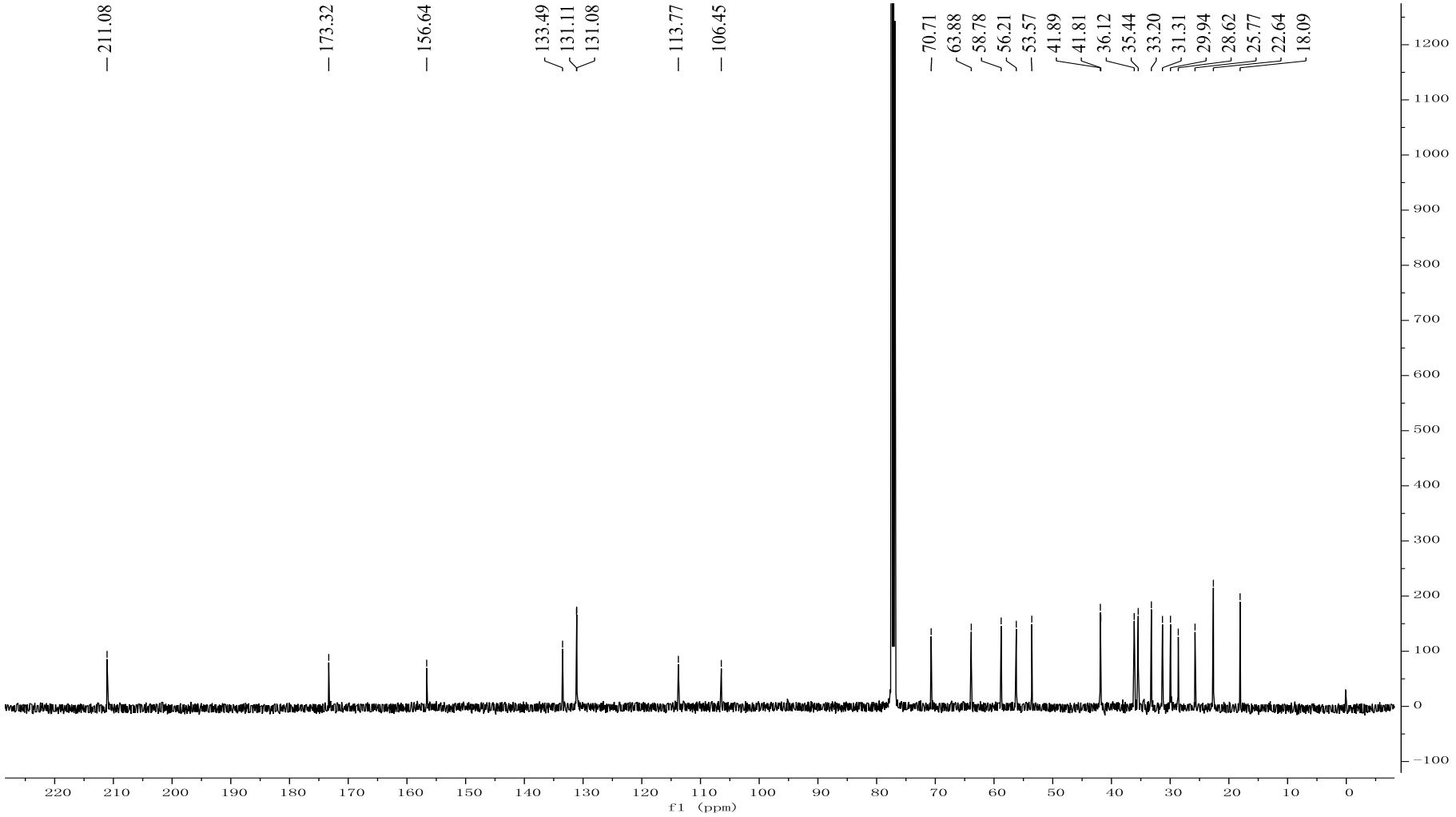


Figure S43. ^{13}C NMR spectrum of (+)-*N*-hydroxyapiosporamide (**9**) in $CDCl_3$ (125 MHz)

