

## Supporting Information

### **Heronamides G-L, polyene macrolactams from *Streptomyces niveus* isolated from Great Khingan Mountains soil**

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Computational details for ECD calculations

Compound **1**

The number of imaginary frequencies: 0

Energy: E(RB3LYP) = -1251.08406970

Cartesian Coordinates:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.106996	0.713665	0.520618
2	6	0	-1.220481	1.049386	-0.147503
3	6	0	-2.636605	1.067005	0.368061
4	6	0	-3.412805	2.270850	-0.109359
5	6	0	-4.665882	2.240487	-0.554684
6	6	0	-5.482442	0.984804	-0.632552
7	1	0	-6.485067	1.180535	-0.230601
8	8	0	-5.613435	0.611056	-2.013869
9	6	0	-4.859636	-0.153488	0.187998
10	1	0	-5.044848	0.056675	1.247510
11	8	0	-5.574796	-1.348197	-0.171857
12	6	0	-3.359316	-0.276261	-0.065723
13	6	0	-2.666079	-1.446384	0.608412
14	6	0	-3.037759	-1.792767	2.025800
15	6	0	-1.569883	-1.911228	-0.016574
16	6	0	-0.432530	-2.614448	0.563280

17	6	0	0.833860	-2.263969	0.284860
18	6	0	1.124694	0.347190	-0.282538
19	1	0	1.067950	0.874850	-1.238376
20	6	0	2.512833	0.655794	0.308632
21	1	0	2.534286	0.534261	1.396057
22	7	0	3.391251	-0.324163	-0.333170
23	6	0	4.767779	0.159231	-0.549112
24	1	0	4.957993	0.146254	-1.627116
25	6	0	5.817954	-0.712179	0.144647
26	6	0	7.249468	-0.248654	-0.129998
27	6	0	4.691876	1.611690	-0.024445
28	6	0	3.196852	1.980412	-0.037501
29	1	0	2.892075	2.294417	-1.042376
30	8	0	2.828691	2.975023	0.913052
31	6	0	2.749320	-1.297699	-1.008513
32	8	0	3.273605	-2.134958	-1.740905
33	1	0	-1.143883	1.149504	-1.229363
34	1	0	-2.627588	1.100791	1.461541
35	1	0	-2.888735	3.221292	-0.065343
36	1	0	-5.147886	3.155021	-0.884460
37	1	0	-5.977975	-0.286999	-2.007390
38	1	0	-4.956222	-2.088624	-0.204324
39	1	0	-2.399905	-2.575887	2.432797
40	1	0	-2.956530	-0.922938	2.686134
41	1	0	-4.073738	-2.136414	2.096146
42	1	0	-1.402769	-1.539691	-1.022679

43	1	0	-0.598703	-3.373312	1.321298
44	1	0	1.632654	-2.774325	0.814189
45	1	0	5.620533	-0.710205	1.221551
46	1	0	5.692706	-1.741485	-0.200116
47	1	0	7.427787	0.760851	0.247995
48	1	0	7.969266	-0.913512	0.351502
49	1	0	7.463906	-0.246560	-1.202318
50	1	0	5.043773	1.655540	1.010187
51	1	0	5.295418	2.299232	-0.616466
52	1	0	3.169550	3.827635	0.617509
53	6	0	-0.021557	0.579805	2.017300
54	1	0	0.680144	1.316029	2.420489
55	1	0	-0.977970	0.740481	2.510243
56	1	0	0.350390	-0.405416	2.309212
57	6	0	1.251860	-1.185882	-0.696855
58	1	0	0.705462	-1.328664	-1.631099
59	1	0	-3.220499	-0.367741	-1.147017

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**Compound 2**

The number of imaginary frequencies: 0

Energy: E(RB3LYP) = -1327.55896690

Cartesian Coordinates:

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

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1	6	0	-0.922069	2.098643	-0.195998
2	6	0	0.400829	2.242867	0.511088
3	6	0	1.615384	2.043183	-0.013935
4	6	0	2.837302	2.093445	0.772676
5	6	0	4.048371	1.643986	0.410286
6	6	0	4.419108	1.058083	-0.918009
7	1	0	3.561319	1.042574	-1.595692
8	8	0	5.475526	1.848922	-1.518737
9	6	0	5.001266	-0.363587	-0.894702
10	1	0	5.415163	-0.522201	-1.897830
11	8	0	6.055172	-0.509191	0.061183
12	6	0	4.001429	-1.517844	-0.694760
13	6	0	3.167079	-1.544085	0.575169
14	6	0	3.890065	-1.773925	1.872703
15	6	0	1.834616	-1.386001	0.460337
16	6	0	0.865743	-1.371941	1.543749
17	6	0	-0.421875	-0.999241	1.472067
18	6	0	-1.176163	-0.482443	0.280593
19	1	0	-0.550733	-0.527959	-0.612531
20	6	0	-1.744356	0.959971	0.475194
21	1	0	-1.760003	1.169395	1.548195
22	6	0	-3.213163	0.884129	-0.004961
23	1	0	-3.370176	1.476429	-0.912002
24	7	0	-3.463529	-0.528604	-0.266413
25	6	0	-4.888689	-0.896152	-0.143273



26	1	0	-4.950537	-1.714299	0.580016
27	6	0	-5.494297	-1.366274	-1.468150
28	6	0	-6.951069	-1.811984	-1.332541
29	6	0	-5.520163	0.397678	0.429952
30	6	0	-4.341610	1.229422	0.970286
31	1	0	-4.065837	0.891598	1.975818
32	8	0	-4.562675	2.636048	0.974956
33	6	0	-2.419611	-1.344247	-0.004478
34	8	0	-2.462582	-2.571047	0.011066
35	1	0	0.331736	2.483646	1.570787
36	1	0	1.702163	1.779937	-1.061415
37	1	0	2.731854	2.492907	1.778702
38	1	0	4.864273	1.714337	1.121868
39	1	0	5.252225	2.781050	-1.404121
40	1	0	6.790109	0.048289	-0.223142
41	1	0	3.315591	-1.474785	-1.542893
42	1	0	4.544200	-2.646425	1.800649
43	1	0	4.529368	-0.920915	2.113349
44	1	0	3.210495	-1.935922	2.706646
45	1	0	1.441960	-1.227621	-0.539317
46	1	0	1.220987	-1.673858	2.523104
47	1	0	-1.004353	-1.043017	2.389157
48	1	0	-5.414736	-0.556044	-2.200282
49	1	0	-4.890809	-2.195987	-1.845693
50	1	0	-7.595247	-0.995187	-0.998337
51	1	0	-7.337157	-2.165958	-2.290499

52	1	0	-7.047260	-2.629263	-0.612393
53	1	0	-6.002457	0.968746	-0.368285
54	1	0	-6.268198	0.188275	1.194221
55	1	0	-5.188830	2.850339	1.676648
56	8	0	4.726946	-2.751014	-0.853041
57	1	0	5.571831	-2.643935	-0.393627
58	6	0	-0.798574	1.971754	-1.717804
59	1	0	-0.264120	2.831837	-2.125706
60	1	0	-0.256236	1.074134	-2.021405
61	1	0	-1.778429	1.941658	-2.195890
62	1	0	-1.489875	3.016087	0.010443

