Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

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Figure S1. Key 2D NMR correlations for chlorahupetone C (**3**)

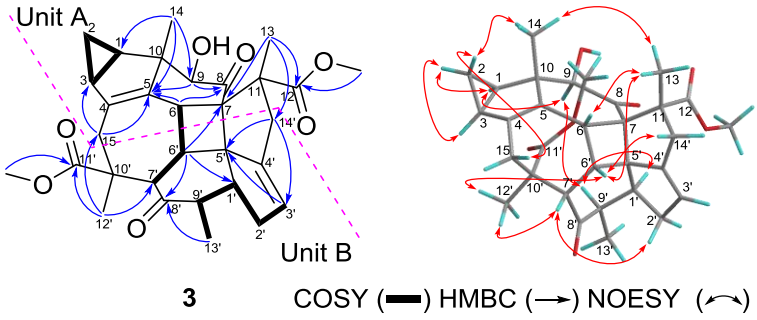


Figure S2. Key 2D NMR correlations for chlorahupetone E (**5**)

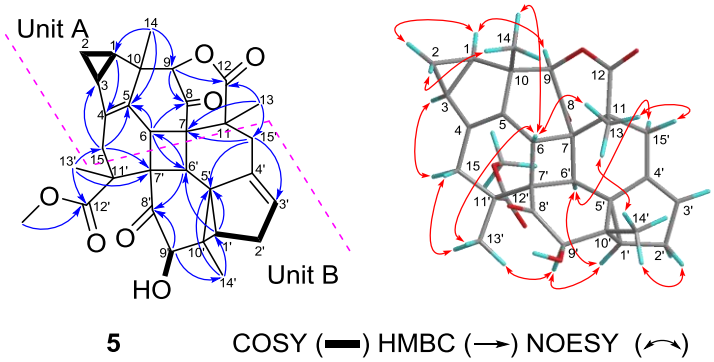
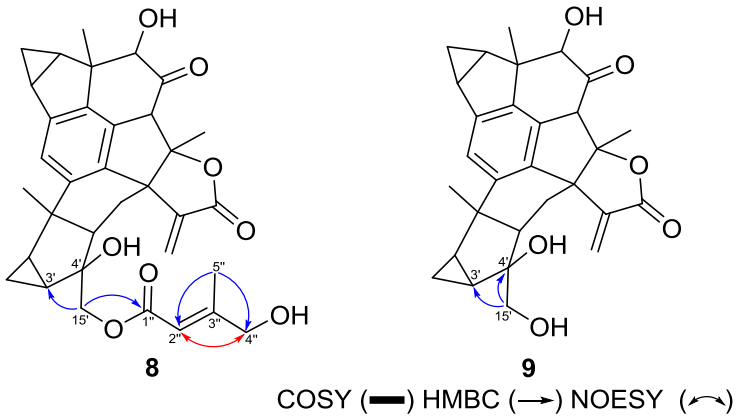


Figure S3. Key 2D NMR correlations for chlorahupetones H−I (**8**–**9**)



ECD calculation details

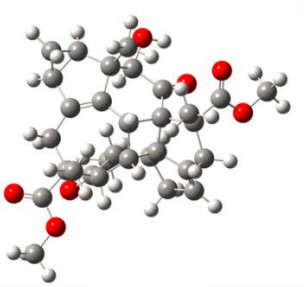
1. Results

Table S1. Gibbs free energiesa and equilibrium populationsb of low-energy conformers of 1*R*, 3*S*, 6*R*, 7*S*, 9*R*, 10*S*, 11*R*, 1'*S*, 5'*R*, 6'*S*, 7'*S*, 9'*R*,10'*R* - **3**.

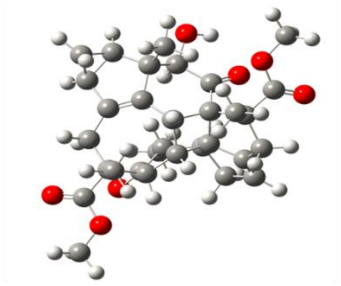
Conformers	In gas	
	G^a	P (%)^b
3-a	-1084934.73980112	15.60
3-b	-1084934.91299388	20.91
3-c	-1084935.02782821	25.38
3-d	-1084934.7448212	15.74
3-e	-1084934.95315452	22.37

[a]B3LYP/6-31G(d, p), in kcal/mol. [b]From *G* values at 298.15K.

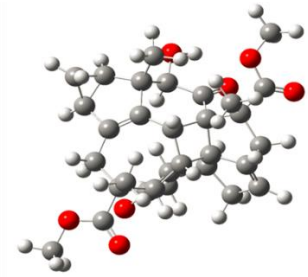
Figure S4. The low-energy reoptimized MMFF conformers of 1*R*, 3*S*, 6*R*, 7*S*, 9*R*, 10*S*, 11*R*, 1'*S*, 5'*R*, 6'*S*, 7'*S*, 9'*R*,10'*R* - **3** at B3LYP/6-31G (d, p) level of theory in gas.



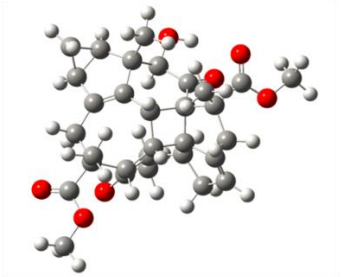
3-a



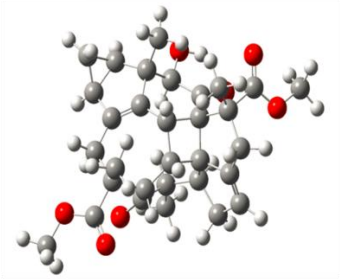
3-b



3-c



3-d



3-e

Table S2. Cartesian coordinates for the low-energy reoptimized MMFF conformers of 1*R*, 3*S*, 6*R*, 7*S*, 9*R*, 10*S*, 11*R*, 1'*S*, 5'*R*, 6'*S*, 7'*S*, 9'*R*,10'*R* - 3 at B3LYP/6-31G (d, p) level of theory in gas.

Conformer **3a**		Standard Orientation (Ångstroms)			
Center number	Atom	Type	X	Y	Z
1.	6.	0.	-0.808171	2.729111	0.164053

2.	6.	0.	0.258743	1.749431	-0.340100
3.	6.	0.	1.508003	2.141718	-0.013441
4.	6.	0.	-1.551175	1.948177	1.265955
5.	6.	0.	-2.151833	0.632579	0.735180
6.	6.	0.	-0.214531	0.512516	-1.041858
7.	6.	0.	-1.499584	-0.136586	-0.399873
8.	6.	0.	2.862742	1.513995	-0.209593
9.	6.	0.	2.981177	0.135913	-0.899284
10.	6.	0.	1.996743	-0.918989	-0.292548
11.	6.	0.	0.554286	-0.825630	-0.823064
12.	6.	0.	-0.601114	-1.359712	0.095736
13.	6.	0.	-0.268774	-1.663077	1.572990
14.	6.	0.	-2.540006	-0.812081	-1.448422
15.	6.	0.	-1.293154	-2.606036	-0.364714
16.	6.	0.	-2.113632	-2.319478	-1.576748
17.	6.	0.	-1.078981	-3.635476	0.457429
18.	6.	0.	-0.187780	-3.223166	1.610477
19.	6.	0.	0.950972	-0.911162	2.137327
20.	6.	0.	2.171595	-1.001491	1.231853
21.	8.	0.	3.295979	-1.123507	1.690936
22.	6.	0.	2.788398	0.261467	-2.431680
23.	6.	0.	1.278109	-1.278617	3.586773
24.	8.	0.	-2.560178	2.713656	1.880770
25.	6.	0.	1.474982	3.472612	0.681485
26.	6.	0.	0.017305	3.872867	0.763540
27.	6.	0.	0.949167	4.633106	-0.142640
28.	6.	0.	-1.817178	3.228242	-0.888520
29.	8.	0.	-3.131873	0.197088	1.327014
30.	6.	0.	-2.537877	-0.153975	-2.844226
31.	6.	0.	-3.988590	-0.660553	-0.939479
32.	8.	0.	-4.474788	-1.772929	-0.360435
33.	8.	0.	-4.642023	0.348728	-1.103841
34.	6.	0.	-5.788792	-1.638033	0.206408
35.	1.	0.	-1.143814	-1.384781	2.172856
36.	6.	0.	4.437758	-0.335095	-0.708467
37.	8.	0.	4.605094	-1.619622	-1.098565
38.	8.	0.	5.354063	0.371753	-0.352166
39.	6.	0.	5.936875	-2.135649	-0.941791
40.	1.	0.	-0.352823	0.747408	-2.101362
41.	1.	0.	2.370525	-1.895737	-0.624678
42.	1.	0.	0.533590	-1.375515	-1.769134
43.	1.	0.	-0.795999	1.652170	2.018296
44.	1.	0.	3.496456	2.226489	-0.753229

45.	1.	0.	3.340718	1.442241	0.775045
46.	1.	0.	-1.503124	-2.428903	-2.483149
47.	1.	0.	-2.973719	-2.980477	-1.687352
48.	1.	0.	-1.477811	-4.638747	0.343188
49.	1.	0.	0.844914	-3.577981	1.467667
50.	1.	0.	-0.519832	-3.629049	2.572406
51.	1.	0.	0.699236	0.160638	2.103033
52.	1.	0.	1.833108	0.728646	-2.678426
53.	1.	0.	2.840150	-0.715796	-2.919248
54.	1.	0.	3.578869	0.891064	-2.852427
55.	1.	0.	1.571970	-2.328730	3.672728
56.	1.	0.	2.108938	-0.677534	3.960629
57.	1.	0.	0.406569	-1.112412	4.227717
58.	1.	0.	-3.253465	2.076689	2.126502
59.	1.	0.	2.190494	3.670918	1.475314
60.	1.	0.	-0.387475	4.383885	1.630913
61.	1.	0.	0.881946	4.499688	-1.218664
62.	1.	0.	1.224047	5.636255	0.170749
63.	1.	0.	-1.306972	3.694096	-1.735595
64.	1.	0.	-2.478493	3.967126	-0.430393
65.	1.	0.	-2.455551	2.425323	-1.269452
66.	1.	0.	-3.280939	-0.650088	-3.476999
67.	1.	0.	-1.569897	-0.264469	-3.338426
68.	1.	0.	-2.803407	0.902555	-2.799440
69.	1.	0.	-5.775970	-0.878968	0.991179
70.	1.	0.	-6.512707	-1.351900	-0.559999
71.	1.	0.	-6.031595	-2.616536	0.620248
72.	1.	0.	5.903383	-3.157633	-1.319258
73.	1.	0.	6.652881	-1.537823	-1.510396
74.	1.	0.	6.221496	-2.125021	0.112900

Conformer **3b**		Standard Orientation (Ångstroms)			
Center number	Atom	Type	X	Y	Z
1.	6.	0.	-1.100344	2.519802	0.197922
2.	6.	0.	0.055670	1.655581	-0.321573
3.	6.	0.	1.261424	2.190722	-0.039205
4.	6.	0.	-1.738388	1.677221	1.320743
5.	6.	0.	-2.198176	0.294211	0.823591
6.	6.	0.	-0.294991	0.363239	-0.995262
7.	6.	0.	-1.479562	-0.412095	-0.306672
8.	6.	0.	2.669800	1.716169	-0.279155

9.	6.	0.	2.917446	0.356695	-0.971849
10.	6.	0.	2.089929	-0.803025	-0.319921
11.	6.	0.	0.620897	-0.880052	-0.777805
12.	6.	0.	-0.430162	-1.499195	0.213025
13.	6.	0.	-0.006407	-1.675529	1.690961
14.	6.	0.	-2.442772	-1.243157	-1.308069
15.	6.	0.	-1.008596	-2.835557	-0.137859
16.	6.	0.	-1.932189	-2.727052	-1.304715
17.	6.	0.	-0.658557	-3.783595	0.734319
18.	6.	0.	0.232003	-3.214860	1.817404
19.	6.	0.	1.161740	-0.784208	2.153965
20.	6.	0.	2.342160	-0.841329	1.196253
21.	8.	0.	3.492316	-0.898890	1.600522
22.	6.	0.	2.648388	0.448052	-2.494735
23.	6.	0.	1.582052	-1.032825	3.604646
24.	8.	0.	-2.818936	2.336821	1.939626
25.	6.	0.	1.100360	3.514241	0.652396
26.	6.	0.	-0.390196	3.751589	0.772572
27.	6.	0.	0.429340	4.607033	-0.157797
28.	6.	0.	-2.165854	2.897998	-0.848711
29.	8.	0.	-3.108944	-0.243638	1.442017
30.	6.	0.	-2.447196	-0.705700	-2.759705
31.	6.	0.	-3.918217	-1.222425	-0.855293
32.	8.	0.	-4.443747	0.017829	-0.988349
33.	8.	0.	-4.572844	-2.185914	-0.529088
34.	6.	0.	-5.801604	0.160043	-0.538944
35.	1.	0.	-0.877601	-1.446750	2.316626
36.	6.	0.	4.425488	0.057947	-0.837833
37.	8.	0.	4.729213	-1.189562	-1.262297
38.	8.	0.	5.263191	0.860612	-0.490821
39.	6.	0.	6.116106	-1.549446	-1.153749
40.	1.	0.	-0.488191	0.564785	-2.052850
41.	1.	0.	2.561323	-1.730886	-0.665117
42.	1.	0.	0.611457	-1.460461	-1.706219
43.	1.	0.	-0.944760	1.476906	2.065026
44.	1.	0.	3.202165	2.492140	-0.844288
45.	1.	0.	3.186350	1.703093	0.688585
46.	1.	0.	-1.402099	-2.925316	-2.245220
47.	1.	0.	-2.771443	-3.421917	-1.245328
48.	1.	0.	-0.966850	-4.824028	0.703178
49.	1.	0.	1.288909	-3.476601	1.652035
50.	1.	0.	-0.022012	-3.587743	2.815719
51.	1.	0.	0.816824	0.257757	2.068264

52.	1.	0.	1.635747	0.798252	-2.702463
53.	1.	0.	2.794728	-0.519939	-2.981104
54.	1.	0.	3.341283	1.162936	-2.950098
55.	1.	0.	1.980534	-2.042769	3.735694
56.	1.	0.	2.365458	-0.334714	3.905982
57.	1.	0.	0.725901	-0.910945	4.275677
58.	1.	0.	-3.400753	1.624880	2.258207
59.	1.	0.	1.809519	3.792783	1.427750
60.	1.	0.	-0.824717	4.218947	1.650224
61.	1.	0.	0.350371	4.466252	-1.232191
62.	1.	0.	0.599887	5.635078	0.149135
63.	1.	0.	-1.718524	3.448622	-1.680130
64.	1.	0.	-2.923182	3.531133	-0.379991
65.	1.	0.	-2.682953	2.023124	-1.253131
66.	1.	0.	-3.161682	-1.284146	-3.355129
67.	1.	0.	-1.468367	-0.827258	-3.230631
68.	1.	0.	-2.741332	0.343304	-2.816203
69.	1.	0.	-6.067627	1.199135	-0.731314
70.	1.	0.	-6.461171	-0.516213	-1.087044
71.	1.	0.	-5.865576	-0.062619	0.528510
72.	1.	0.	6.190367	-2.560527	-1.553975
73.	1.	0.	6.740267	-0.860634	-1.727604
74.	1.	0.	6.428217	-1.526685	-0.107136

Conformer **3c**		Standard Orientation (Ångstroms)			
Center number	Atom	Type	X	Y	Z
1.	6.	0.	-0.839936	2.543284	0.286714
2.	6.	0.	0.210837	1.591287	-0.299869
3.	6.	0.	1.472026	1.999950	-0.043888
4.	6.	0.	-1.532523	1.725396	1.393862
5.	6.	0.	-2.142701	0.415076	0.856647
6.	6.	0.	-0.286093	0.365642	-1.006557
7.	6.	0.	-1.535206	-0.310745	-0.326581
8.	6.	0.	2.825724	1.413459	-0.359347
9.	6.	0.	2.910402	0.024664	-1.035564
10.	6.	0.	1.963248	-1.017137	-0.355621
11.	6.	0.	0.507786	-0.965493	-0.843368
12.	6.	0.	-0.602508	-1.535054	0.107476
13.	6.	0.	-0.202259	-1.873382	1.560667
14.	6.	0.	-2.605527	-0.972840	-1.346254
15.	6.	0.	-1.303762	-2.779081	-0.345908

16.	6.	0.	-2.215517	-2.485941	-1.489171
17.	6.	0.	-1.022135	-3.827655	0.430631
18.	6.	0.	-0.071774	-3.429940	1.539631
19.	6.	0.	1.005567	-1.101339	2.116804
20.	6.	0.	2.192566	-1.030368	1.162043
21.	8.	0.	3.334148	-0.958569	1.590060
22.	6.	0.	2.629608	0.132531	-2.555887
23.	6.	0.	1.423540	-1.549565	3.521066
24.	8.	0.	-2.528335	2.464656	2.063596
25.	6.	0.	1.459442	3.306017	0.698036
26.	6.	0.	0.003466	3.678057	0.880469
27.	6.	0.	0.869933	4.487494	-0.048642
28.	6.	0.	-1.892913	3.065560	-0.710734
29.	8.	0.	-3.085043	-0.053171	1.483989
30.	6.	0.	-2.628195	-0.315772	-2.747192
31.	6.	0.	-4.052035	-0.885517	-0.813759
32.	8.	0.	-4.507874	0.387847	-0.862600
33.	8.	0.	-4.745177	-1.823490	-0.492475
34.	6.	0.	-5.831528	0.584538	-0.338266
35.	1.	0.	-1.066553	-1.650294	2.198254
36.	6.	0.	4.336774	-0.558448	-0.957327
37.	8.	0.	5.271461	0.361700	-0.653332
38.	8.	0.	4.603797	-1.707852	-1.241333
39.	6.	0.	6.619120	-0.135860	-0.588444
40.	1.	0.	-0.470520	0.619989	-2.054430
41.	1.	0.	2.351553	-1.998894	-0.663556
42.	1.	0.	0.470261	-1.501894	-1.796589
43.	1.	0.	-0.747554	1.421148	2.111216
44.	1.	0.	3.374806	2.139147	-0.974118
45.	1.	0.	3.388067	1.374711	0.579569
46.	1.	0.	-1.698690	-2.631250	-2.446704
47.	1.	0.	-3.106369	-3.115865	-1.494205
48.	1.	0.	-1.412244	-4.833646	0.312104
49.	1.	0.	0.959712	-3.748277	1.321383
50.	1.	0.	-0.332521	-3.876341	2.505481
51.	1.	0.	0.697511	-0.045862	2.182134
52.	1.	0.	1.660779	0.593916	-2.755643
53.	1.	0.	2.661669	-0.852045	-3.029976
54.	1.	0.	3.393577	0.758695	-3.028171
55.	1.	0.	1.777822	-2.584516	3.517049
56.	1.	0.	2.237046	-0.927283	3.897237
57.	1.	0.	0.576756	-1.480566	4.211088
58.	1.	0.	-3.170476	1.801588	2.371538

59.	1.	0.	2.216104	3.486528	1.457312
60.	1.	0.	-0.356256	4.149969	1.788933
61.	1.	0.	0.742284	4.394320	-1.123421
62.	1.	0.	1.147427	5.482886	0.286677
63.	1.	0.	-1.418467	3.568768	-1.557105
64.	1.	0.	-2.546006	3.779224	-0.202921
65.	1.	0.	-2.531529	2.266694	-1.098175
66.	1.	0.	-3.417956	-0.777839	-3.349098
67.	1.	0.	-1.687033	-0.481993	-3.277373
68.	1.	0.	-2.828068	0.755592	-2.705570
69.	1.	0.	-6.044884	1.645222	-0.468757
70.	1.	0.	-6.555583	-0.025295	-0.883039
71.	1.	0.	-5.857764	0.313056	0.719435
72.	1.	0.	7.239044	0.726920	-0.345641
73.	1.	0.	6.700686	-0.899655	0.188041
74.	1.	0.	6.916985	-0.568731	-1.546213

Conformer **3d**		Standard Orientation (Ångstroms)			
Center number	Atom	Type	X	Y	Z
1.	6.	0.	-0.808292	2.729011	0.164016
2.	6.	0.	0.258660	1.749361	-0.340107
3.	6.	0.	1.507906	2.141697	-0.013464
4.	6.	0.	-1.551302	1.948078	1.265935
5.	6.	0.	-2.151922	0.632472	0.735158
6.	6.	0.	-0.214567	0.512403	-1.041831
7.	6.	0.	-1.499581	-0.136716	-0.399817
8.	6.	0.	2.862670	1.514036	-0.209670
9.	6.	0.	2.981139	0.135961	-0.899371
10.	6.	0.	1.996796	-0.919001	-0.292582
11.	6.	0.	0.554290	-0.825713	-0.822980
12.	6.	0.	-0.601053	-1.359727	0.095960
13.	6.	0.	-0.268604	-1.662834	1.573243
14.	6.	0.	-2.539916	-0.812384	-1.448327
15.	6.	0.	-1.293090	-2.606150	-0.364238
16.	6.	0.	-2.113640	-2.319847	-1.576280
17.	6.	0.	-1.078853	-3.635445	0.458070
18.	6.	0.	-0.187603	-3.222923	1.611001
19.	6.	0.	0.951221	-0.910875	2.137373
20.	6.	0.	2.171755	-1.001457	1.231812
21.	8.	0.	3.296156	-1.123618	1.690812
22.	6.	0.	2.788279	0.261502	-2.431757

23.	6.	0.	1.278444	-1.278131	3.586850
24.	8.	0.	-2.560315	2.713521	1.880764
25.	6.	0.	1.474843	3.472594	0.681456
26.	6.	0.	0.017143	3.872797	0.763501
27.	6.	0.	0.948978	4.633066	-0.142675
28.	6.	0.	-1.817291	3.228077	-0.888587
29.	8.	0.	-3.131991	0.196981	1.326930
30.	6.	0.	-2.537566	-0.154608	-2.844297
31.	6.	0.	-3.988558	-0.660568	-0.939630
32.	8.	0.	-4.475082	-1.772822	-0.360622
33.	8.	0.	-4.641754	0.348843	-1.104125
34.	6.	0.	-5.789167	-1.637645	0.205968
35.	1.	0.	-1.143586	-1.384429	2.173143
36.	6.	0.	4.437743	-0.334985	-0.708614
37.	8.	0.	4.605148	-1.619463	-1.098841
38.	8.	0.	5.354008	0.371873	-0.352233
39.	6.	0.	5.936944	-2.135445	-0.942024
40.	1.	0.	-0.352880	0.747256	-2.101343
41.	1.	0.	2.370623	-1.895720	-0.624737
42.	1.	0.	0.533503	-1.375686	-1.768997
43.	1.	0.	-0.796115	1.652084	2.018274
44.	1.	0.	3.496320	2.226560	-0.753341
45.	1.	0.	3.340702	1.442308	0.774941
46.	1.	0.	-1.503219	-2.429560	-2.482707
47.	1.	0.	-2.973784	-2.980810	-1.686625
48.	1.	0.	-1.477667	-4.638745	0.344019
49.	1.	0.	0.845088	-3.577754	1.468222
50.	1.	0.	-0.519615	-3.628630	2.573019
51.	1.	0.	0.699541	0.160930	2.102935
52.	1.	0.	1.832964	0.728655	-2.678453
53.	1.	0.	2.840031	-0.715761	-2.919325
54.	1.	0.	3.578711	0.891118	-2.852550
55.	1.	0.	1.572358	-2.328217	3.672936
56.	1.	0.	2.109266	-0.676964	3.960591
57.	1.	0.	0.406932	-1.111869	4.227819
58.	1.	0.	-3.253665	2.076568	2.126359
59.	1.	0.	2.190326	3.670937	1.475301
60.	1.	0.	-0.387648	4.383803	1.630877
61.	1.	0.	0.881772	4.499618	-1.218698
62.	1.	0.	1.223812	5.636237	0.170684
63.	1.	0.	-1.307085	3.694142	-1.735548
64.	1.	0.	-2.478790	3.966771	-0.430420
65.	1.	0.	-2.455459	2.425081	-1.269691

66.	1.	0.	-3.280566	-0.650849	-3.477045
67.	1.	0.	-1.569528	-0.265277	-3.338346
68.	1.	0.	-2.803047	0.901945	-2.799807
69.	1.	0.	-5.776381	-0.878462	0.990622
70.	1.	0.	-6.512902	-1.351527	-0.560615
71.	1.	0.	-6.032185	-2.616051	0.619912
72.	1.	0.	5.903294	-3.157700	-1.318745
73.	1.	0.	6.652827	-1.538088	-1.511283
74.	1.	0.	6.221853	-2.124046	0.112574

Conformer **3e**		Standard Orientation (Ångstroms)			
Center number	Atom	Type	X	Y	Z
1.	6.	0.	-0.557746	2.723271	0.248256
2.	6.	0.	0.398011	1.665116	-0.316663
3.	6.	0.	1.687919	1.930381	-0.017651
4.	6.	0.	-1.355366	1.978473	1.335639
5.	6.	0.	-2.094639	0.748366	0.771025
6.	6.	0.	-0.209764	0.505092	-1.047102
7.	6.	0.	-1.543692	-0.039570	-0.405156
8.	6.	0.	2.979219	1.198929	-0.287631
9.	6.	0.	2.935559	-0.185381	-0.975854
10.	6.	0.	1.855708	-1.120795	-0.342844
11.	6.	0.	0.434117	-0.903715	-0.880775
12.	6.	0.	-0.763936	-1.369479	0.016958
13.	6.	0.	-0.459298	-1.792971	1.468554
14.	6.	0.	-2.663742	-0.561721	-1.460287
15.	6.	0.	-1.561889	-2.520055	-0.515767
16.	6.	0.	-2.356784	-2.084168	-1.699466
17.	6.	0.	-1.420491	-3.617362	0.230534
18.	6.	0.	-0.489408	-3.353510	1.396734
19.	6.	0.	0.797261	-1.160677	2.088633
20.	6.	0.	2.023690	-1.180095	1.181105
21.	8.	0.	3.148525	-1.219135	1.655112
22.	6.	0.	2.723523	-0.034837	-2.503744
23.	6.	0.	1.114829	-1.680660	3.494853
24.	8.	0.	-2.272372	2.816521	1.997864
25.	6.	0.	1.796742	3.230074	0.727294
26.	6.	0.	0.385840	3.759763	0.868090
27.	6.	0.	1.361655	4.468508	-0.033784
28.	6.	0.	-1.531037	3.356952	-0.765085
29.	8.	0.	-3.103181	0.394388	1.369111

30.	6.	0.	-2.656677	0.184914	-2.809903
31.	6.	0.	-4.081391	-0.350097	-0.888915
32.	8.	0.	-4.596617	-1.453398	-0.316541
33.	8.	0.	-4.690641	0.693122	-1.000493
34.	6.	0.	-5.875033	-1.270216	0.313759
35.	1.	0.	-1.320525	-1.498875	2.081189
36.	6.	0.	4.285402	-0.922221	-0.853705
37.	8.	0.	5.305333	-0.110192	-0.517600
38.	8.	0.	4.433479	-2.094494	-1.131605
39.	6.	0.	6.587842	-0.751979	-0.412484
40.	1.	0.	-0.340792	0.786300	-2.096292
41.	1.	0.	2.143845	-2.136498	-0.651955
42.	1.	0.	0.378024	-1.418448	-1.844574
43.	1.	0.	-0.621522	1.581075	2.061985
44.	1.	0.	3.628510	1.863627	-0.872925
45.	1.	0.	3.496180	1.091580	0.671846
46.	1.	0.	-1.755242	-2.174539	-2.614097
47.	1.	0.	-3.266351	-2.665625	-1.854361
48.	1.	0.	-1.893235	-4.578248	0.052339
49.	1.	0.	0.512858	-3.770248	1.211173
50.	1.	0.	-0.838862	-3.801440	2.333550
51.	1.	0.	0.592537	-0.081490	2.172286
52.	1.	0.	1.817458	0.529832	-2.731328
53.	1.	0.	2.667181	-1.012951	-2.988866
54.	1.	0.	3.566892	0.510113	-2.940133
55.	1.	0.	1.365205	-2.745554	3.476767
56.	1.	0.	1.970449	-1.151076	3.916649
57.	1.	0.	0.252912	-1.543214	4.155261
58.	1.	0.	-3.020788	2.242017	2.236223
59.	1.	0.	2.546774	3.327341	1.508078
60.	1.	0.	0.052309	4.268942	1.766308
61.	1.	0.	1.254656	4.389310	-1.111945
62.	1.	0.	1.736864	5.427665	0.311828
63.	1.	0.	-0.992878	3.800063	-1.606957
64.	1.	0.	-2.108346	4.139982	-0.268368
65.	1.	0.	-2.250829	2.634009	-1.159971
66.	1.	0.	-3.449587	-0.218622	-3.447805
67.	1.	0.	-1.713239	0.043733	-3.342073
68.	1.	0.	-2.849604	1.251216	-2.691252
69.	1.	0.	-6.148615	-2.247175	0.711853
70.	1.	0.	-5.788158	-0.536040	1.117342
71.	1.	0.	-6.617222	-0.926298	-0.410285
72.	1.	0.	7.290445	0.038005	-0.148067

73.	1.	0.	6.561519	-1.519746	0.363926
74.	1.	0.	6.866407	-1.215203	-1.361832

Table S3. Gibbs free energiesa and equilibrium populationsb of low-energy conformers of 1*S*, 3*R*, 6*S*, 7*R*, 9*S*, 10*R*, 11*S*, 1'*R*, 5'*S*, 6'*R*, 7'*R*, 9'*S*,10'*S* - **3**.

Conformers	In gas	
	G^a	P (%)[b]
3-f	-1084934.73980112	15.60
3-g	-1084934.91299388	20.91
3-h	-1084935.02782821	25.38
3-i	-1084934.7448212	15.74
3-j	-1084934.95315452	22.37

[a]B3LYP/6-31G(d,p), in kcal/mol. [b]From *G* values at 298.15K.

Figure S5. The low-energy reoptimized MMFF conformers of 1*S*, 3*R*, 6*S*, 7*R*, 9*S*, 10*R*, 11*S*, 1'*R*, 5'*S*, 6'*R*, 7'*R*, 9'*S*,10'*S* - **3** at B3LYP/6-31G(d,p) level of theory in gas.

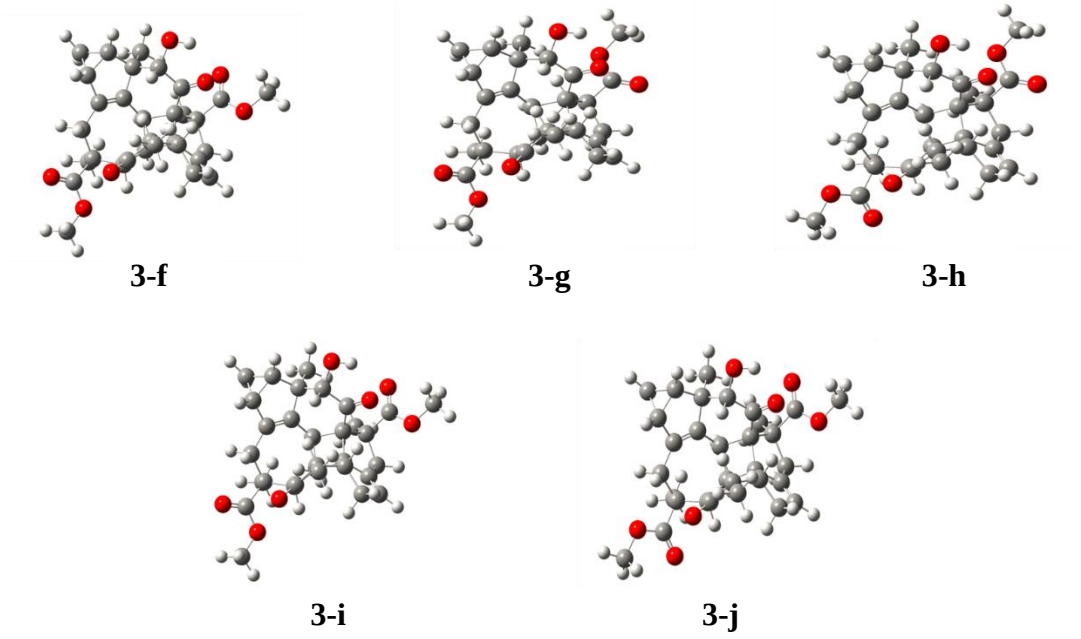


Table S4. Cartesian coordinates for the low-energy reoptimized MMFF conformers of 1*S*, 3*R*, 6*S*, 7*R*, 9*S*, 10*R*, 11*S*, 1'*R*, 5'*S*, 6'*R*, 7'*R*, 9'*S*,10'*S* – **3** at B3LYP/6-31G (d, p) level of theory in gas.

Conformer **3f**		Standard Orientation (Ångstroms)			
Center number	Atom	Type	X	Y	Z
1.	6.	0.	-0.808171	2.729111	-0.164050

2.	6.	0.	0.258743	1.749431	0.340100
3.	6.	0.	1.508003	2.141718	0.013441
4.	6.	0.	-1.551175	1.948177	-1.265960
5.	6.	0.	-2.151833	0.632579	-0.735180
6.	6.	0.	-0.214531	0.512516	1.041858
7.	6.	0.	-1.499584	-0.136586	0.399873
8.	6.	0.	2.862742	1.513995	0.209593
9.	6.	0.	2.981177	0.135913	0.899284
10.	6.	0.	1.996743	-0.918989	0.292548
11.	6.	0.	0.554286	-0.825630	0.823064
12.	6.	0.	-0.601114	-1.359712	-0.095740
13.	6.	0.	-0.268774	-1.663077	-1.572990
14.	6.	0.	-2.540006	-0.812081	1.448422
15.	6.	0.	-1.293154	-2.606036	0.364714
16.	6.	0.	-2.113632	-2.319478	1.576748
17.	6.	0.	-1.078981	-3.635476	-0.457430
18.	6.	0.	-0.187780	-3.223166	-1.610480
19.	6.	0.	0.950972	-0.911162	-2.137330
20.	6.	0.	2.171595	-1.001491	-1.231850
21.	8.	0.	3.295979	-1.123507	-1.690940
22.	6.	0.	2.788398	0.261467	2.431680
23.	6.	0.	1.278109	-1.278617	-3.586770
24.	8.	0.	-2.560178	2.713656	-1.880770
25.	6.	0.	1.474982	3.472612	-0.681490
26.	6.	0.	0.017305	3.872867	-0.763540
27.	6.	0.	0.949167	4.633106	0.142640
28.	6.	0.	-1.817178	3.228242	0.888520
29.	8.	0.	-3.131873	0.197088	-1.327010
30.	6.	0.	-2.537877	-0.153975	2.844226
31.	6.	0.	-3.988590	-0.660553	0.939479
32.	8.	0.	-4.474788	-1.772929	0.360435
33.	8.	0.	-4.642023	0.348728	1.103841
34.	6.	0.	-5.788792	-1.638033	-0.206410
35.	1.	0.	-1.143814	-1.384781	-2.172860
36.	6.	0.	4.437758	-0.335095	0.708467
37.	8.	0.	4.605094	-1.619622	1.098565
38.	8.	0.	5.354063	0.371753	0.352166
39.	6.	0.	5.936875	-2.135649	0.941791
40.	1.	0.	-0.352823	0.747408	2.101362
41.	1.	0.	2.370525	-1.895737	0.624678
42.	1.	0.	0.533590	-1.375515	1.769134
43.	1.	0.	-0.795999	1.652170	-2.018300
44.	1.	0.	3.496456	2.226489	0.753229

45.	1.	0.	3.340718	1.442241	-0.775050
46.	1.	0.	-1.503124	-2.428903	2.483149
47.	1.	0.	-2.973719	-2.980477	1.687352
48.	1.	0.	-1.477811	-4.638747	-0.343190
49.	1.	0.	0.844914	-3.577981	-1.467670
50.	1.	0.	-0.519832	-3.629049	-2.572410
51.	1.	0.	0.699236	0.160638	-2.103030
52.	1.	0.	1.833108	0.728646	2.678426
53.	1.	0.	2.840150	-0.715796	2.919248
54.	1.	0.	3.578869	0.891064	2.852427
55.	1.	0.	1.571970	-2.328730	-3.672730
56.	1.	0.	2.108938	-0.677534	-3.960630
57.	1.	0.	0.406569	-1.112412	-4.227720
58.	1.	0.	-3.253465	2.076689	-2.126500
59.	1.	0.	2.190494	3.670918	-1.475310
60.	1.	0.	-0.387475	4.383885	-1.630910
61.	1.	0.	0.881946	4.499688	1.218664
62.	1.	0.	1.224047	5.636255	-0.170750
63.	1.	0.	-1.306972	3.694096	1.735595
64.	1.	0.	-2.478493	3.967126	0.430393
65.	1.	0.	-2.455551	2.425323	1.269452
66.	1.	0.	-3.280939	-0.650088	3.476999
67.	1.	0.	-1.569897	-0.264469	3.338426
68.	1.	0.	-2.803407	0.902555	2.799440
69.	1.	0.	-5.775970	-0.878968	-0.991180
70.	1.	0.	-6.512707	-1.351900	0.559999
71.	1.	0.	-6.031595	-2.616536	-0.620250
72.	1.	0.	5.903383	-3.157633	1.319258
73.	1.	0.	6.652881	-1.537823	1.510396
74.	1.	0.	6.221496	-2.125021	-0.112900

Conformer **3g**		Standard Orientation (Ångstroms)			
Center number	Atom	Type	X	Y	Z
1.	6.	0.	-1.100344	2.519802	-0.19792
2.	6.	0.	0.055670	1.655581	0.321573
3.	6.	0.	1.261424	2.190722	0.039205
4.	6.	0.	-1.738388	1.677221	-1.32074
5.	6.	0.	-2.198176	0.294211	-0.82359
6.	6.	0.	-0.294991	0.363239	0.995262
7.	6.	0.	-1.479562	-0.412095	0.306672
8.	6.	0.	2.669800	1.716169	0.279155

9.	6.	0.	2.917446	0.356695	0.971849
10.	6.	0.	2.089929	-0.803025	0.319921
11.	6.	0.	0.620897	-0.880052	0.777805
12.	6.	0.	-0.430162	-1.499195	-0.21303
13.	6.	0.	-0.006407	-1.675529	-1.69096
14.	6.	0.	-2.442772	-1.243157	1.308069
15.	6.	0.	-1.008596	-2.835557	0.137859
16.	6.	0.	-1.932189	-2.727052	1.304715
17.	6.	0.	-0.658557	-3.783595	-0.73432
18.	6.	0.	0.232003	-3.214860	-1.8174
19.	6.	0.	1.161740	-0.784208	-2.15397
20.	6.	0.	2.342160	-0.841329	-1.19625
21.	8.	0.	3.492316	-0.898890	-1.60052
22.	6.	0.	2.648388	0.448052	2.494735
23.	6.	0.	1.582052	-1.032825	-3.60465
24.	8.	0.	-2.818936	2.336821	-1.93963
25.	6.	0.	1.100360	3.514241	-0.6524
26.	6.	0.	-0.390196	3.751589	-0.77257
27.	6.	0.	0.429340	4.607033	0.157797
28.	6.	0.	-2.165854	2.897998	0.848711
29.	8.	0.	-3.108944	-0.243638	-1.44202
30.	6.	0.	-2.447196	-0.705700	2.759705
31.	6.	0.	-3.918217	-1.222425	0.855293
32.	8.	0.	-4.443747	0.017829	0.988349
33.	8.	0.	-4.572844	-2.185914	0.529088
34.	6.	0.	-5.801604	0.160043	0.538944
35.	1.	0.	-0.877601	-1.446750	-2.31663
36.	6.	0.	4.425488	0.057947	0.837833
37.	8.	0.	4.729213	-1.189562	1.262297
38.	8.	0.	5.263191	0.860612	0.490821
39.	6.	0.	6.116106	-1.549446	1.153749
40.	1.	0.	-0.488191	0.564785	2.05285
41.	1.	0.	2.561323	-1.730886	0.665117
42.	1.	0.	0.611457	-1.460461	1.706219
43.	1.	0.	-0.944760	1.476906	-2.06503
44.	1.	0.	3.202165	2.492140	0.844288
45.	1.	0.	3.186350	1.703093	-0.68859
46.	1.	0.	-1.402099	-2.925316	2.24522
47.	1.	0.	-2.771443	-3.421917	1.245328
48.	1.	0.	-0.966850	-4.824028	-0.70318
49.	1.	0.	1.288909	-3.476601	-1.65204
50.	1.	0.	-0.022012	-3.587743	-2.81572
51.	1.	0.	0.816824	0.257757	-2.06826