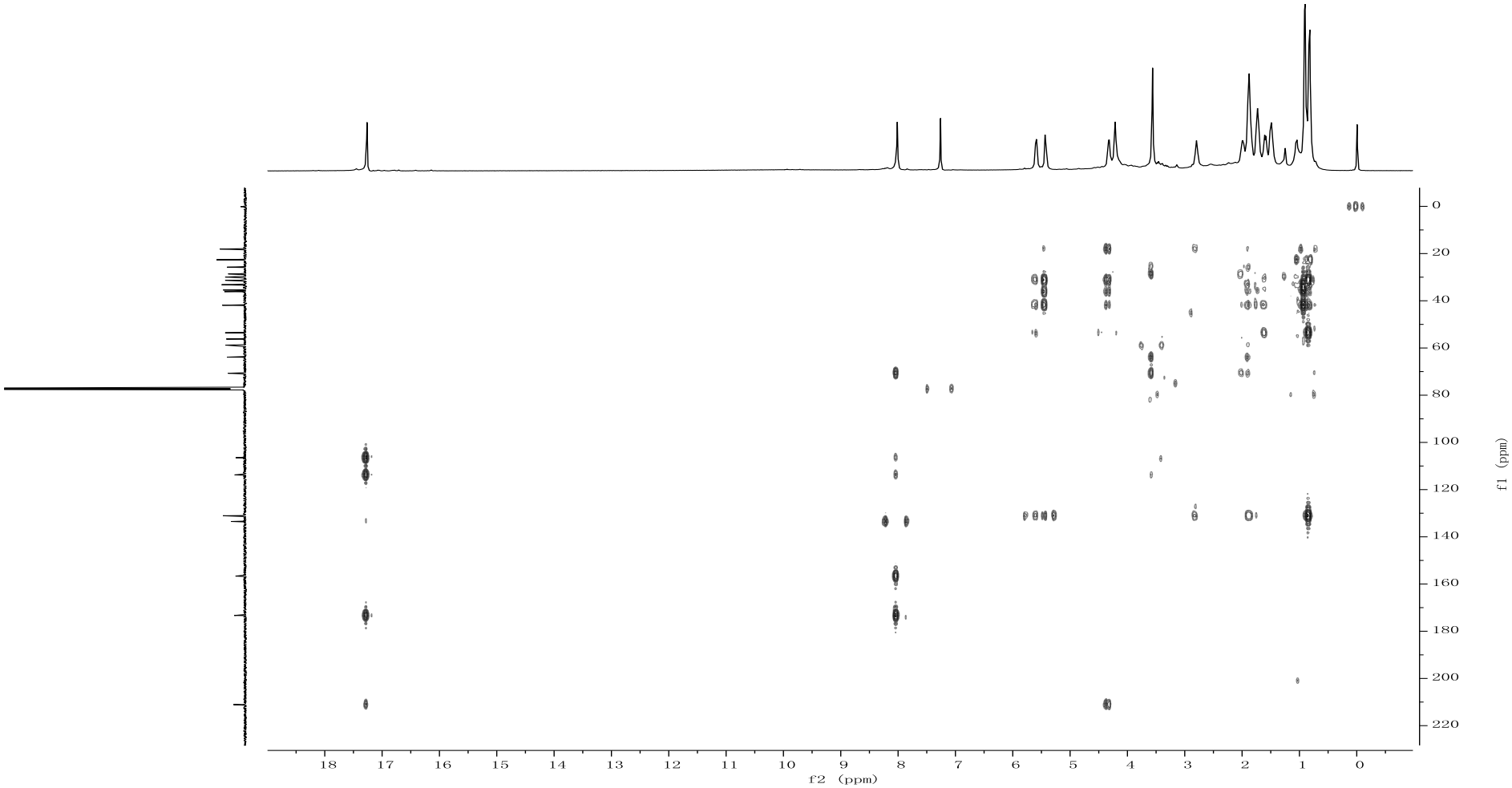


Figure S44. HMBC spectrum of (+)-*N*-hydroxyapiosporamide (**9**) in $CDCl_3$

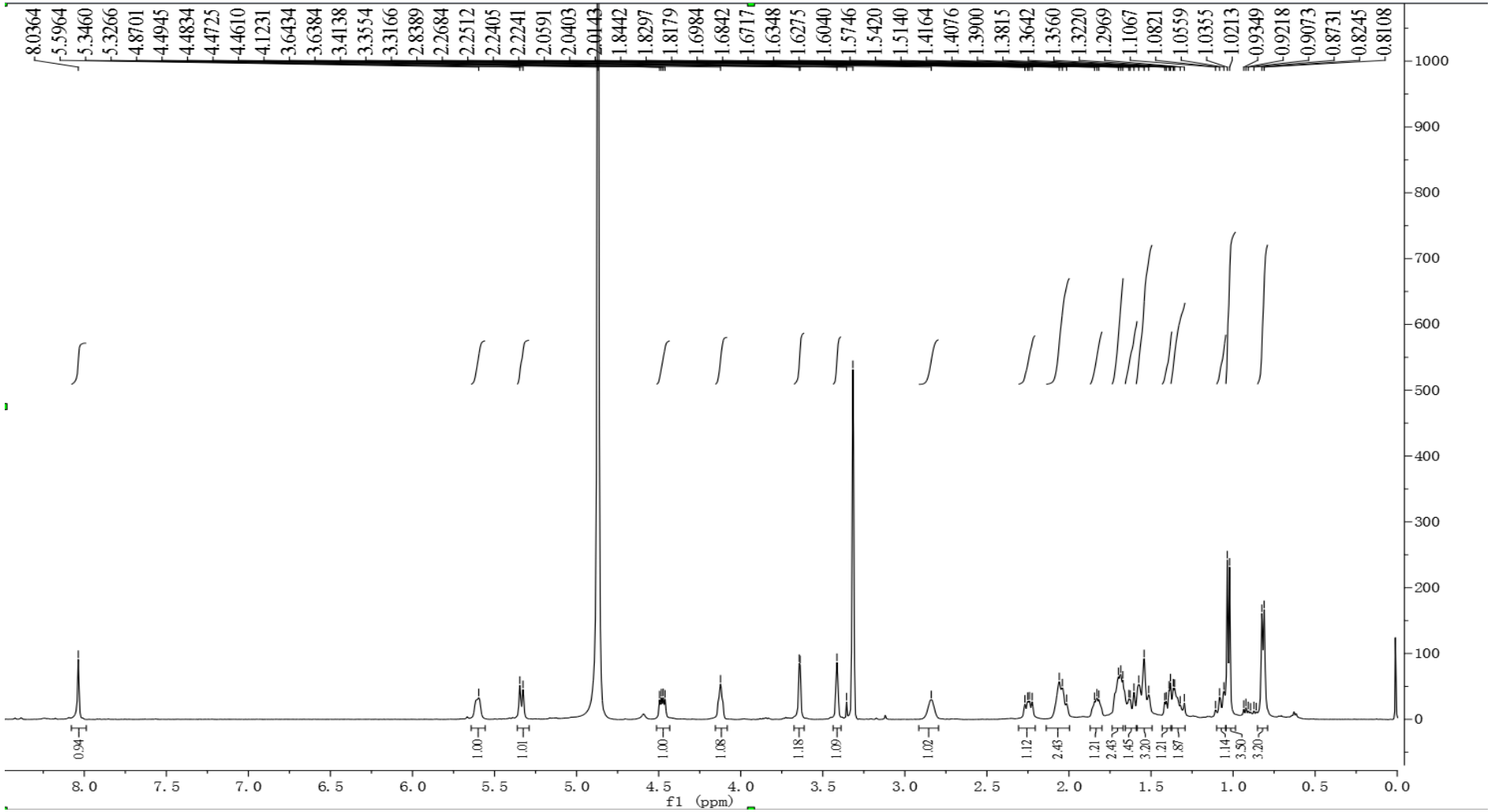


Figure S45. ^{1}H NMR spectrum of didymellamide F (**10**) in CD_3OD (500 MHz)