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**Compound 3**

The number of imaginary frequencies: 0

Energy: E(RB3LYP) = -1402.79456774

Cartesian Coordinates:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	3.512190	2.584729	-0.626720
2	6	0	3.099572	1.585913	-0.022238
3	7	0	3.764313	0.398109	-0.058849
4	6	0	3.210848	-0.911594	0.399363
5	6	0	4.310576	-1.915129	0.004292

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6	1	0	3.871566	-2.876944	-0.269128
7	8	0	5.157748	-2.084951	1.149705
8	6	0	5.027434	-1.251950	-1.173370
9	6	0	4.989424	0.255807	-0.878771
10	1	0	4.846167	0.826946	-1.798206
11	6	0	6.228800	0.811789	-0.159759
12	6	0	7.454966	0.900127	-1.070093
13	1	0	3.135559	-0.916147	1.485845
14	6	0	1.868989	-1.179765	-0.231639
15	6	0	0.730067	-1.528633	0.394180
16	6	0	0.655608	-1.915491	1.848563
17	6	0	-0.525999	-1.382806	-0.348085
18	6	0	-1.748837	-1.310035	0.191939
19	6	0	-2.972720	-0.942118	-0.592688
20	1	0	-2.698355	-0.988639	-1.647205
21	6	0	-3.642587	0.492832	-0.409971
22	6	0	-5.152525	0.203824	-0.227923
23	1	0	-5.406930	0.133365	0.831752
24	8	0	-6.004260	1.155500	-0.864540
25	6	0	-5.379690	-1.169855	-0.857560
26	1	0	-6.299966	-1.640535	-0.493400
27	8	0	-5.403566	-1.087887	-2.281281
28	6	0	-4.136603	-1.948556	-0.427284
29	1	0	-3.980249	-2.832549	-1.051975
30	8	0	-4.242766	-2.326395	0.949052
31	1	0	-3.549182	0.987570	-1.379363

32	6	0	-3.099259	1.545985	0.601908
33	8	0	-4.019837	2.667208	0.391732
34	6	0	-3.174261	1.135461	2.071174
35	6	0	-1.731428	2.011682	0.164949
36	6	0	-0.590948	1.916444	0.857174
37	6	0	0.713909	2.162857	0.271245
38	6	0	1.832164	1.604315	0.754058
39	1	0	5.867019	-2.695767	0.914066
40	1	0	6.039455	-1.636904	-1.300713
41	1	0	4.476801	-1.470607	-2.091414
42	1	0	5.982283	1.810011	0.209049
43	1	0	6.446353	0.190154	0.711905
44	1	0	8.306803	1.319452	-0.530325
45	1	0	7.757014	-0.079974	-1.447634
46	1	0	7.259780	1.542620	-1.933413
47	1	0	1.809891	-0.925415	-1.286934
48	1	0	0.120031	-1.163473	2.435606
49	1	0	0.105243	-2.853197	1.961700
50	1	0	1.637134	-2.056652	2.295638
51	1	0	-0.417064	-1.182822	-1.412213
52	1	0	-1.880688	-1.496653	1.249989
53	1	0	-5.685460	2.027609	-0.586779
54	1	0	-5.838444	-0.251160	-2.502154
55	1	0	-4.950483	-2.977106	1.032883
56	1	0	-3.756786	3.392606	0.972809
57	1	0	-2.543878	0.275788	2.289706

58	1	0	-2.849340	1.960721	2.708882
59	1	0	-4.198370	0.886816	2.344959
60	1	0	-1.702989	2.403025	-0.849628
61	1	0	-0.595721	1.497147	1.857963
62	1	0	0.751271	2.687916	-0.679283
63	1	0	1.790252	1.023770	1.668598

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**Compound 4**

The number of imaginary frequencies: 0

Energy: E(RB3LYP) = -1402.79168094

Cartesian Coordinates:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	2.757187	2.370666	0.583223
2	6	0	2.313473	1.430899	-0.079576
3	6	0	1.036092	1.555635	-0.850509
4	6	0	0.044054	2.339534	-0.413641
5	6	0	-1.273727	2.564155	-1.124288
6	1	0	-1.118196	2.367388	-2.197299
7	8	0	-1.711559	3.918010	-0.949130
8	6	0	-2.372307	1.615708	-0.666594
9	1	0	-2.580059	0.830361	-1.390570
10	6	0	-3.063921	1.604779	0.484515

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11	6	0	-2.853224	2.589719	1.609351
12	6	0	-4.133087	0.550958	0.741019
13	1	0	-4.704949	0.871417	1.620492
14	6	0	-3.656400	-0.924298	1.098360
15	6	0	-4.986317	-1.683532	0.936736
16	1	0	-5.666032	-1.382545	1.752563
17	8	0	-4.804660	-3.087096	0.935952
18	6	0	-5.565699	-1.139213	-0.377945
19	1	0	-5.028857	-1.624124	-1.203578
20	8	0	-6.937476	-1.423946	-0.557669
21	6	0	-5.223232	0.376136	-0.361256
22	1	0	-4.871756	0.712813	-1.342182
23	8	0	-6.428981	1.074558	-0.022632
24	1	0	-3.315068	-0.940053	2.139214
25	6	0	-2.553800	-1.447130	0.224770
26	6	0	-1.264593	-1.455542	0.599779
27	6	0	-0.111182	-1.649780	-0.281923
28	6	0	-0.361648	-2.086645	-1.705581
29	6	0	1.101923	-1.292862	0.191456
30	6	0	2.370355	-1.053281	-0.589059
31	1	0	2.178789	-1.047256	-1.666030
32	7	0	2.982256	0.232813	-0.165847
33	6	0	4.245487	0.057620	0.580285
34	1	0	4.168420	0.616737	1.518040
35	6	0	5.445564	0.618986	-0.219455
36	6	0	6.738635	0.553641	0.544537

37	6	0	7.833848	-0.106658	0.154740
38	6	0	9.132769	-0.158248	0.908088
39	6	0	4.294617	-1.460135	0.829881
40	6	0	3.495560	-2.078067	-0.325283
41	1	0	3.071834	-3.057727	-0.065843
42	8	0	4.252416	-2.171906	-1.534280
43	1	0	0.935389	0.995136	-1.778618
44	1	0	0.169502	2.860226	0.534778
45	1	0	-0.962087	4.489944	-1.184070
46	1	0	-2.145361	3.375622	1.346835
47	1	0	-3.802295	3.069065	1.885593
48	1	0	-2.495330	2.070755	2.510164
49	1	0	-5.668802	-3.470219	0.710267
50	1	0	-7.406129	-0.606929	-0.304868
51	1	0	-6.362010	1.984413	-0.346505
52	1	0	-2.816406	-1.739631	-0.789383
53	1	0	-1.024300	-1.154929	1.620365
54	1	0	-0.930153	-3.024167	-1.722432
55	1	0	-0.959031	-1.343541	-2.250642
56	1	0	0.562529	-2.253906	-2.262825
57	1	0	1.168403	-1.002325	1.239917
58	1	0	5.527045	0.075861	-1.166930
59	1	0	5.206277	1.665177	-0.450630
60	1	0	6.765360	1.099895	1.490705
61	1	0	7.809003	-0.644770	-0.795589
62	1	0	9.074525	0.400083	1.848685