52.	1.	0.	1.635747	0.798252	2.702463
53.	1.	0.	2.794728	-0.519939	2.981104
54.	1.	0.	3.341283	1.162936	2.950098
55.	1.	0.	1.980534	-2.042769	-3.73569
56.	1.	0.	2.365458	-0.334714	-3.90598
57.	1.	0.	0.725901	-0.910945	-4.27568
58.	1.	0.	-3.400753	1.624880	-2.25821
59.	1.	0.	1.809519	3.792783	-1.42775
60.	1.	0.	-0.824717	4.218947	-1.65022
61.	1.	0.	0.350371	4.466252	1.232191
62.	1.	0.	0.599887	5.635078	-0.14914
63.	1.	0.	-1.718524	3.448622	1.68013
64.	1.	0.	-2.923182	3.531133	0.379991
65.	1.	0.	-2.682953	2.023124	1.253131
66.	1.	0.	-3.161682	-1.284146	3.355129
67.	1.	0.	-1.468367	-0.827258	3.230631
68.	1.	0.	-2.741332	0.343304	2.816203
69.	1.	0.	-6.067627	1.199135	0.731314
70.	1.	0.	-6.461171	-0.516213	1.087044
71.	1.	0.	-5.865576	-0.062619	-0.52851
72.	1.	0.	6.190367	-2.560527	1.553975
73.	1.	0.	6.740267	-0.860634	1.727604
74.	1.	0.	6.428217	-1.526685	0.107136

Conformer **3h**		Standard Orientation (Ångstroms)			
Center number	Atom number	Type	X	Y	Z
1.	6.	0.	-0.839936	2.543284	-0.28671
2.	6.	0.	0.210837	1.591287	0.299869
3.	6.	0.	1.472026	1.999950	0.043888
4.	6.	0.	-1.532523	1.725396	-1.39386
5.	6.	0.	-2.142701	0.415076	-0.85665
6.	6.	0.	-0.286093	0.365642	1.006557
7.	6.	0.	-1.535206	-0.310745	0.326581
8.	6.	0.	2.825724	1.413459	0.359347
9.	6.	0.	2.910402	0.024664	1.035564
10.	6.	0.	1.963248	-1.017137	0.355621
11.	6.	0.	0.507786	-0.965493	0.843368
12.	6.	0.	-0.602508	-1.535054	-0.10748
13.	6.	0.	-0.202259	-1.873382	-1.56067
14.	6.	0.	-2.605527	-0.972840	1.346254
15.	6.	0.	-1.303762	-2.779081	0.345908

16.	6.	0.	-2.215517	-2.485941	1.489171
17.	6.	0.	-1.022135	-3.827655	-0.43063
18.	6.	0.	-0.071774	-3.429940	-1.53963
19.	6.	0.	1.005567	-1.101339	-2.1168
20.	6.	0.	2.192566	-1.030368	-1.16204
21.	8.	0.	3.334148	-0.958569	-1.59006
22.	6.	0.	2.629608	0.132531	2.555887
23.	6.	0.	1.423540	-1.549565	-3.52107
24.	8.	0.	-2.528335	2.464656	-2.0636
25.	6.	0.	1.459442	3.306017	-0.69804
26.	6.	0.	0.003466	3.678057	-0.88047
27.	6.	0.	0.869933	4.487494	0.048642
28.	6.	0.	-1.892913	3.065560	0.710734
29.	8.	0.	-3.085043	-0.053171	-1.48399
30.	6.	0.	-2.628195	-0.315772	2.747192
31.	6.	0.	-4.052035	-0.885517	0.813759
32.	8.	0.	-4.507874	0.387847	0.8626
33.	8.	0.	-4.745177	-1.823490	0.492475
34.	6.	0.	-5.831528	0.584538	0.338266
35.	1.	0.	-1.066553	-1.650294	-2.19825
36.	6.	0.	4.336774	-0.558448	0.957327
37.	8.	0.	5.271461	0.361700	0.653332
38.	8.	0.	4.603797	-1.707852	1.241333
39.	6.	0.	6.619120	-0.135860	0.588444
40.	1.	0.	-0.470520	0.619989	2.05443
41.	1.	0.	2.351553	-1.998894	0.663556
42.	1.	0.	0.470261	-1.501894	1.796589
43.	1.	0.	-0.747554	1.421148	-2.11122
44.	1.	0.	3.374806	2.139147	0.974118
45.	1.	0.	3.388067	1.374711	-0.57957
46.	1.	0.	-1.698690	-2.631250	2.446704
47.	1.	0.	-3.106369	-3.115865	1.494205
48.	1.	0.	-1.412244	-4.833646	-0.3121
49.	1.	0.	0.959712	-3.748277	-1.32138
50.	1.	0.	-0.332521	-3.876341	-2.50548
51.	1.	0.	0.697511	-0.045862	-2.18213
52.	1.	0.	1.660779	0.593916	2.755643
53.	1.	0.	2.661669	-0.852045	3.029976
54.	1.	0.	3.393577	0.758695	3.028171
55.	1.	0.	1.777822	-2.584516	-3.51705
56.	1.	0.	2.237046	-0.927283	-3.89724
57.	1.	0.	0.576756	-1.480566	-4.21109
58.	1.	0.	-3.170476	1.801588	-2.37154

59.	1.	0.	2.216104	3.486528	-1.45731
60.	1.	0.	-0.356256	4.149969	-1.78893
61.	1.	0.	0.742284	4.394320	1.123421
62.	1.	0.	1.147427	5.482886	-0.28668
63.	1.	0.	-1.418467	3.568768	1.557105
64.	1.	0.	-2.546006	3.779224	0.202921
65.	1.	0.	-2.531529	2.266694	1.098175
66.	1.	0.	-3.417956	-0.777839	3.349098
67.	1.	0.	-1.687033	-0.481993	3.277373
68.	1.	0.	-2.828068	0.755592	2.70557
69.	1.	0.	-6.044884	1.645222	0.468757
70.	1.	0.	-6.555583	-0.025295	0.883039
71.	1.	0.	-5.857764	0.313056	-0.71944
72.	1.	0.	7.239044	0.726920	0.345641
73.	1.	0.	6.700686	-0.899655	-0.18804
74.	1.	0.	6.916985	-0.568731	1.546213

Conformer **3i**		Standard Orientation (Ångstroms)			
Center number	Atom	Type	X	Y	Z
1.	6.	0.	-0.808292	2.729011	-0.16402
2.	6.	0.	0.258660	1.749361	0.340107
3.	6.	0.	1.507906	2.141697	0.013464
4.	6.	0.	-1.551302	1.948078	-1.26594
5.	6.	0.	-2.151922	0.632472	-0.73516
6.	6.	0.	-0.214567	0.512403	1.041831
7.	6.	0.	-1.499581	-0.136716	0.399817
8.	6.	0.	2.862670	1.514036	0.20967
9.	6.	0.	2.981139	0.135961	0.899371
10.	6.	0.	1.996796	-0.919001	0.292582
11.	6.	0.	0.554290	-0.825713	0.82298
12.	6.	0.	-0.601053	-1.359727	-0.09596
13.	6.	0.	-0.268604	-1.662834	-1.57324
14.	6.	0.	-2.539916	-0.812384	1.448327
15.	6.	0.	-1.293090	-2.606150	0.364238
16.	6.	0.	-2.113640	-2.319847	1.57628
17.	6.	0.	-1.078853	-3.635445	-0.45807
18.	6.	0.	-0.187603	-3.222923	-1.611
19.	6.	0.	0.951221	-0.910875	-2.13737
20.	6.	0.	2.171755	-1.001457	-1.23181
21.	8.	0.	3.296156	-1.123618	-1.69081
22.	6.	0.	2.788279	0.261502	2.431757

23.	6.	0.	1.278444	-1.278131	-3.58685
24.	8.	0.	-2.560315	2.713521	-1.88076
25.	6.	0.	1.474843	3.472594	-0.68146
26.	6.	0.	0.017143	3.872797	-0.7635
27.	6.	0.	0.948978	4.633066	0.142675
28.	6.	0.	-1.817291	3.228077	0.888587
29.	8.	0.	-3.131991	0.196981	-1.32693
30.	6.	0.	-2.537566	-0.154608	2.844297
31.	6.	0.	-3.988558	-0.660568	0.93963
32.	8.	0.	-4.475082	-1.772822	0.360622
33.	8.	0.	-4.641754	0.348843	1.104125
34.	6.	0.	-5.789167	-1.637645	-0.20597
35.	1.	0.	-1.143586	-1.384429	-2.17314
36.	6.	0.	4.437743	-0.334985	0.708614
37.	8.	0.	4.605148	-1.619463	1.098841
38.	8.	0.	5.354008	0.371873	0.352233
39.	6.	0.	5.936944	-2.135445	0.942024
40.	1.	0.	-0.352880	0.747256	2.101343
41.	1.	0.	2.370623	-1.895720	0.624737
42.	1.	0.	0.533503	-1.375686	1.768997
43.	1.	0.	-0.796115	1.652084	-2.01827
44.	1.	0.	3.496320	2.226560	0.753341
45.	1.	0.	3.340702	1.442308	-0.77494
46.	1.	0.	-1.503219	-2.429560	2.482707
47.	1.	0.	-2.973784	-2.980810	1.686625
48.	1.	0.	-1.477667	-4.638745	-0.34402
49.	1.	0.	0.845088	-3.577754	-1.46822
50.	1.	0.	-0.519615	-3.628630	-2.57302
51.	1.	0.	0.699541	0.160930	-2.10294
52.	1.	0.	1.832964	0.728655	2.678453
53.	1.	0.	2.840031	-0.715761	2.919325
54.	1.	0.	3.578711	0.891118	2.85255
55.	1.	0.	1.572358	-2.328217	-3.67294
56.	1.	0.	2.109266	-0.676964	-3.96059
57.	1.	0.	0.406932	-1.111869	-4.22782
58.	1.	0.	-3.253665	2.076568	-2.12636
59.	1.	0.	2.190326	3.670937	-1.4753
60.	1.	0.	-0.387648	4.383803	-1.63088
61.	1.	0.	0.881772	4.499618	1.218698
62.	1.	0.	1.223812	5.636237	-0.17068
63.	1.	0.	-1.307085	3.694142	1.735548
64.	1.	0.	-2.478790	3.966771	0.43042
65.	1.	0.	-2.455459	2.425081	1.269691

66.	1.	0.	-3.280566	-0.650849	3.477045
67.	1.	0.	-1.569528	-0.265277	3.338346
68.	1.	0.	-2.803047	0.901945	2.799807
69.	1.	0.	-5.776381	-0.878462	-0.99062
70.	1.	0.	-6.512902	-1.351527	0.560615
71.	1.	0.	-6.032185	-2.616051	-0.61991
72.	1.	0.	5.903294	-3.157700	1.318745
73.	1.	0.	6.652827	-1.538088	1.511283
74.	1.	0.	6.221853	-2.124046	-0.11257

Conformer **3j**		Standard Orientation (Ångstroms)			
Center number	Atom	Type	X	Y	Z
1.	6.	0.	-0.557746	2.723271	-0.24826
2.	6.	0.	0.398011	1.665116	0.316663
3.	6.	0.	1.687919	1.930381	0.017651
4.	6.	0.	-1.355366	1.978473	-1.33564
5.	6.	0.	-2.094639	0.748366	-0.77103
6.	6.	0.	-0.209764	0.505092	1.047102
7.	6.	0.	-1.543692	-0.039570	0.405156
8.	6.	0.	2.979219	1.198929	0.287631
9.	6.	0.	2.935559	-0.185381	0.975854
10.	6.	0.	1.855708	-1.120795	0.342844
11.	6.	0.	0.434117	-0.903715	0.880775
12.	6.	0.	-0.763936	-1.369479	-0.01696
13.	6.	0.	-0.459298	-1.792971	-1.46855
14.	6.	0.	-2.663742	-0.561721	1.460287
15.	6.	0.	-1.561889	-2.520055	0.515767
16.	6.	0.	-2.356784	-2.084168	1.699466
17.	6.	0.	-1.420491	-3.617362	-0.23053
18.	6.	0.	-0.489408	-3.353510	-1.39673
19.	6.	0.	0.797261	-1.160677	-2.08863
20.	6.	0.	2.023690	-1.180095	-1.18111
21.	8.	0.	3.148525	-1.219135	-1.65511
22.	6.	0.	2.723523	-0.034837	2.503744
23.	6.	0.	1.114829	-1.680660	-3.49485
24.	8.	0.	-2.272372	2.816521	-1.99786
25.	6.	0.	1.796742	3.230074	-0.72729
26.	6.	0.	0.385840	3.759763	-0.86809
27.	6.	0.	1.361655	4.468508	0.033784
28.	6.	0.	-1.531037	3.356952	0.765085
29.	8.	0.	-3.103181	0.394388	-1.36911

30.	6.	0.	-2.656677	0.184914	2.809903
31.	6.	0.	-4.081391	-0.350097	0.888915
32.	8.	0.	-4.596617	-1.453398	0.316541
33.	8.	0.	-4.690641	0.693122	1.000493
34.	6.	0.	-5.875033	-1.270216	-0.31376
35.	1.	0.	-1.320525	-1.498875	-2.08119
36.	6.	0.	4.285402	-0.922221	0.853705
37.	8.	0.	5.305333	-0.110192	0.5176
38.	8.	0.	4.433479	-2.094494	1.131605
39.	6.	0.	6.587842	-0.751979	0.412484
40.	1.	0.	-0.340792	0.786300	2.096292
41.	1.	0.	2.143845	-2.136498	0.651955
42.	1.	0.	0.378024	-1.418448	1.844574
43.	1.	0.	-0.621522	1.581075	-2.06199
44.	1.	0.	3.628510	1.863627	0.872925
45.	1.	0.	3.496180	1.091580	-0.67185
46.	1.	0.	-1.755242	-2.174539	2.614097
47.	1.	0.	-3.266351	-2.665625	1.854361
48.	1.	0.	-1.893235	-4.578248	-0.05234
49.	1.	0.	0.512858	-3.770248	-1.21117
50.	1.	0.	-0.838862	-3.801440	-2.33355
51.	1.	0.	0.592537	-0.081490	-2.17229
52.	1.	0.	1.817458	0.529832	2.731328
53.	1.	0.	2.667181	-1.012951	2.988866
54.	1.	0.	3.566892	0.510113	2.940133
55.	1.	0.	1.365205	-2.745554	-3.47677
56.	1.	0.	1.970449	-1.151076	-3.91665
57.	1.	0.	0.252912	-1.543214	-4.15526
58.	1.	0.	-3.020788	2.242017	-2.23622
59.	1.	0.	2.546774	3.327341	-1.50808
60.	1.	0.	0.052309	4.268942	-1.76631
61.	1.	0.	1.254656	4.389310	1.111945
62.	1.	0.	1.736864	5.427665	-0.31183
63.	1.	0.	-0.992878	3.800063	1.606957
64.	1.	0.	-2.108346	4.139982	0.268368
65.	1.	0.	-2.250829	2.634009	1.159971
66.	1.	0.	-3.449587	-0.218622	3.447805
67.	1.	0.	-1.713239	0.043733	3.342073
68.	1.	0.	-2.849604	1.251216	2.691252
69.	1.	0.	-6.148615	-2.247175	-0.71185
70.	1.	0.	-5.788158	-0.536040	-1.11734
71.	1.	0.	-6.617222	-0.926298	0.410285
72.	1.	0.	7.290445	0.038005	0.148067

73.	1.	0.	6.561519	-1.519746	-0.36393
74.	1.	0.	6.866407	-1.215203	1.361832

Figure S6. ^{1}H NMR spectrum of chlorahupetone A (**1**) in $CDCl_3$

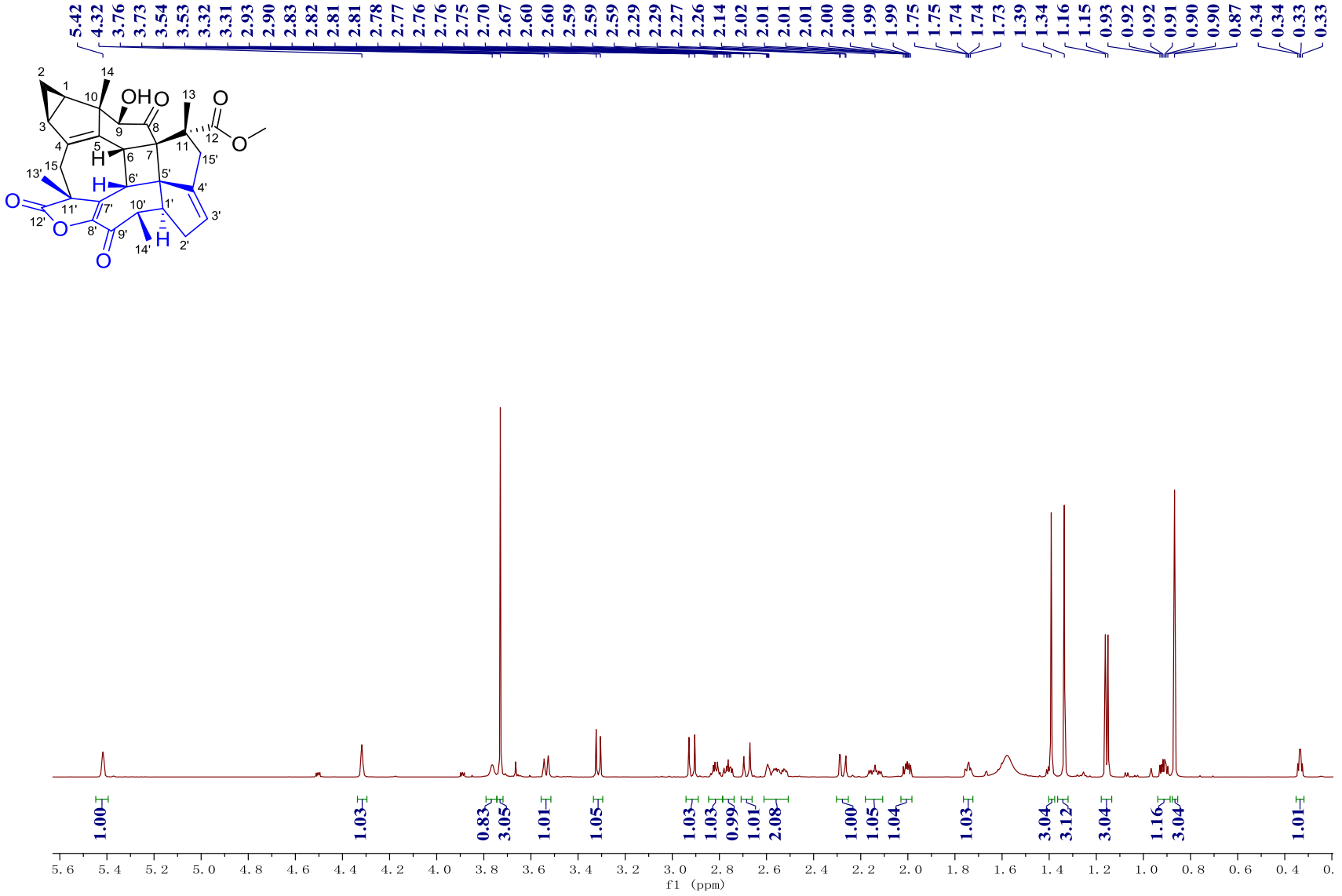


Figure S7. ^{13}C NMR and DEPT spectrum of chlorahupetone A (**1**) in $CDCl_3$

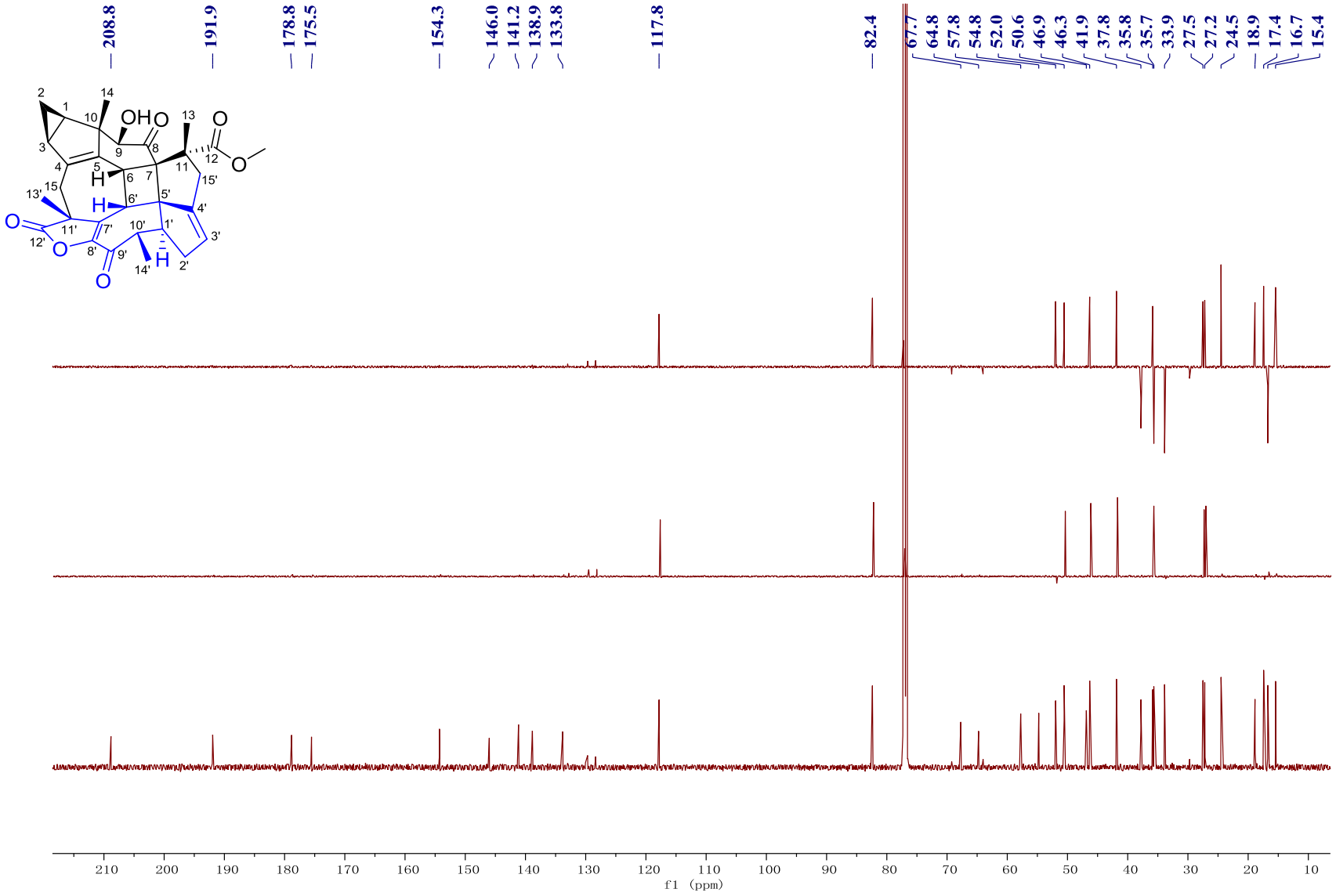


Figure S8. HSQC spectrum of chlorahupetone A (**1**) in $CDCl_3$

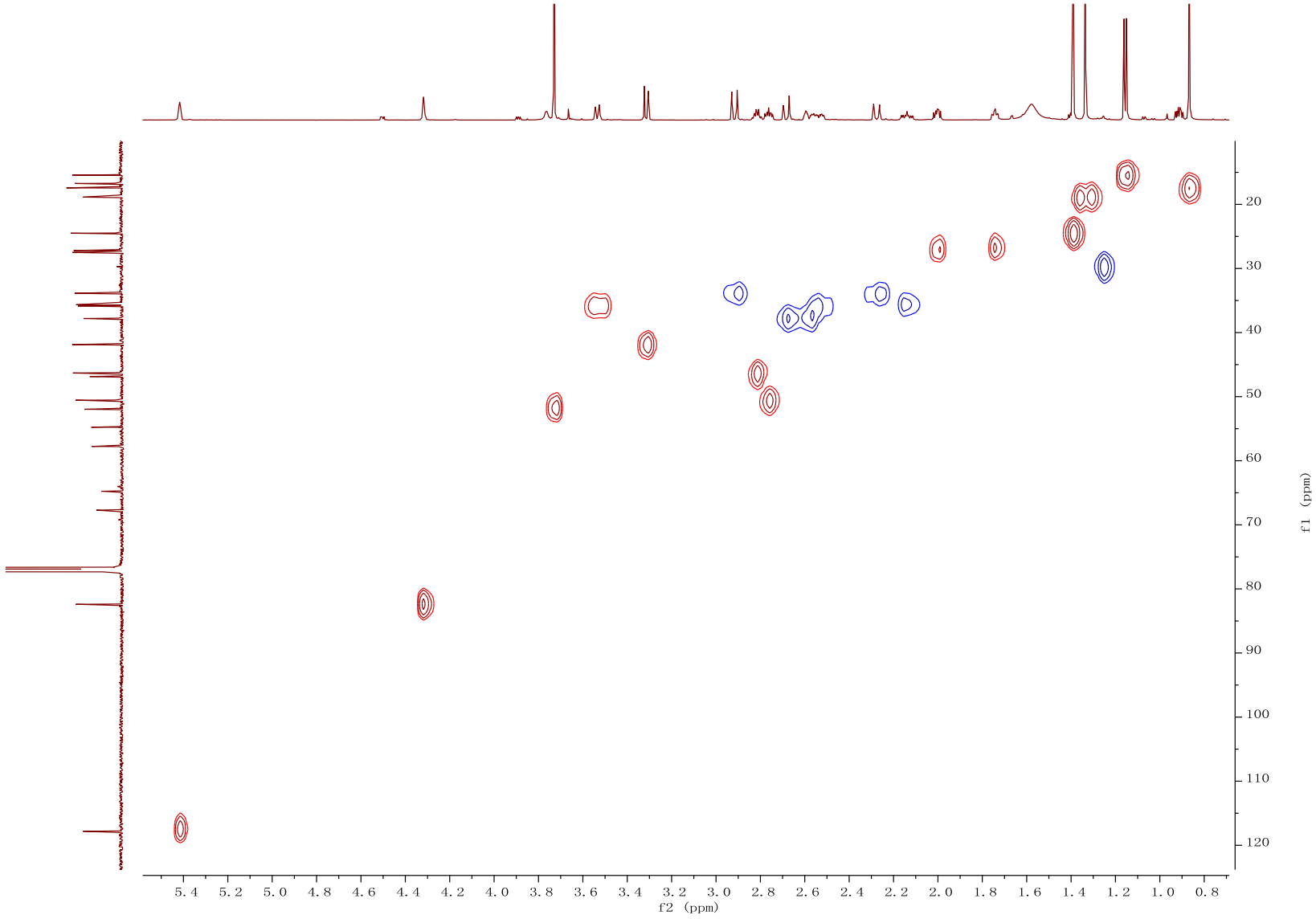


Figure S9. HMBC spectrum of chlorahupetone A (**1**) in $CDCl_3$

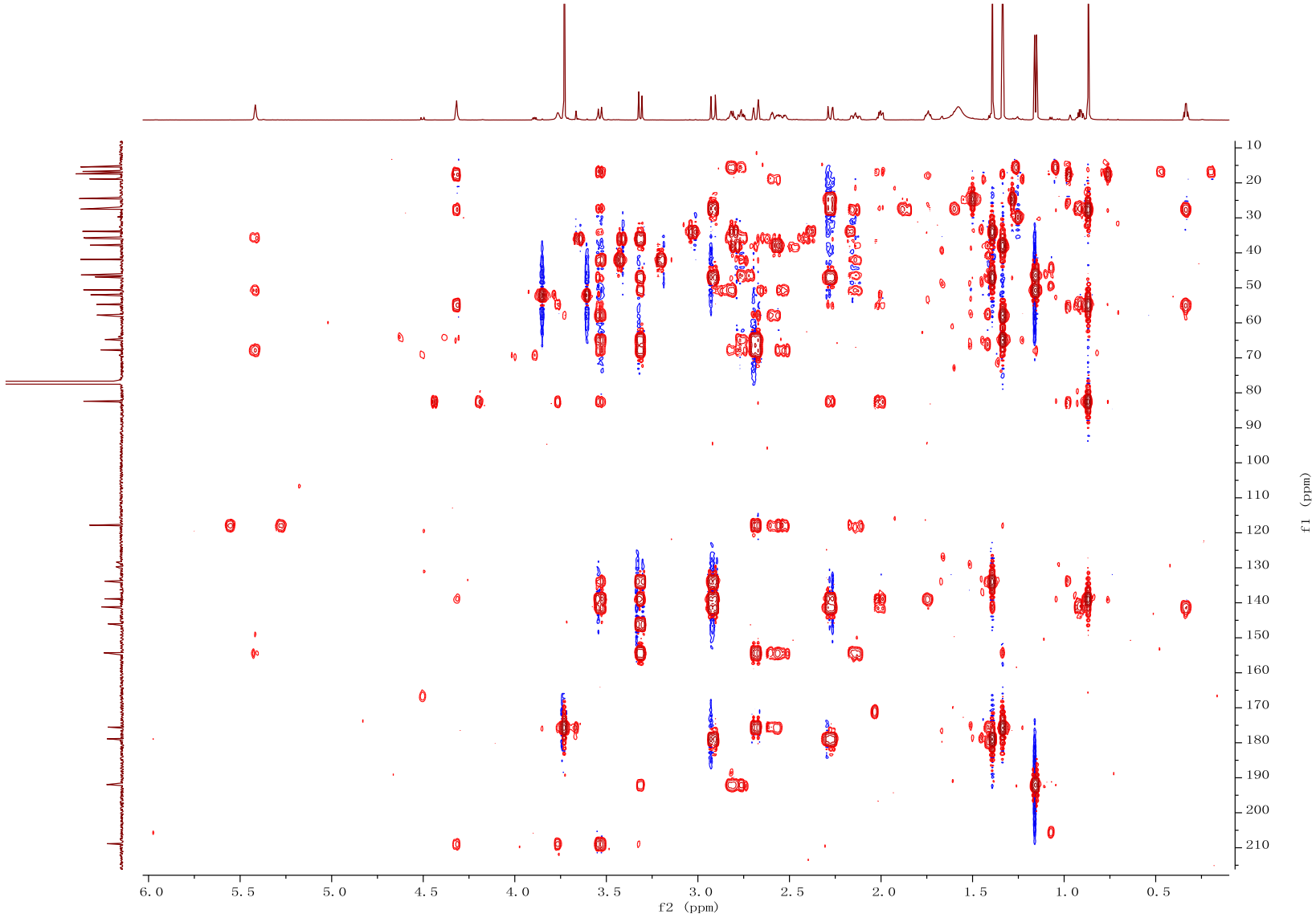


Figure S10. ^{1}H-^{1}H COSY spectrum of chlorahupetone A (**1**) in $CDCl_3$

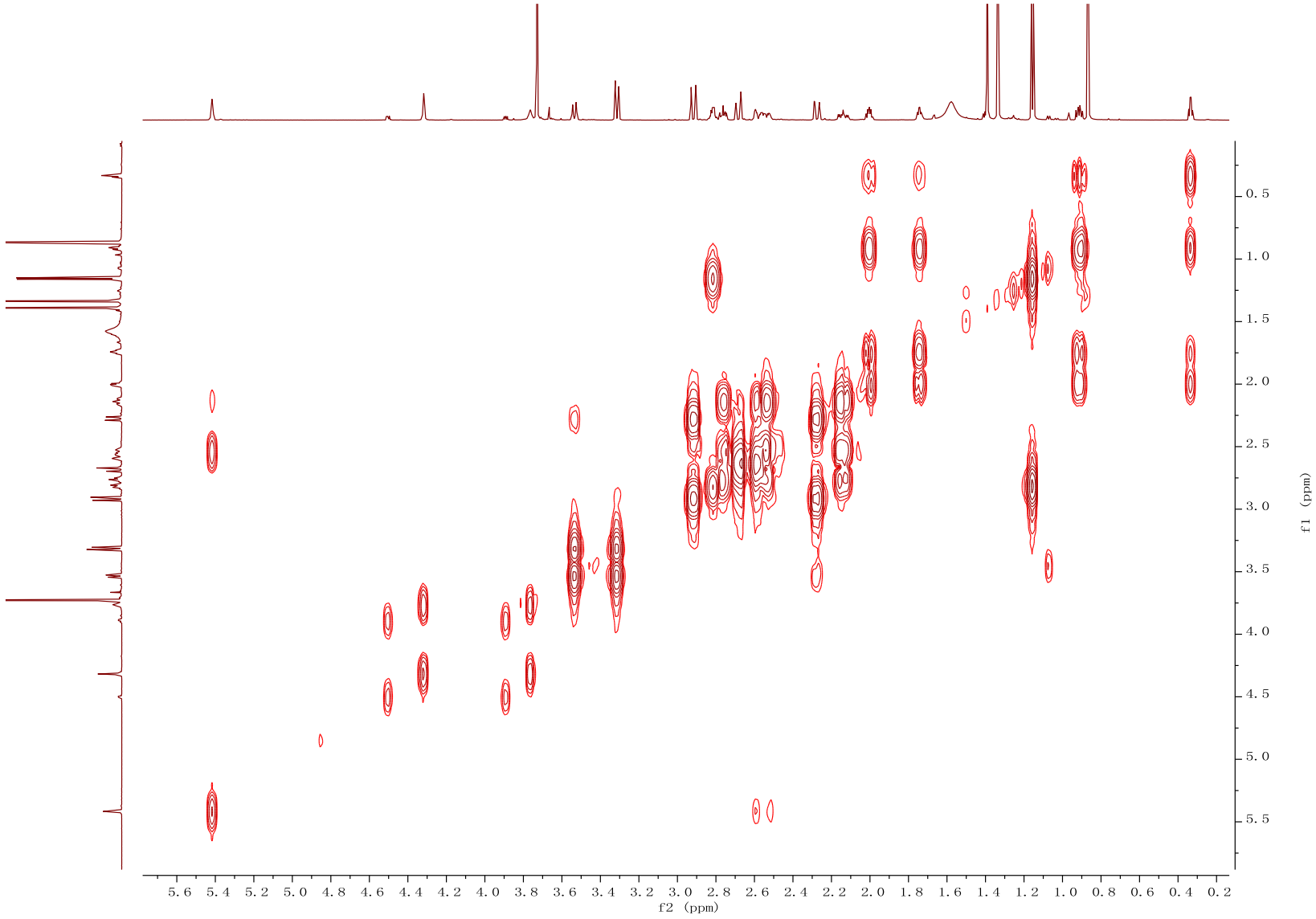


Figure S11. NOESY spectrum of chlorahupetone A (**1**) in $CDCl_3$

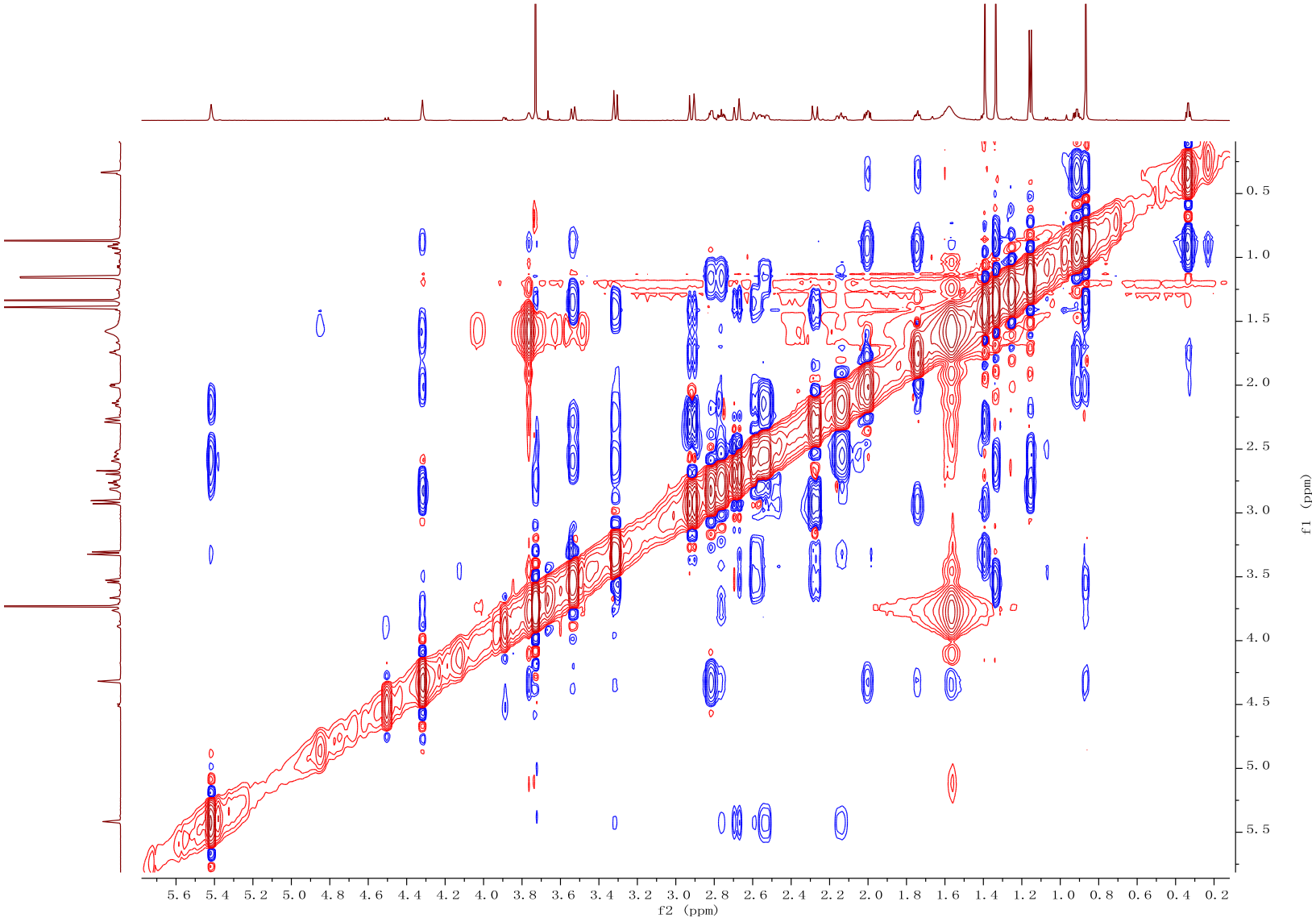


Figure S12. (-)-HRESIMS spectrum of chlorahupetone A (**1**)

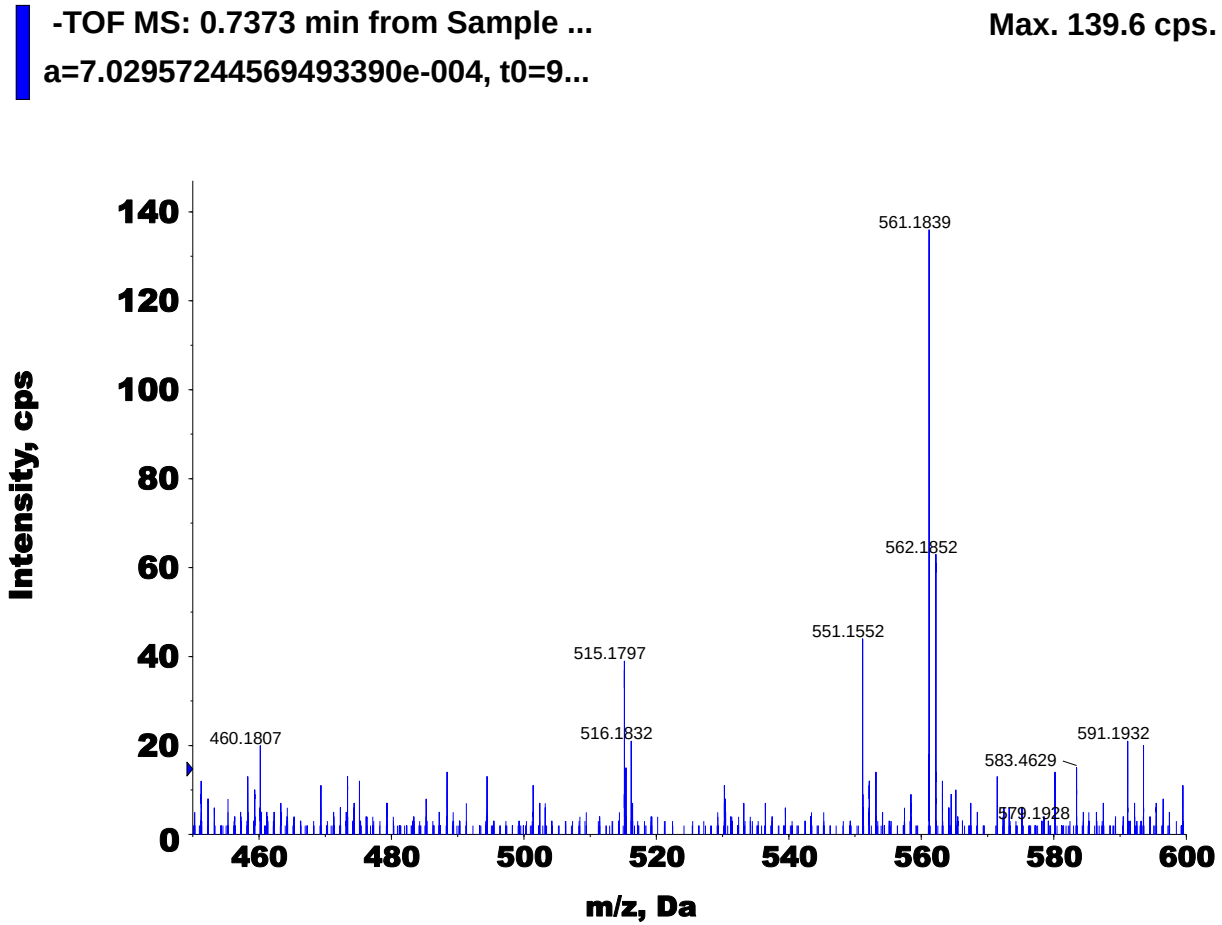


Figure S13. IR spectrum of chlorahupetone A (**1**)