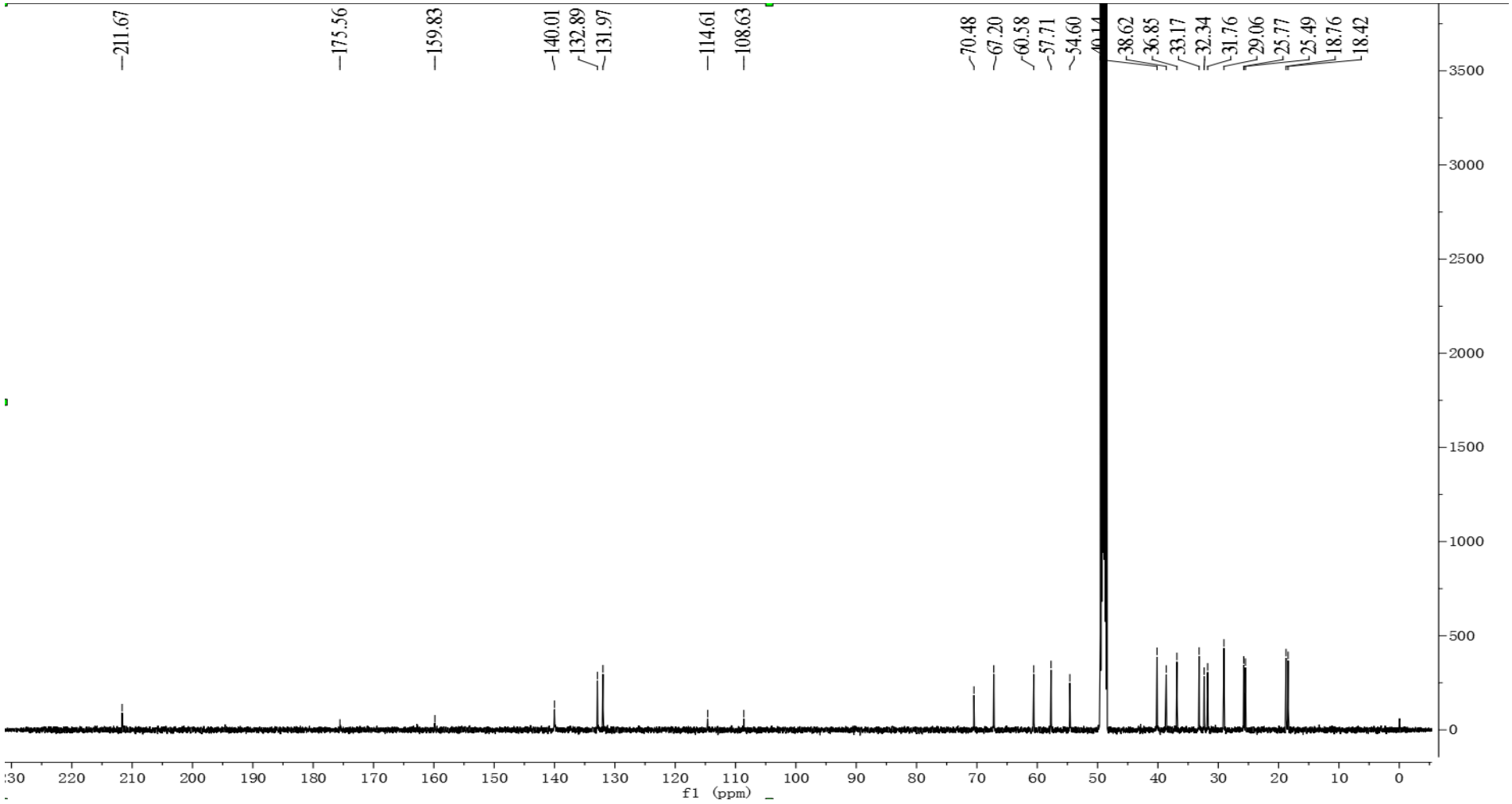


Figure S46. ^{13}C NMR spectrum of didymellamide F (**10**) in CD_3OD (125 MHz)