63	1	0	9.419091	-1.192320	1.144599
64	1	0	9.954670	0.264761	0.314344
65	1	0	5.320798	-1.839463	0.880653
66	1	0	3.805624	-1.707726	1.779909
67	1	0	5.028909	-2.724300	-1.352346

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**Compound 5**

The number of imaginary frequencies: 0

Energy: E(RB3LYP) = -1327.56401830

Cartesian Coordinates:

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	8	0	3.262301	-2.736857	-1.120339
2	6	0	3.636616	-1.612343	-0.771582
3	6	0	2.670889	-0.427633	-0.802734
4	1	0	2.666380	-0.096625	-1.848279
5	6	0	1.275316	-0.828596	-0.413353
6	6	0	0.185276	-0.277557	-0.948309
7	6	0	-1.189632	-0.332445	-0.362594
8	1	0	-1.217515	-1.137745	0.378032
9	6	0	-1.624923	0.968955	0.431000
10	6	0	-3.157665	0.787381	0.566834
11	6	0	-3.669174	0.238758	1.924772

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12	1	0	-4.017525	1.043764	2.577191
13	8	0	-2.636488	-0.506927	2.580111
14	6	0	-4.823045	-0.692129	1.541018
15	1	0	-5.047952	-1.414117	2.333754
16	8	0	-5.974577	0.104677	1.264454
17	6	0	-4.306380	-1.374554	0.271304
18	1	0	-3.590775	-2.144490	0.572408
19	8	0	-5.420358	-1.981514	-0.388176
20	1	0	-3.659434	1.739736	0.402963
21	6	0	-3.612776	-0.244451	-0.516475
22	1	0	-4.351870	0.190127	-1.190761
23	6	0	-2.358414	-0.599187	-1.343564
24	6	0	-2.333642	-2.002249	-1.944941
25	8	0	-2.355862	0.369061	-2.418877
26	1	0	-1.160767	0.894192	1.414795
27	6	0	-1.260547	2.313160	-0.166829
28	6	0	-0.042835	2.887088	-0.181970
29	6	0	0.194171	4.219228	-0.846059
30	6	0	1.105447	2.134897	0.339653
31	6	0	2.298448	1.985817	-0.246685
32	6	0	3.172470	0.804721	0.058835
33	1	0	3.048253	0.535349	1.111627
34	6	0	4.653758	1.042004	-0.241205
35	6	0	5.526756	-0.160974	0.117955
36	1	0	6.487823	-0.051437	-0.394659
37	6	0	5.817276	-0.266178	1.625627

38	6	0	6.756369	-1.412674	2.003760
39	7	0	4.916692	-1.391386	-0.405970
40	1	0	1.181438	-1.460527	0.467058
41	1	0	0.317615	0.380440	-1.803827
42	1	0	-2.956128	-0.762980	3.453641
43	1	0	-6.519539	-0.393014	0.638584
44	1	0	-5.130661	-2.379137	-1.216997
45	1	0	-2.354164	-2.778342	-1.177716
46	1	0	-3.179340	-2.146637	-2.621492
47	1	0	-1.418802	-2.146683	-2.525675
48	1	0	-1.582120	0.210626	-2.973870
49	1	0	-2.070665	2.856140	-0.645622
50	1	0	0.636523	4.933822	-0.145513
51	1	0	0.891022	4.128928	-1.685091
52	1	0	-0.736949	4.640783	-1.227303
53	1	0	0.889611	1.483733	1.181615
54	1	0	2.552245	2.560715	-1.135058
55	1	0	4.768335	1.268308	-1.306187
56	1	0	5.015196	1.912867	0.309323
57	1	0	6.265402	0.682691	1.935793
58	1	0	4.875210	-0.365415	2.172761
59	1	0	6.979905	-1.389857	3.072244
60	1	0	6.316977	-2.389072	1.786235
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62	1	0	5.497646	-2.218795	-0.436366