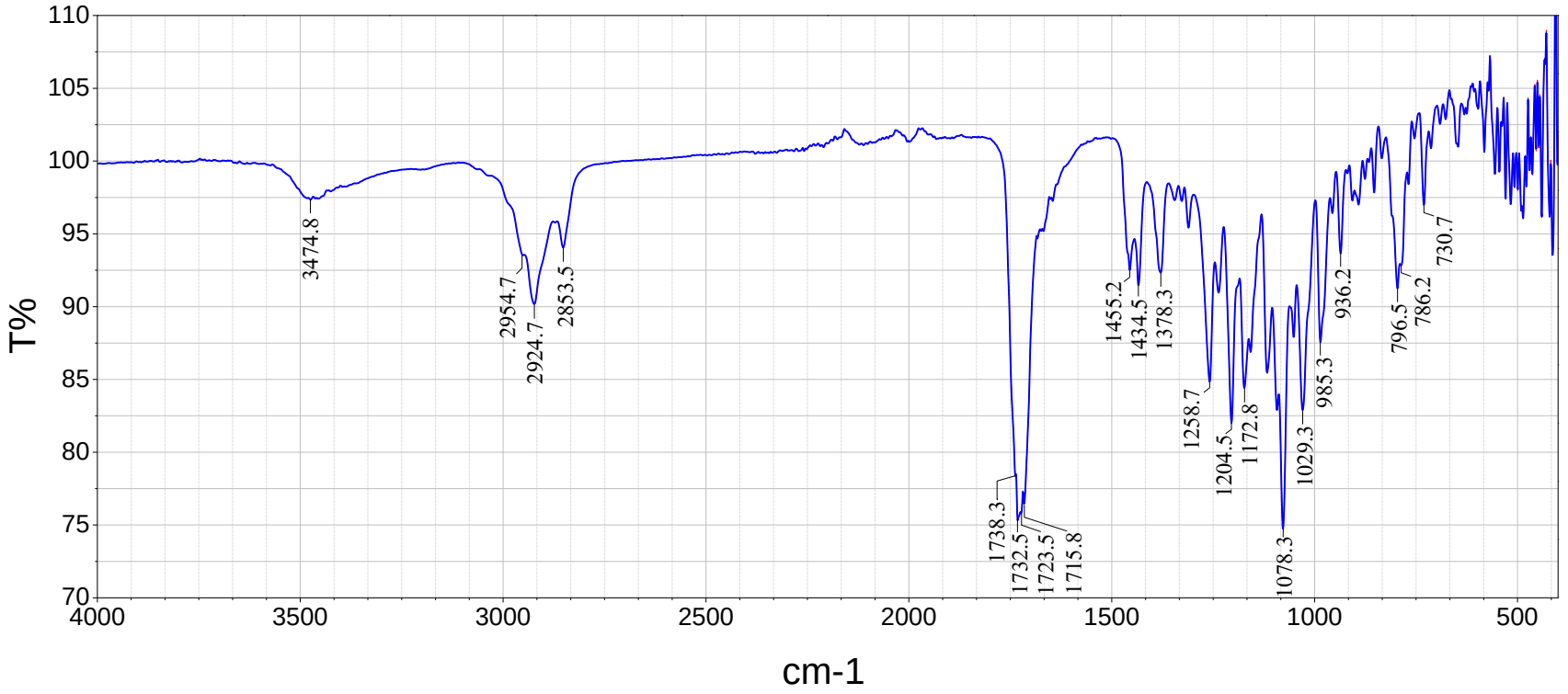


Figure S14. ^{1}H NMR spectrum of chlorahupetone B (**2**) in pyridine-d_5

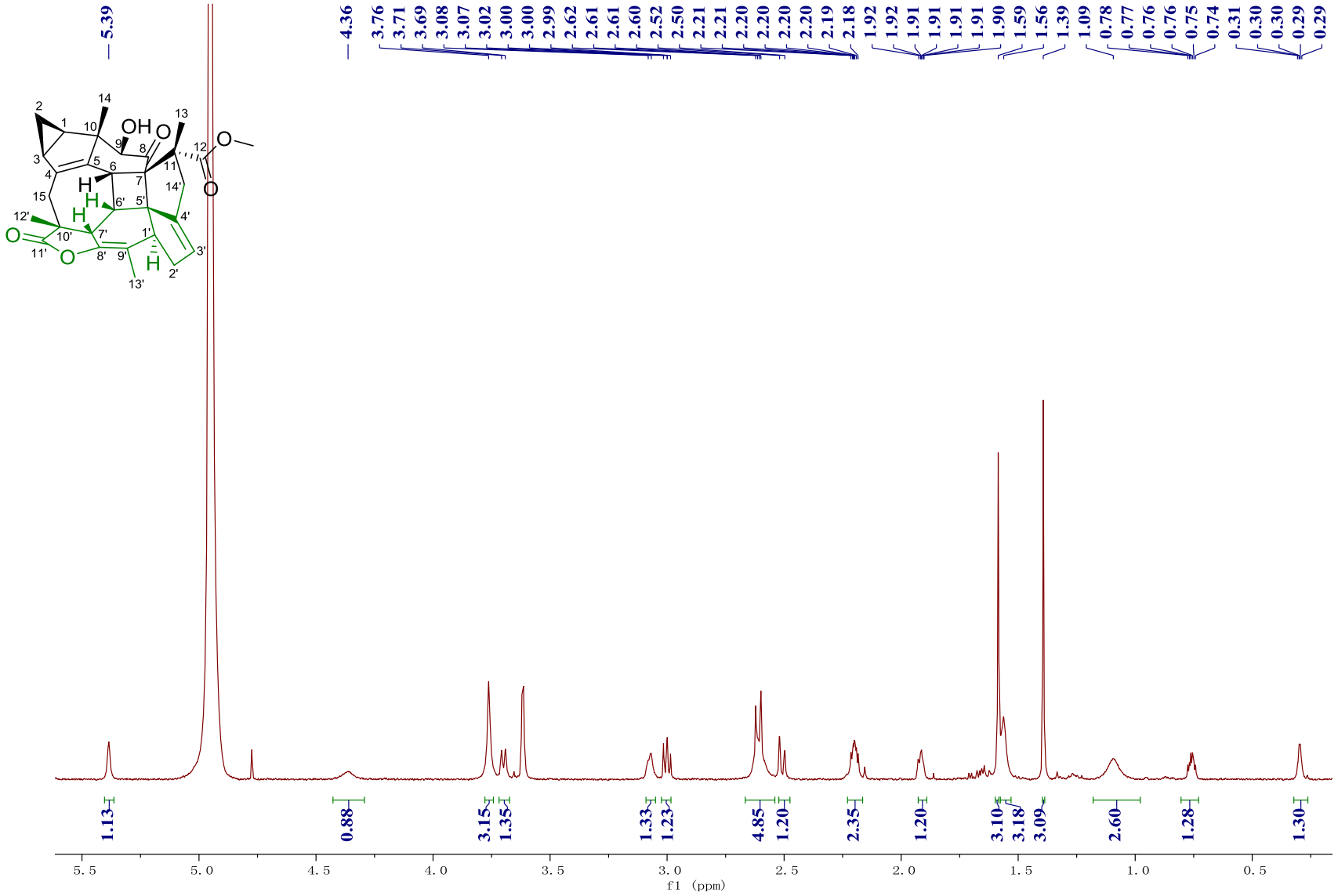


Figure S15. ^{13}C NMR spectrum of chlorahupetone B (**2**) in pyridine-d_5

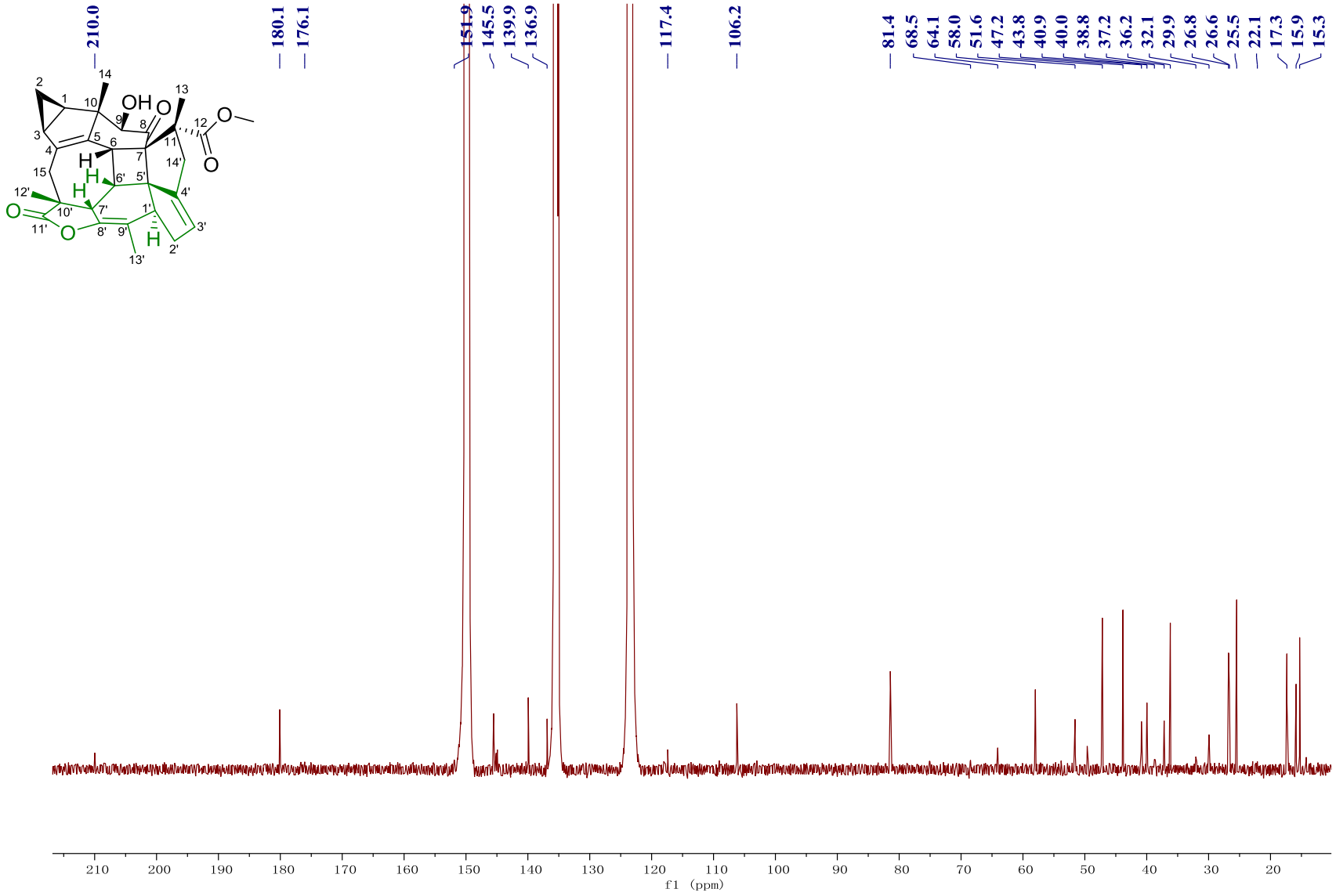


Figure S16. HSQC spectrum of chlorahupetone B (**2**) in pyridine-d_5

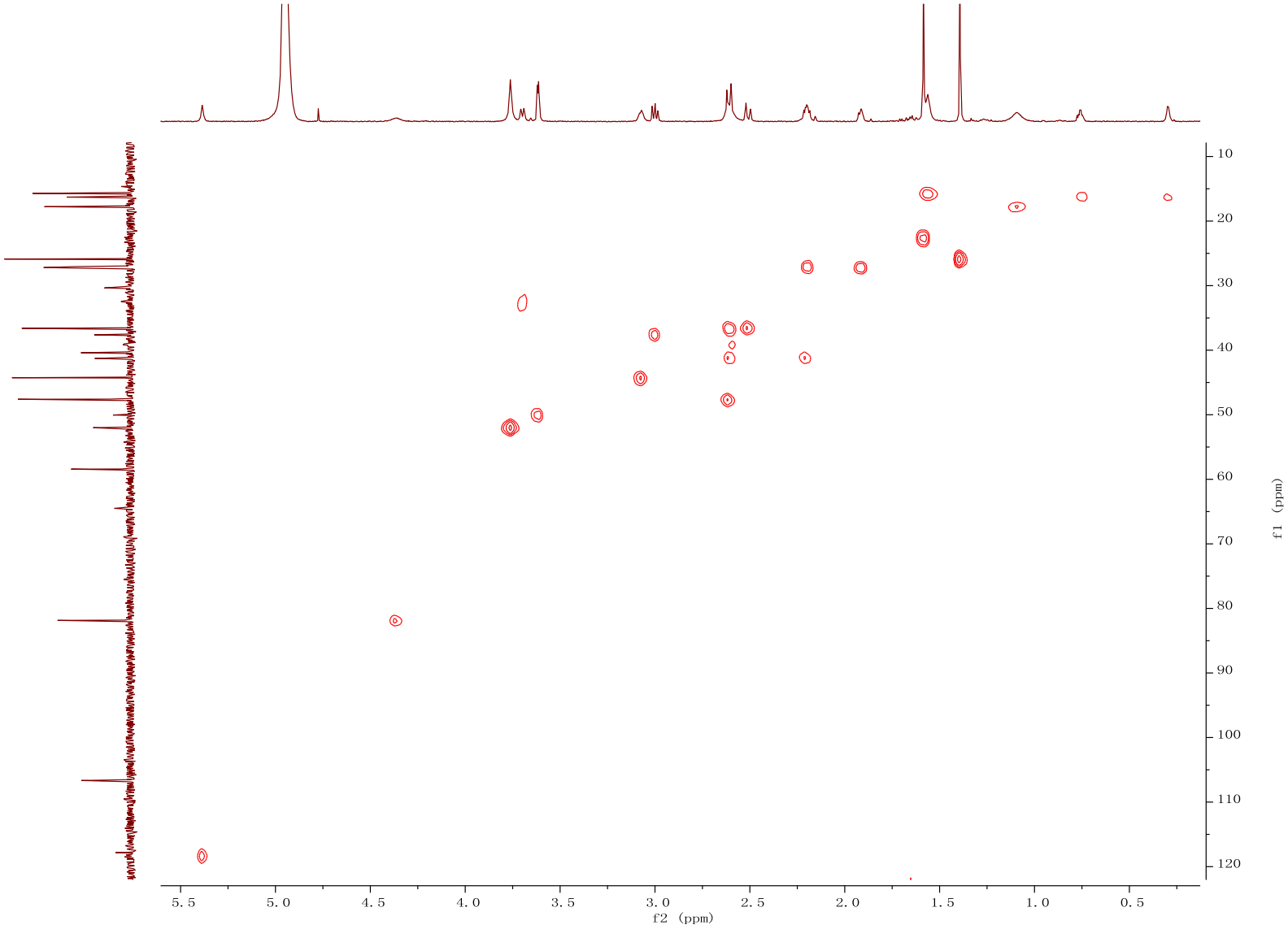


Figure S17. HMBC spectrum of chlorahupetone B (**2**) in pyridine-d_5

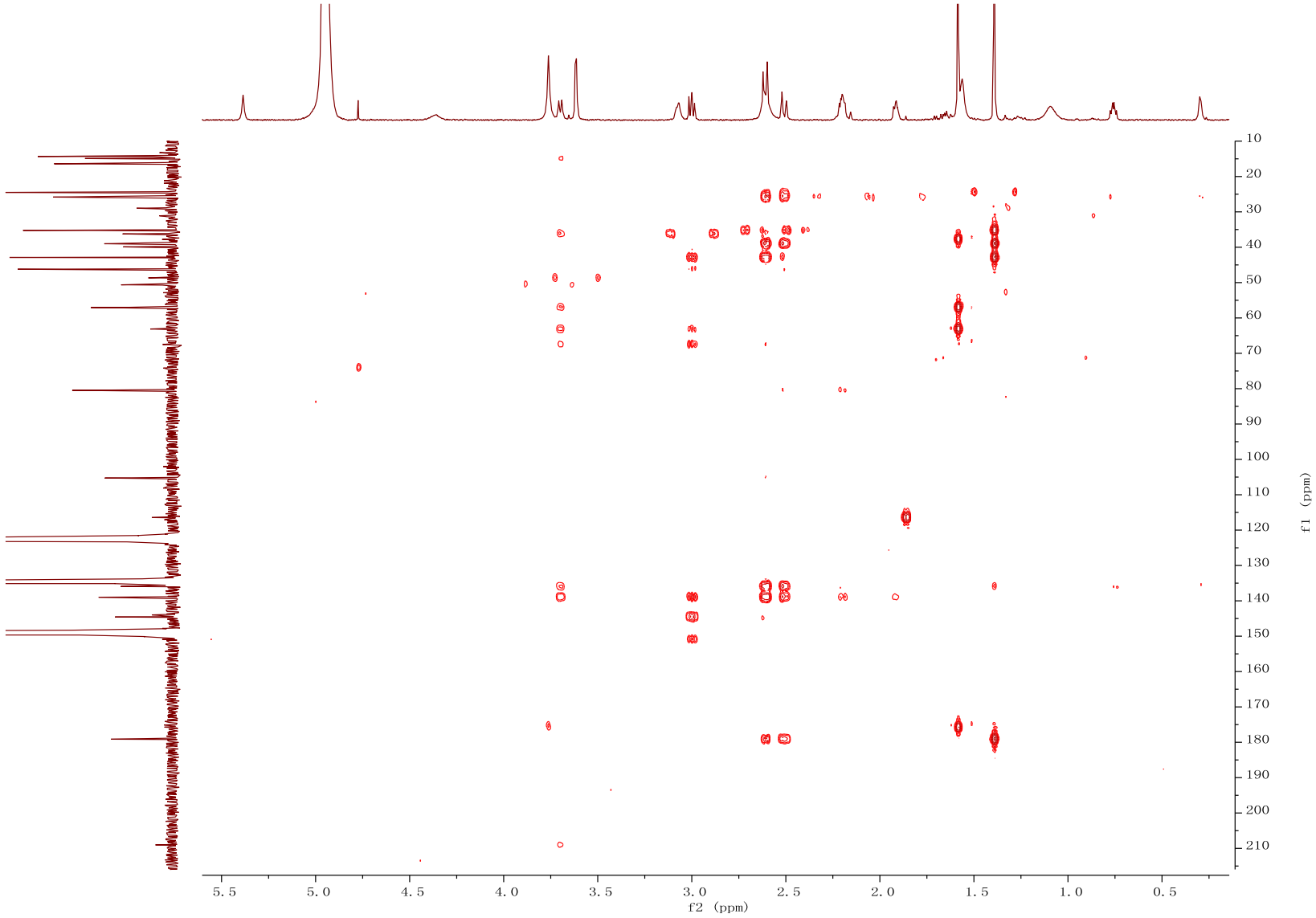


Figure S18. ^{1}H-^{1}H COSY spectrum of chlorahupetone B (**2**) in pyridine-d_5

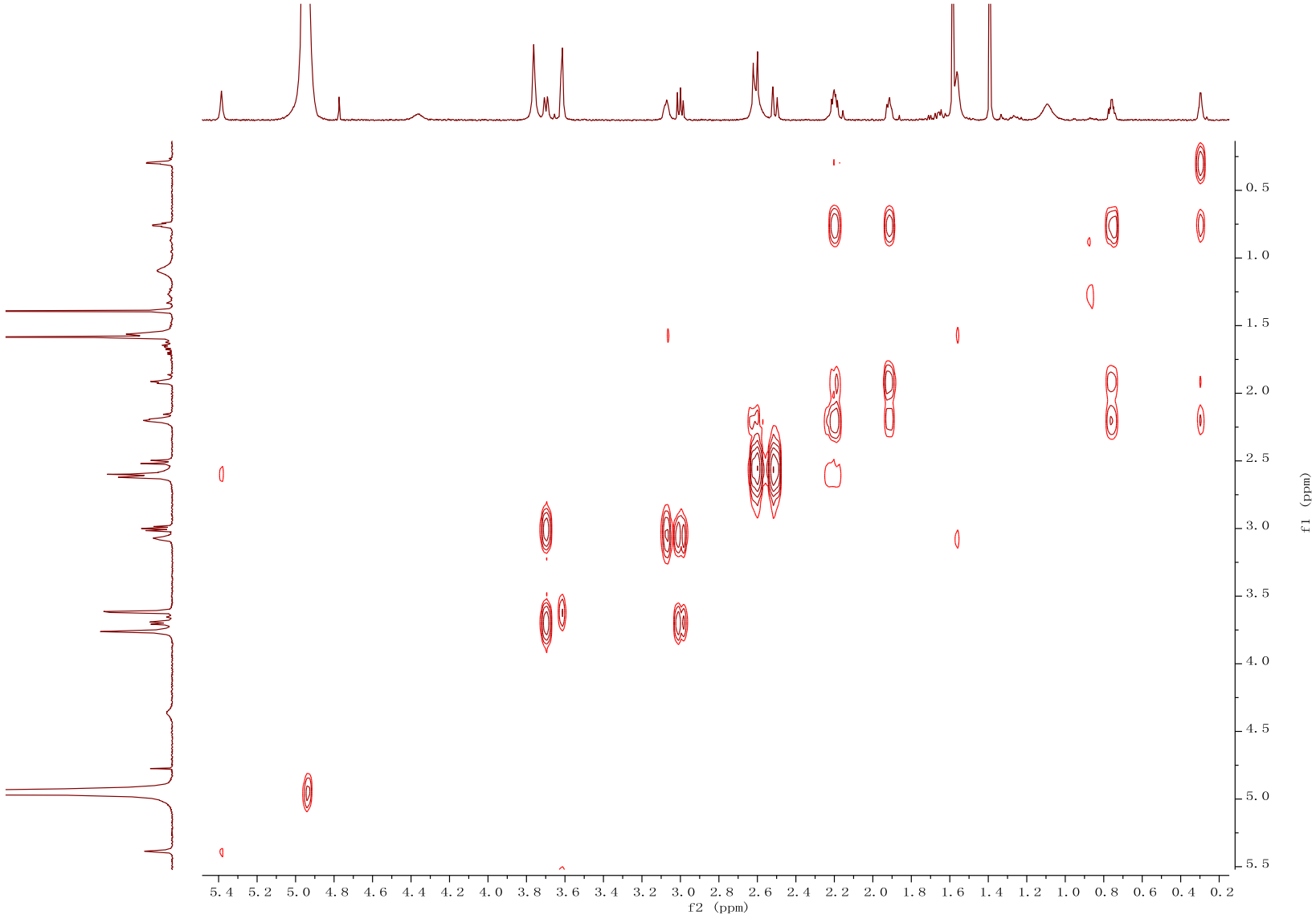


Figure S19. NOESY spectrum of chlorahupetone B (**2**) in pyridine-d_5

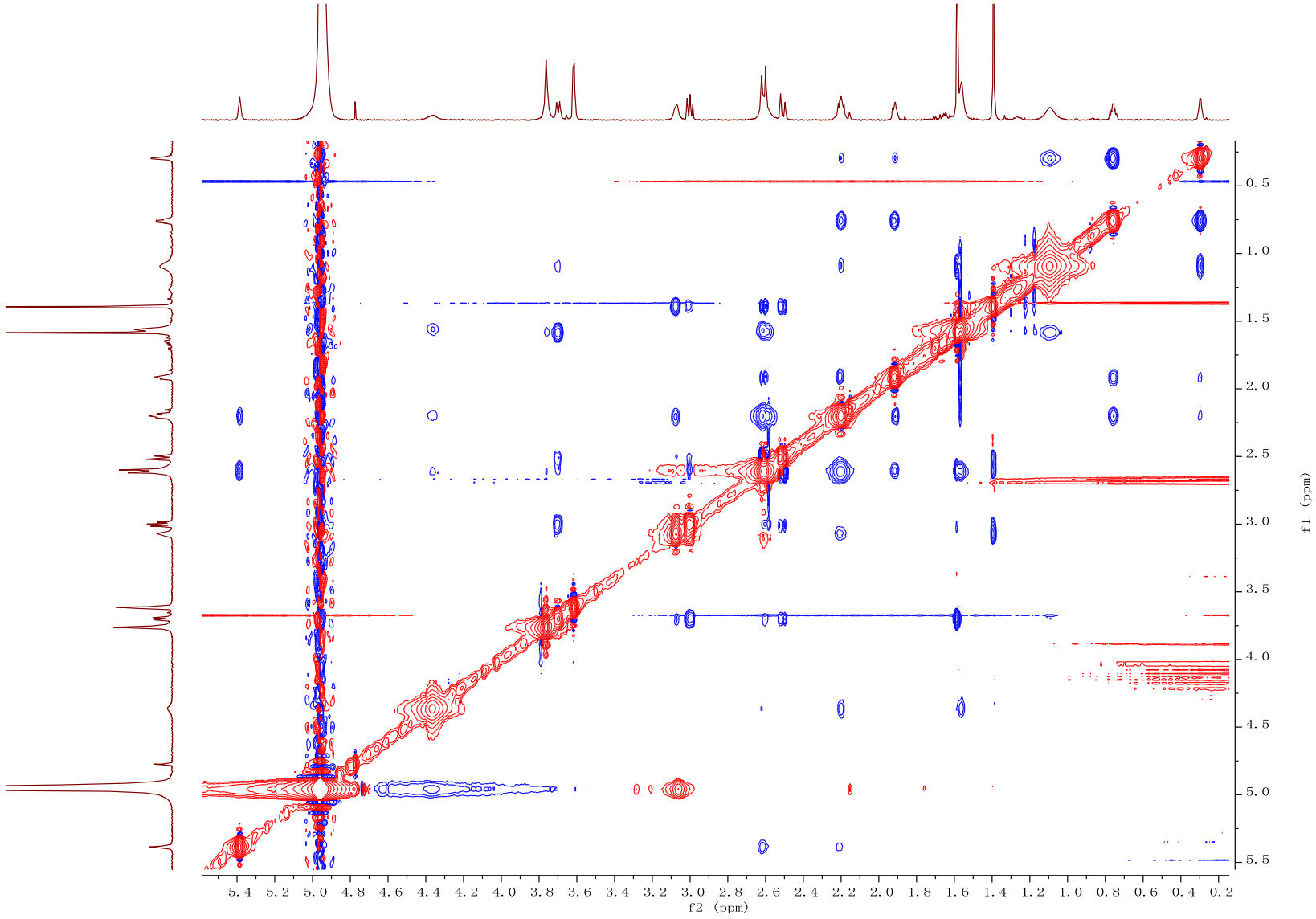


Figure S20. (+)-HRESIMS spectrum of chlorahupetone B (**2**)

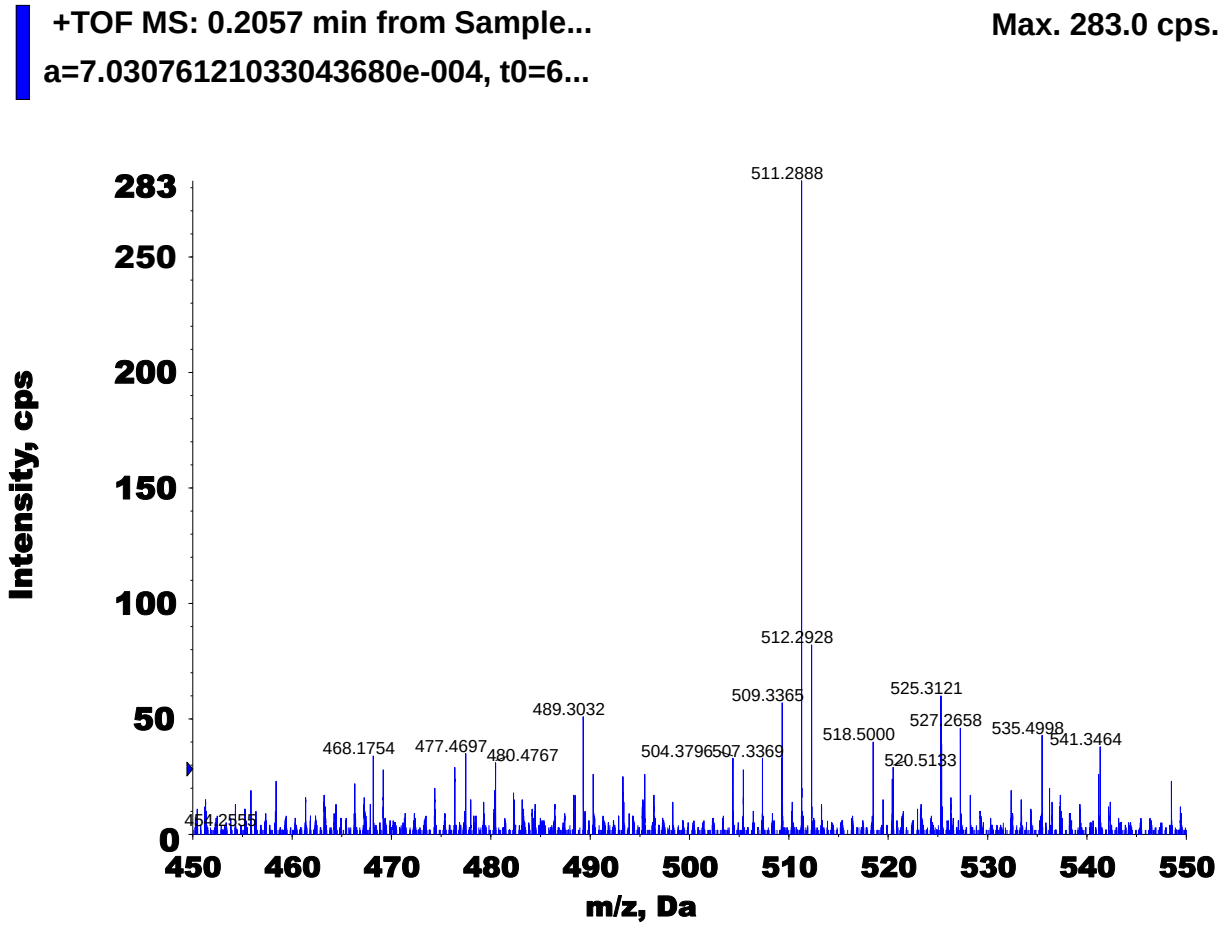


Figure S21. IR spectrum of chlorahupetone B (**2**)