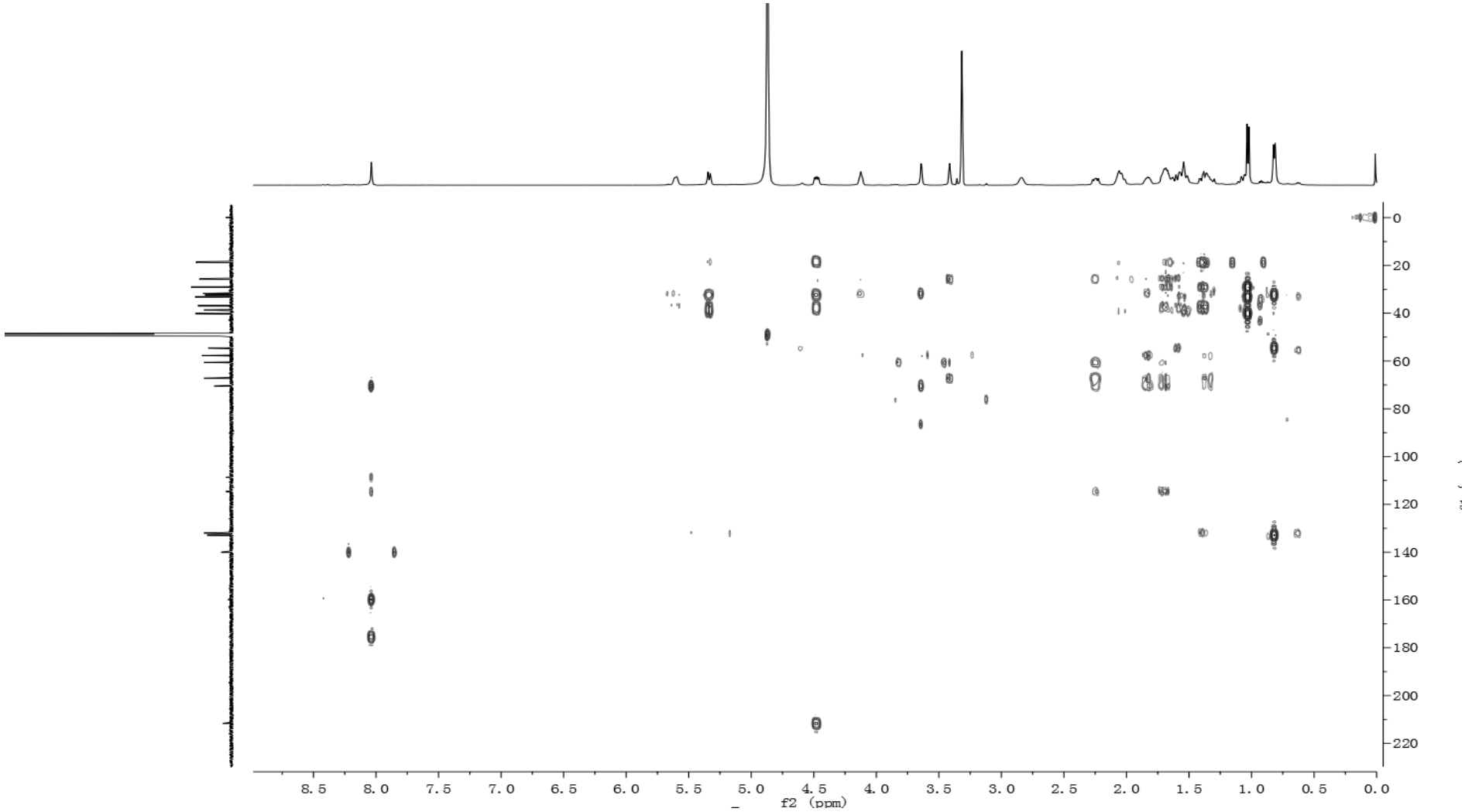


Figure S47. HMBC spectrum of didymellamide F (**10**) in CD_3OD

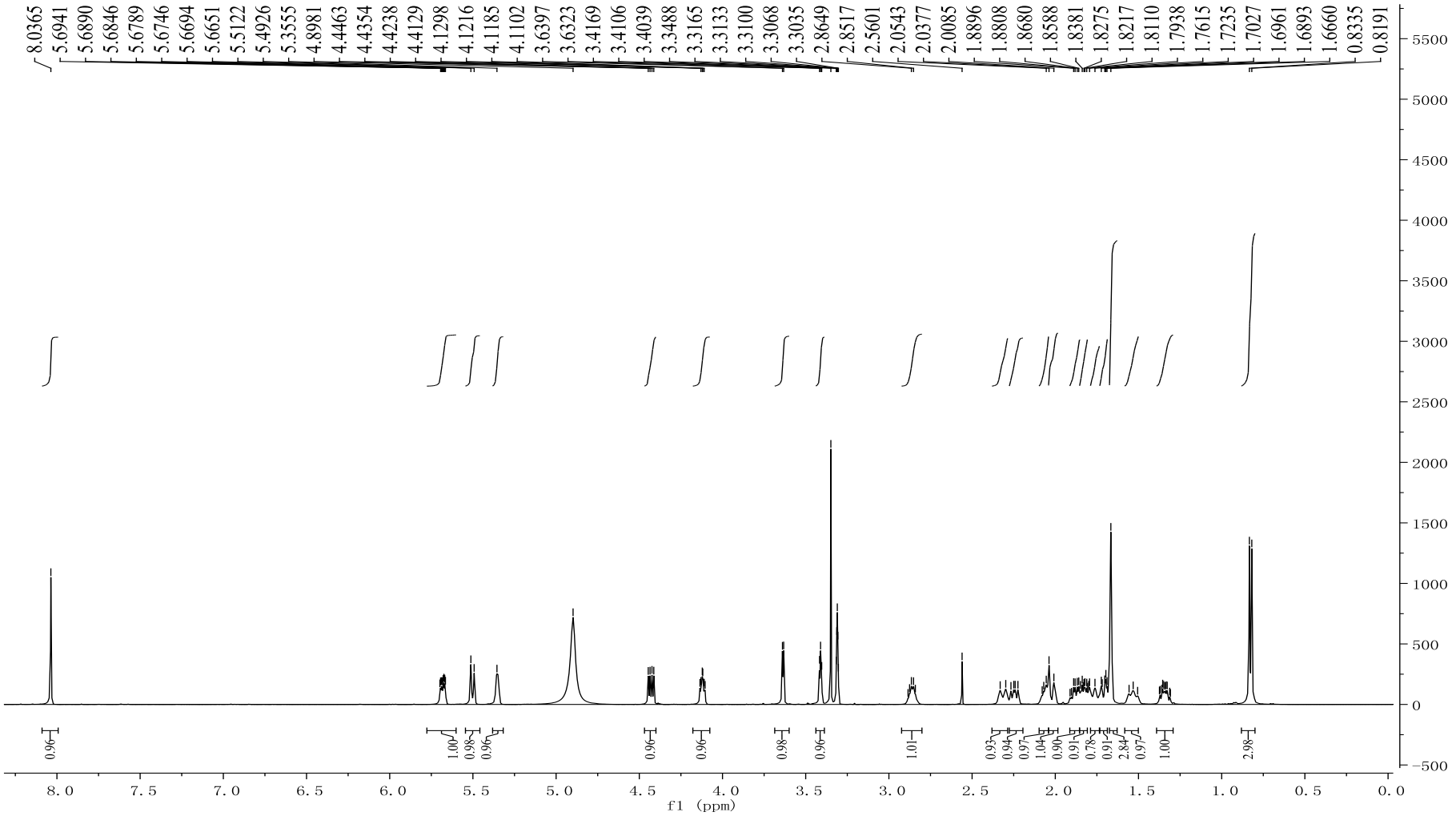


Figure S48. ^{1}H NMR spectrum of didymellamide G (**11**) in CD_3OD (500 MHz)