## User Spectra

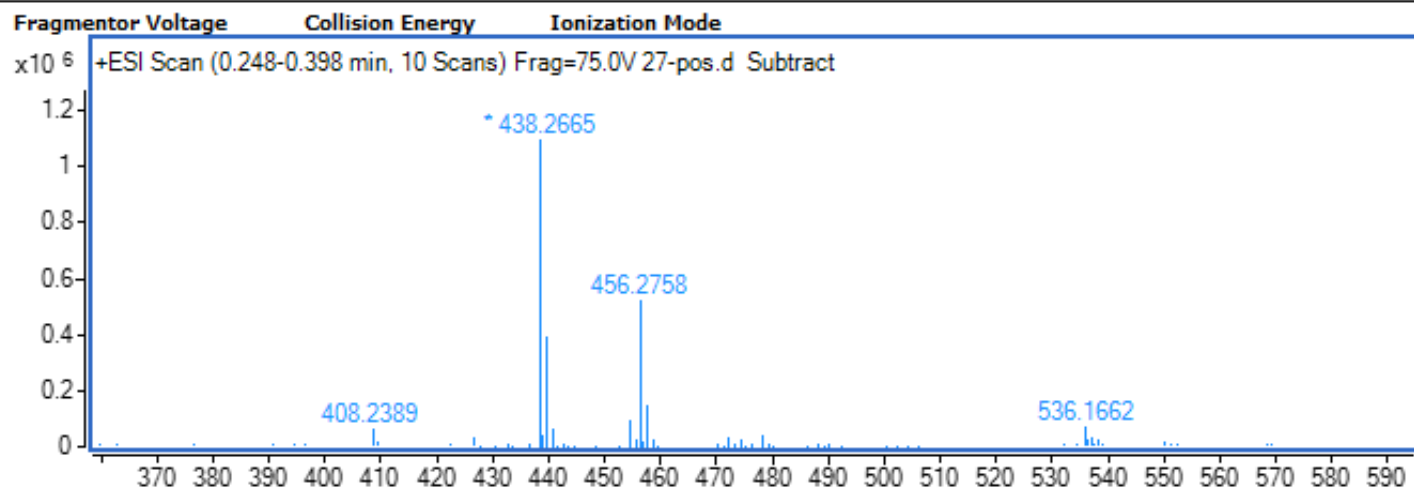
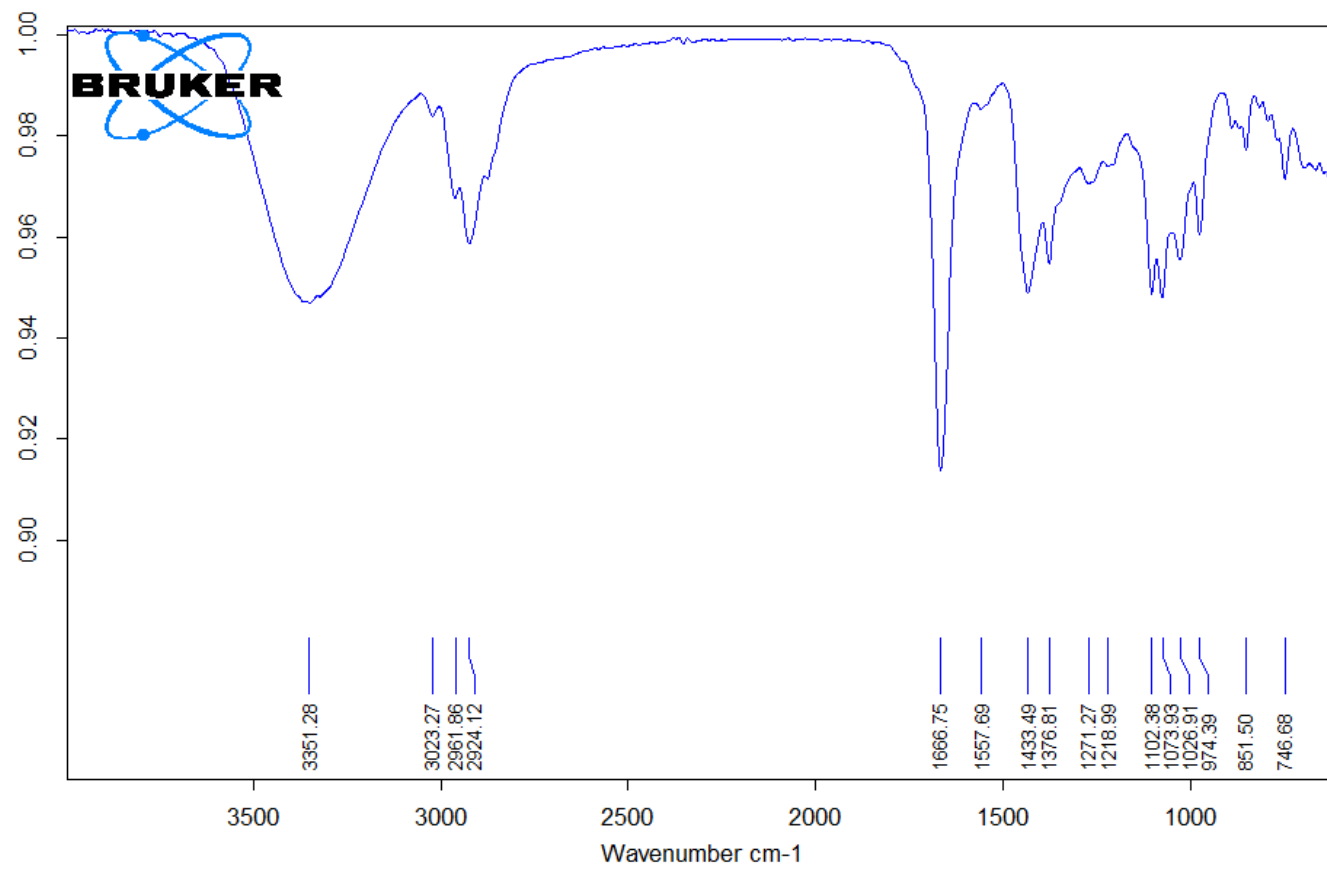
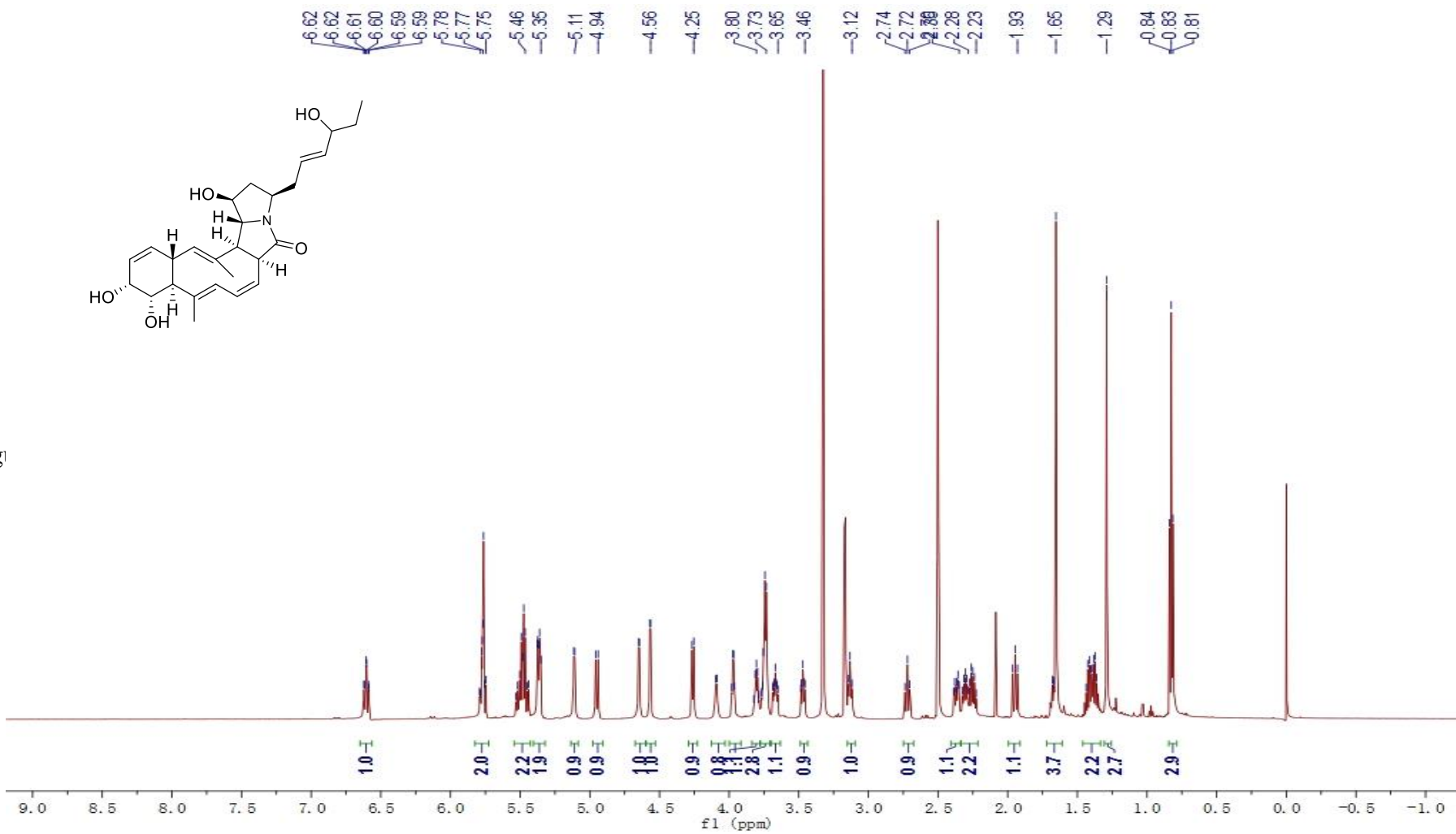
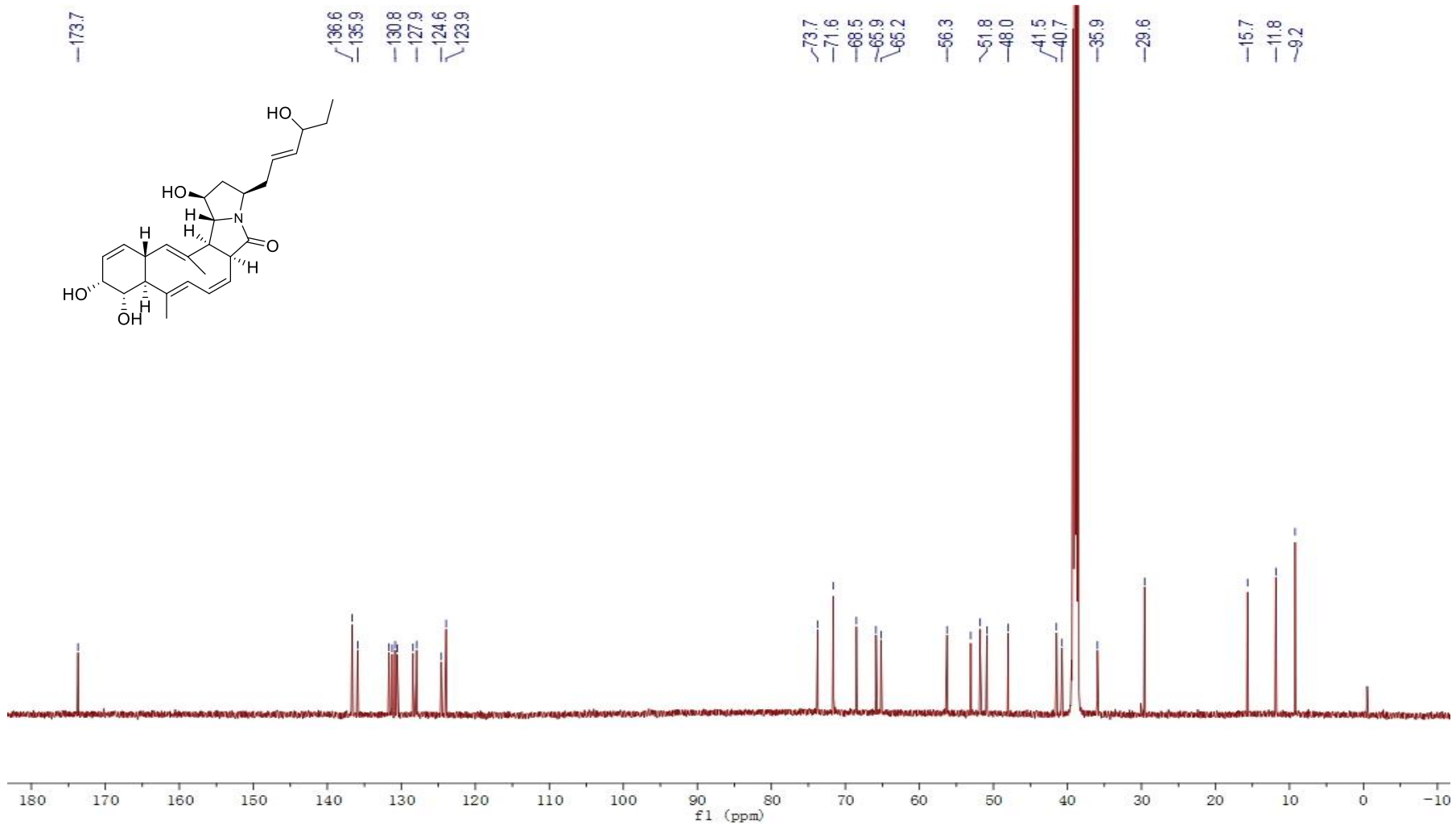
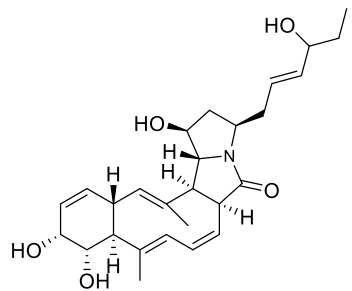