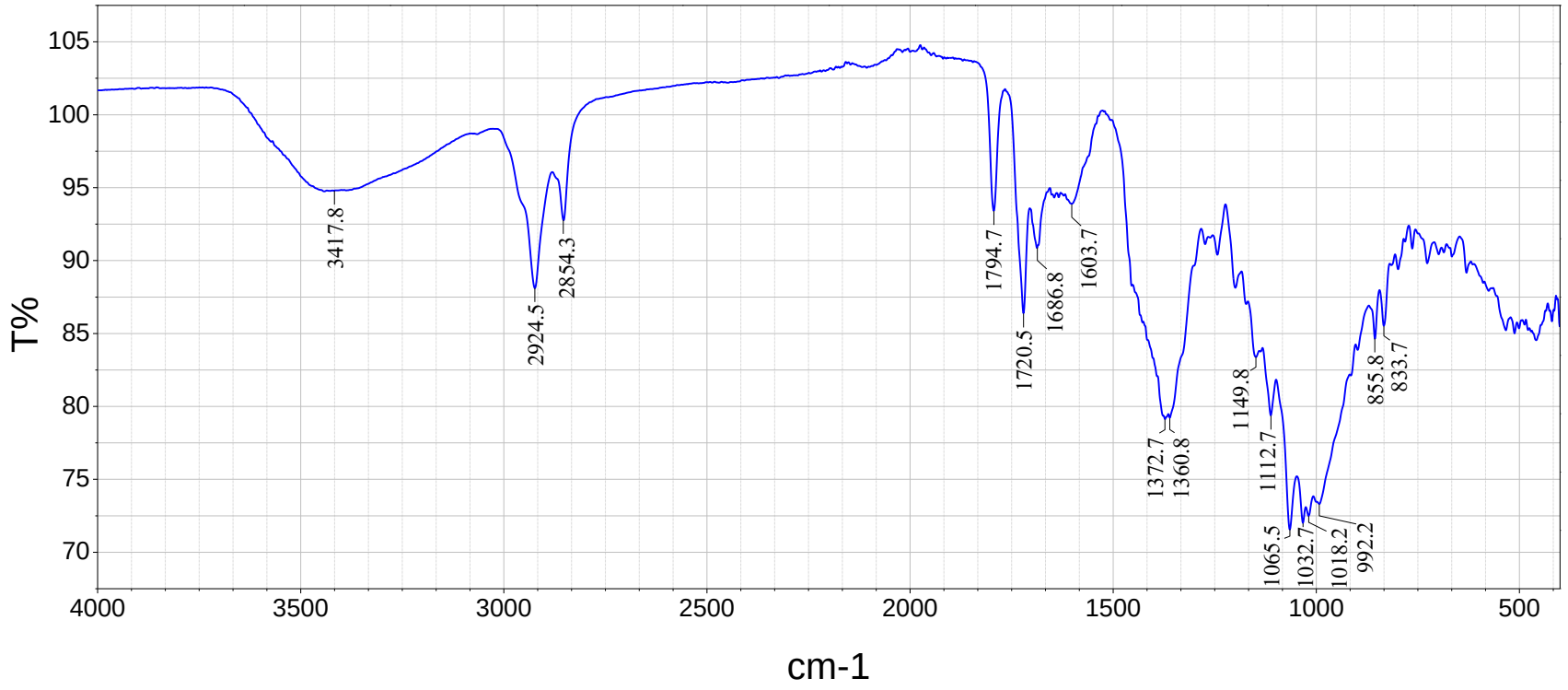


Figure S22. ^{1}H NMR spectrum of chlorahupetone C (**3**) in $CDCl_3$

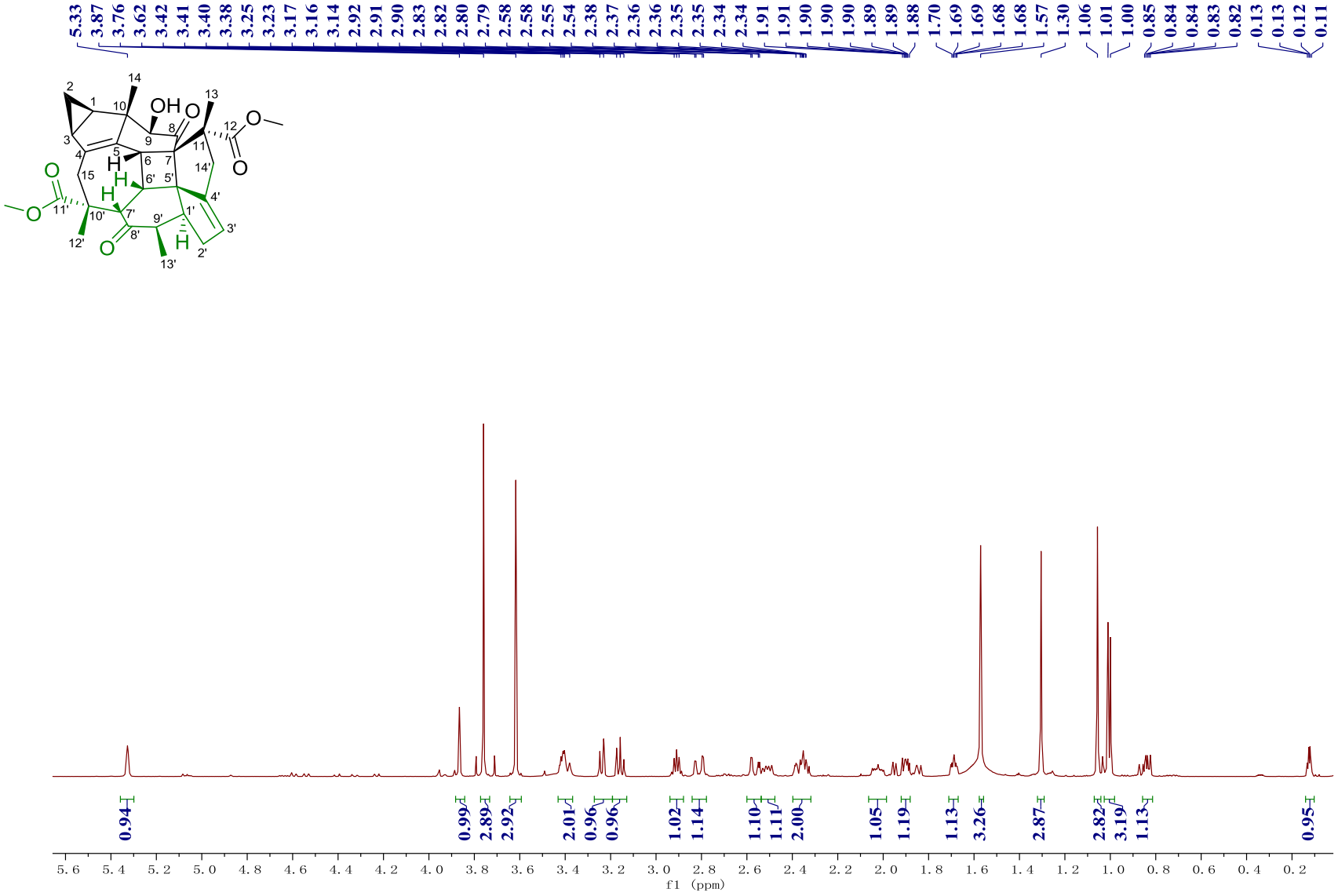


Figure S23. ^{13}C NMR and DEPT spectrum of chlorahupetone C (**3**) in $CDCl_3$

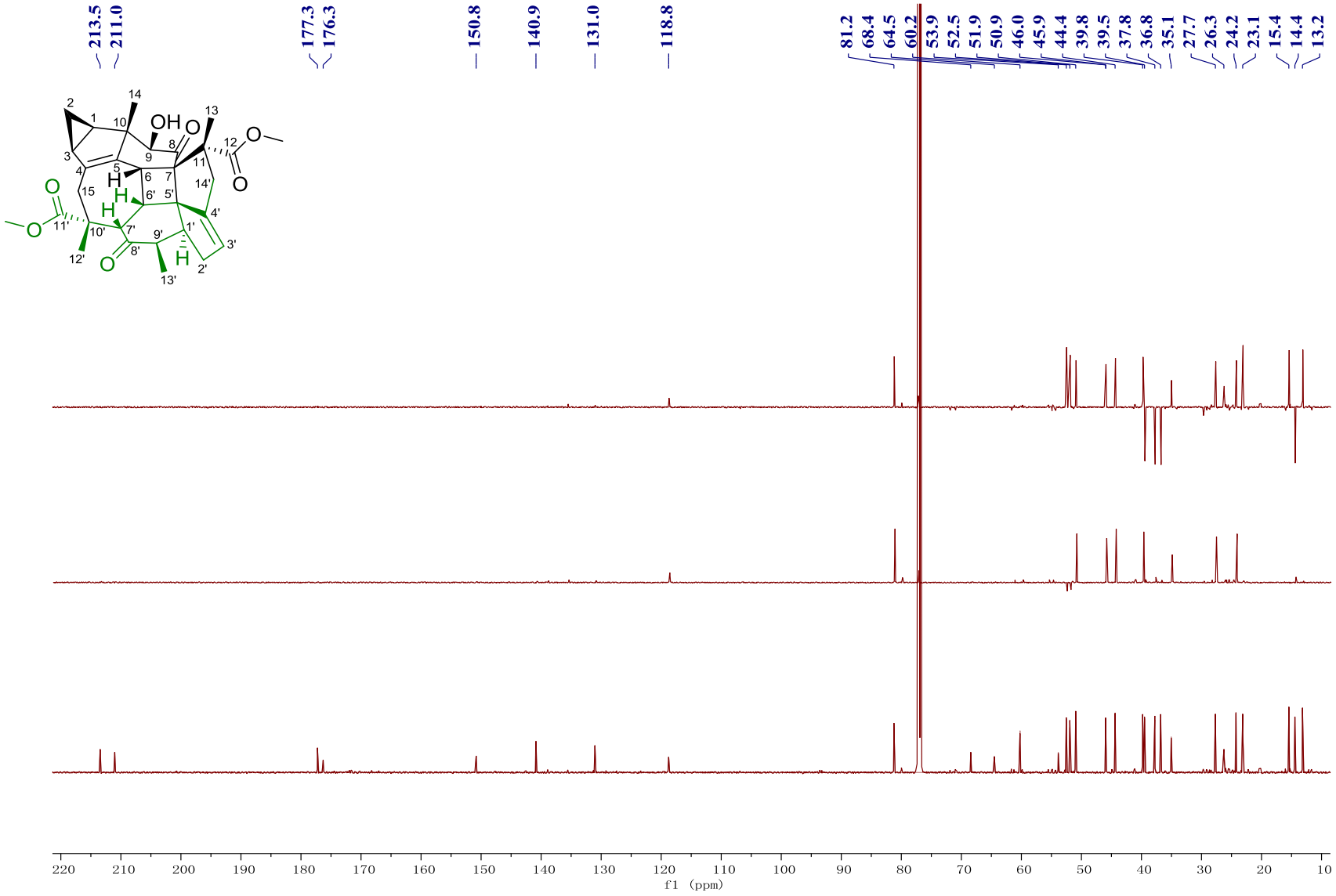


Figure S24. HSQC spectrum of chlorahupetone C (**3**) in $CDCl_3$

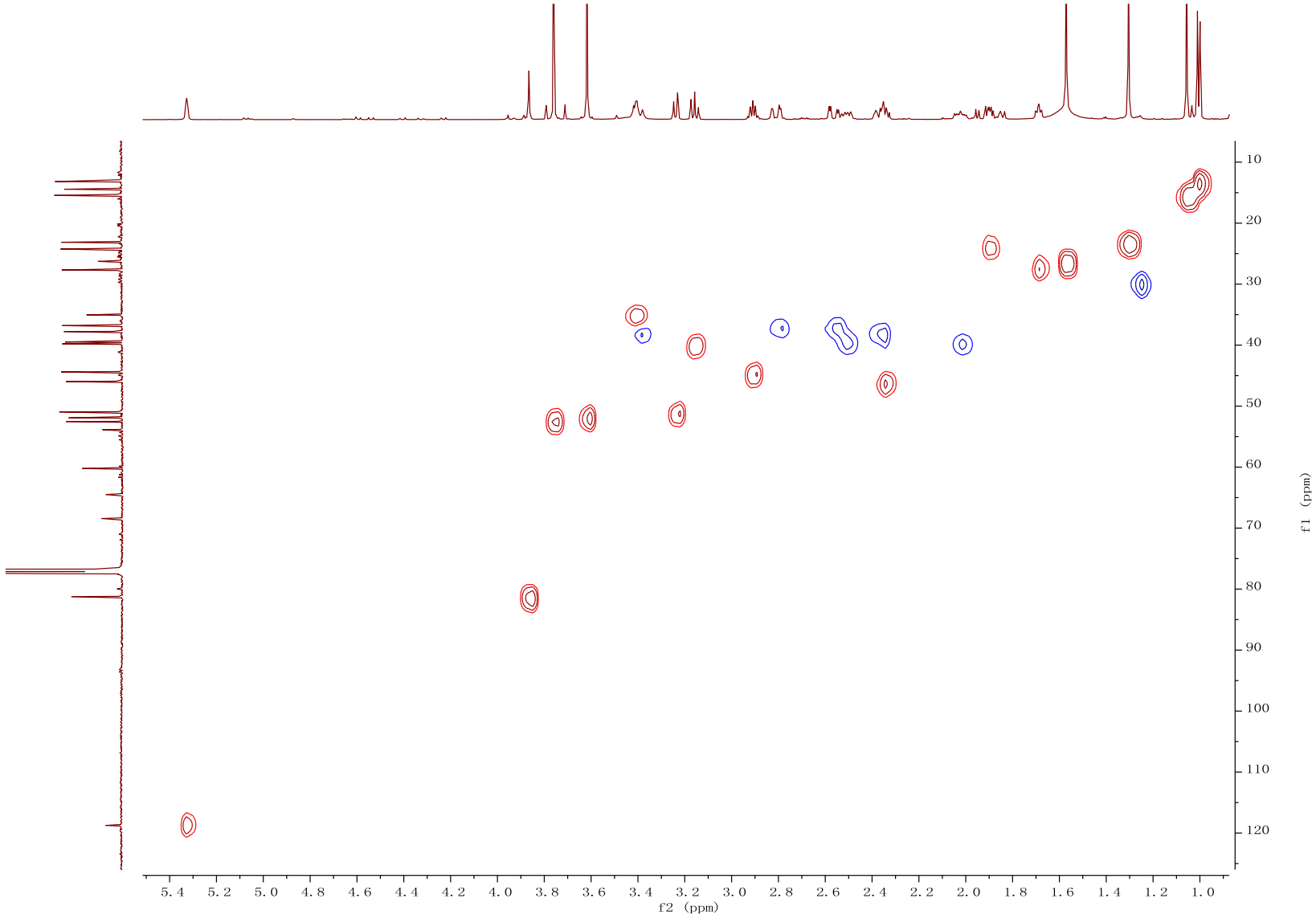


Figure S25. HMBC spectrum of chlorahupetone C (**3**) in $CDCl_3$

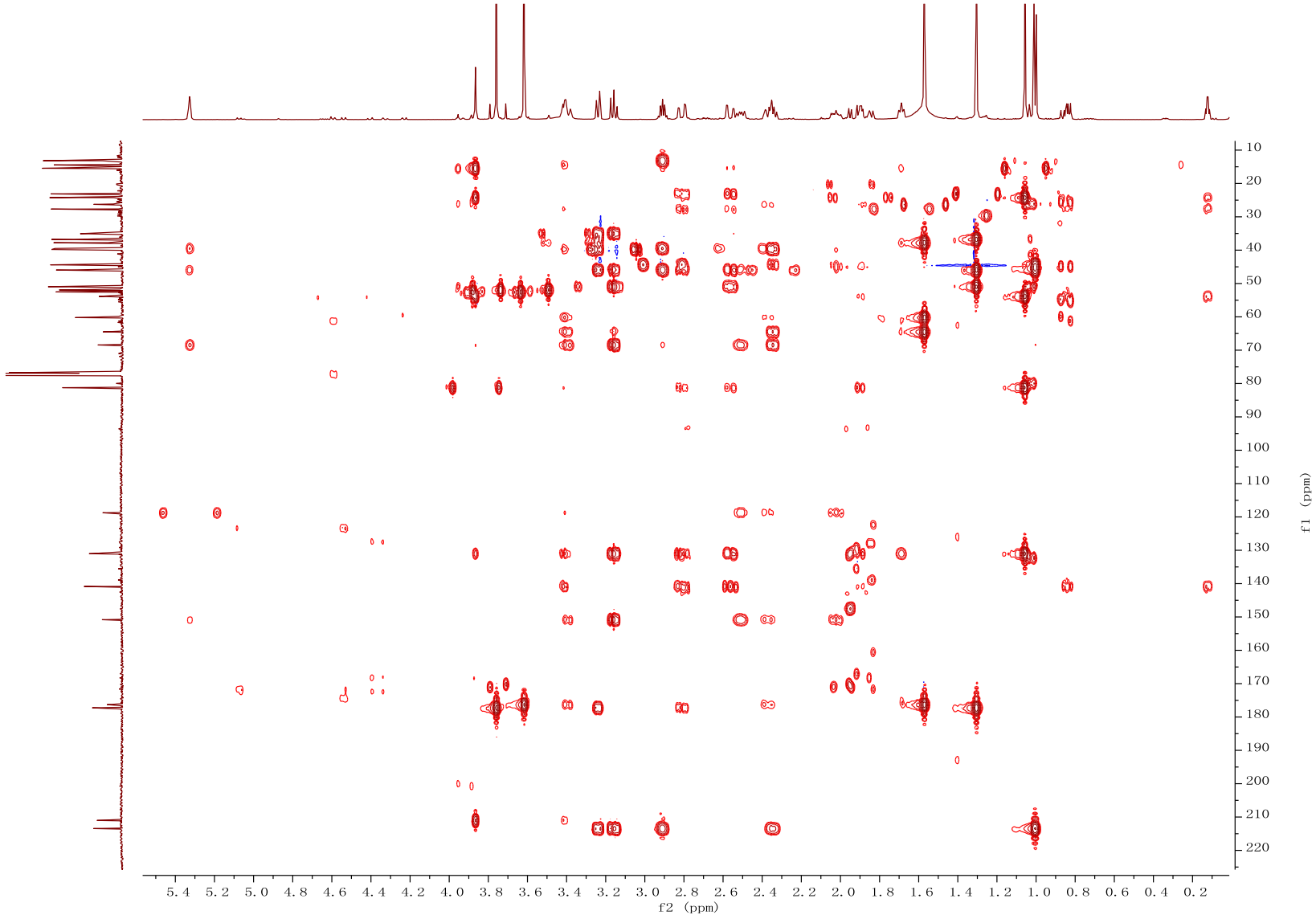


Figure S26. ^{1}H-^{1}H COSY spectrum of chlorahupetone C (**3**) in $CDCl_3$

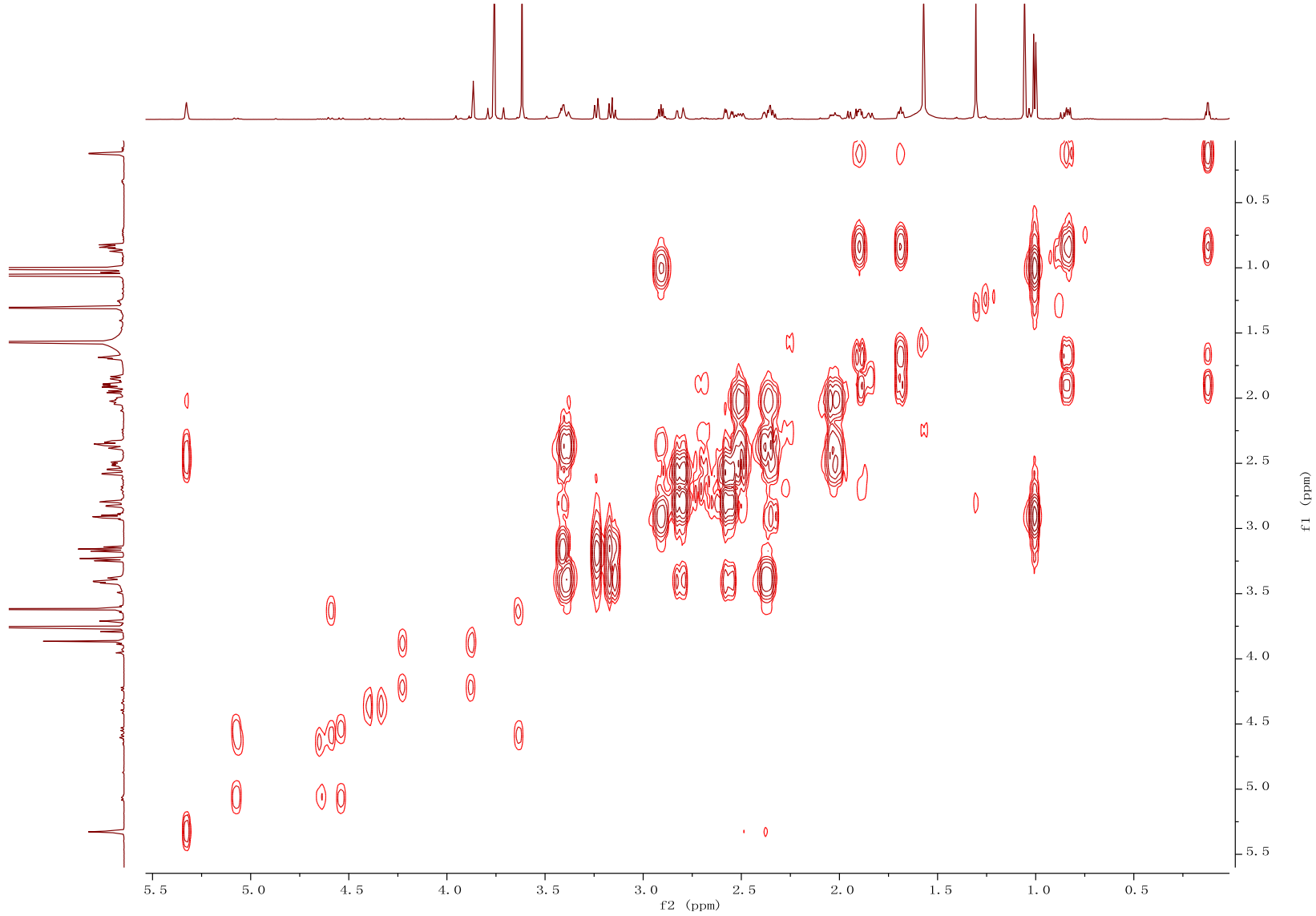


Figure S27. NOESY spectrum of chlorahupetone C (**3**) in $CDCl_3$

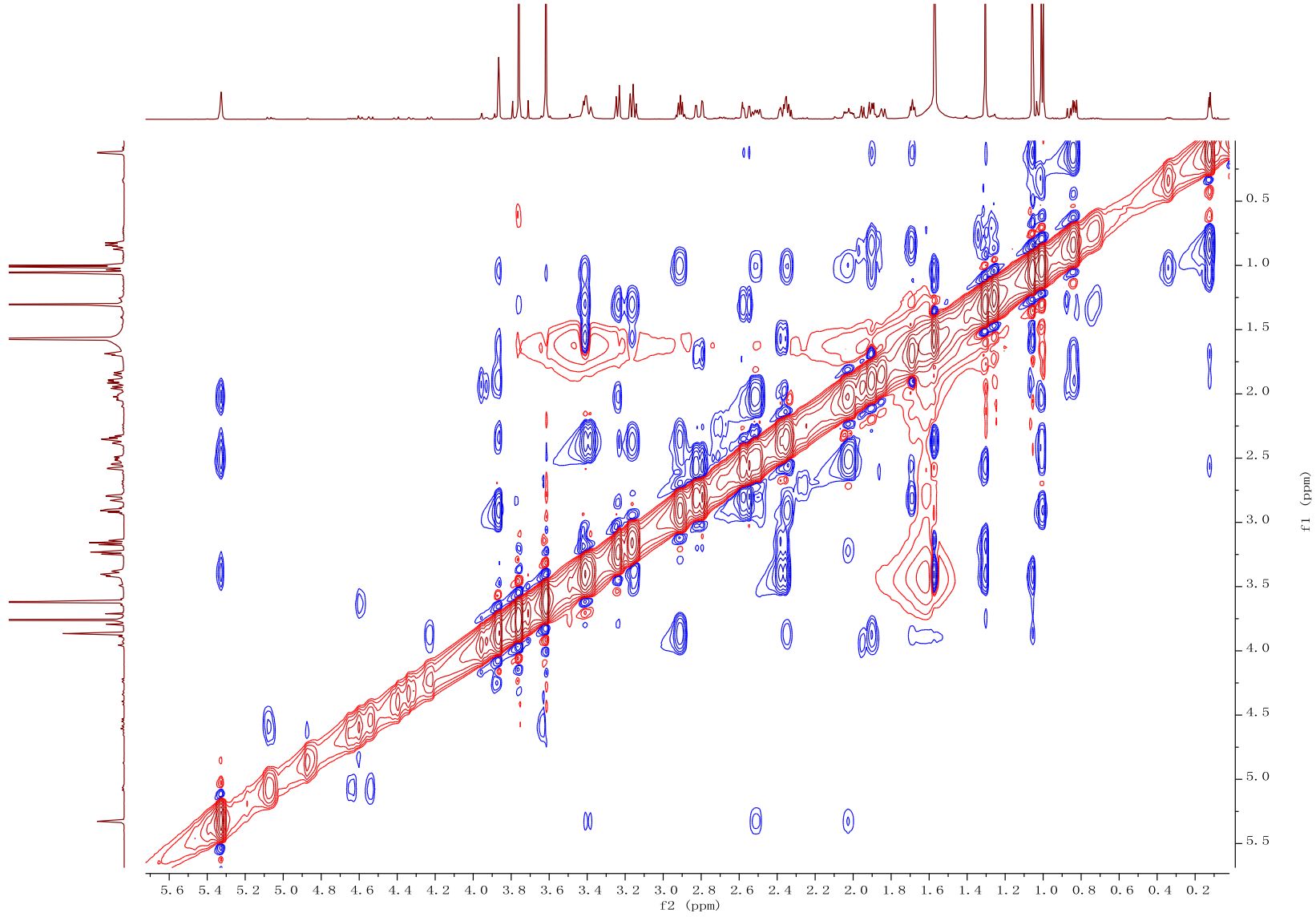


Figure S28. (+)-HRESIMS spectrum of chlorahupetone C (**3**)

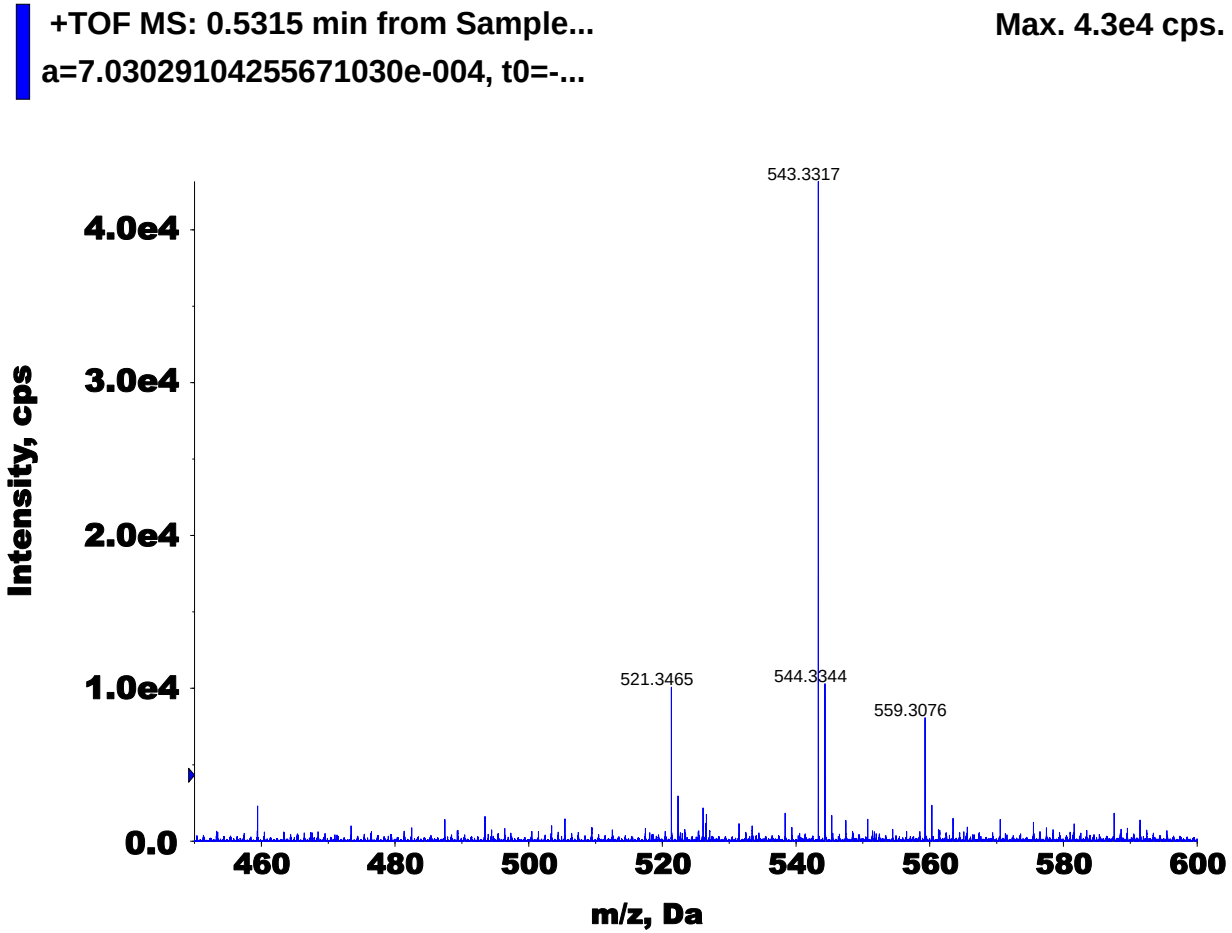


Figure S29. IR spectrum of chlorahupetone C (**3**)

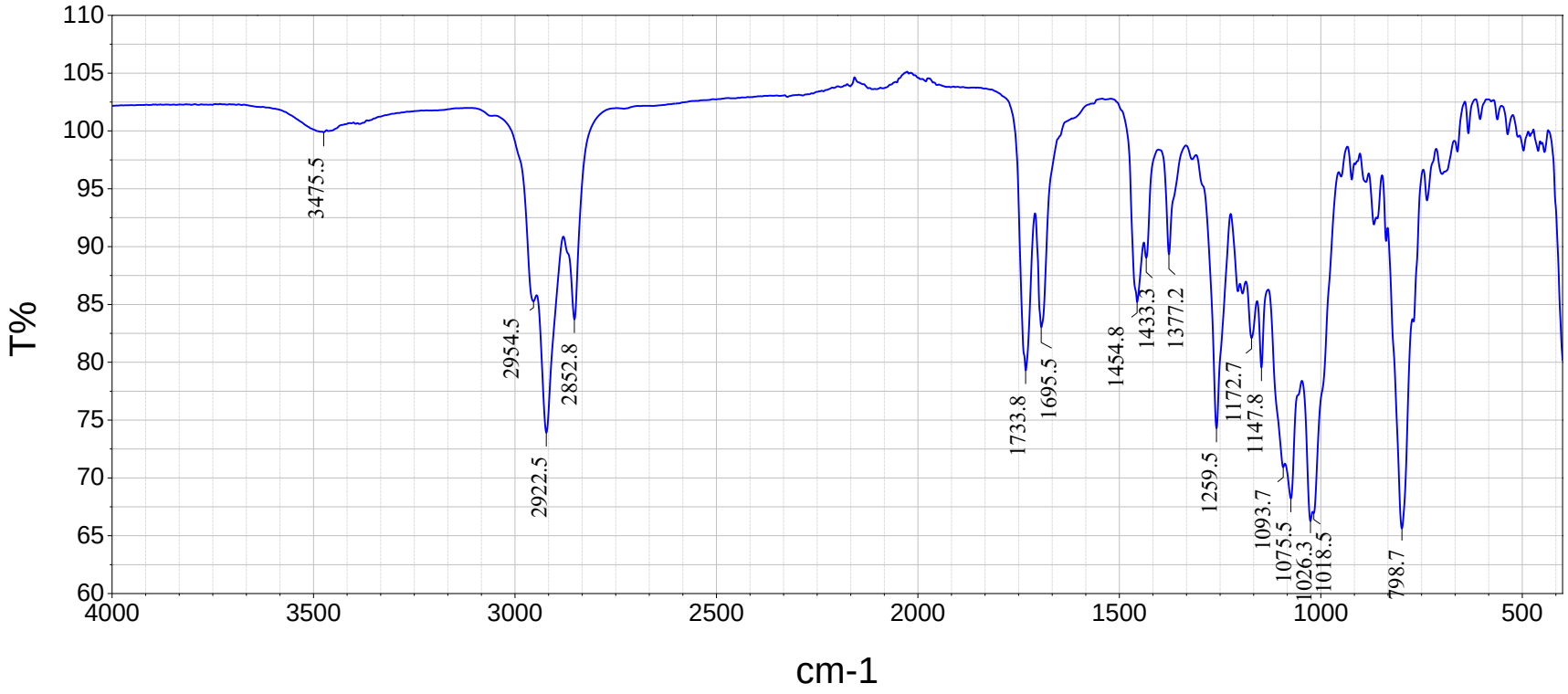


Figure S30. ^{1}H NMR spectrum of chlorahupetone D (**4**) in pyridine-d_5

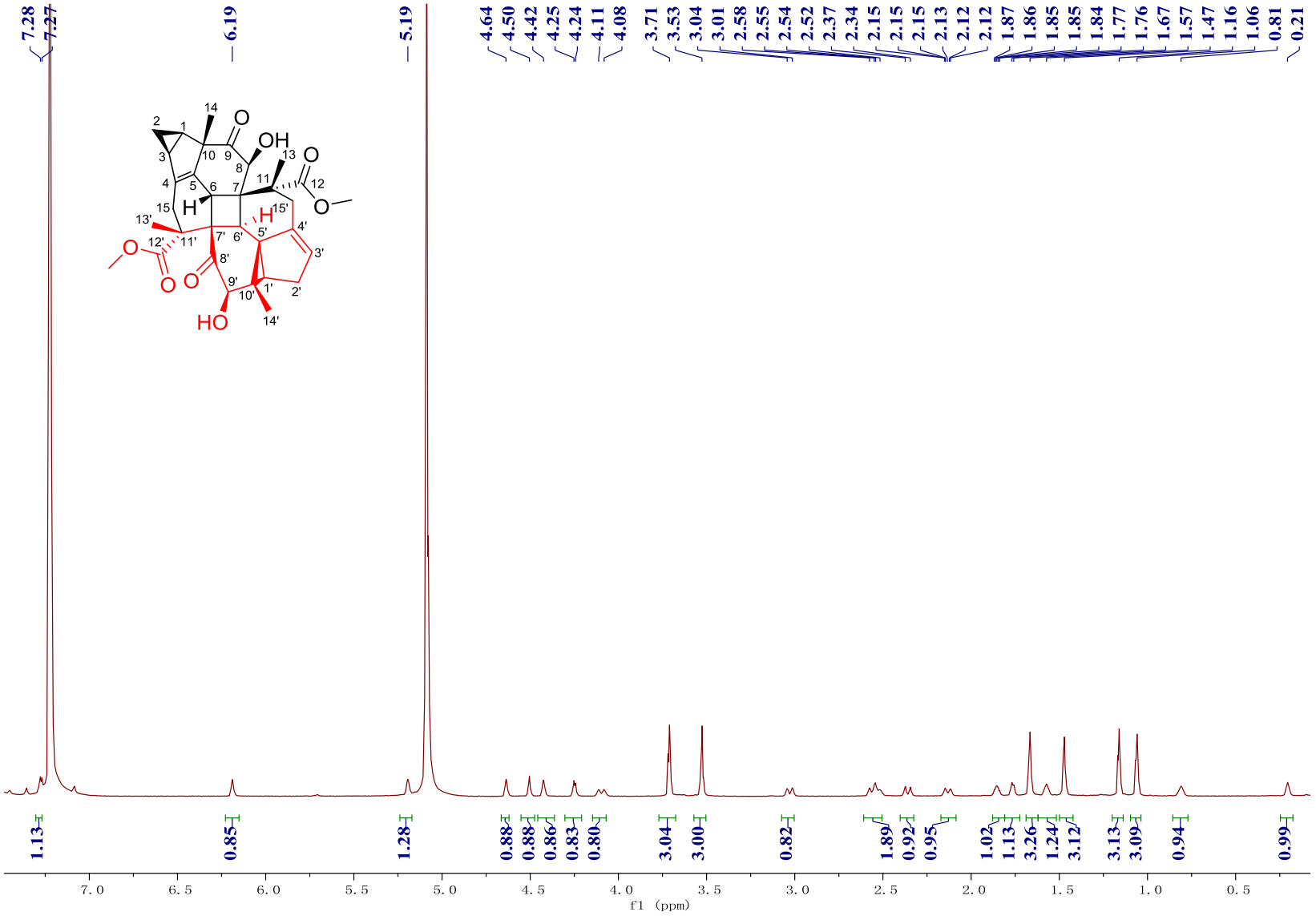


Figure S31. ^{13}C NMR and DEPT spectrum of chlorahupetone D (**4**) in pyridine-d_5

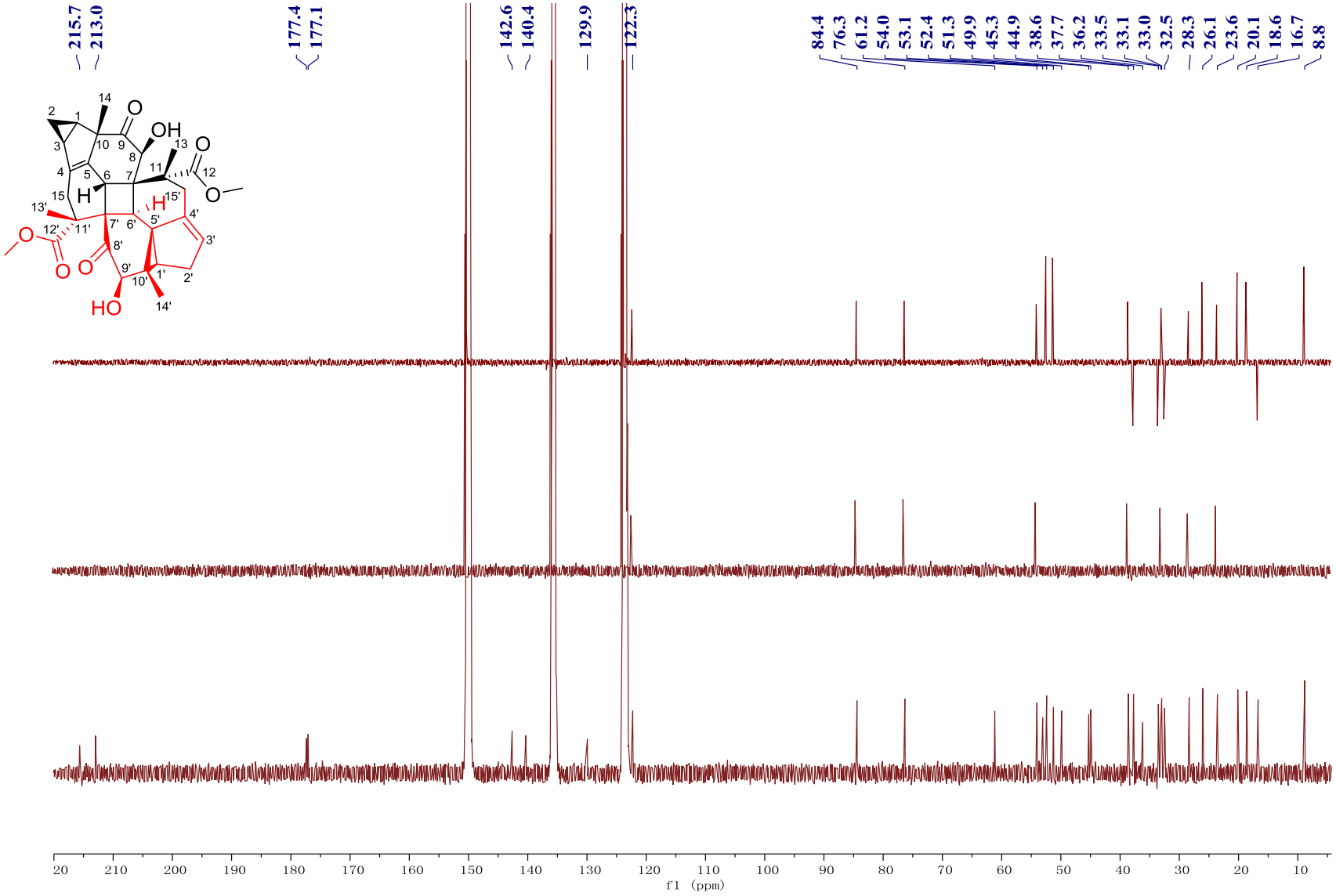


Figure S32. HSQC spectrum of chlorahupetone D (**4**) in pyridine-d_5

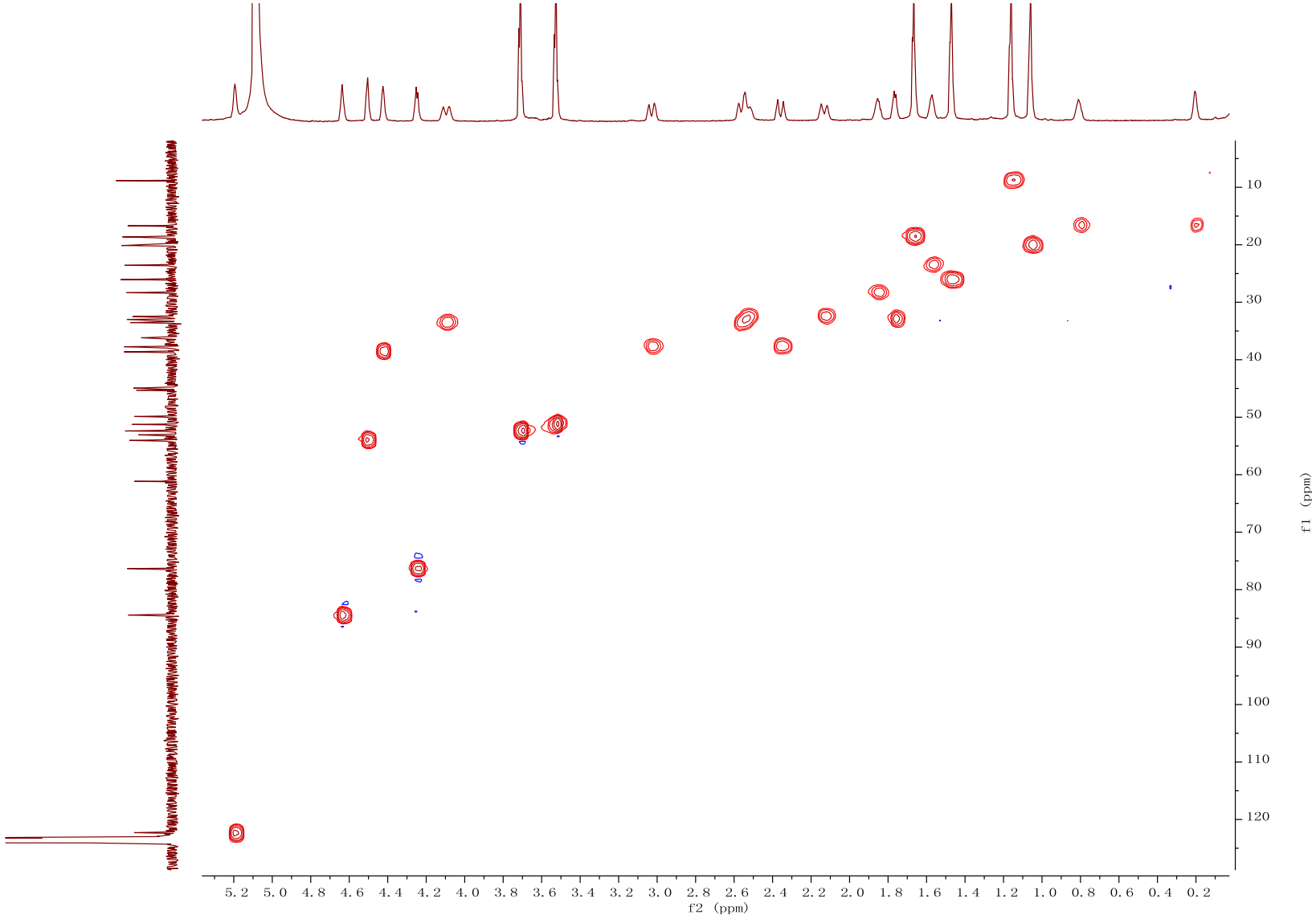


Figure S33. HMBC spectrum of chlorahupetone D (**4**) in pyridine-d_5

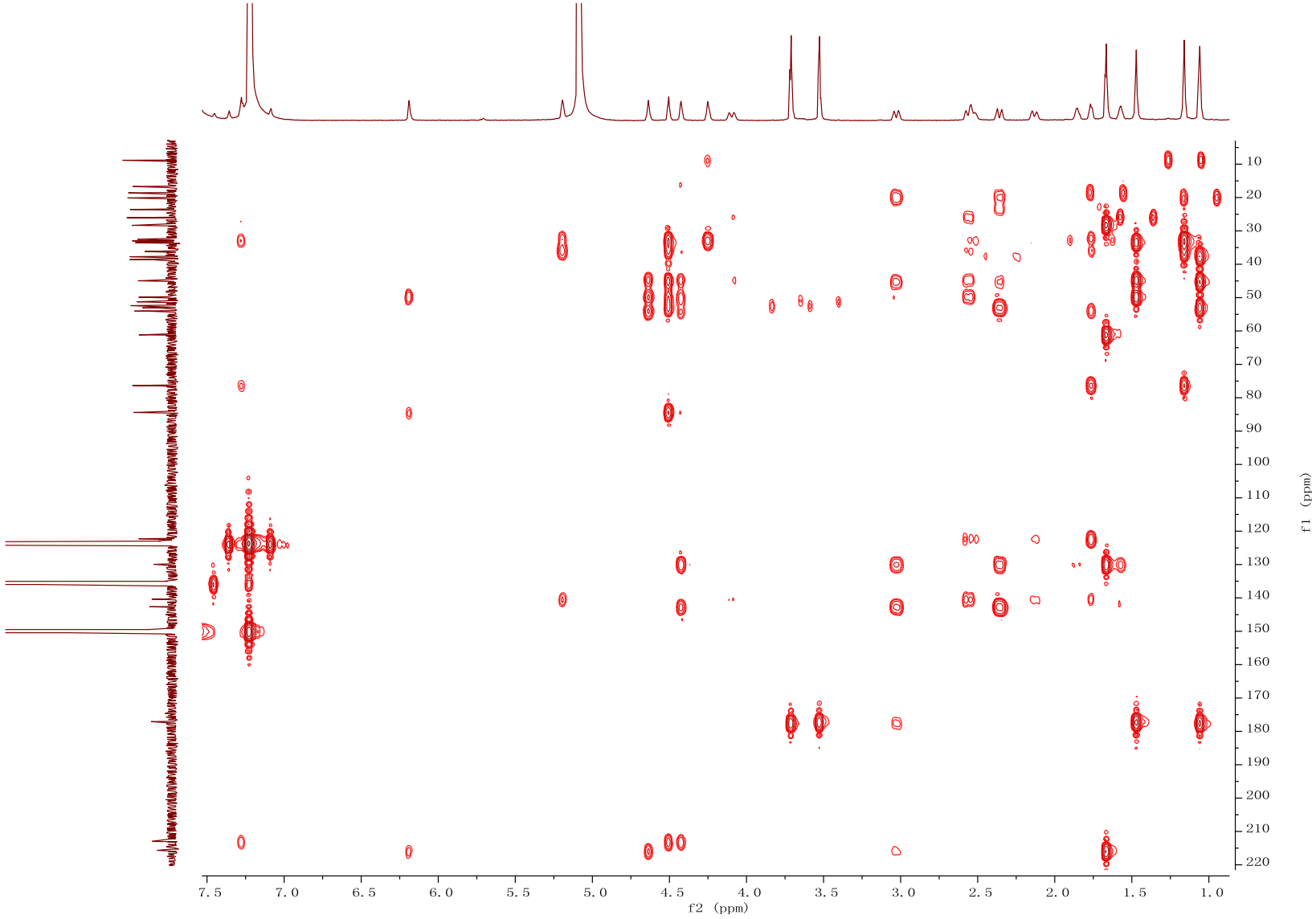


Figure S34. ^{1}H-^{1}H COSY spectrum of chlorahupetone D (**4**) in pyridine-d_5