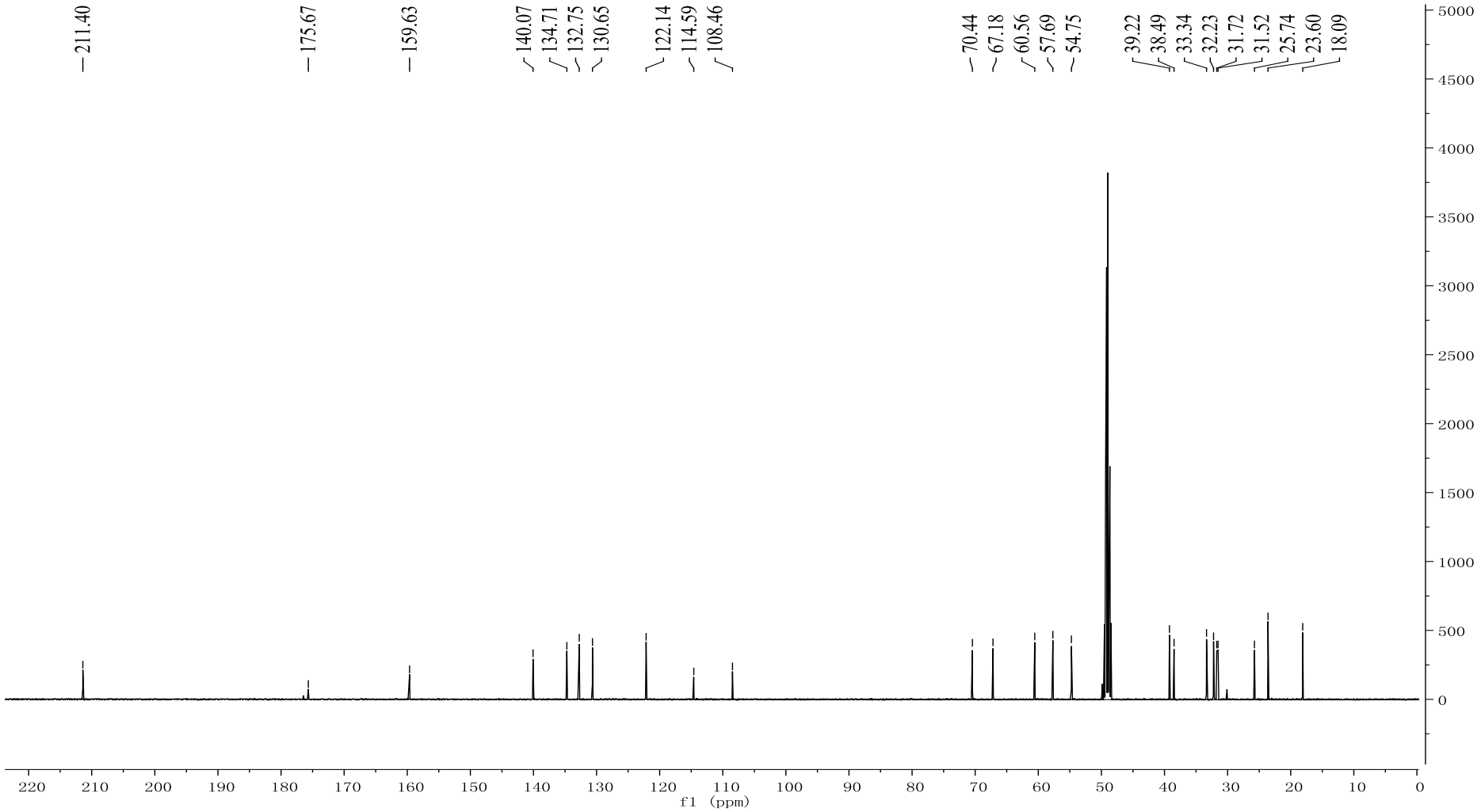


Figure S49. ^{13}C NMR spectrum of didymellamide G (**11**) in CD_3OD (125 MHz)