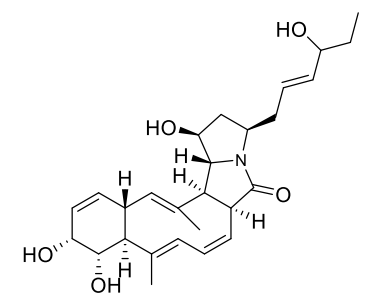
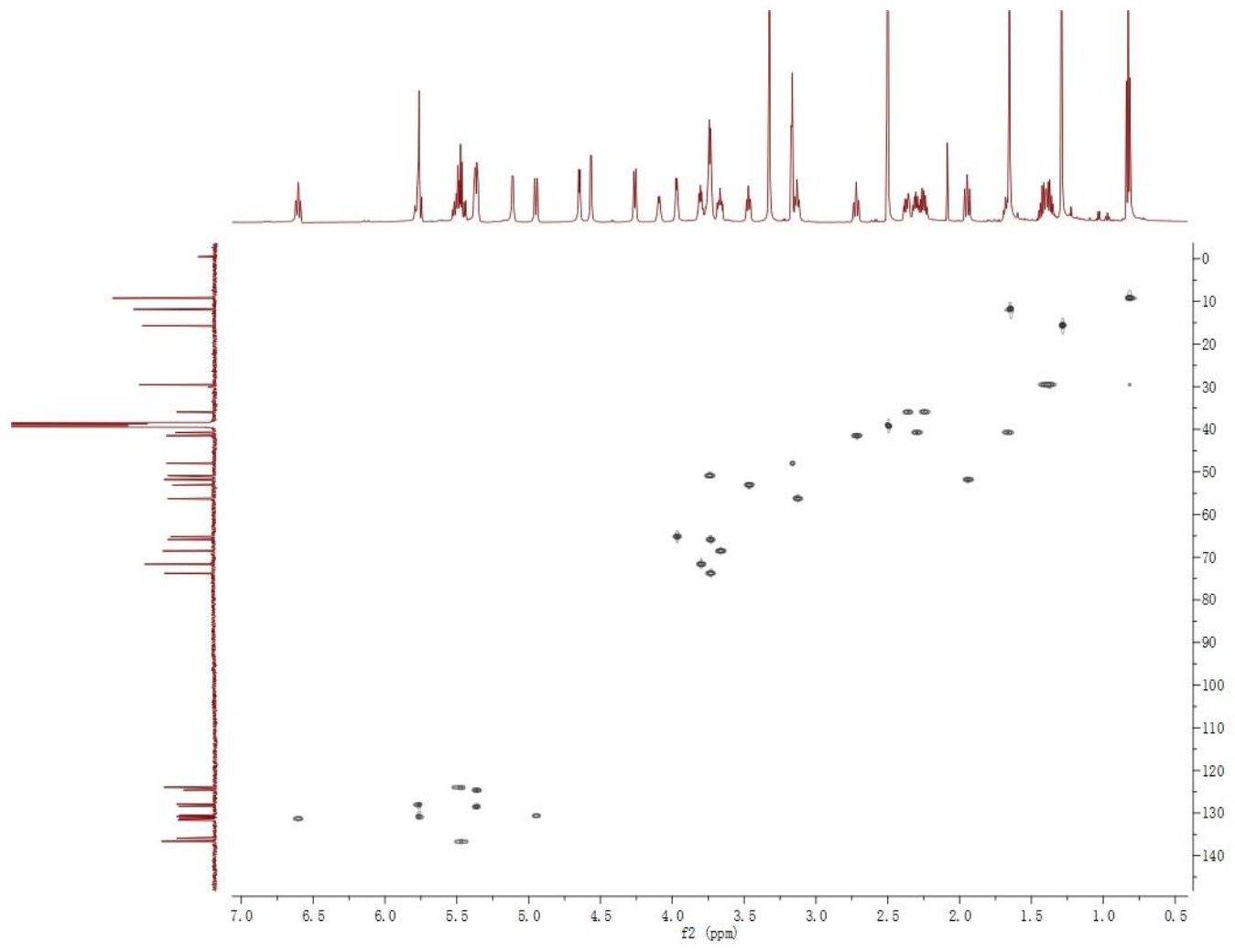
Figure S1. HRESIMS spectrum of compound **1**