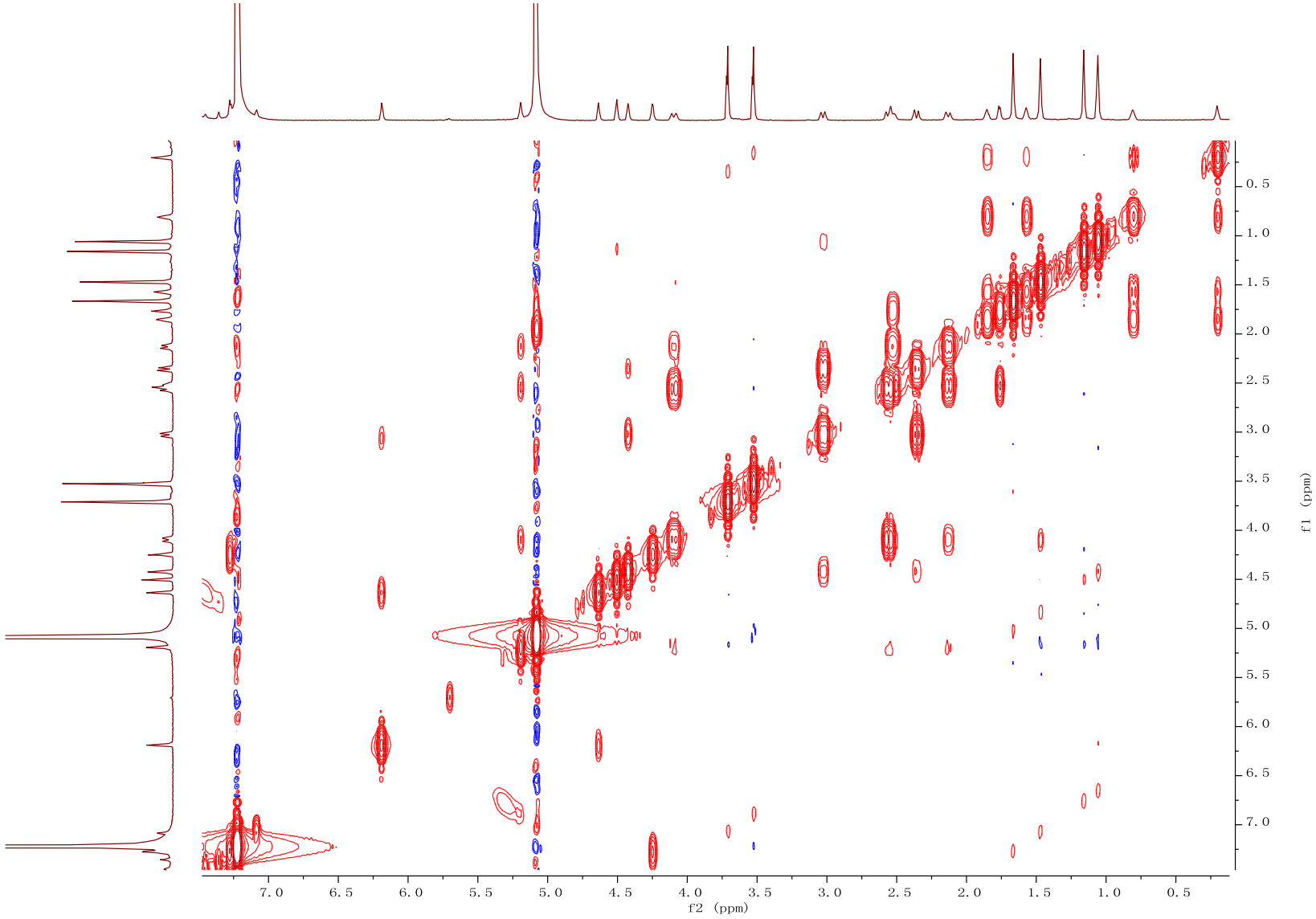


Figure S35. NOESY spectrum of chlorahupetone D (**4**) in pyridine-d_5

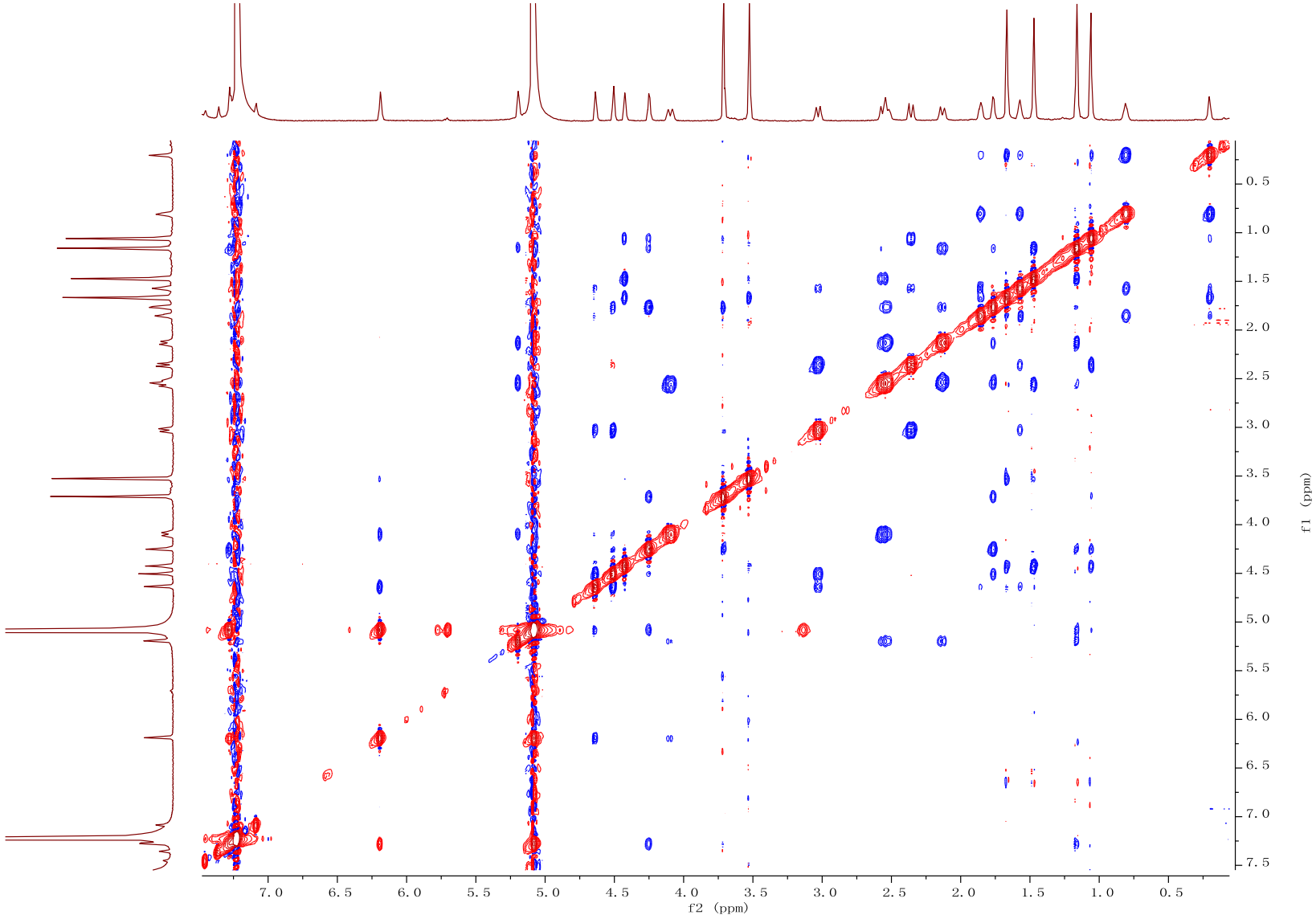


Figure S36. (+)-HRESIMS spectrum of chlorahupetone D (**4**)

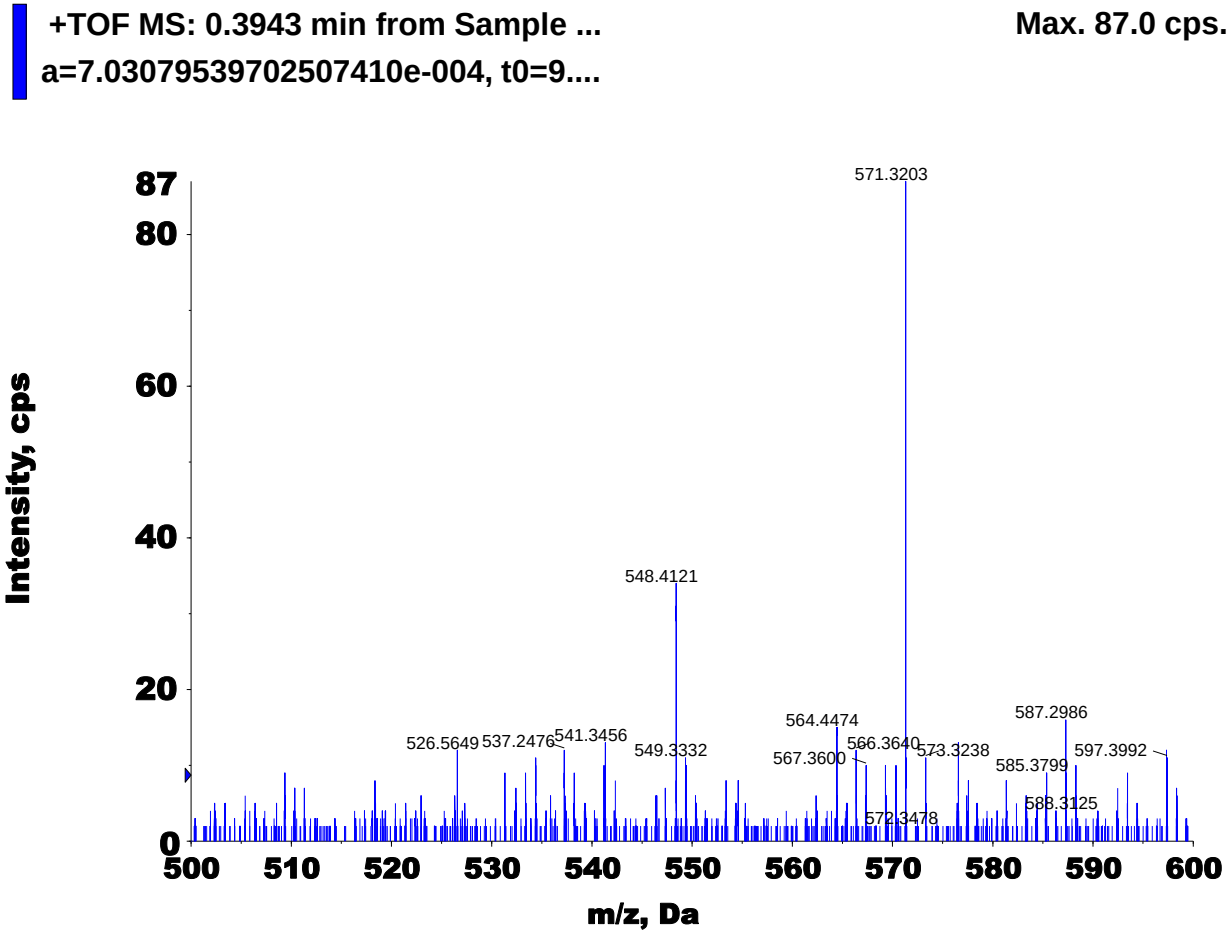


Figure S37. IR spectrum of chlorahupetone D (**4**)

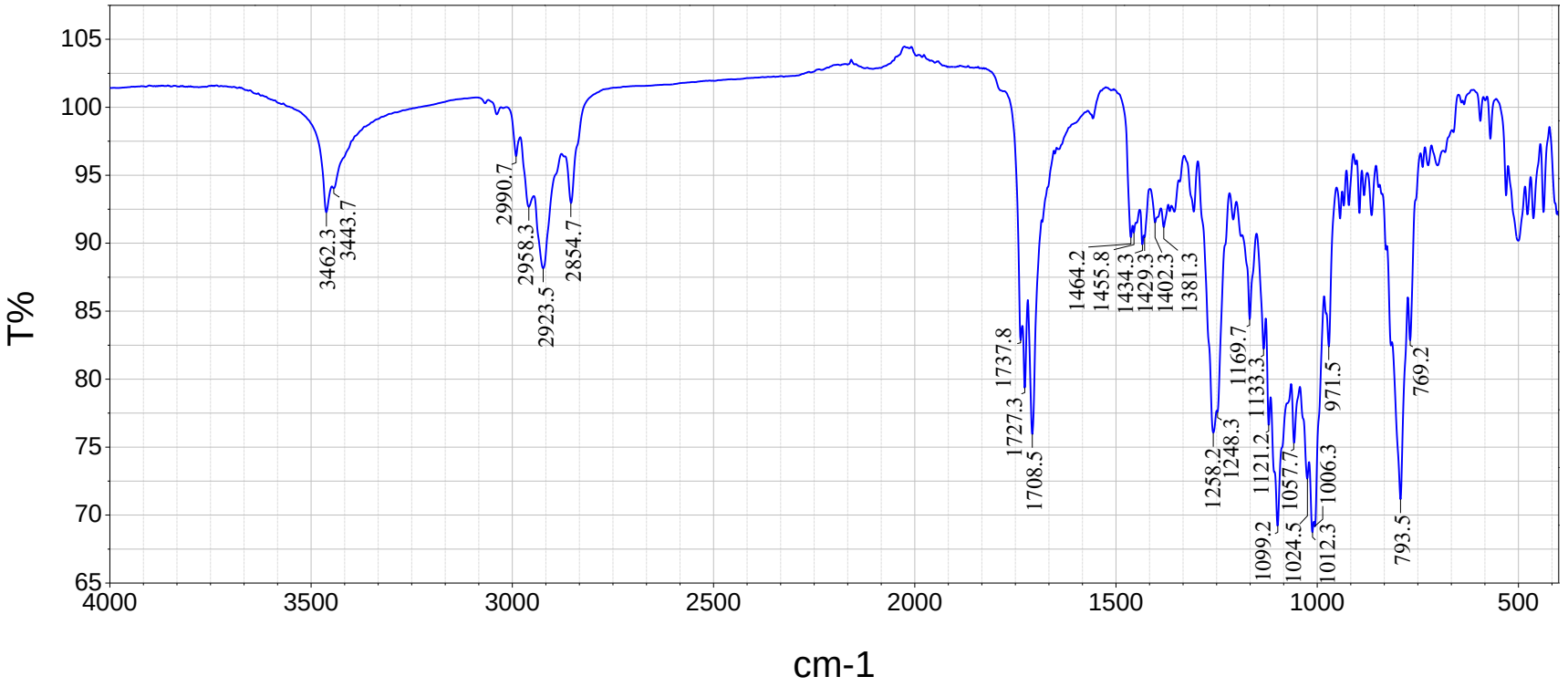


Figure S38. ^{1}H NMR spectrum of chlorahupetone E (**5**) in $CDCl_3$

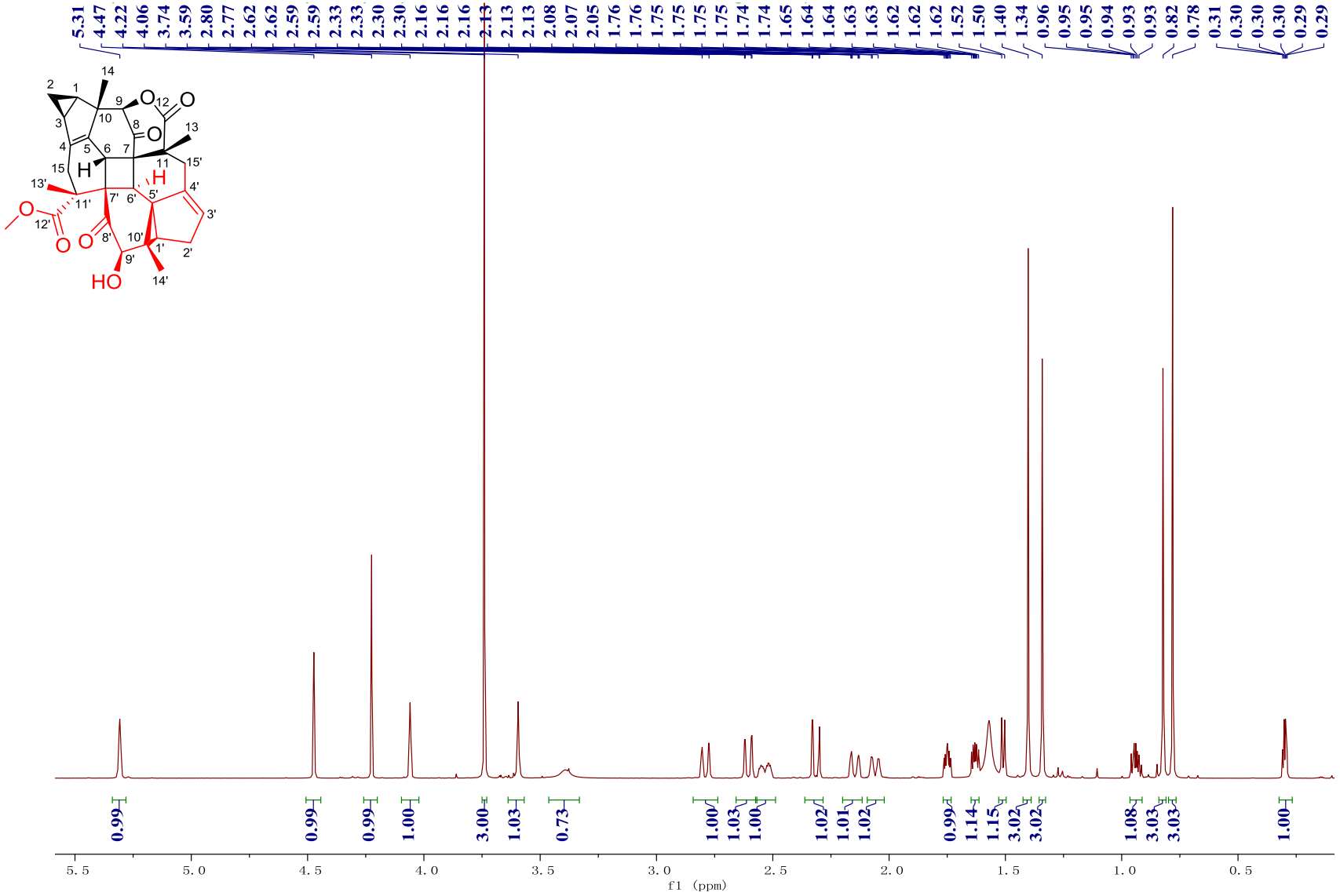


Figure S39. ^{13}C NMR and DEPT spectrum of chlorahupetone E (**5**) in $CDCl_3$

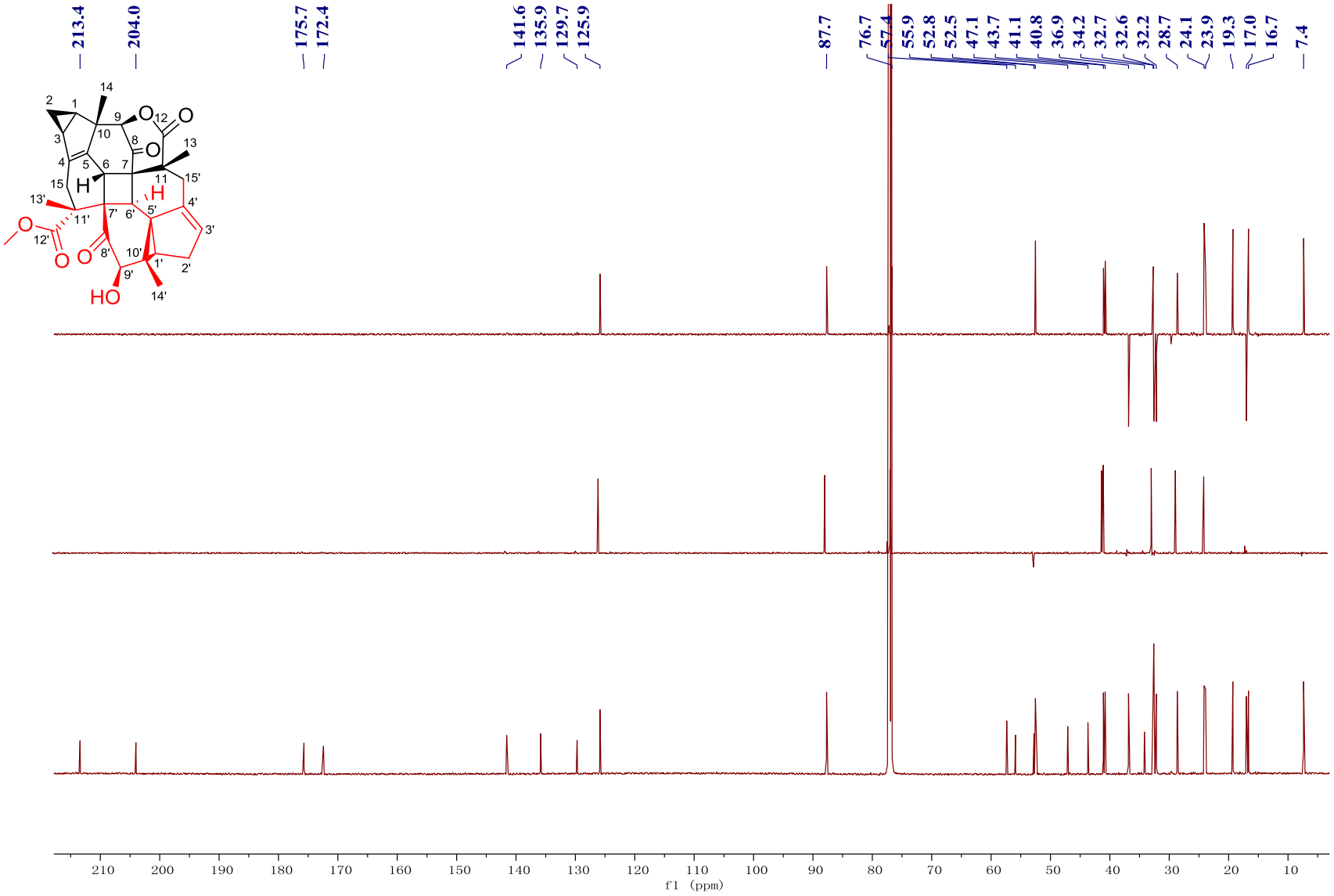


Figure S40. HSQC spectrum of chlorahupetone E (**5**) in $CDCl_3$

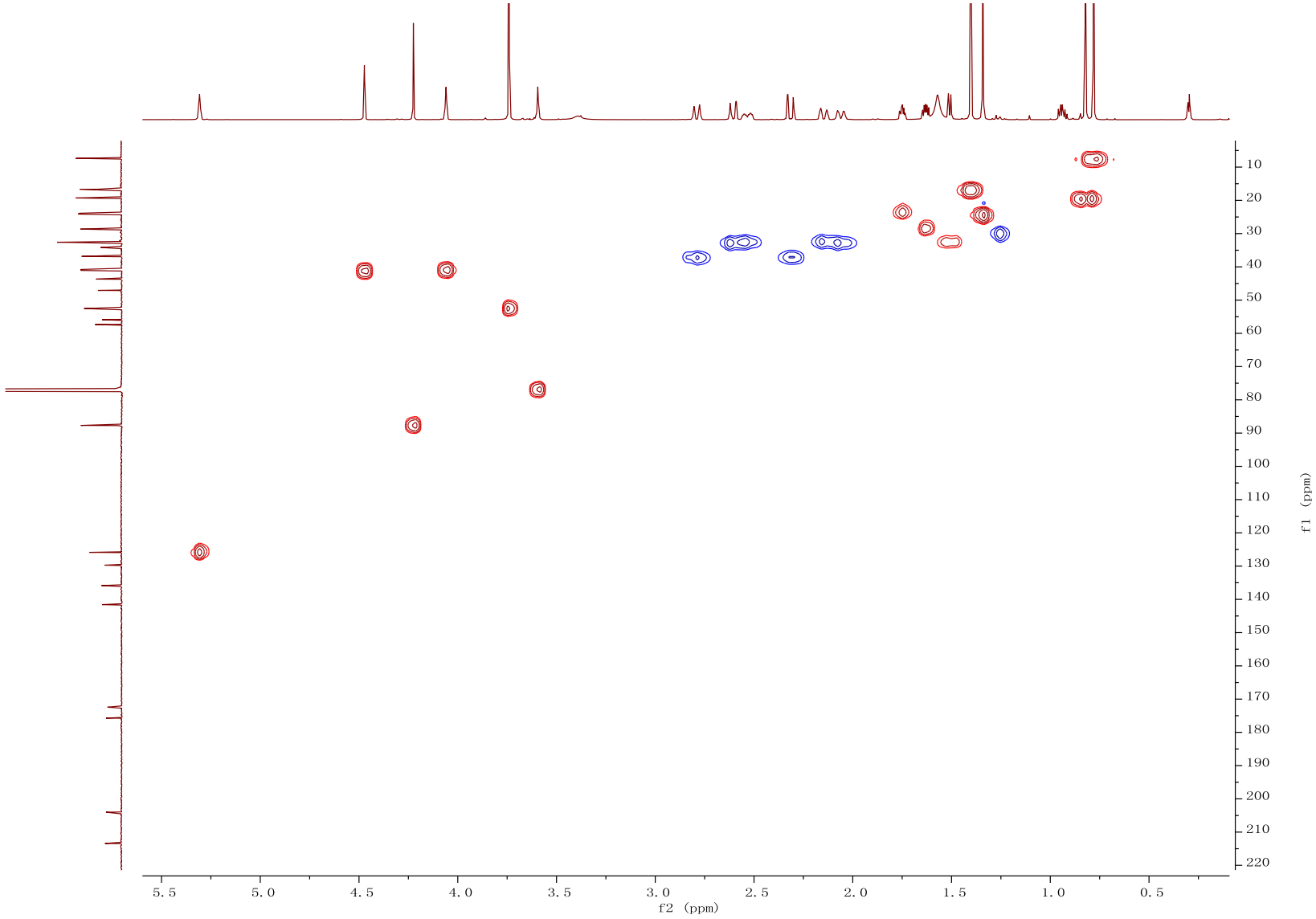


Figure S41. HMBC spectrum of chlorahupetone E (**5**) in $CDCl_3$

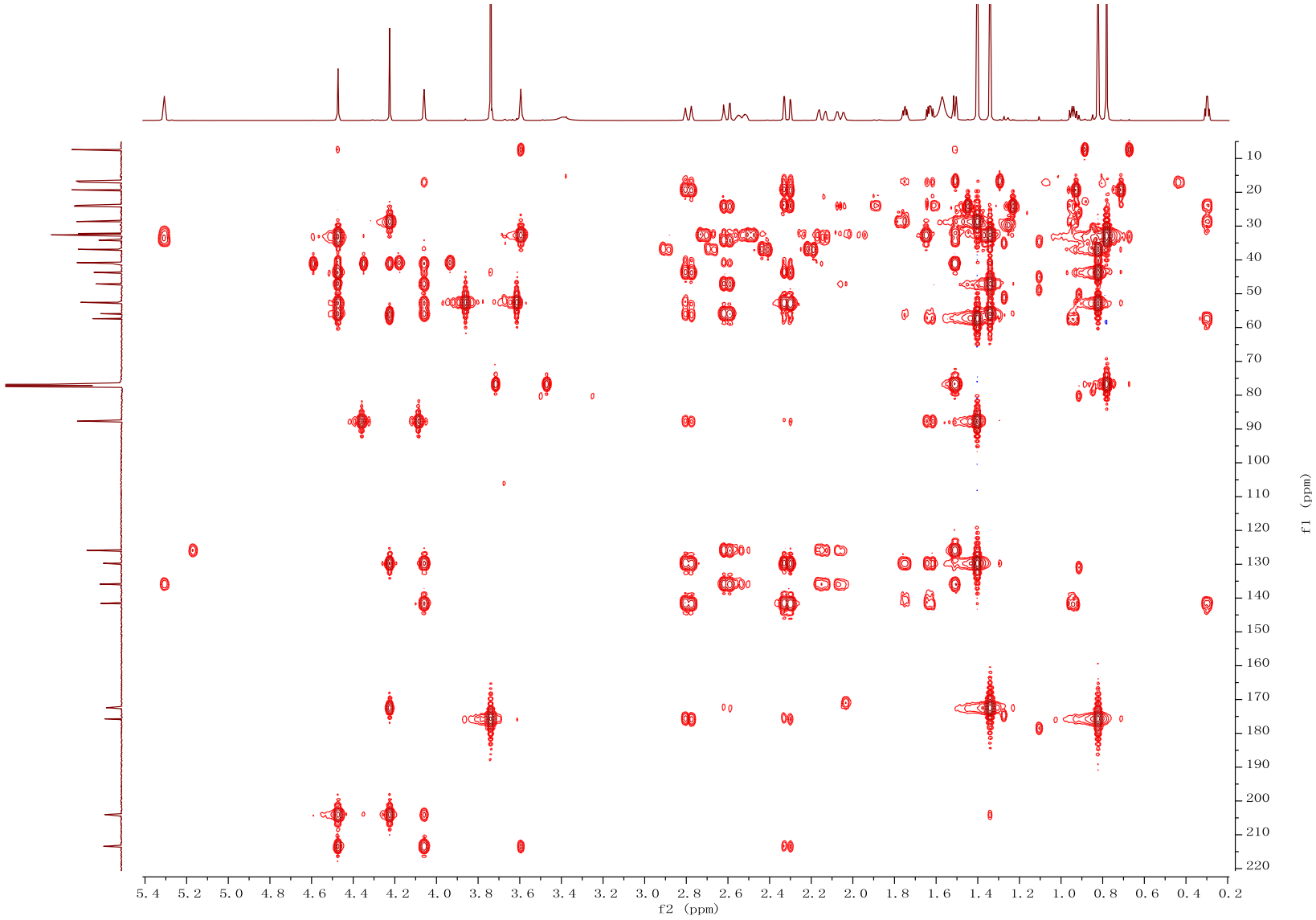


Figure S42. ^{1}H-^{1}H COSY spectrum of chlorahupetone E (**5**) in $CDCl_3$

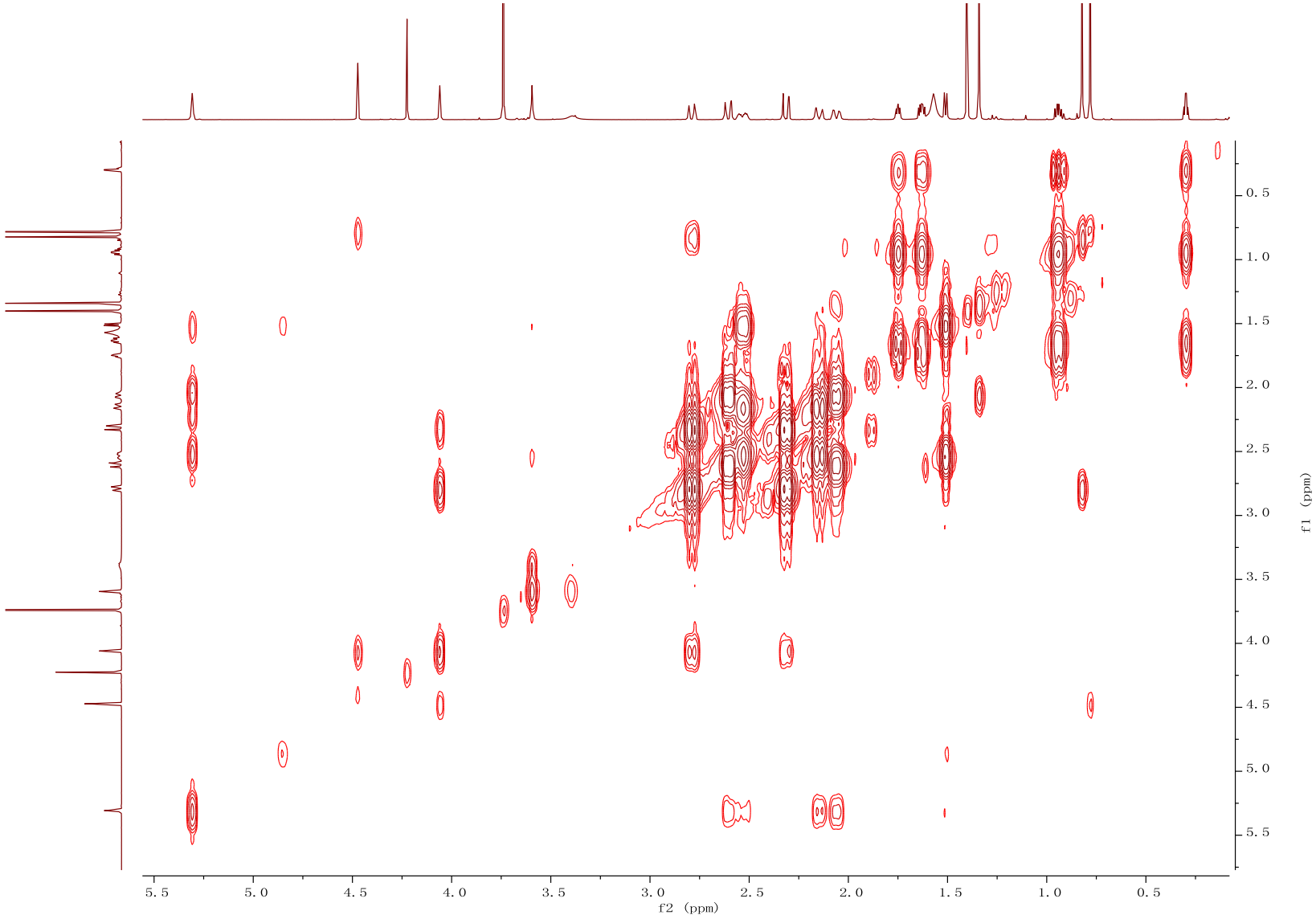


Figure S43. NOESY spectrum of chlorahupetone E (**5**) in $CDCl_3$

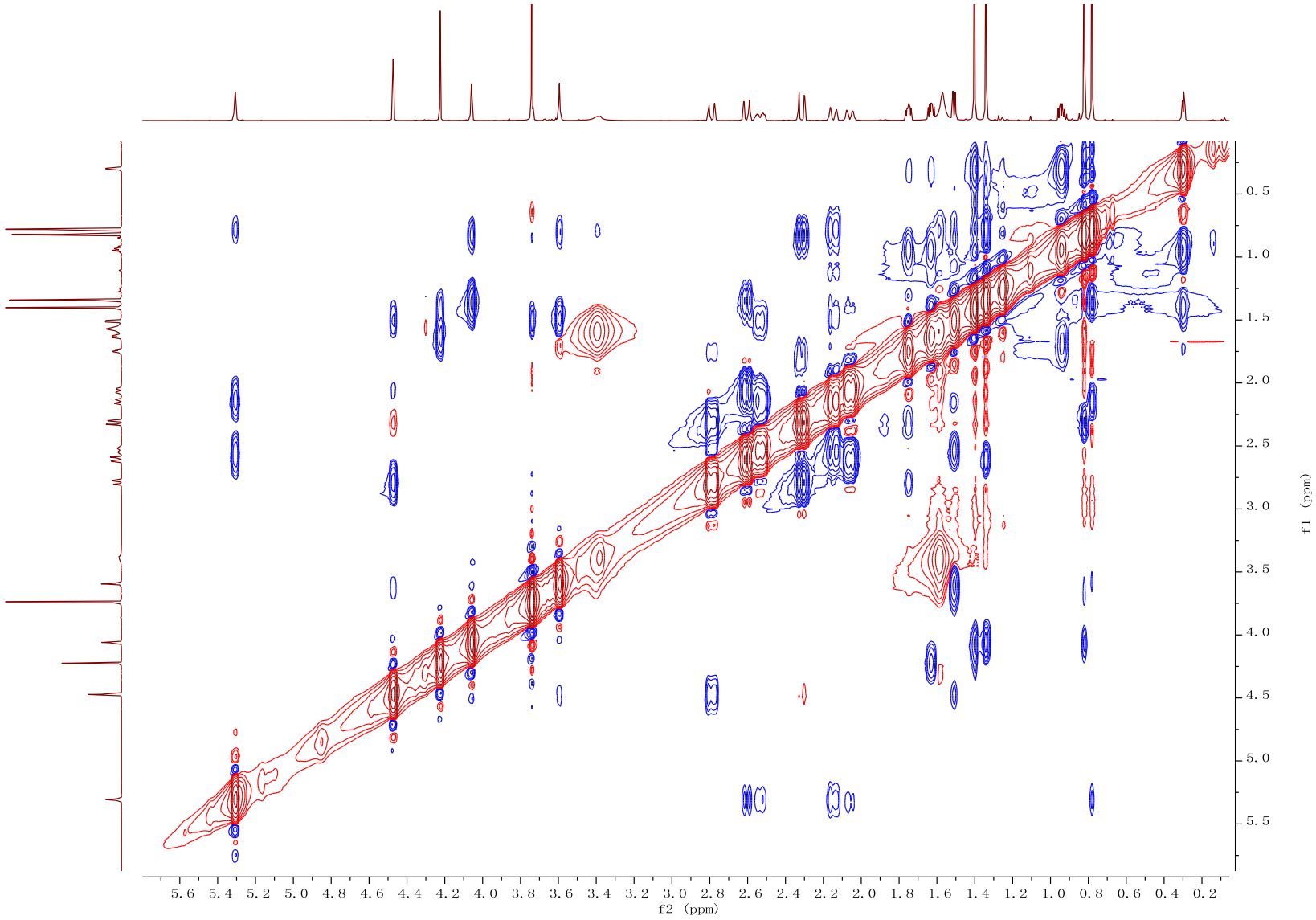


Figure S44. (+)-HRESIMS spectrum of chlorahupetone E (**5**)

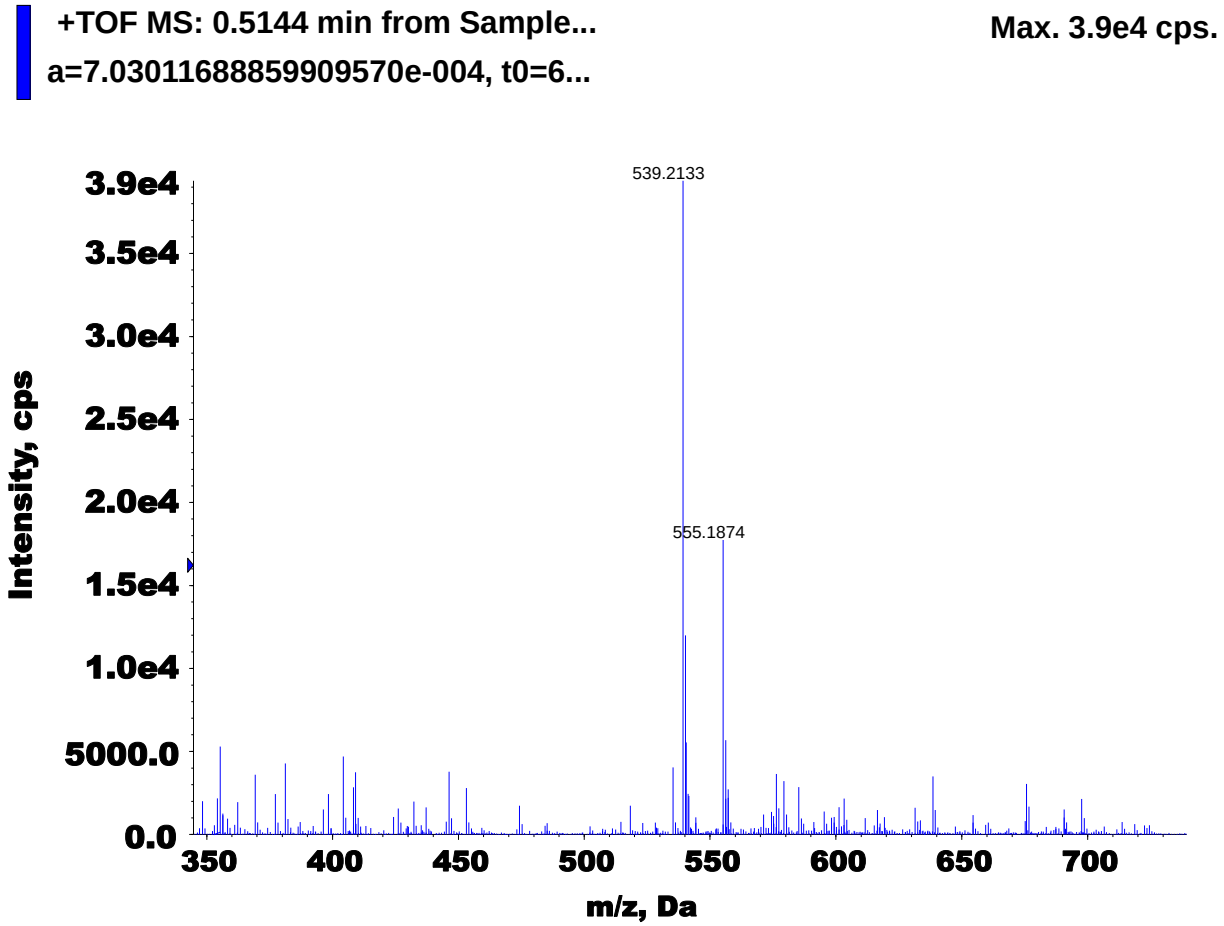


Figure S45. IR spectrum of chlorahupetone E (**5**)