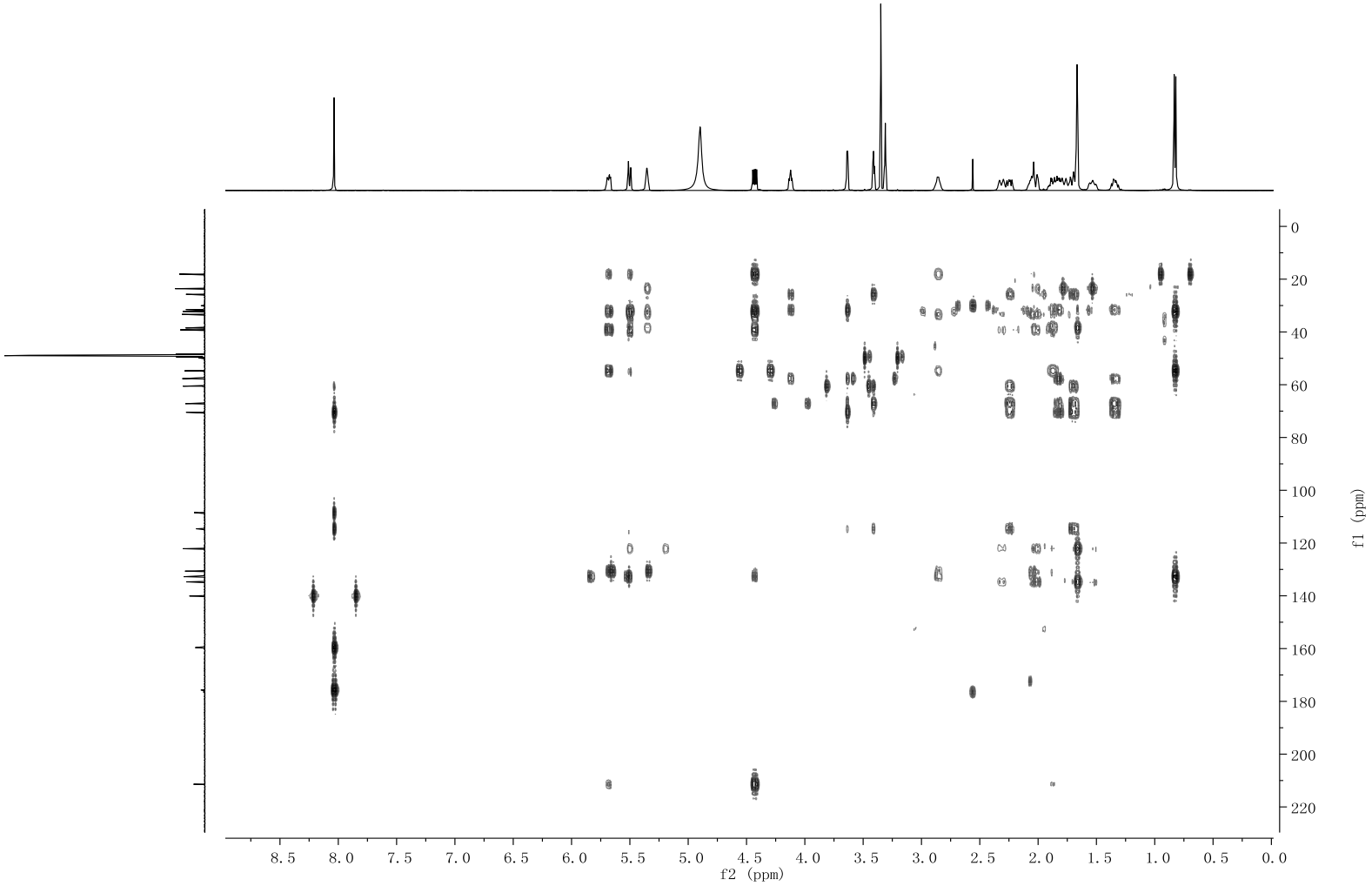


Figure S50. HMBC spectrum of didymellamide G (**11**) in CD_3OD

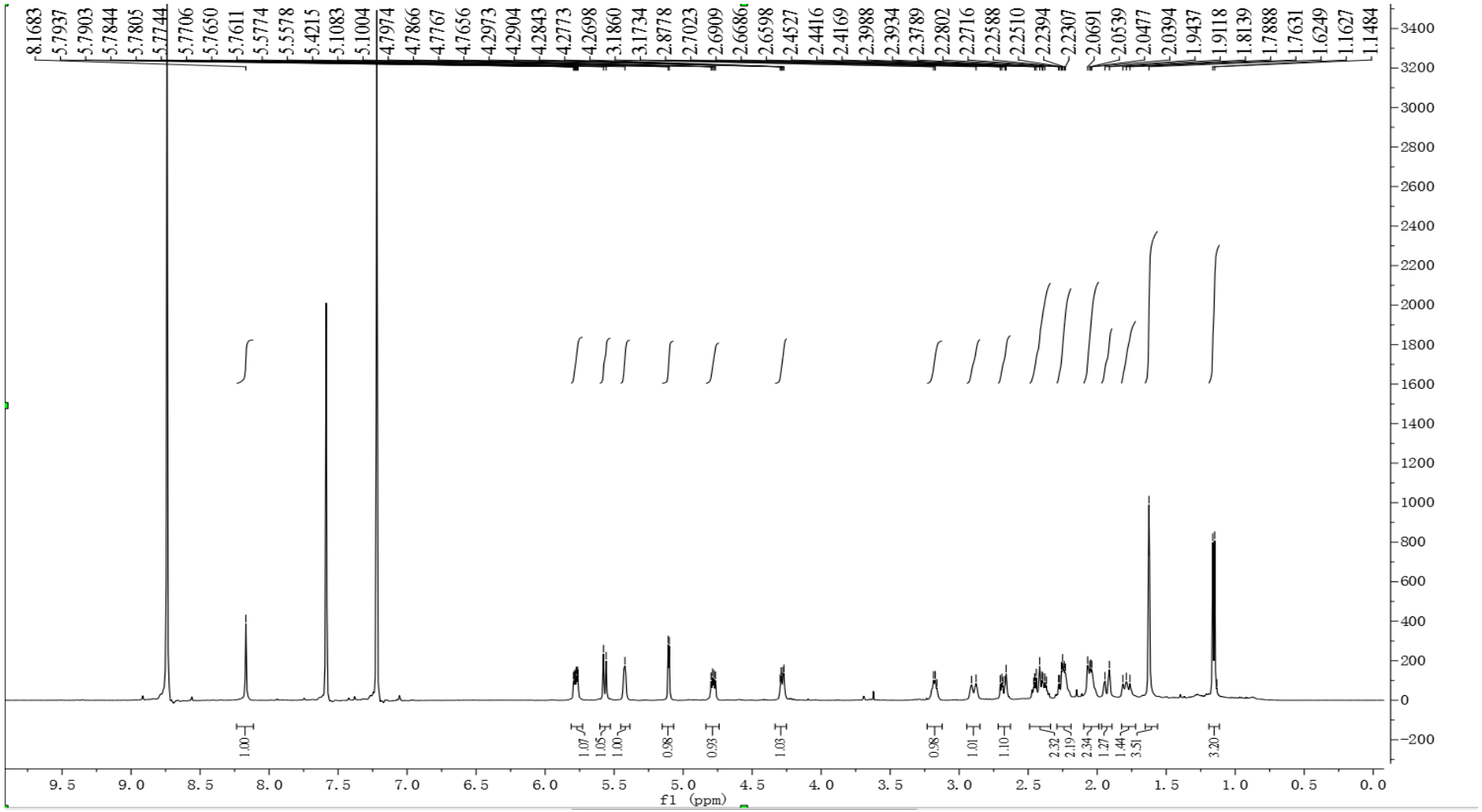


Figure S51. ^{1}H NMR spectrum of didymellamide H (**12**) in pyridine-d_5 (500 MHz)