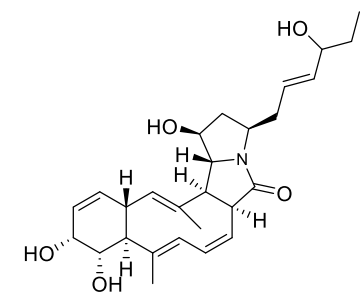
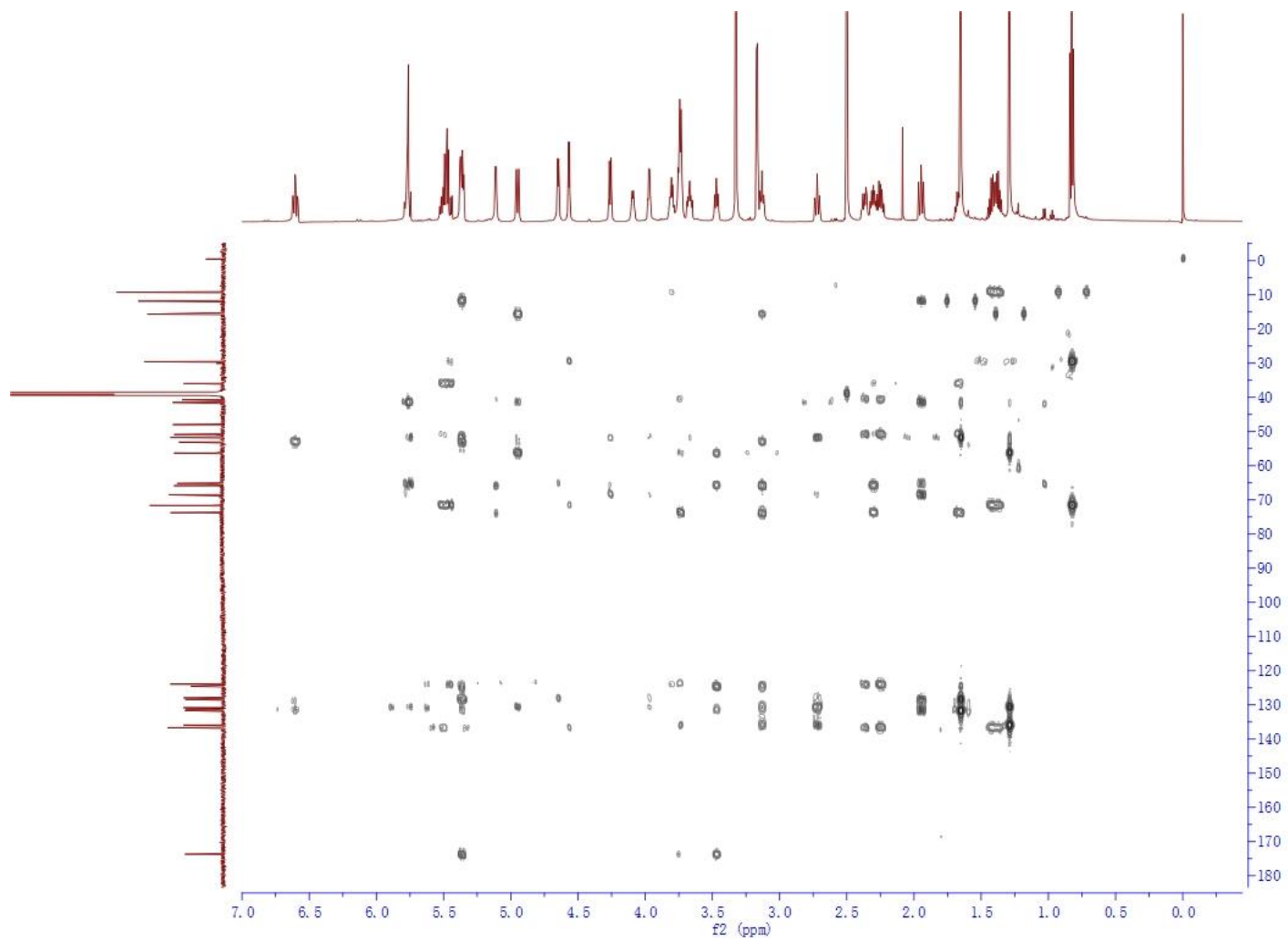