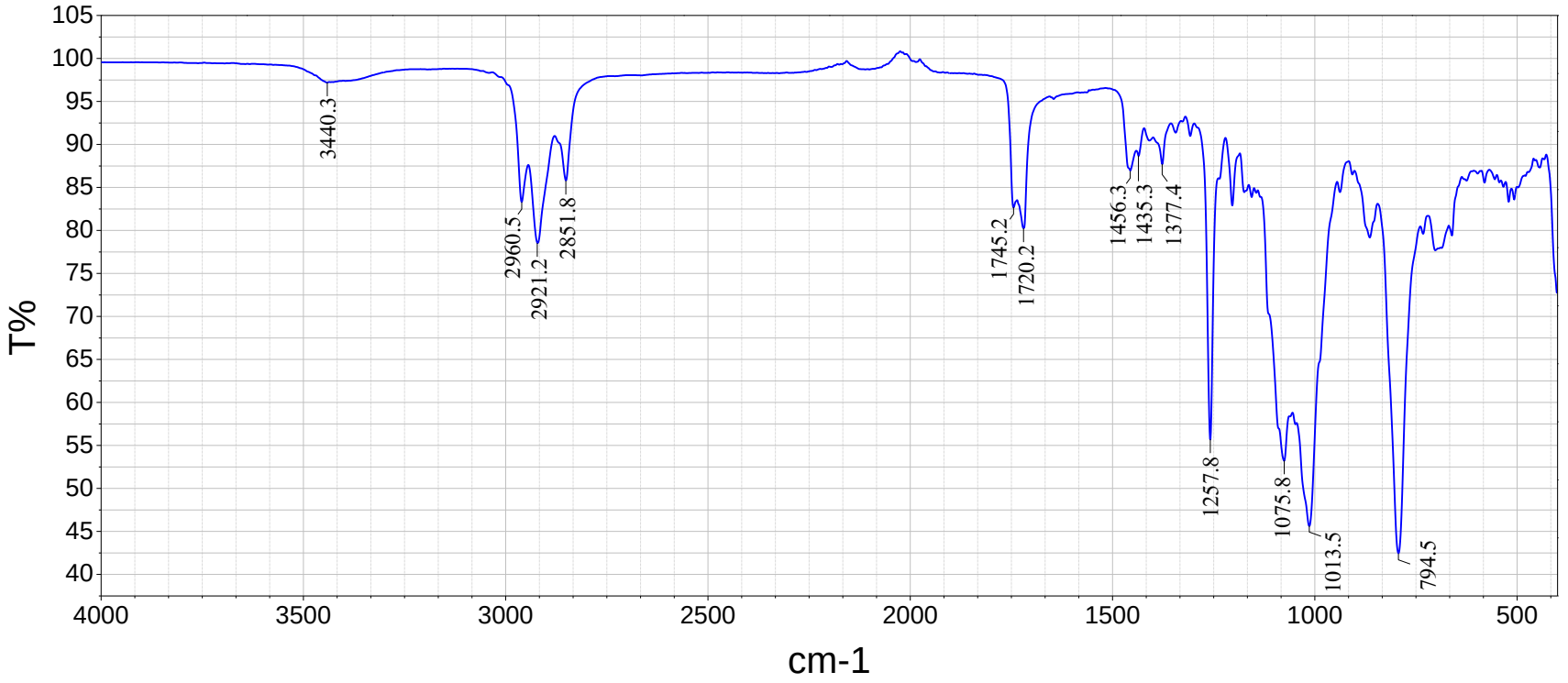


Figure S46. ^{1}H NMR spectrum of chlorahupetone F (**6**) in $CDCl_3$

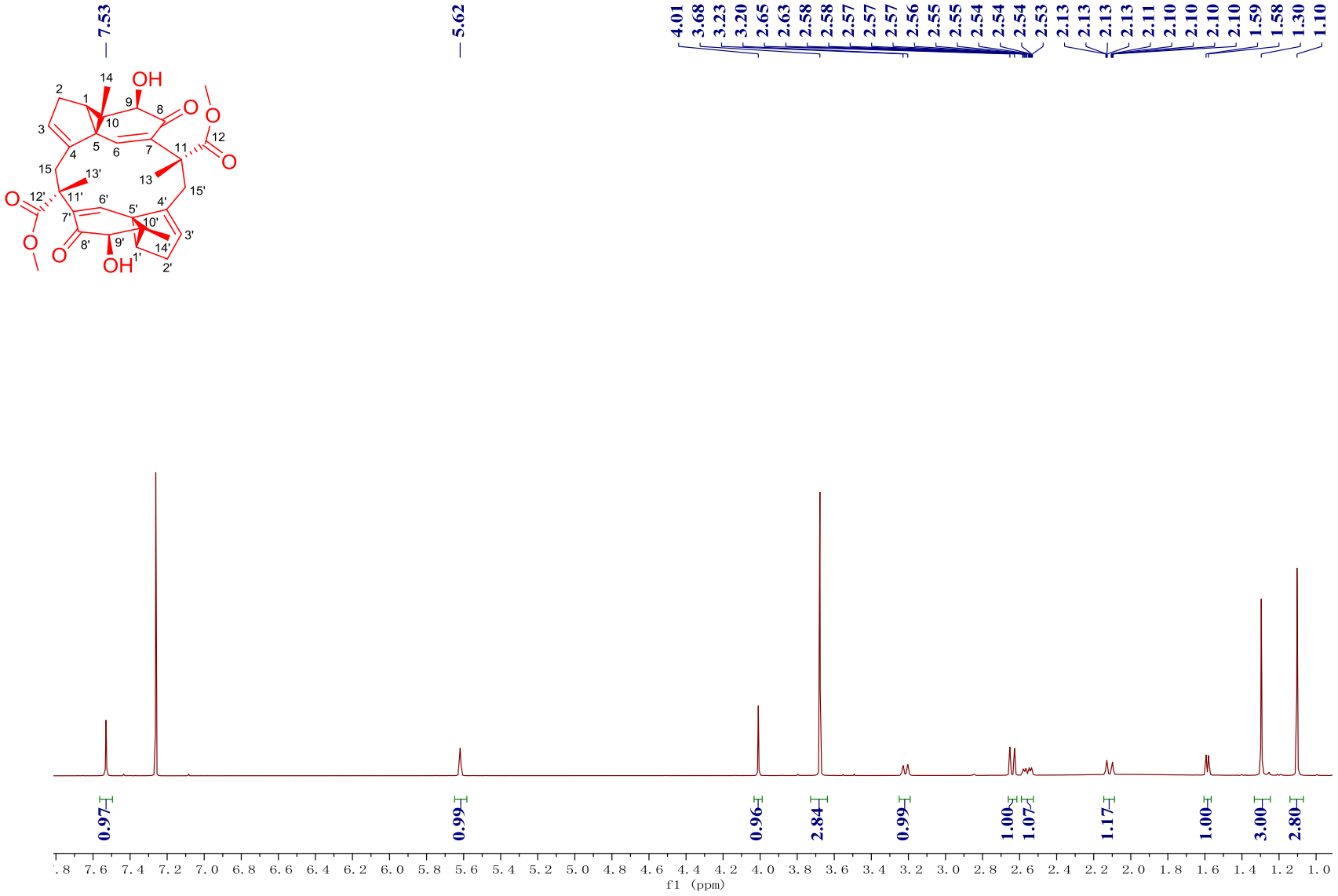


Figure S47. ^{13}C NMR and DEPT spectrum of chlorahupetone F (**6**) in $CDCl_3$

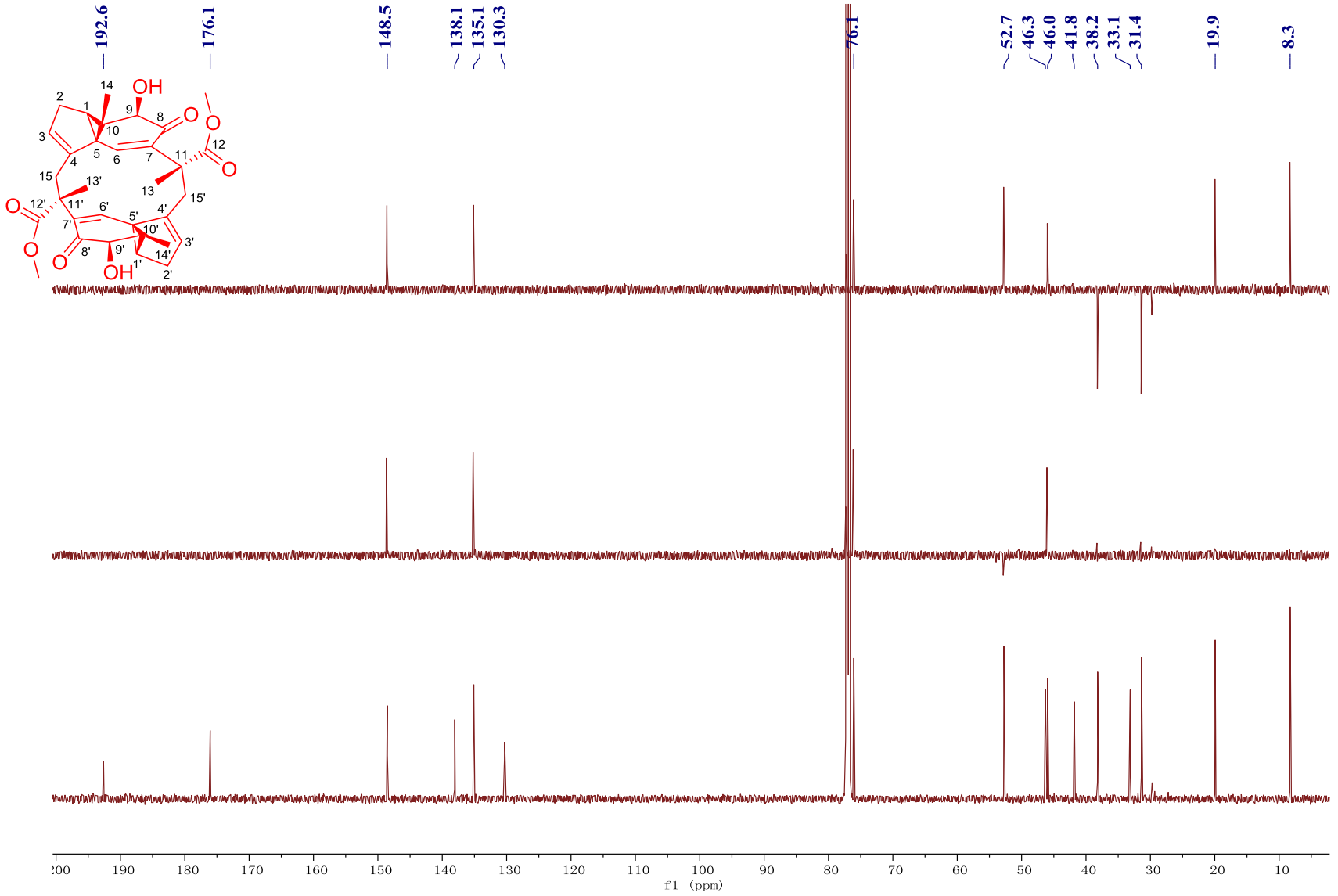


Figure S48. HSQC spectrum of chlorahupetone F (**6**) in $CDCl_3$

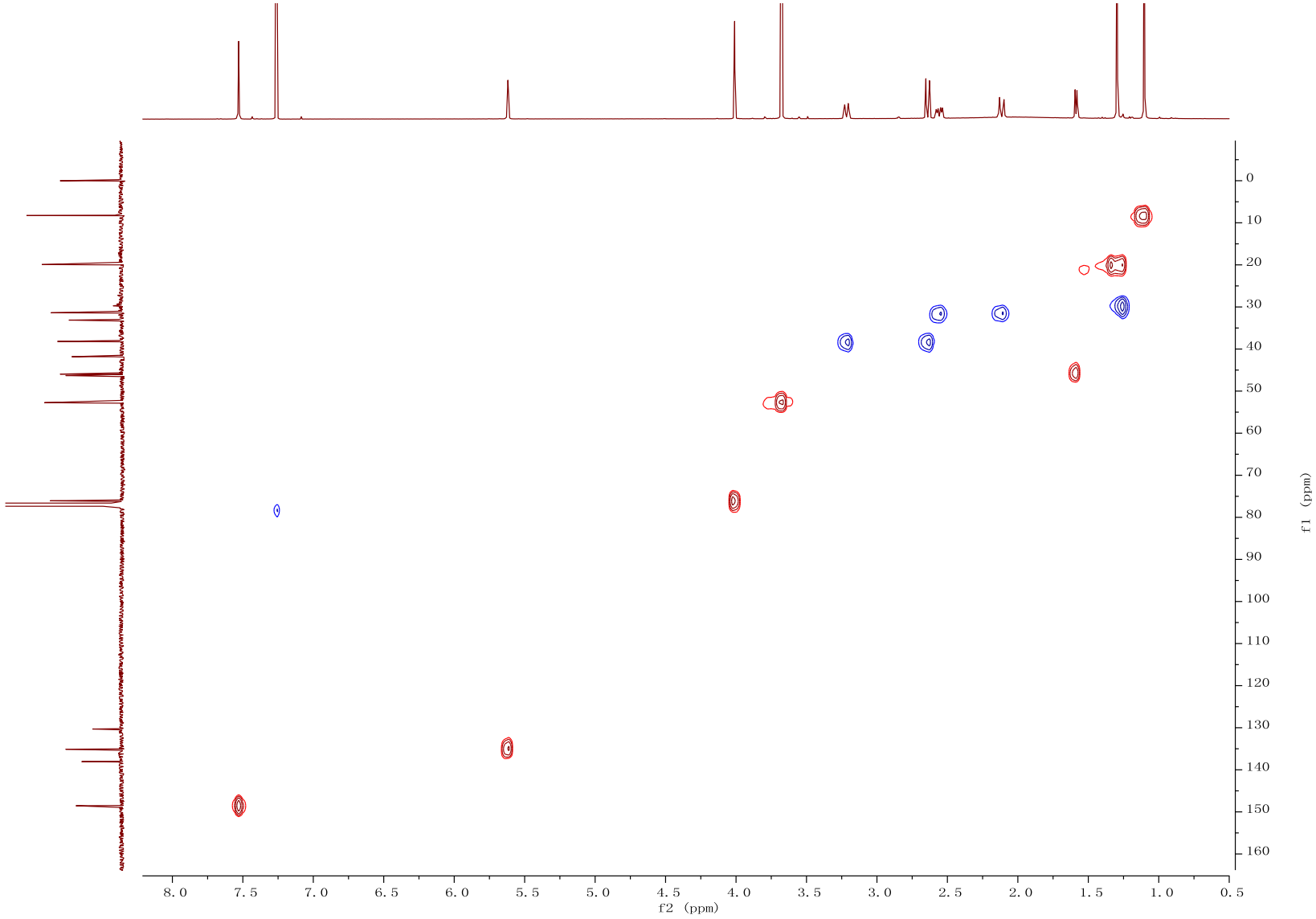


Figure S49. HMBC spectrum of chlorahupetone F (**6**) in $CDCl_3$

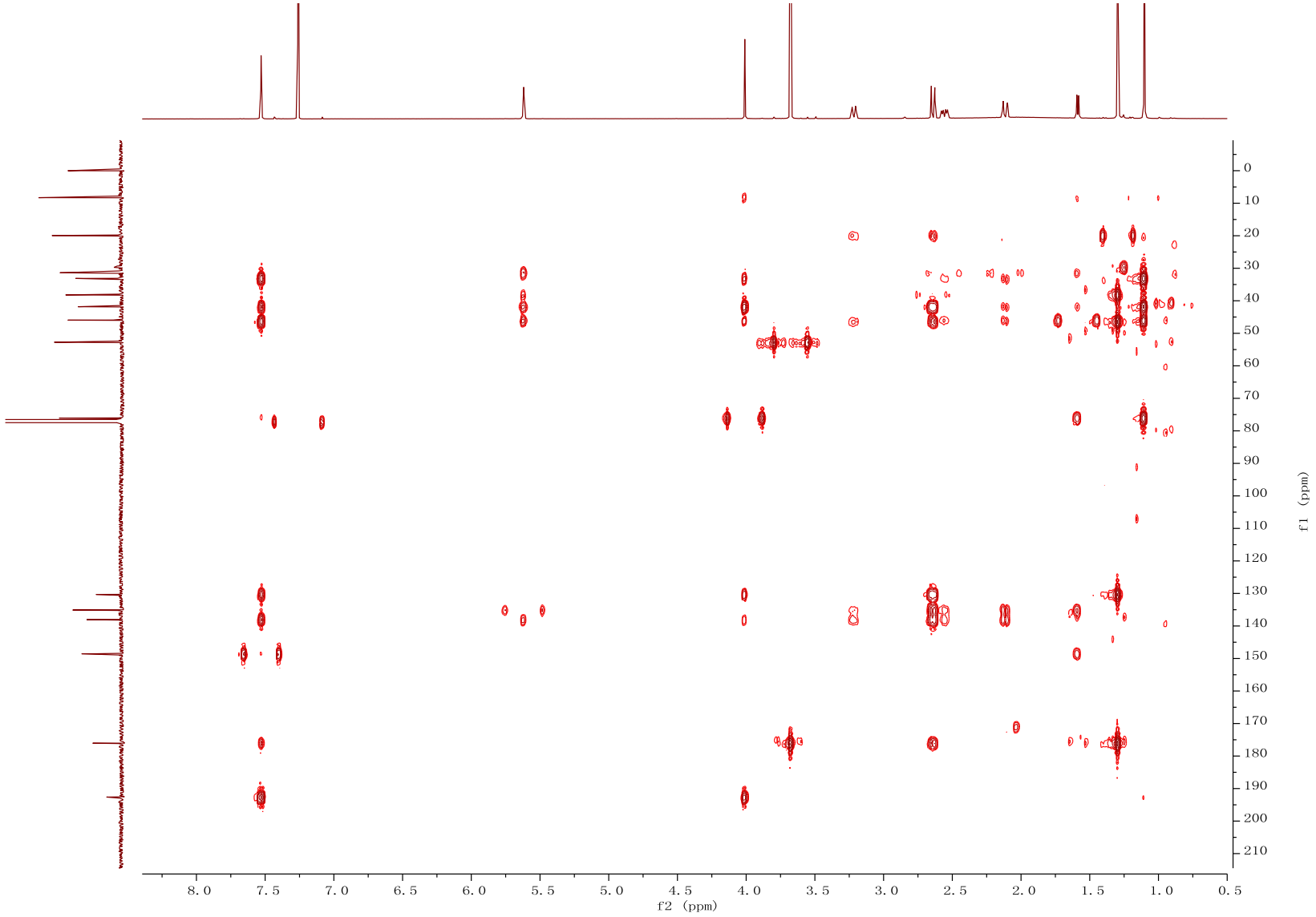


Figure S50. ^{1}H-^{1}H COSY spectrum of chlorahupetone F (**6**) in $CDCl_3$

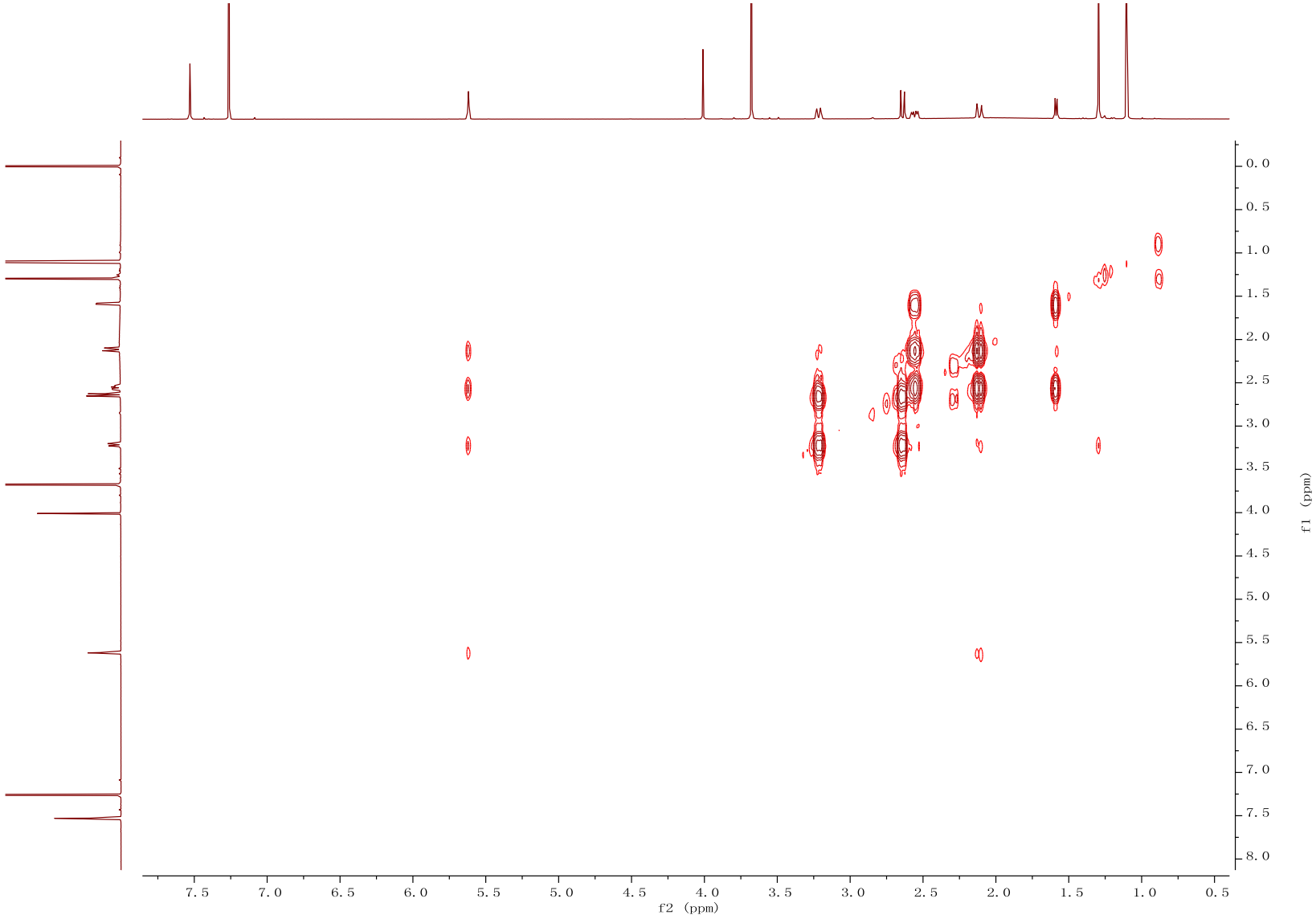


Figure S51. NOESY spectrum of chlorahupetone F (**6**) in $CDCl_3$

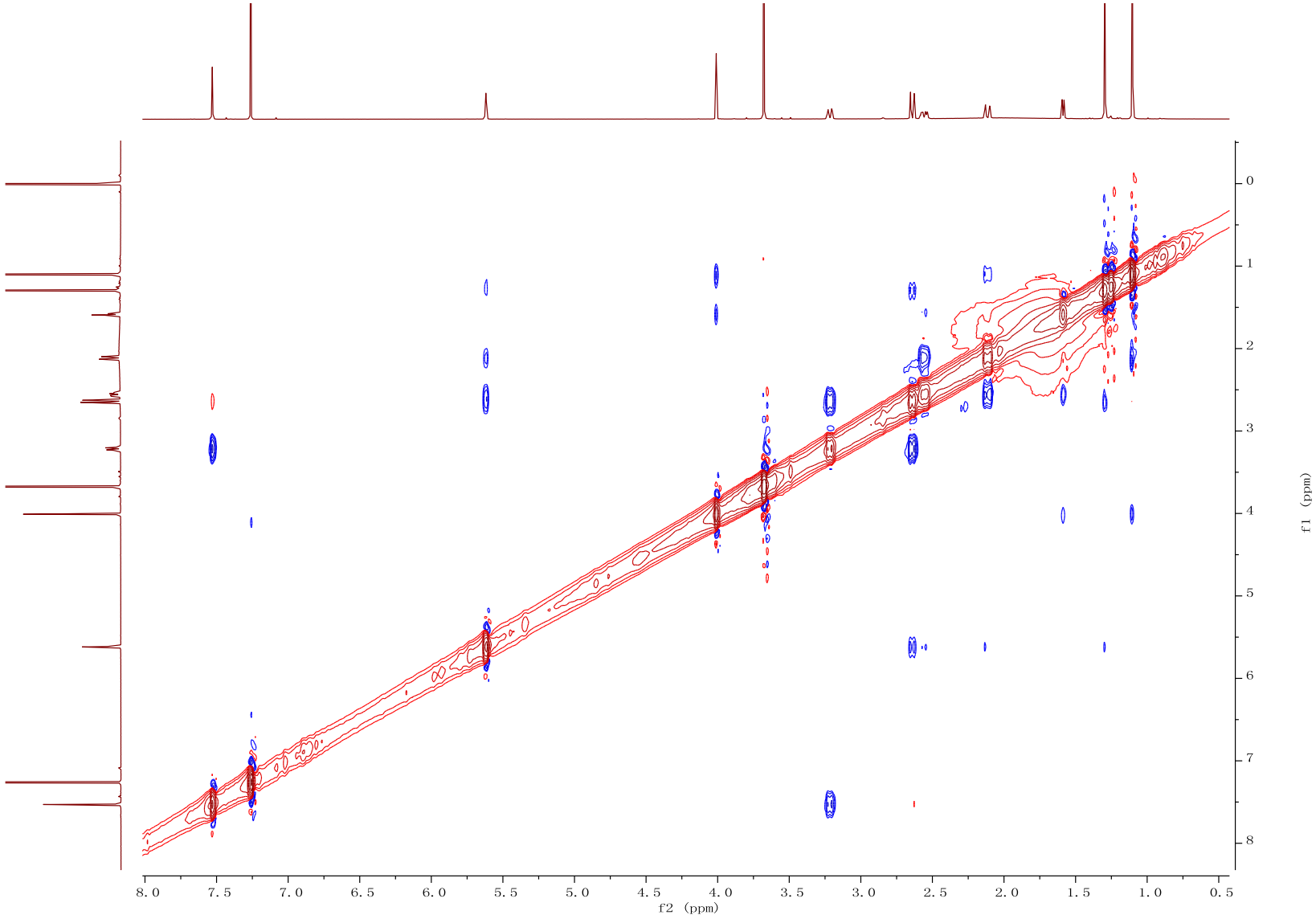


Figure S52. (+)-HRESIMS spectrum of chlorahupetone F (**6**)

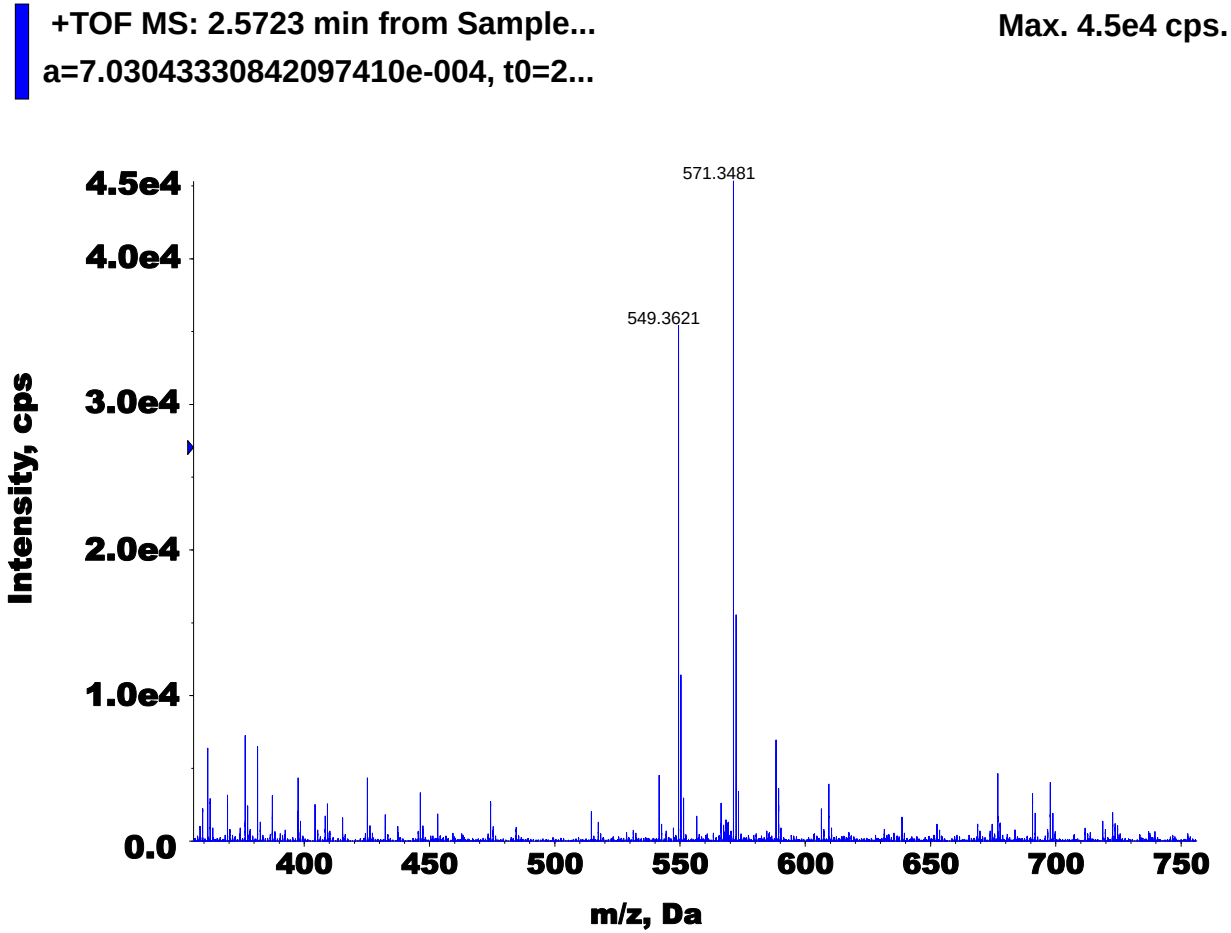


Figure S53. IR spectrum of chlorahupetone F (**6**)