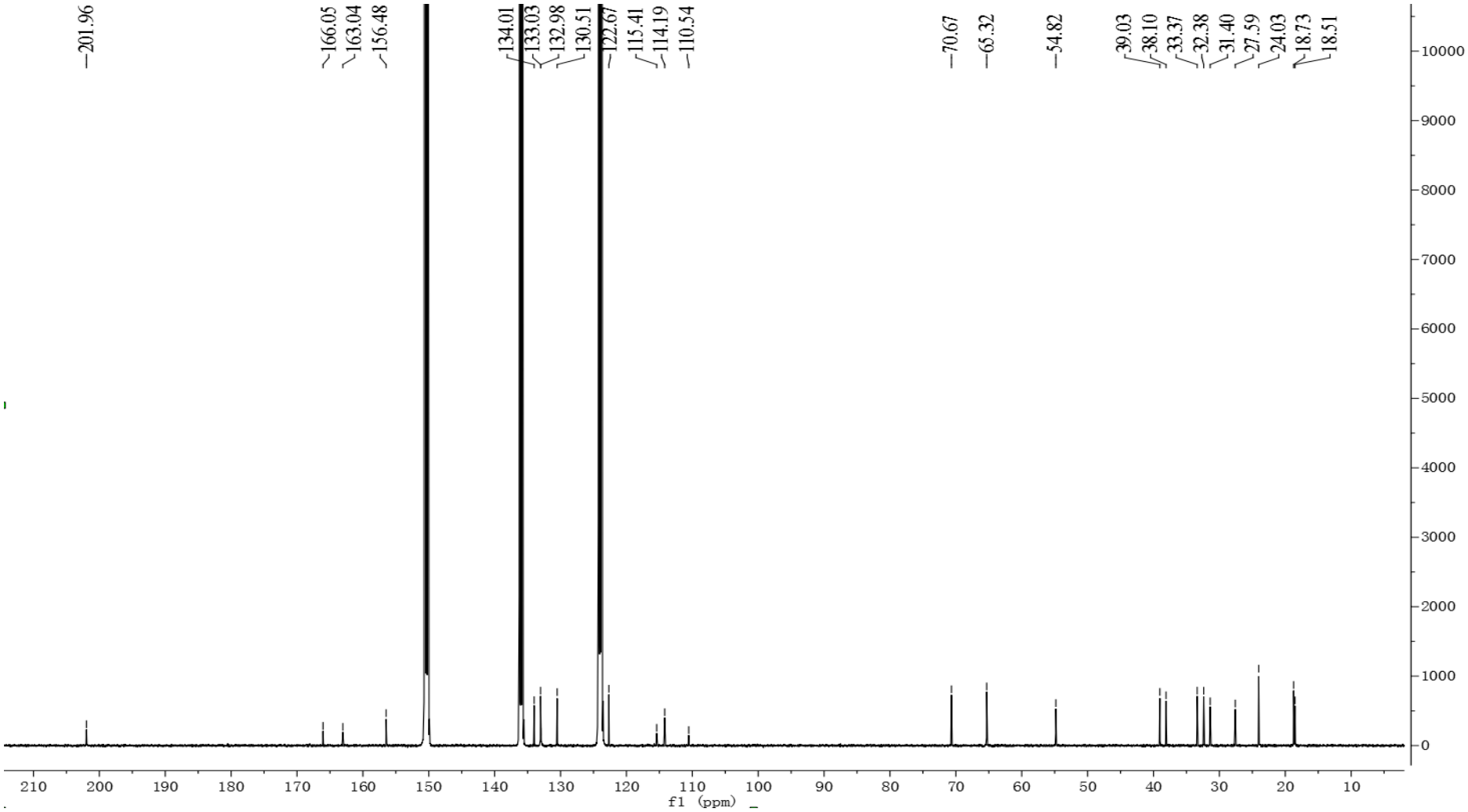


Figure S52. ^{13}C NMR spectrum of didymellamide H (**12**) in pyridine-d_5 (125 MHz)