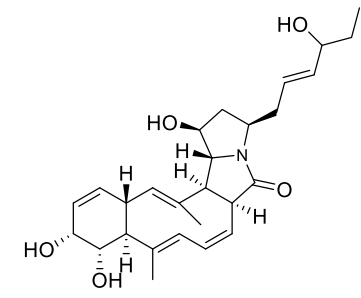
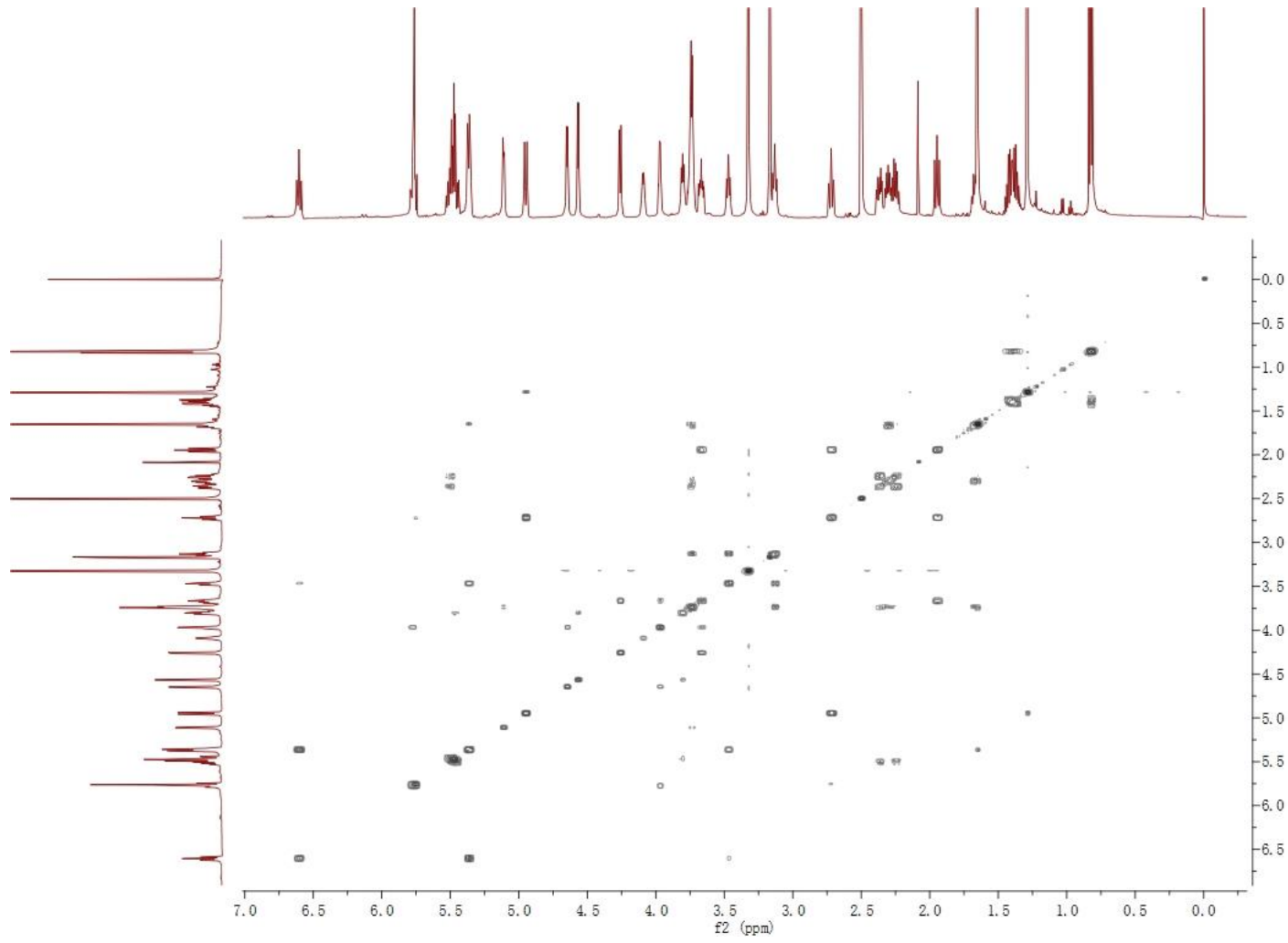
Fig