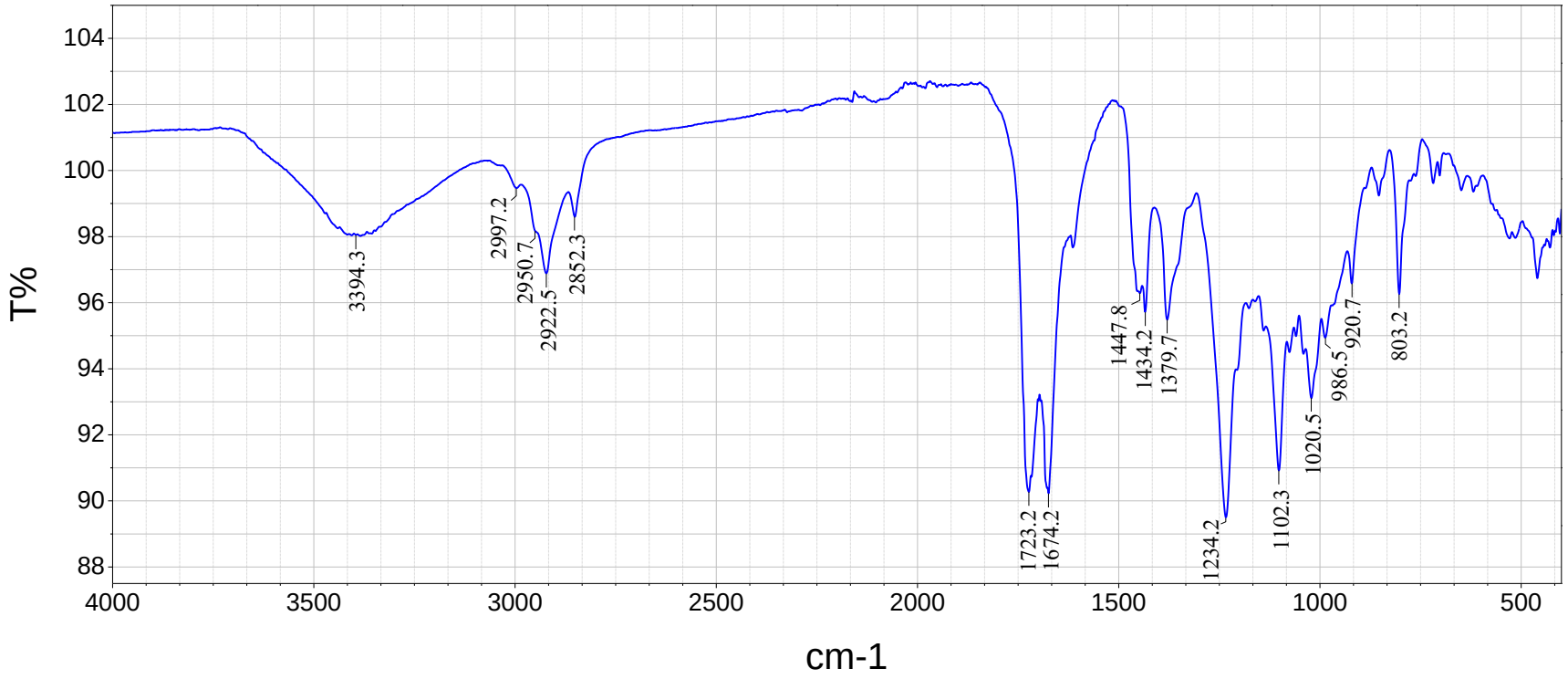


Figure S54. ^{1}H NMR spectrum of chlorahupetone G (**7**) in $CDCl_3$

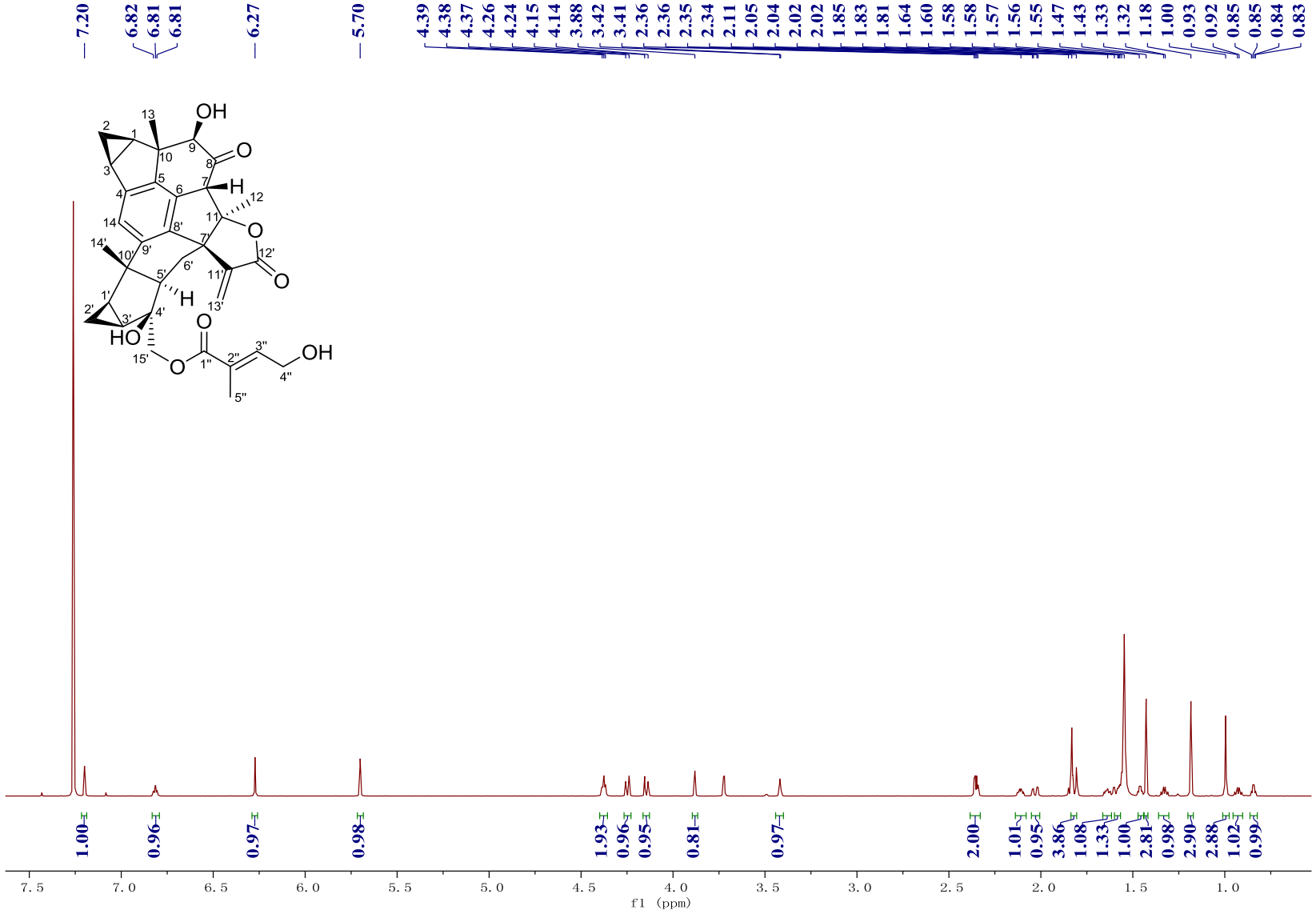


Figure S55. ^{13}C NMR and DEPT spectrum of chlorahupetone G (**7**) in $CDCl_3$

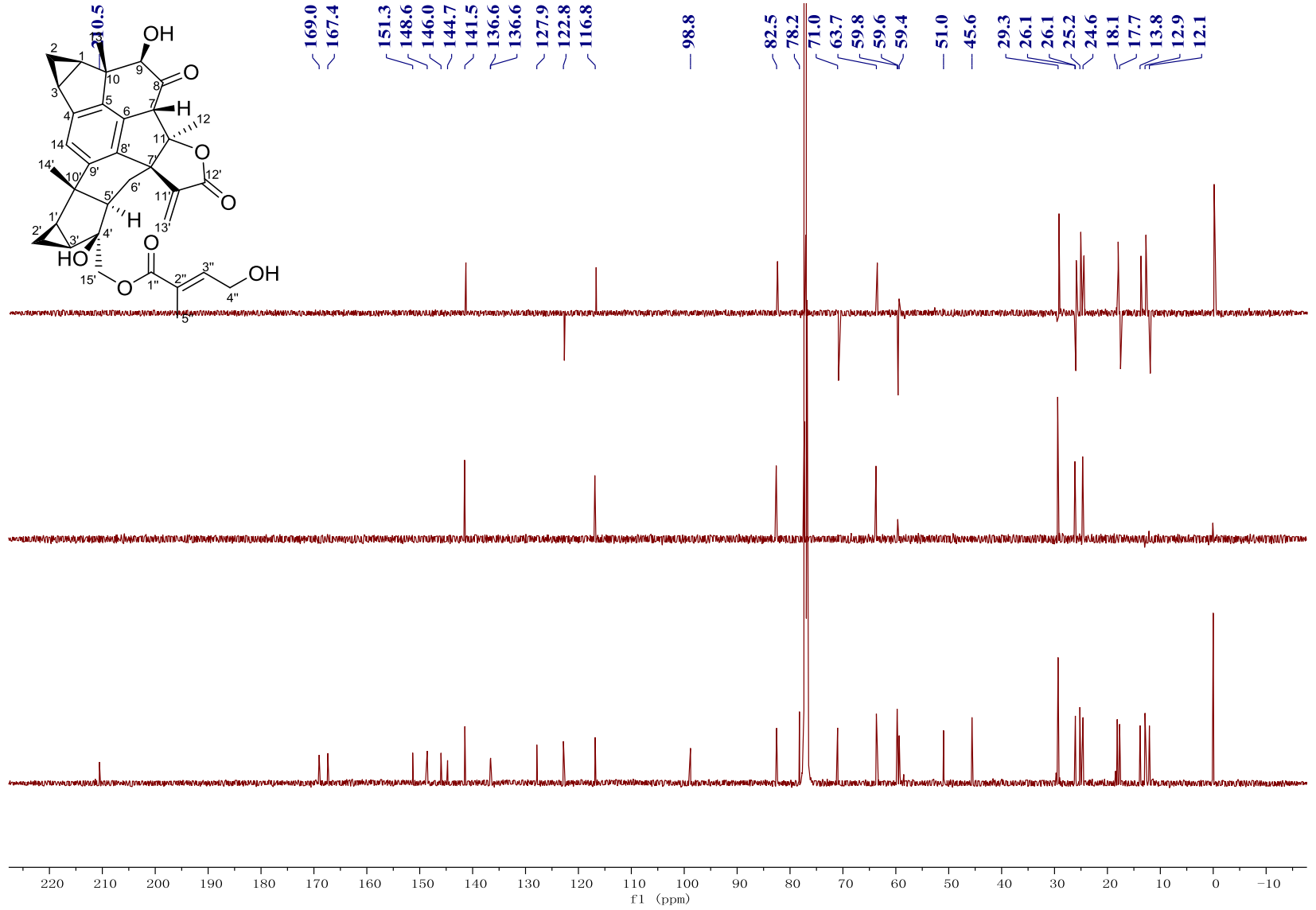


Figure S56. HSQC spectrum of chlorahupetone G (**7**) in $CDCl_3$

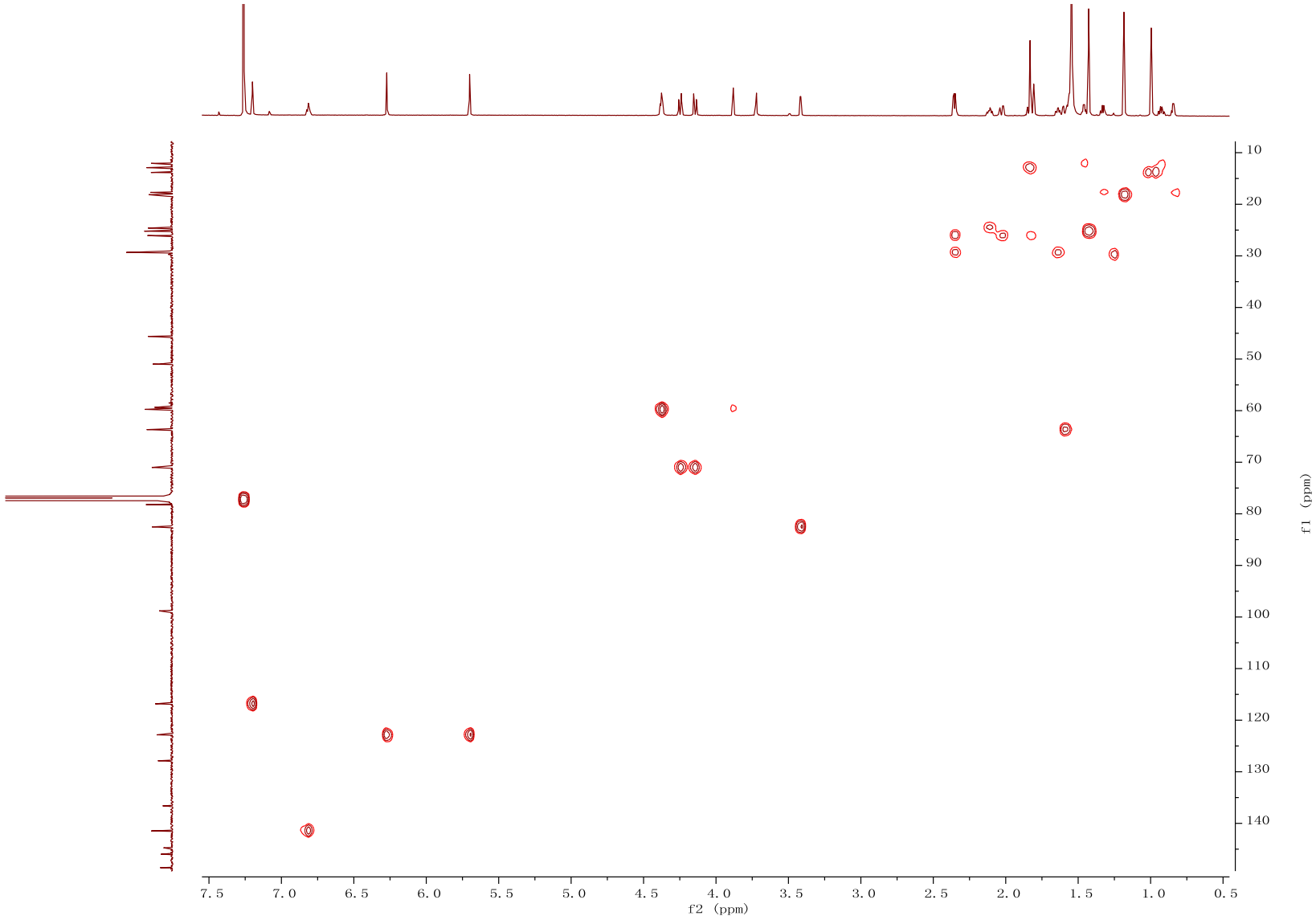


Figure S57. HMBC spectrum of chlorahupetone G (**7**) in $CDCl_3$

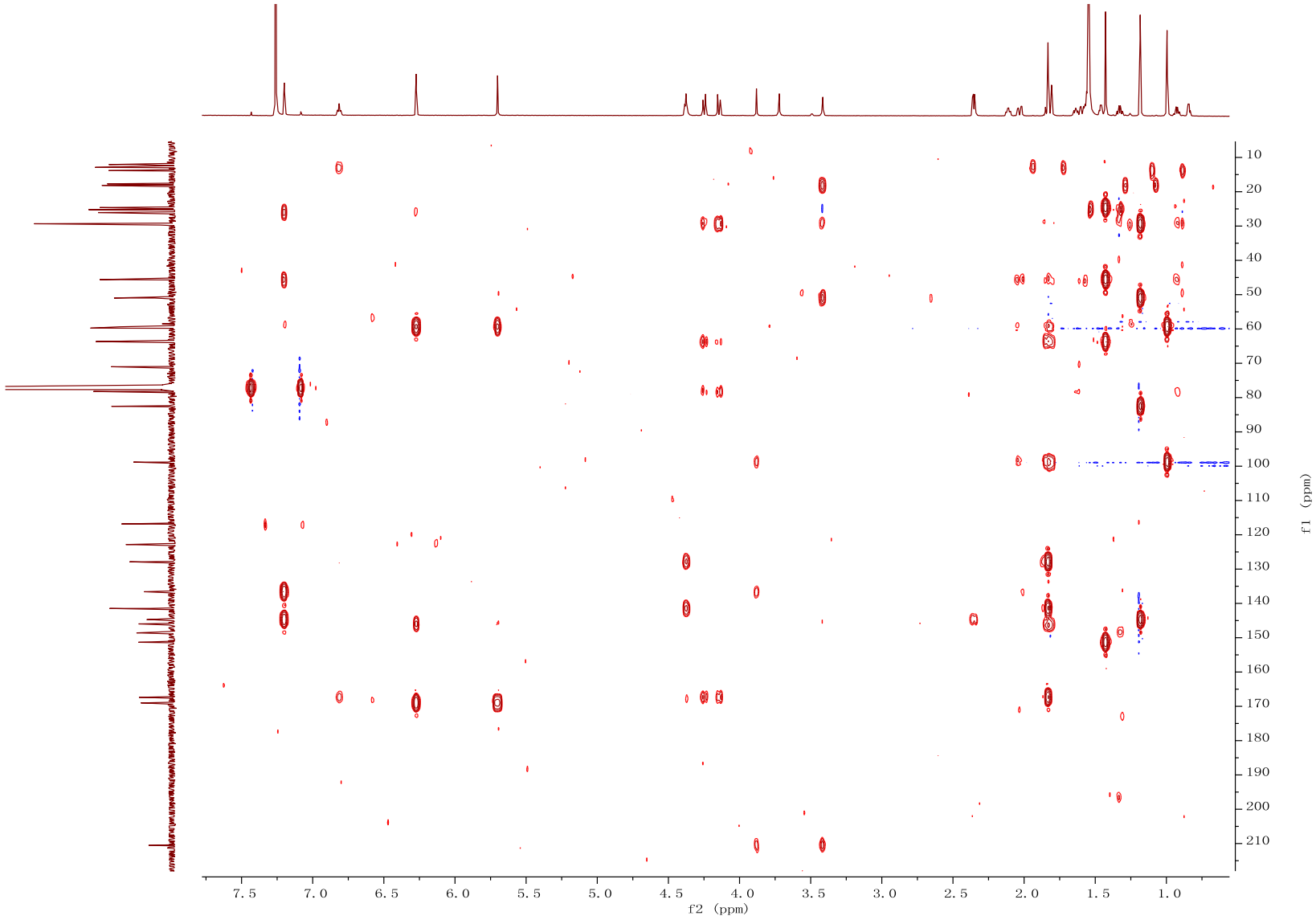


Figure S58. ^{1}H-^{1}H COSY spectrum of chlorahupetone G (**7**) in $CDCl_3$

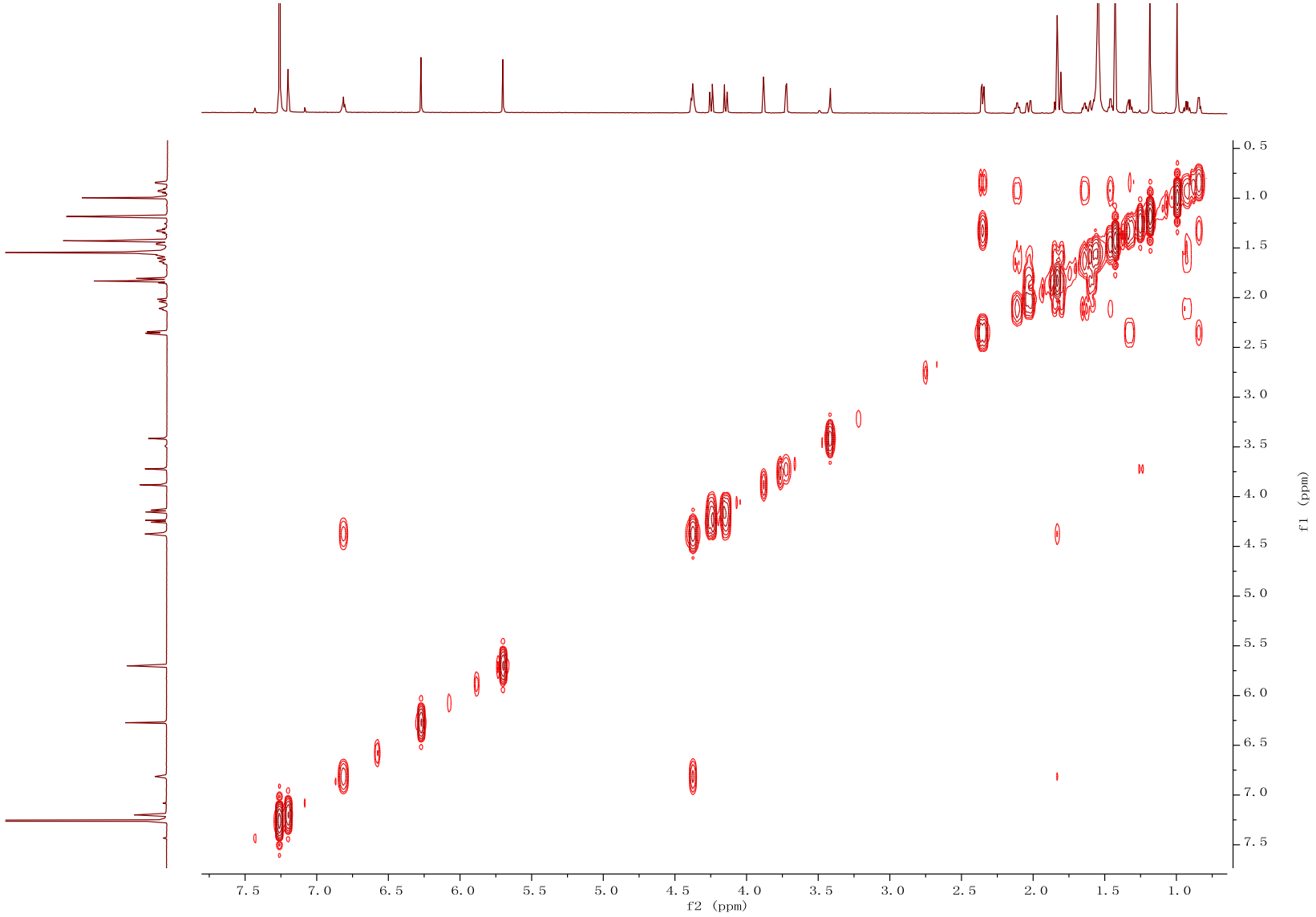


Figure S59. NOESY spectrum of chlorahupetone G (**7**) in $CDCl_3$

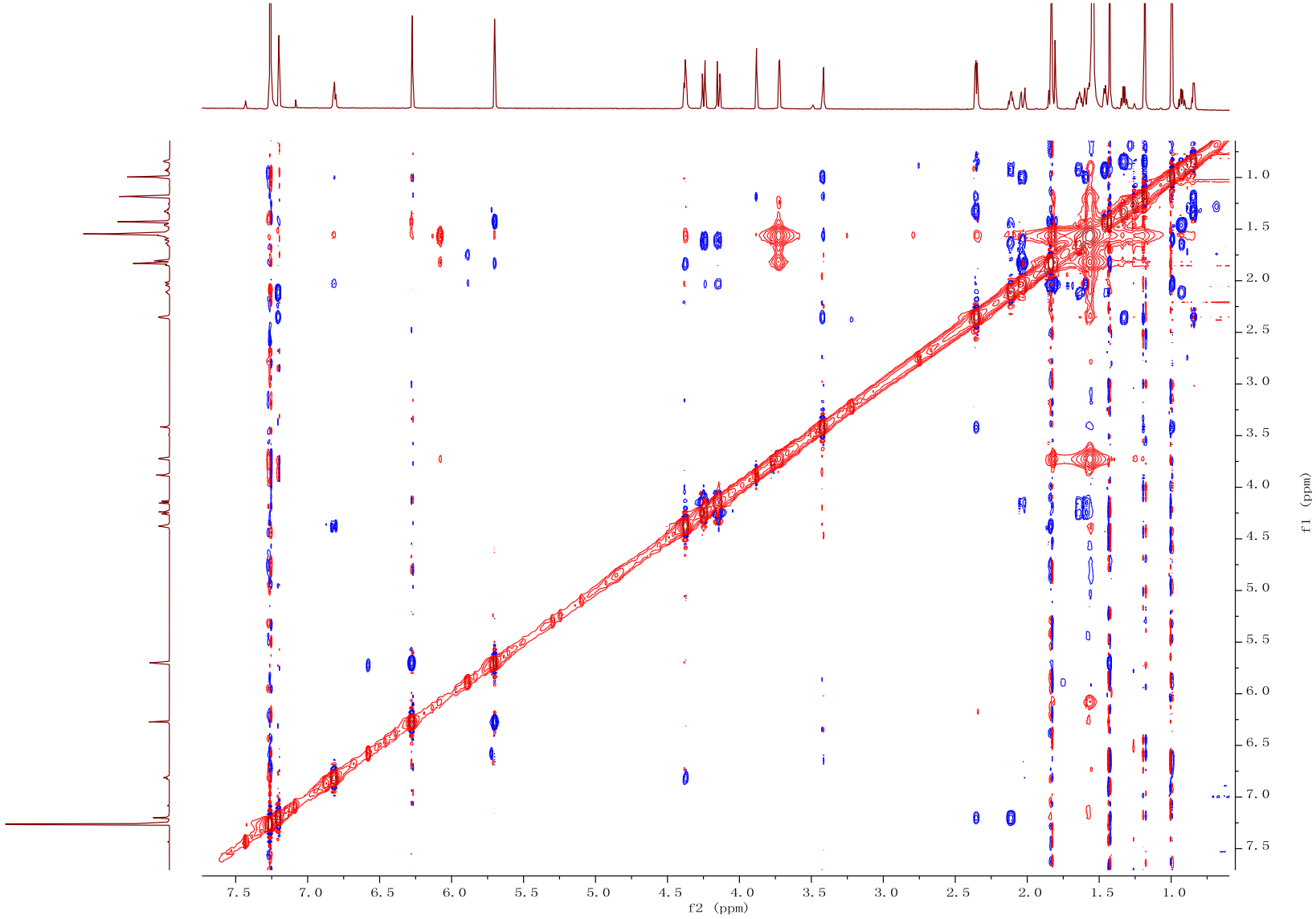


Figure S60. (-)-HRESIMS spectrum of chlorahupetone G (**7**)

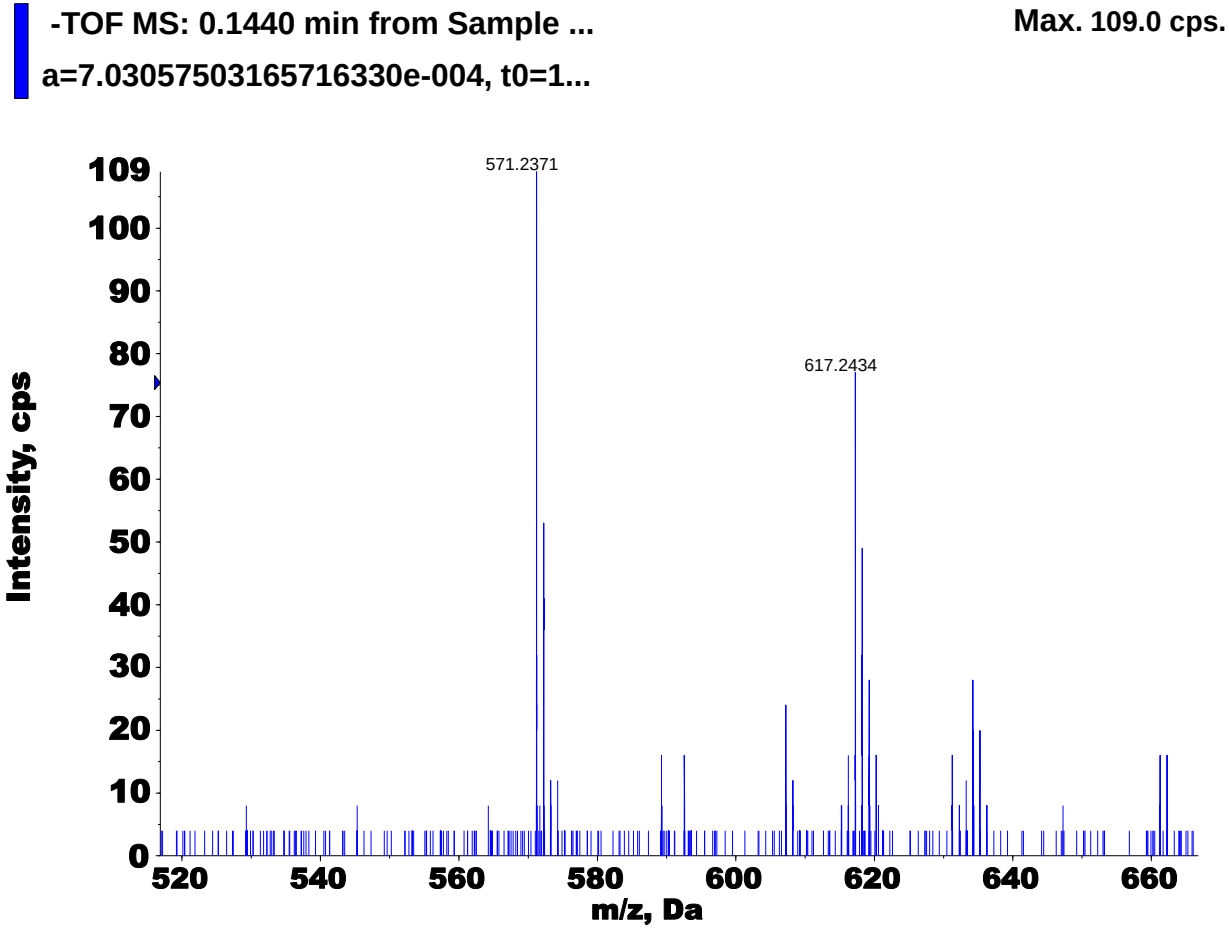


Figure S61. IR spectrum of chlorahupetone G (**7**)