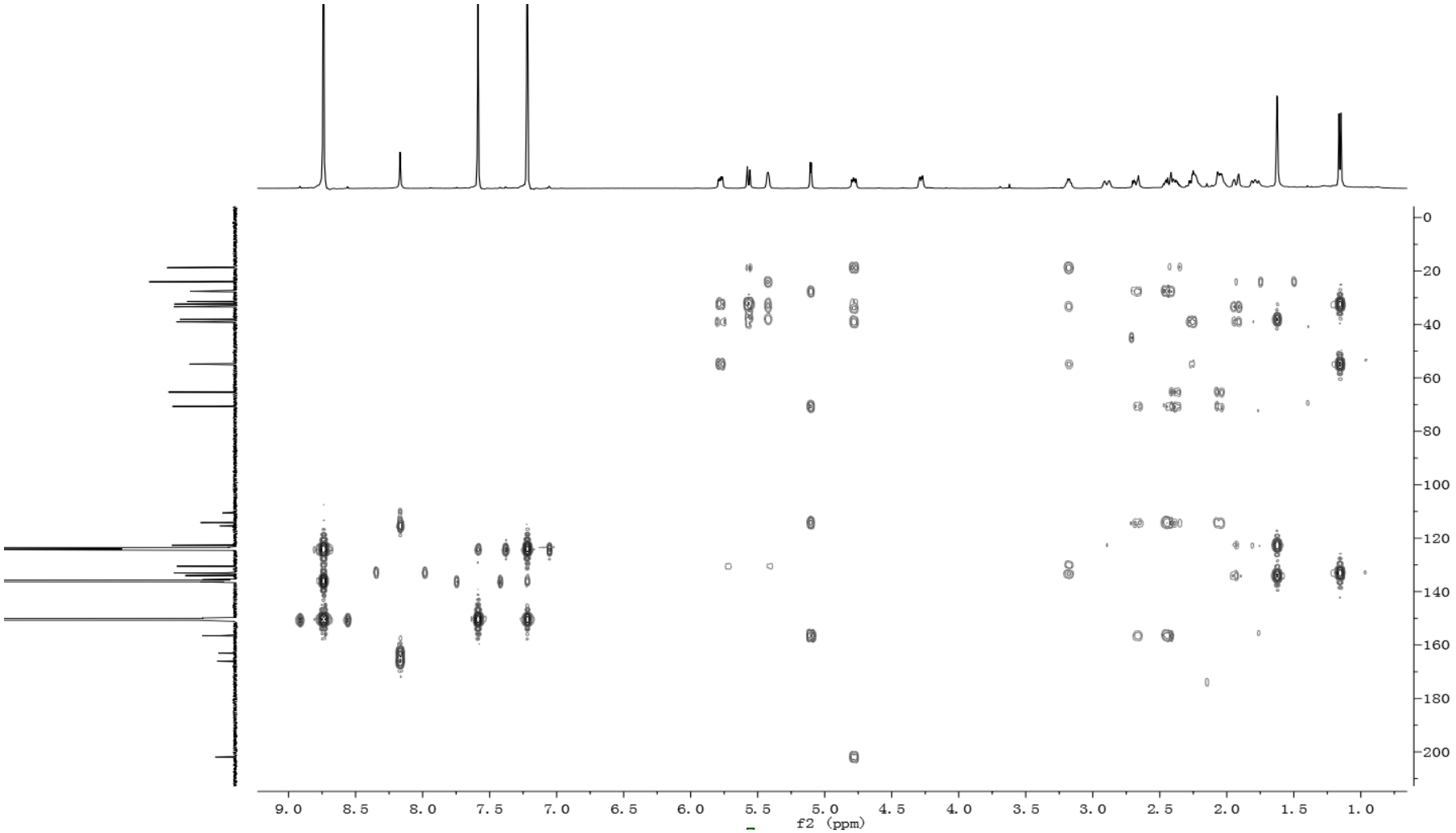


Figure S53. HMBC spectrum of didymellamide H (**12**) in pyridine-d_5

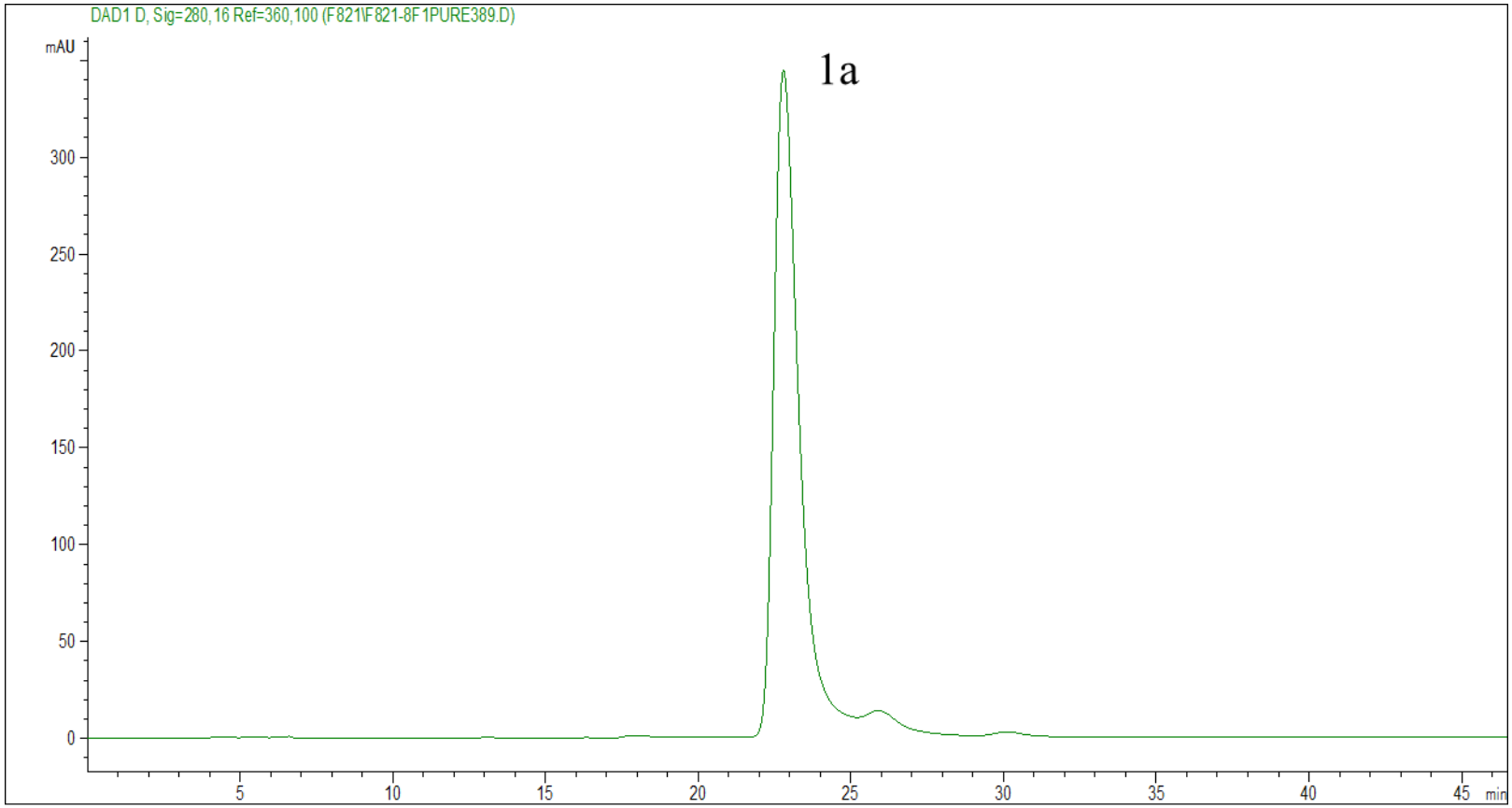


Figure S54. HPLC analysis of the enantiomer **1a** treated by the similar isolation procedure as described for **1** (1mg) using a Kromasil 5-CelluCoat column with an elution of isopropanol/n-hexane (15:85) containing 0.005% TFA.