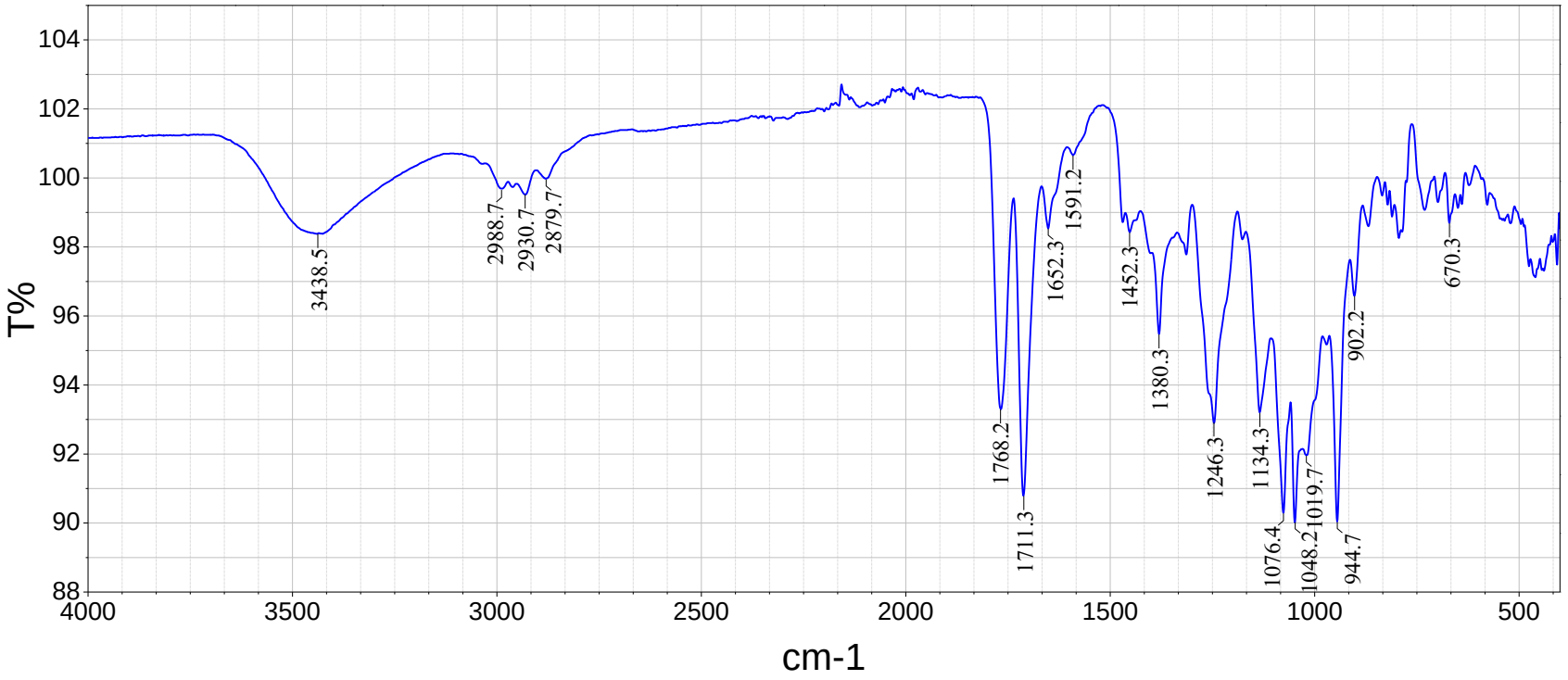


Figure S62. ^{1}H NMR spectrum of chlorahupetone H (**8**) in $CDCl_3$

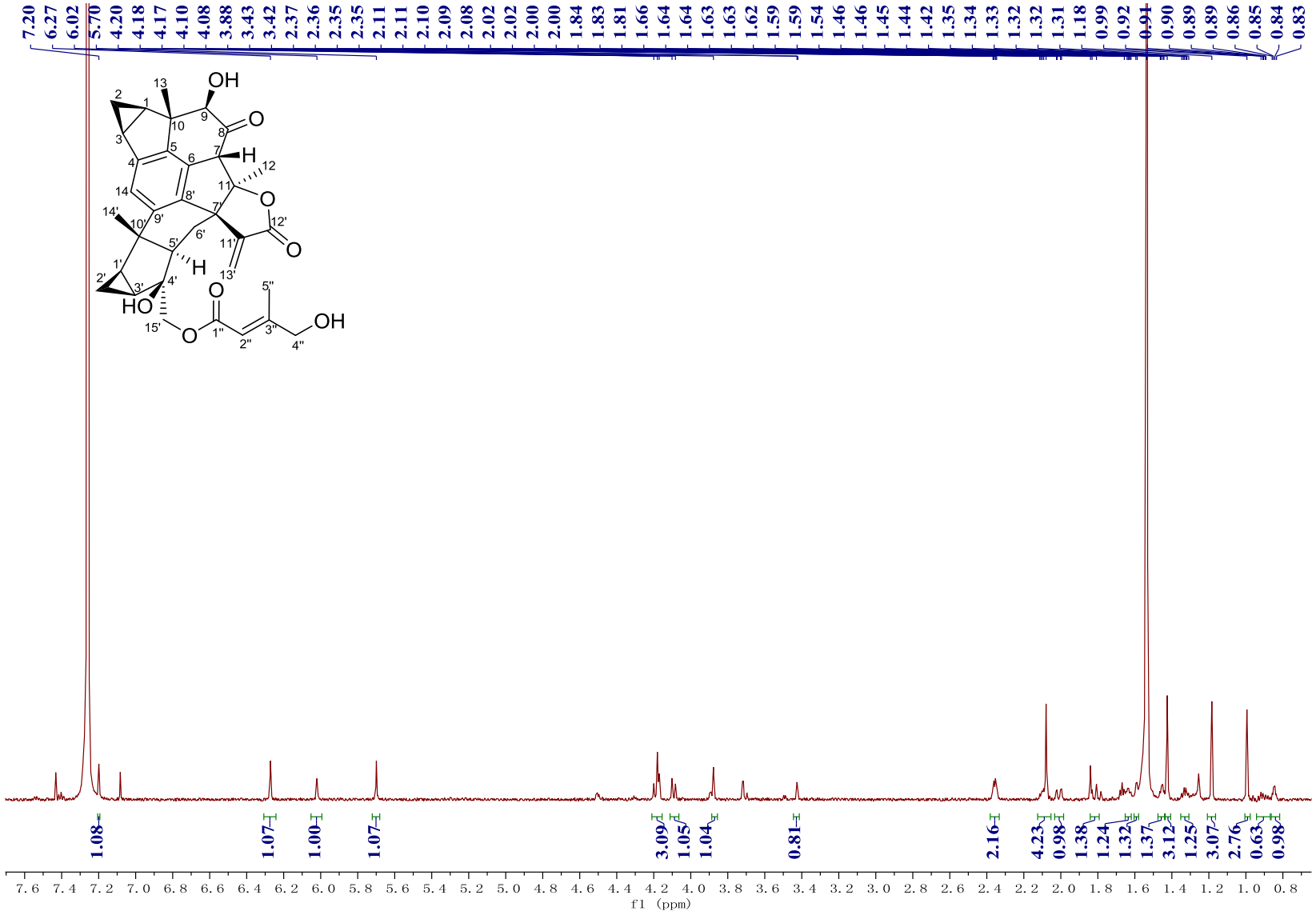


Figure S63. ^{13}C NMR and DEPT spectrum of chlorahupetone H (**8**) in $CDCl_3$

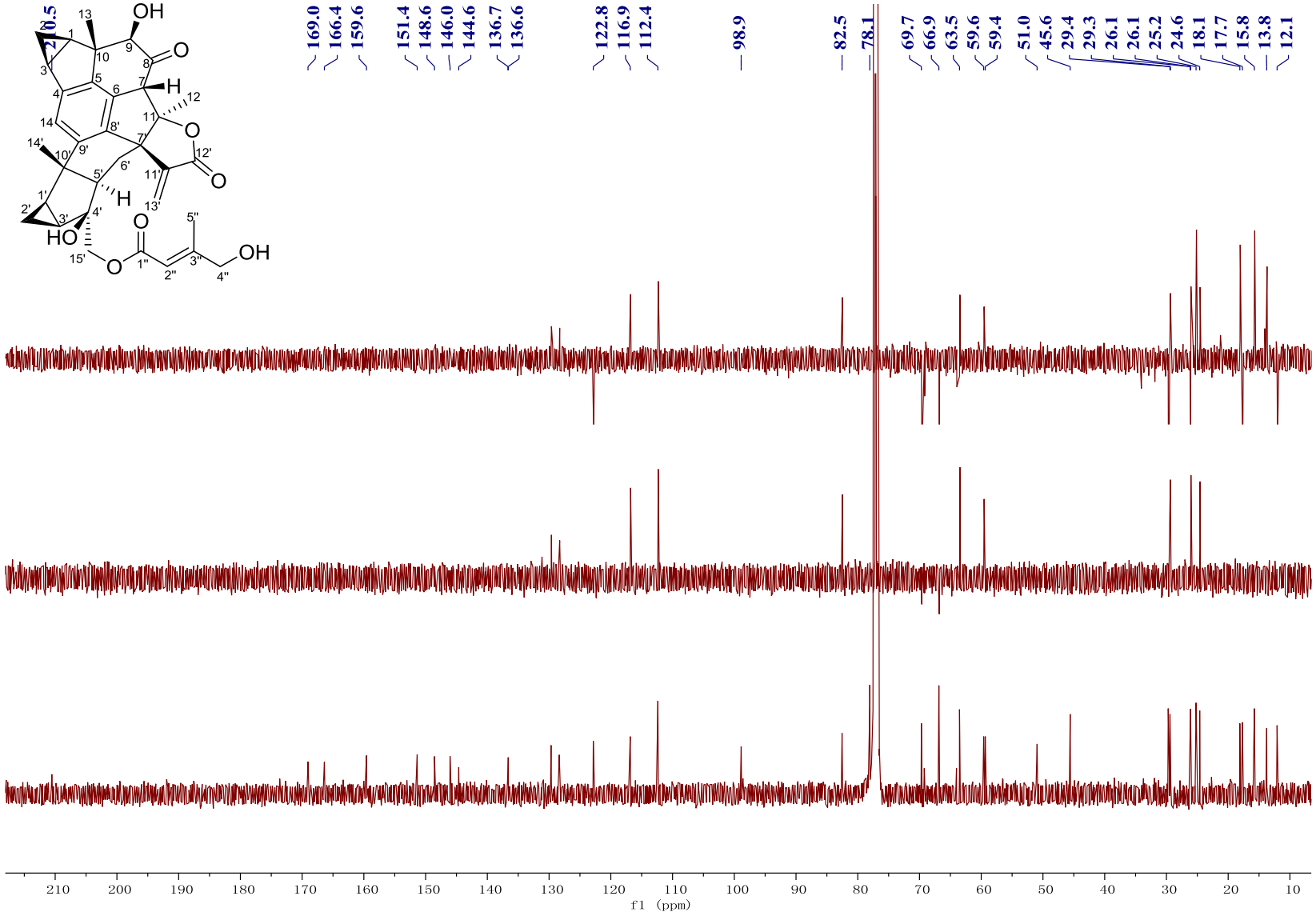


Figure S64. HSQC spectrum of chlorahupetone H (**8**) in $CDCl_3$

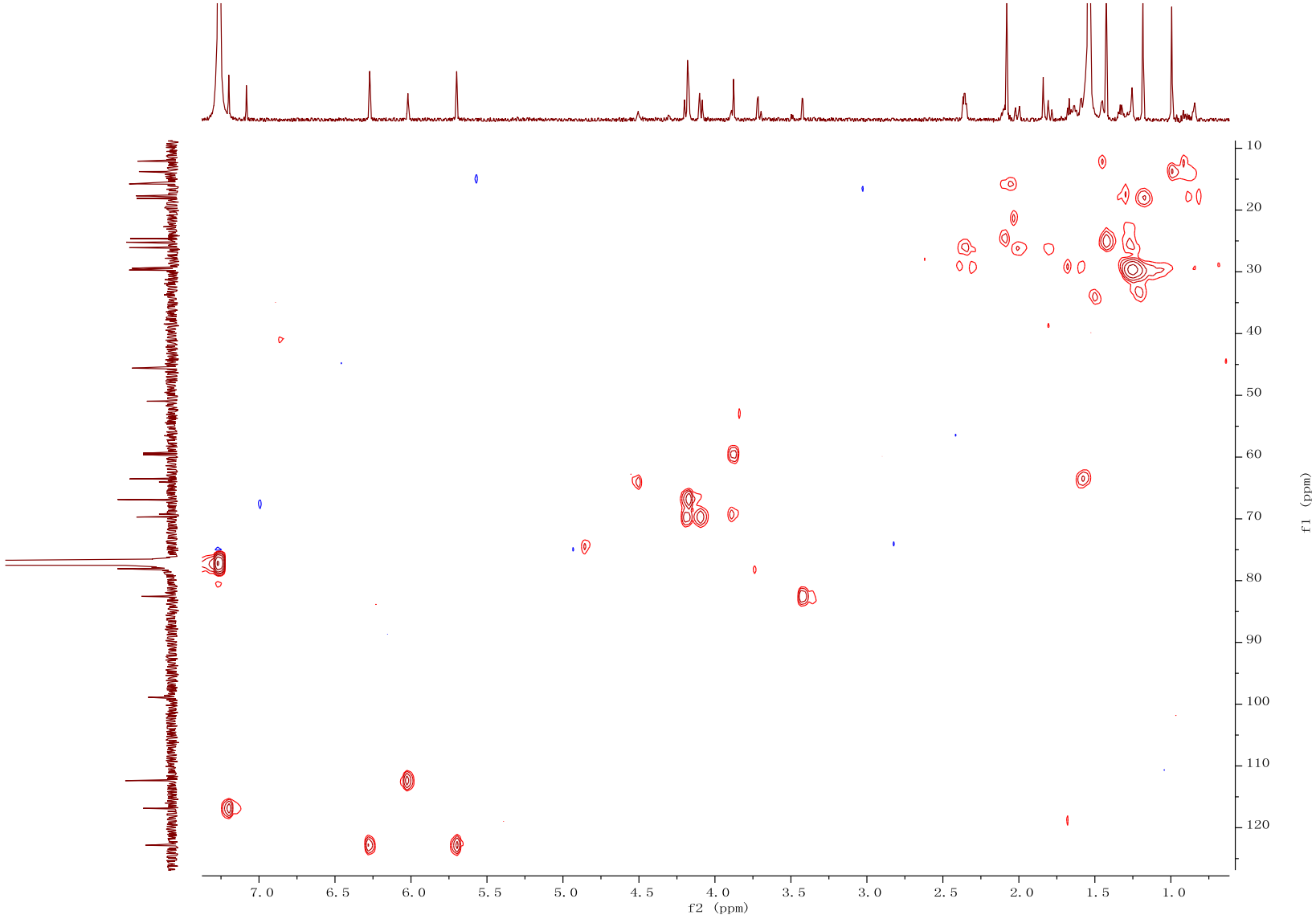


Figure S65. HMBC spectrum of chlorahupetone H (**8**) in $CDCl_3$

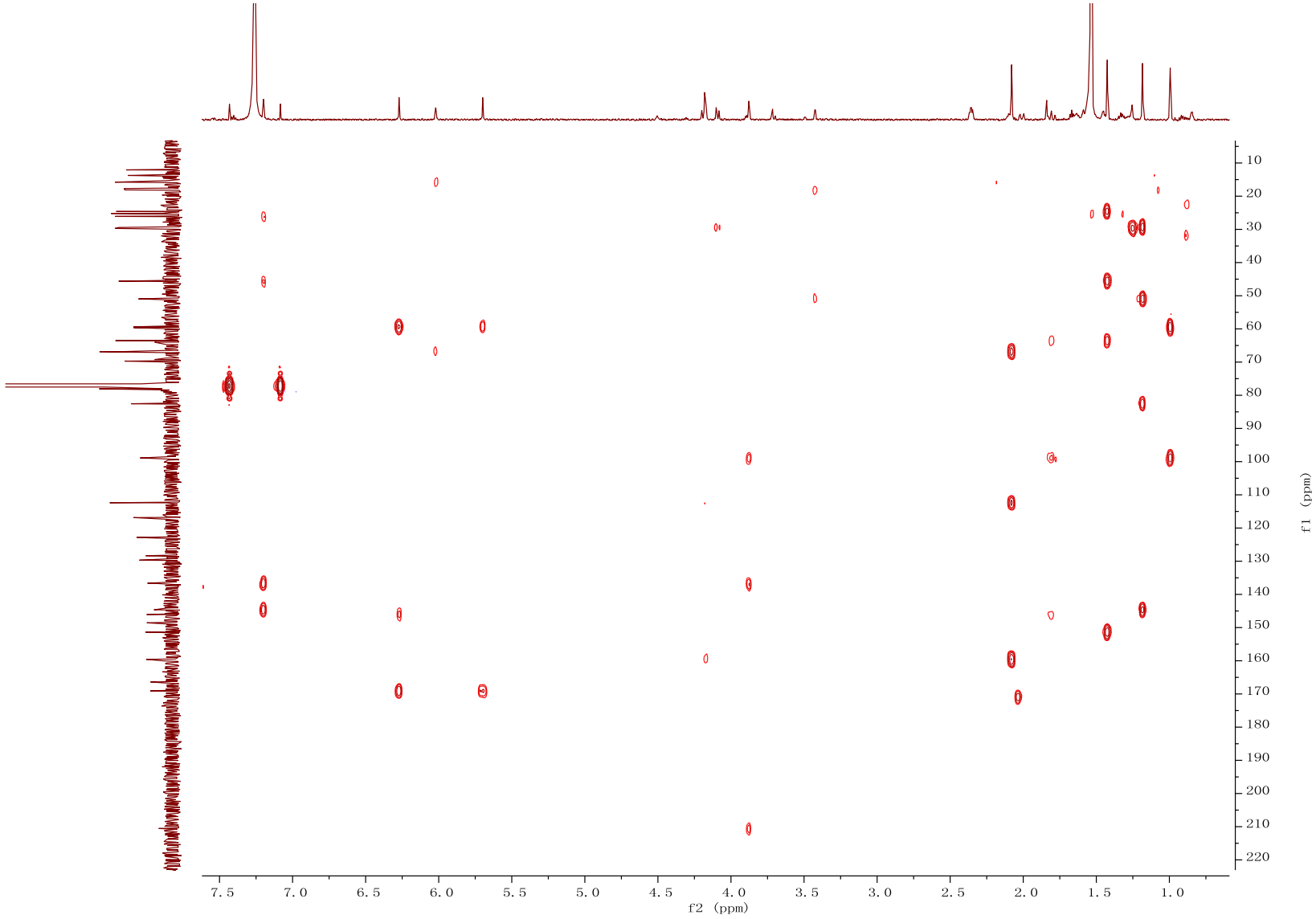


Figure S66. ^{1}H-^{1}H COSY spectrum of chlorahupetone H (**8**) in $CDCl_3$

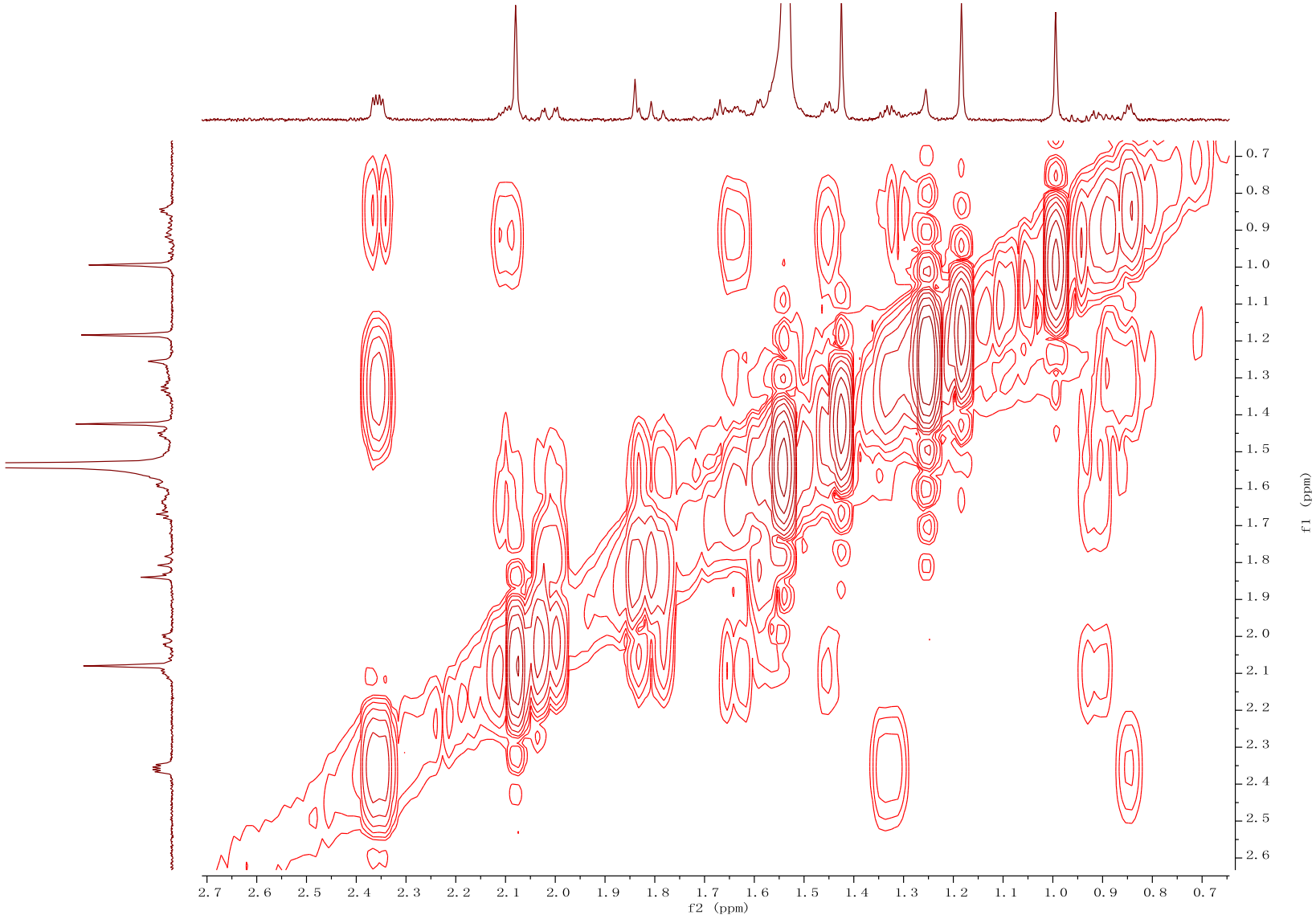


Figure S67. NOESY spectrum of chlorahupetone H (**8**) in $CDCl_3$

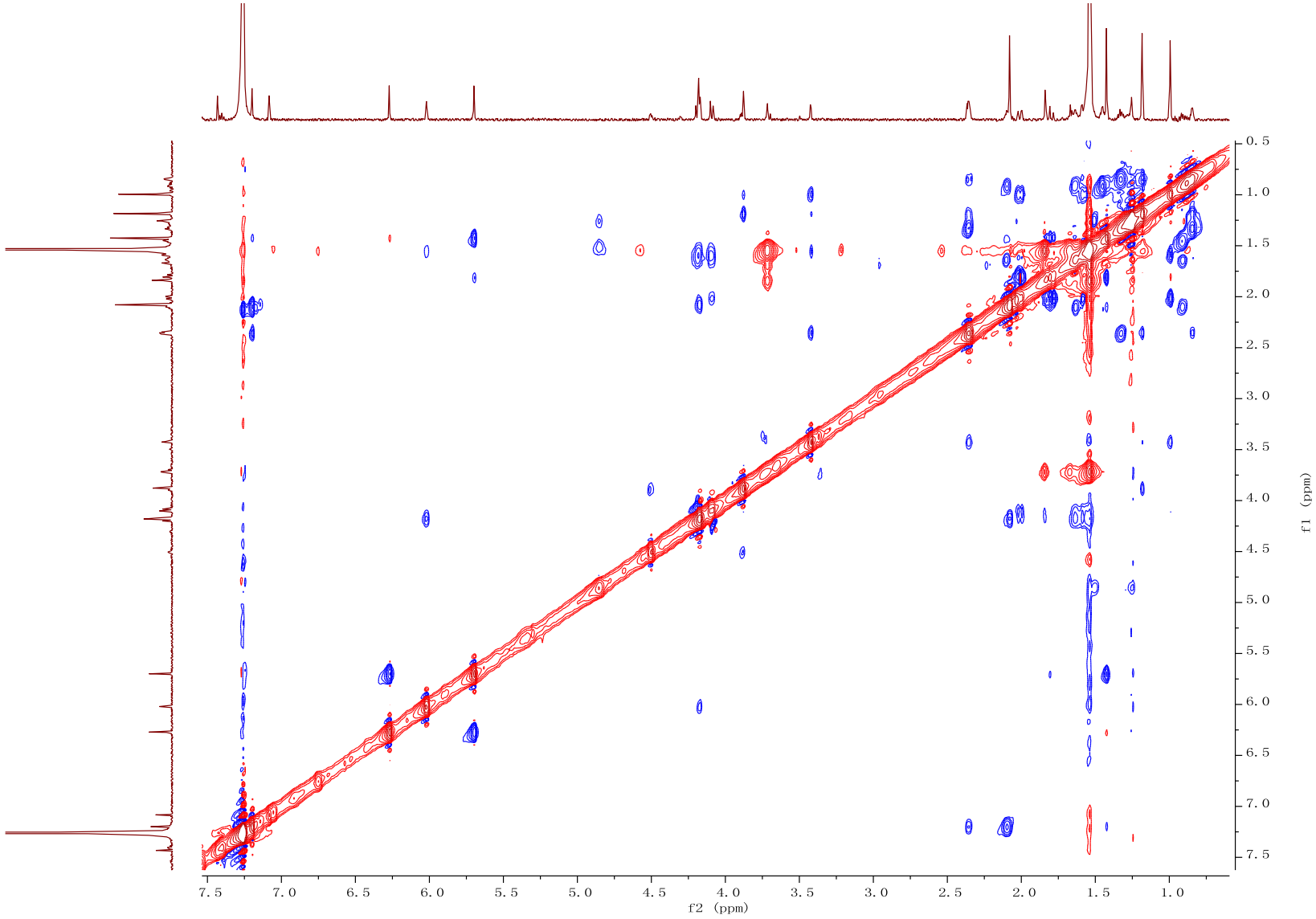


Figure S68. (+)-HRESIMS spectrum of chlorahupetone H (**8**)

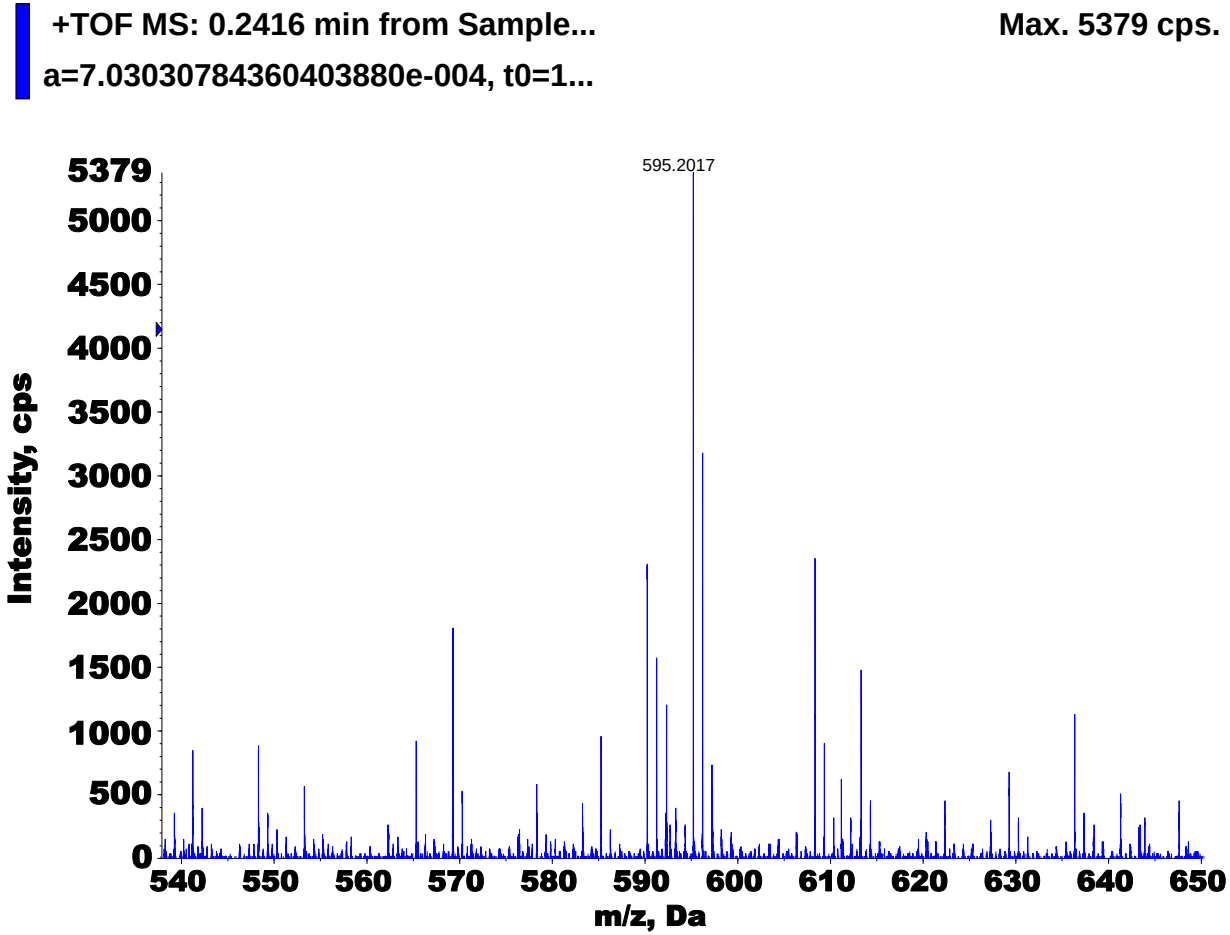


Figure S69. IR spectrum of chlorahupetone H (**8**)

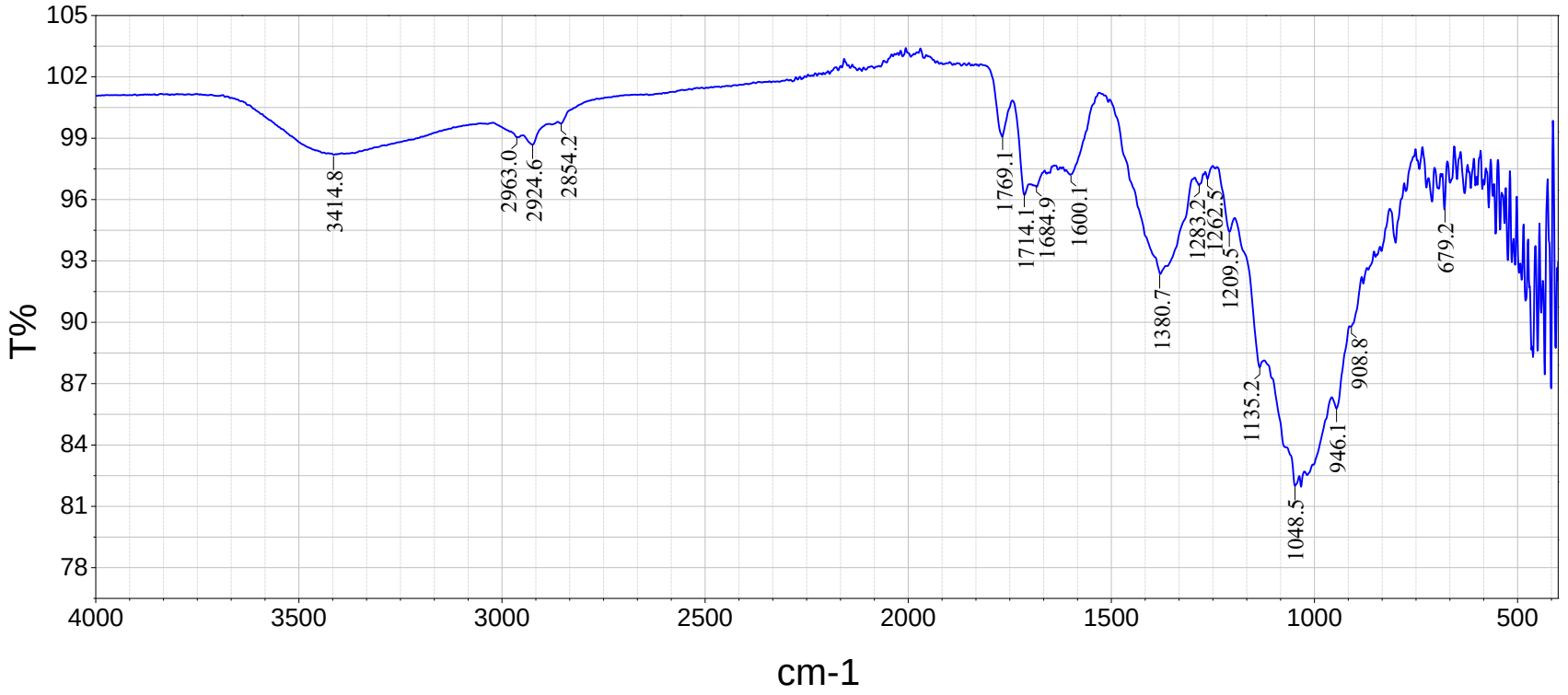


Figure S70. ^{1}H NMR spectrum of chlorahupetone I (**9**) in $CDCl_3$

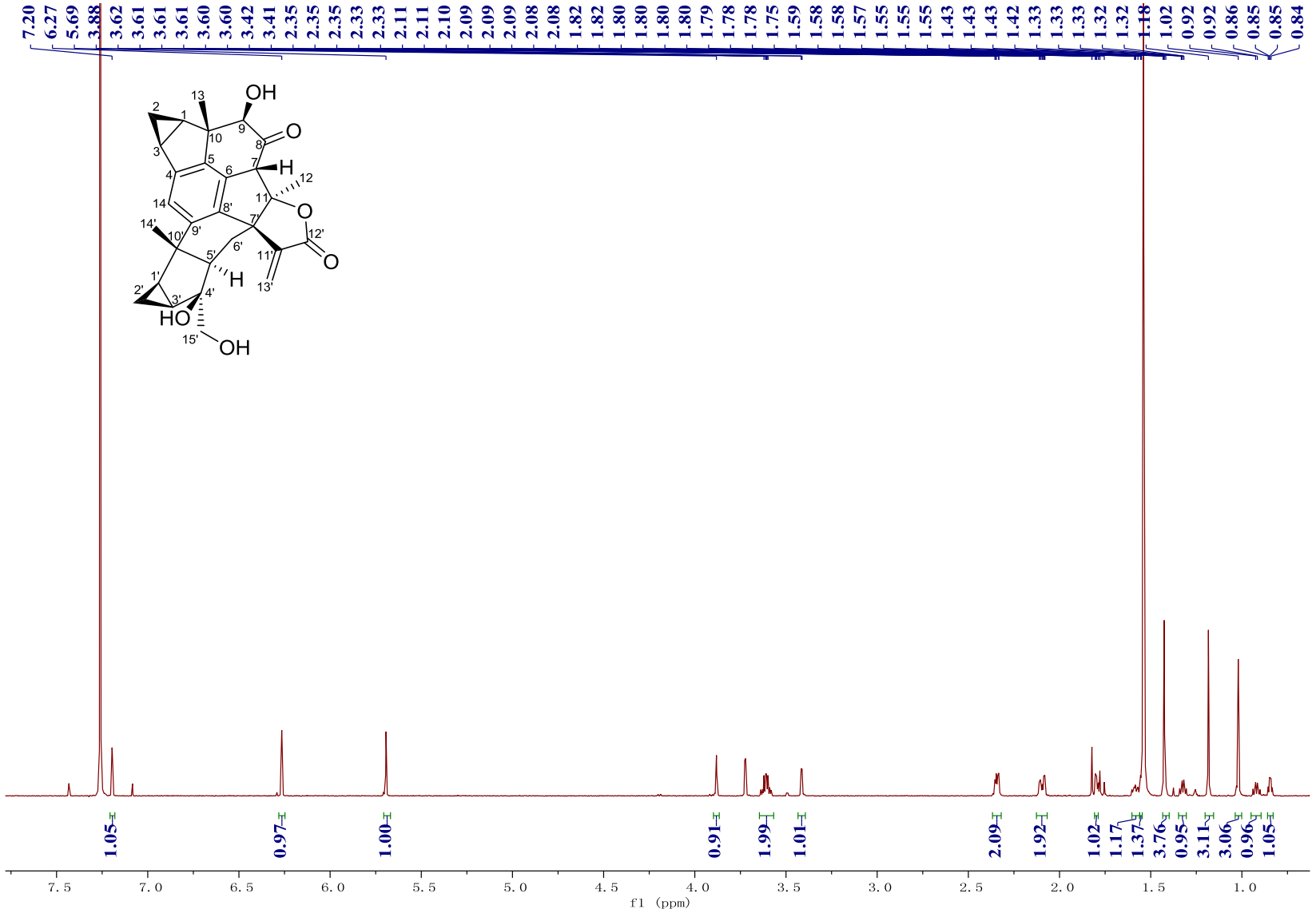


Figure S71. ^{13}C NMR and DEPT spectrum of chlorahupetone I (**9**) in $CDCl_3$

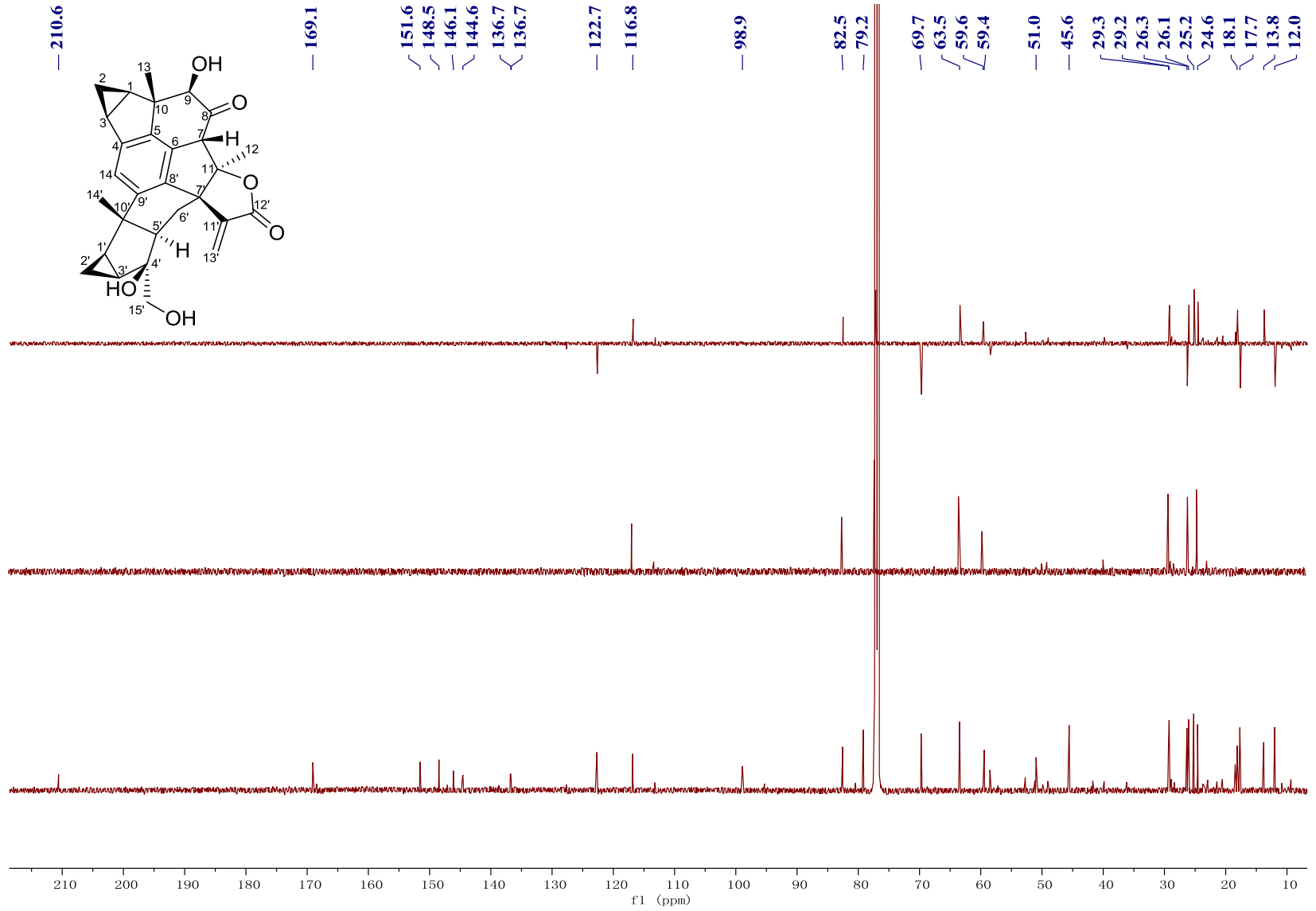


Figure S72. HSQC spectrum of chlorahupetone I (**9**) in $CDCl_3$

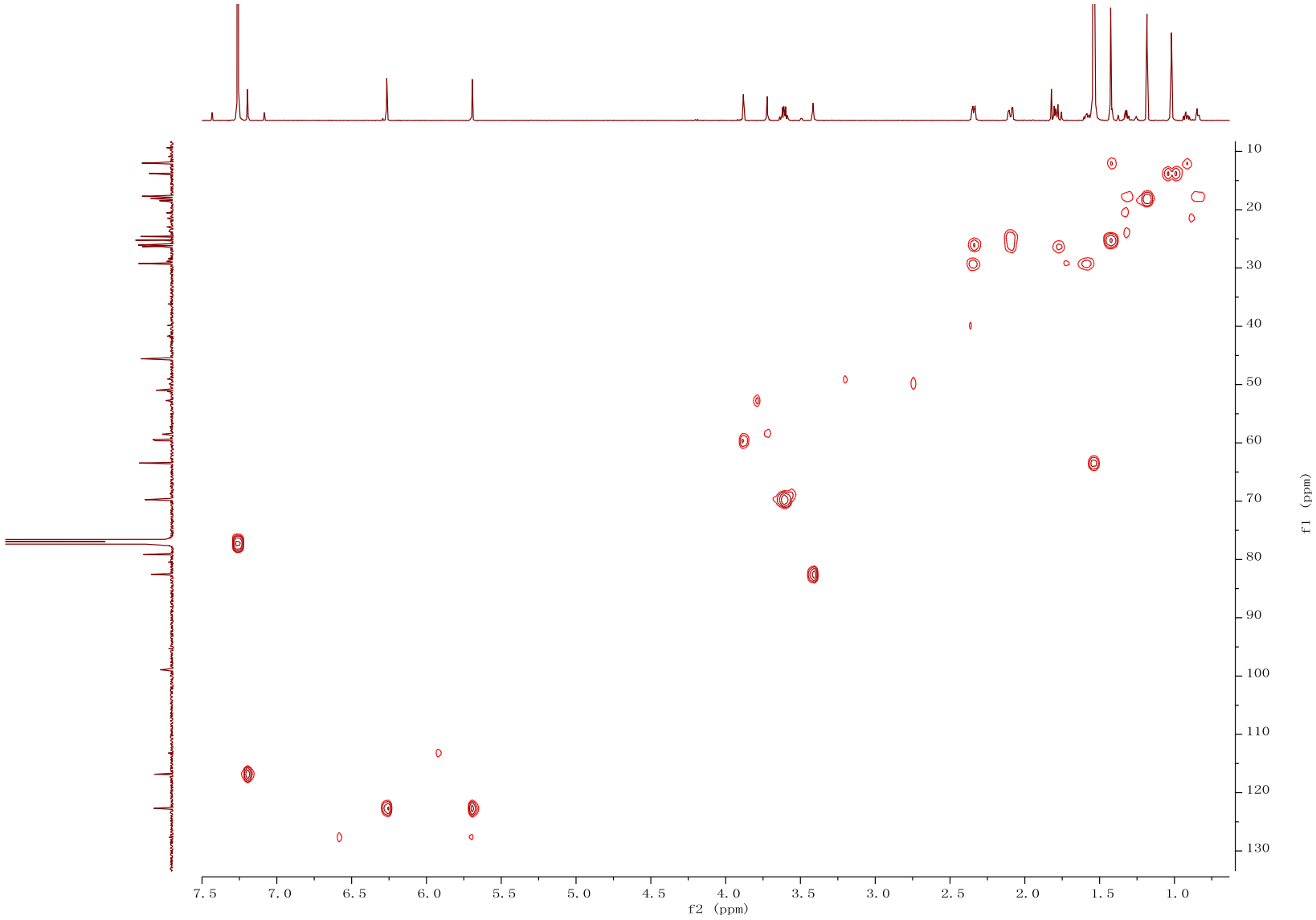


Figure S73. HMBC spectrum of chlorahupetone I (**9**) in $CDCl_3$

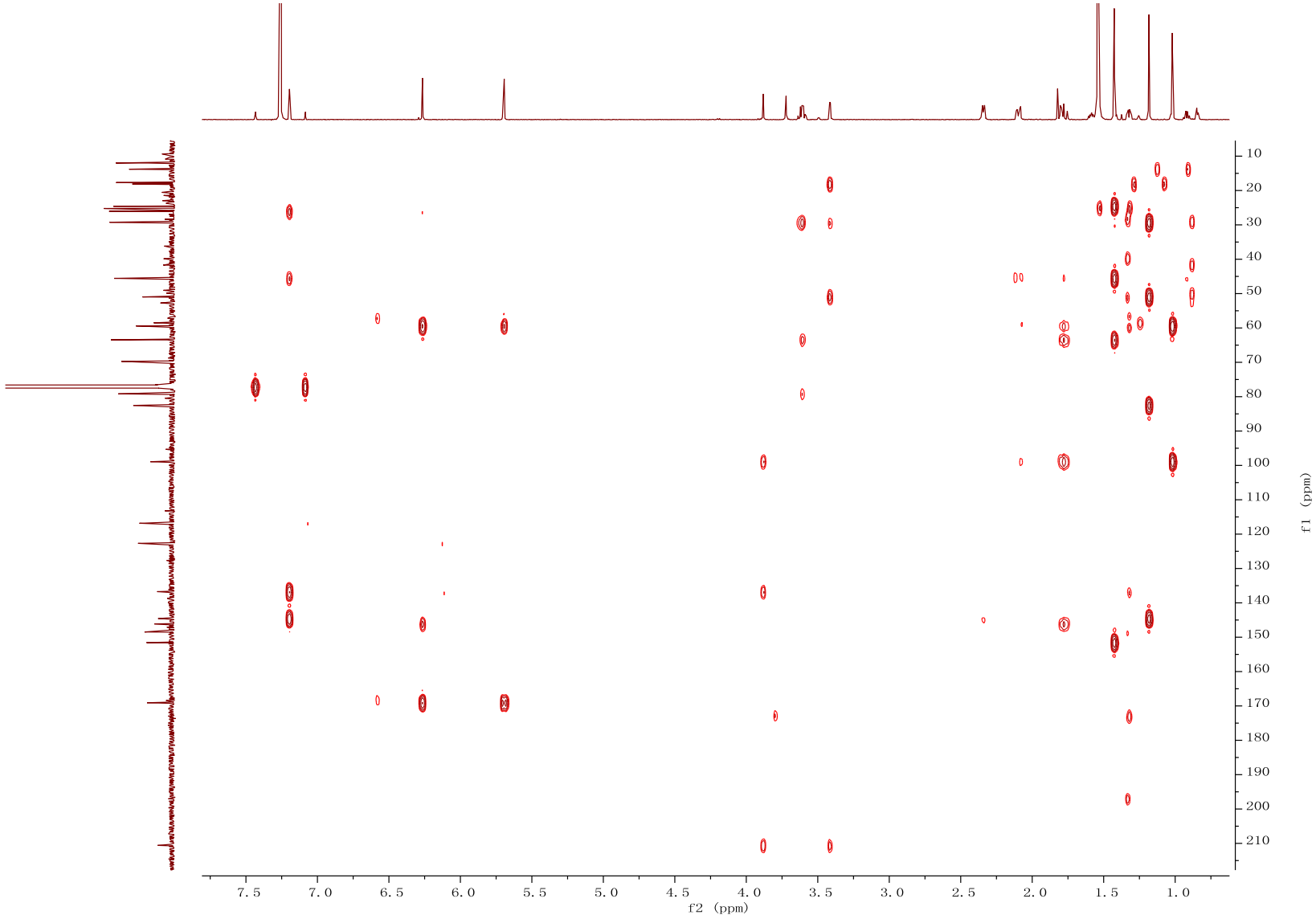


Figure S74. ^{1}H-^{1}H COSY spectrum of chlorahupetone I (**9**) in $CDCl_3$

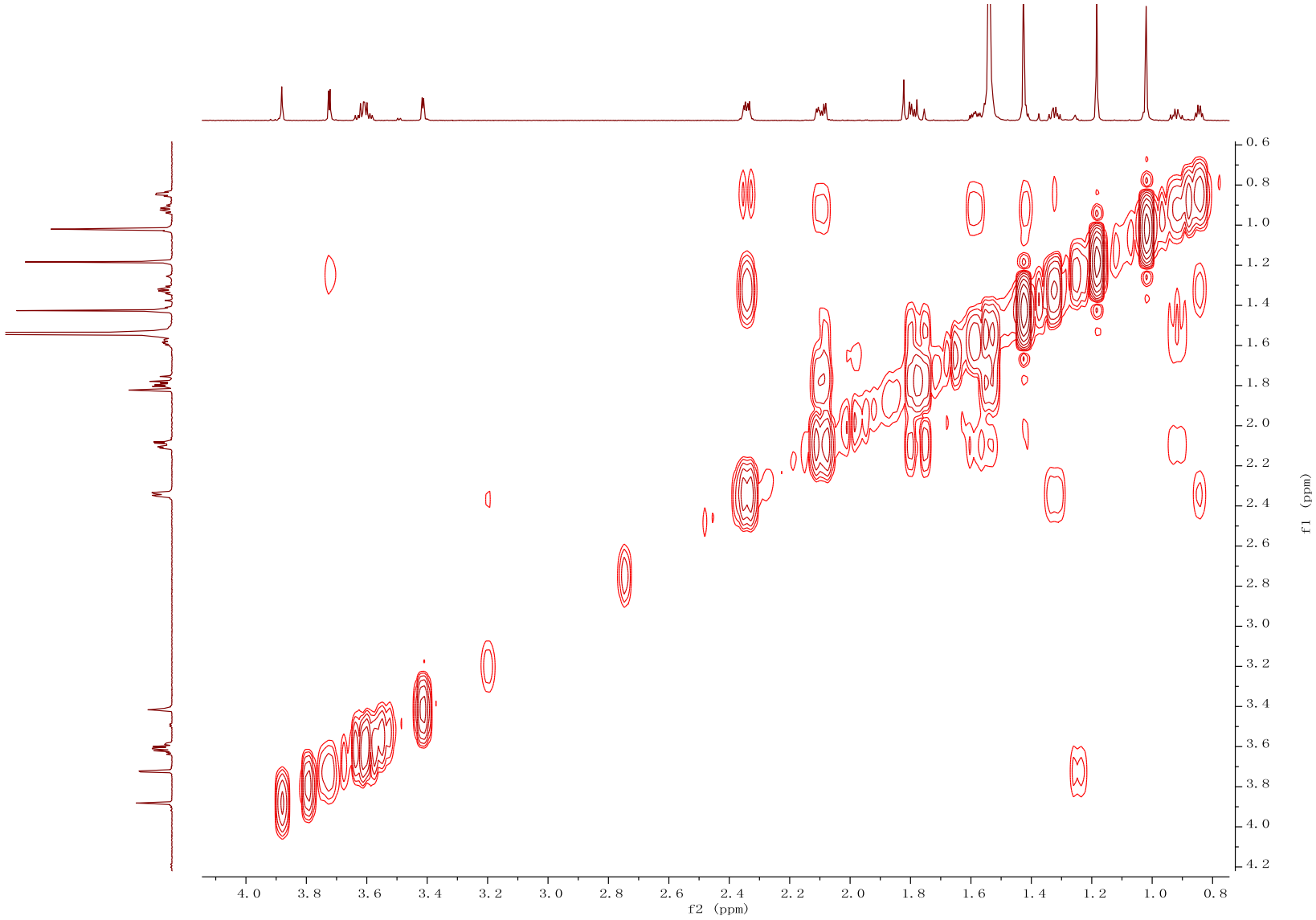


Figure S75. NOESY spectrum of chlorahupetone I (**9**) in $CDCl_3$

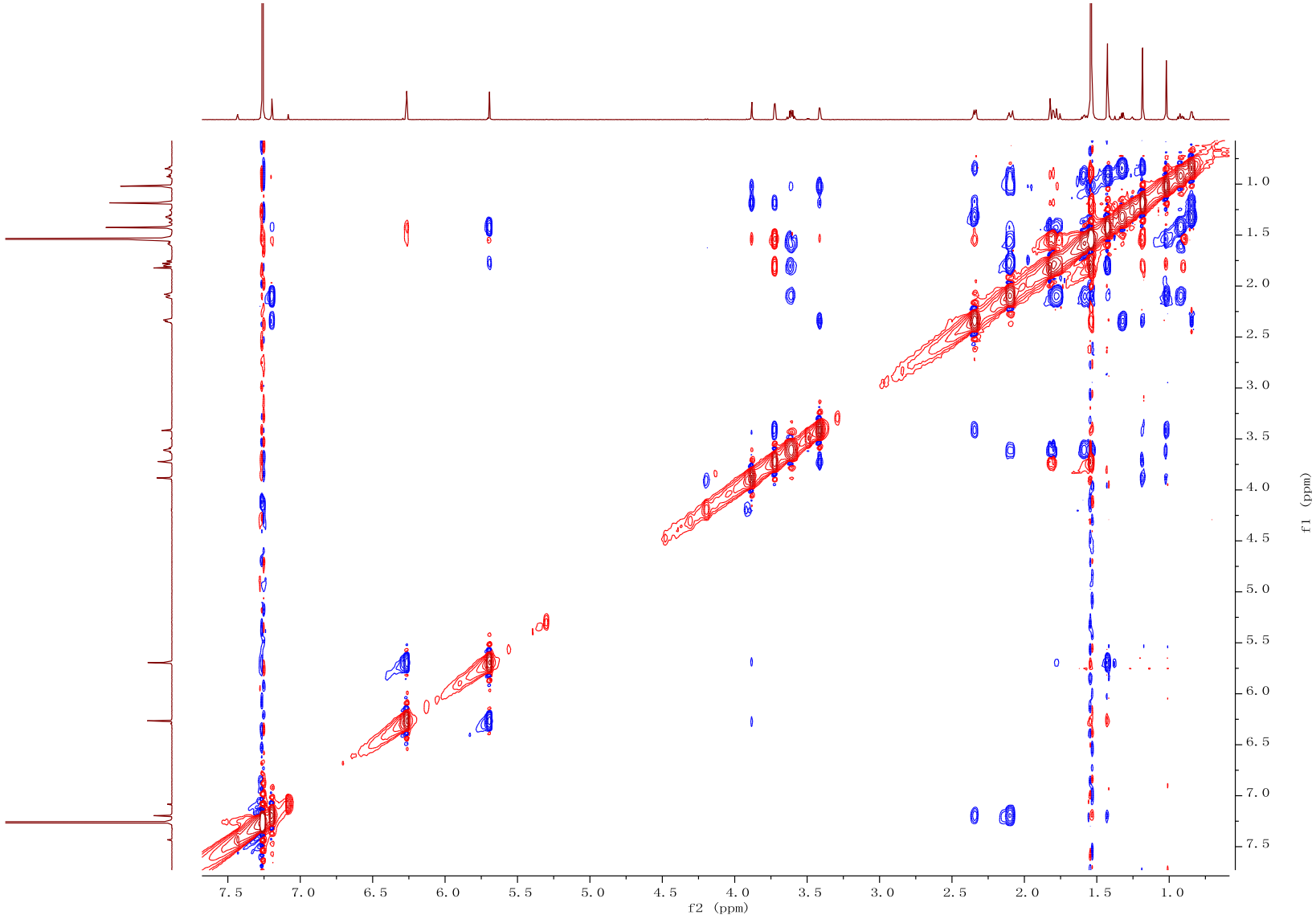


Figure S76. (+)-HRESIMS spectrum of chlorahupetone I (**9**)

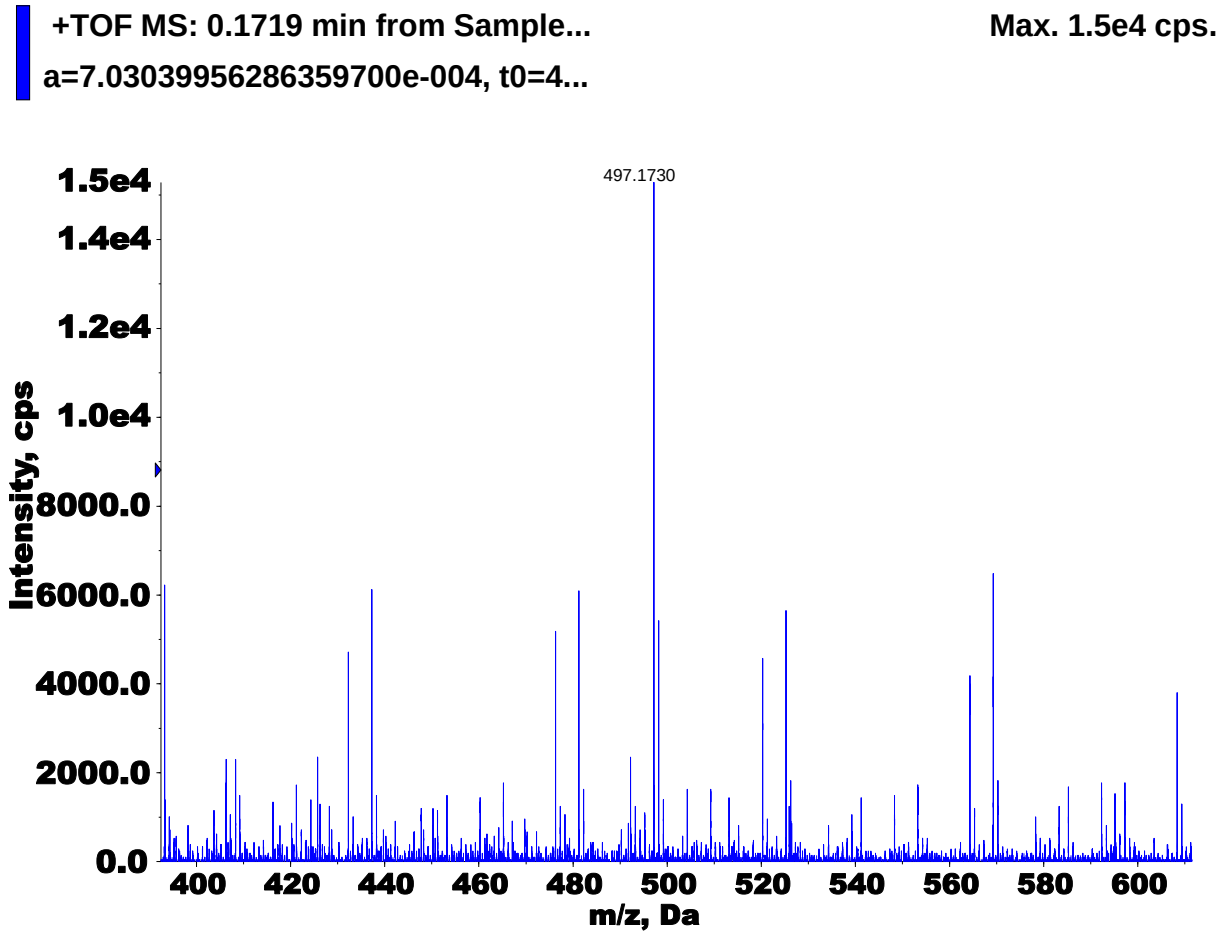


Figure S77. IR spectrum of chlorahupetone I (**9**)