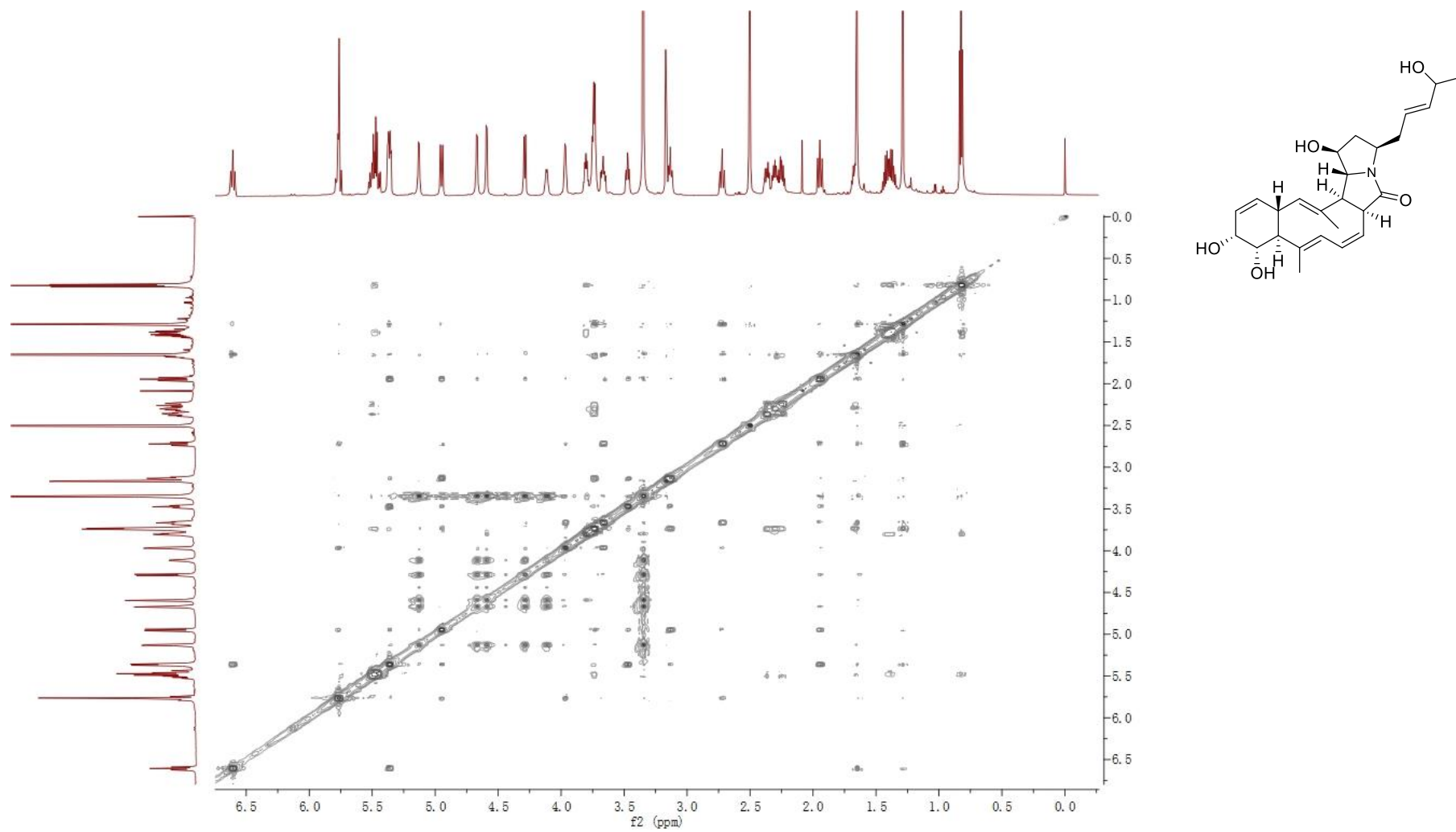


Figure S8. NOESY spectrum of compound **1**

## User Spectra

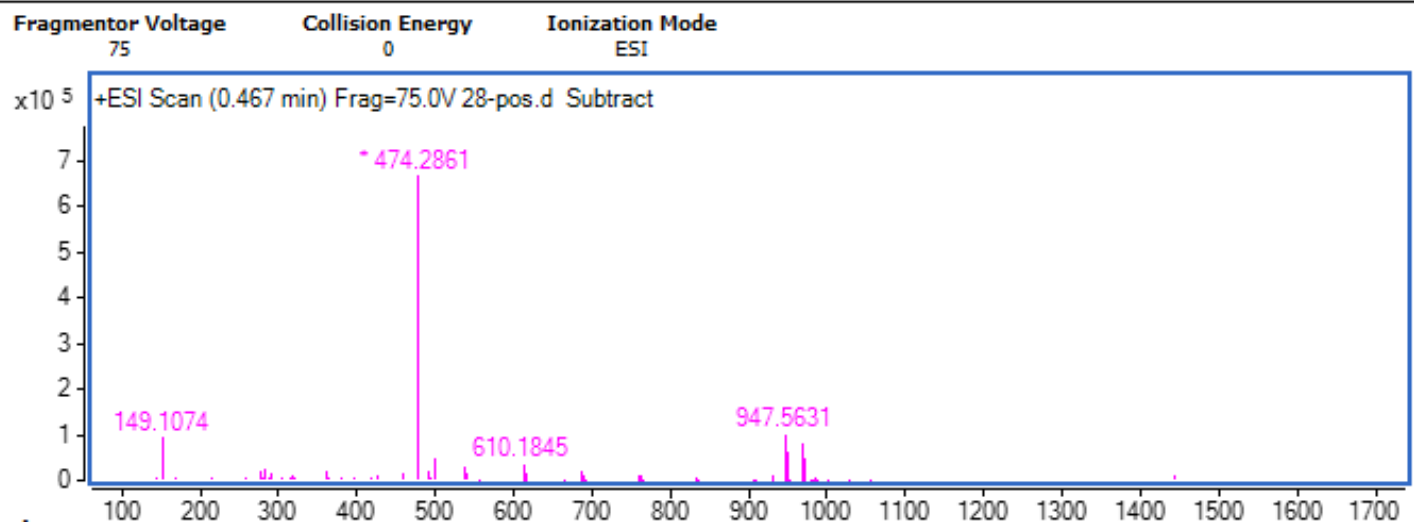


Figure S9. HRESIMS spectrum of compound **2**

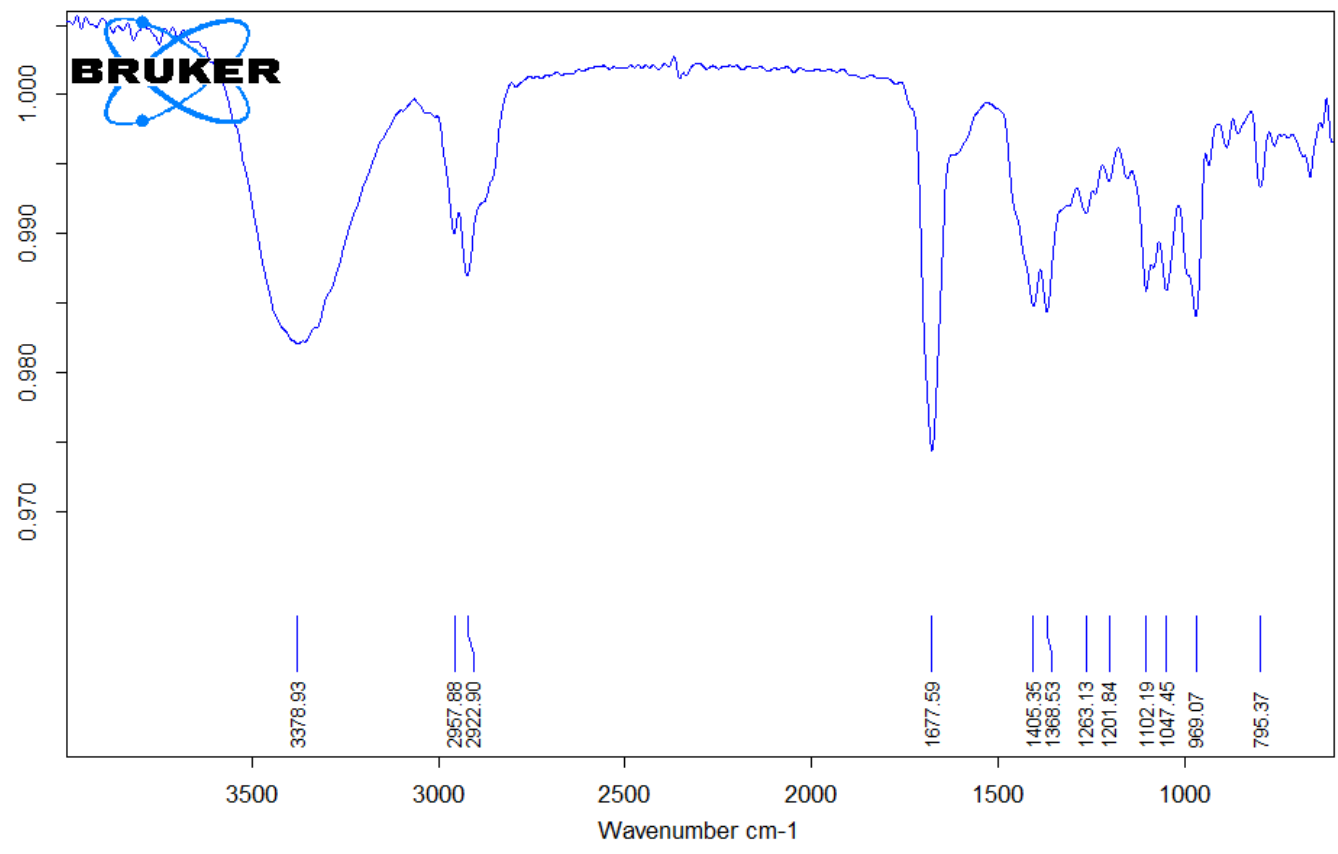


Figure S10. IR spectrum of compound **2**

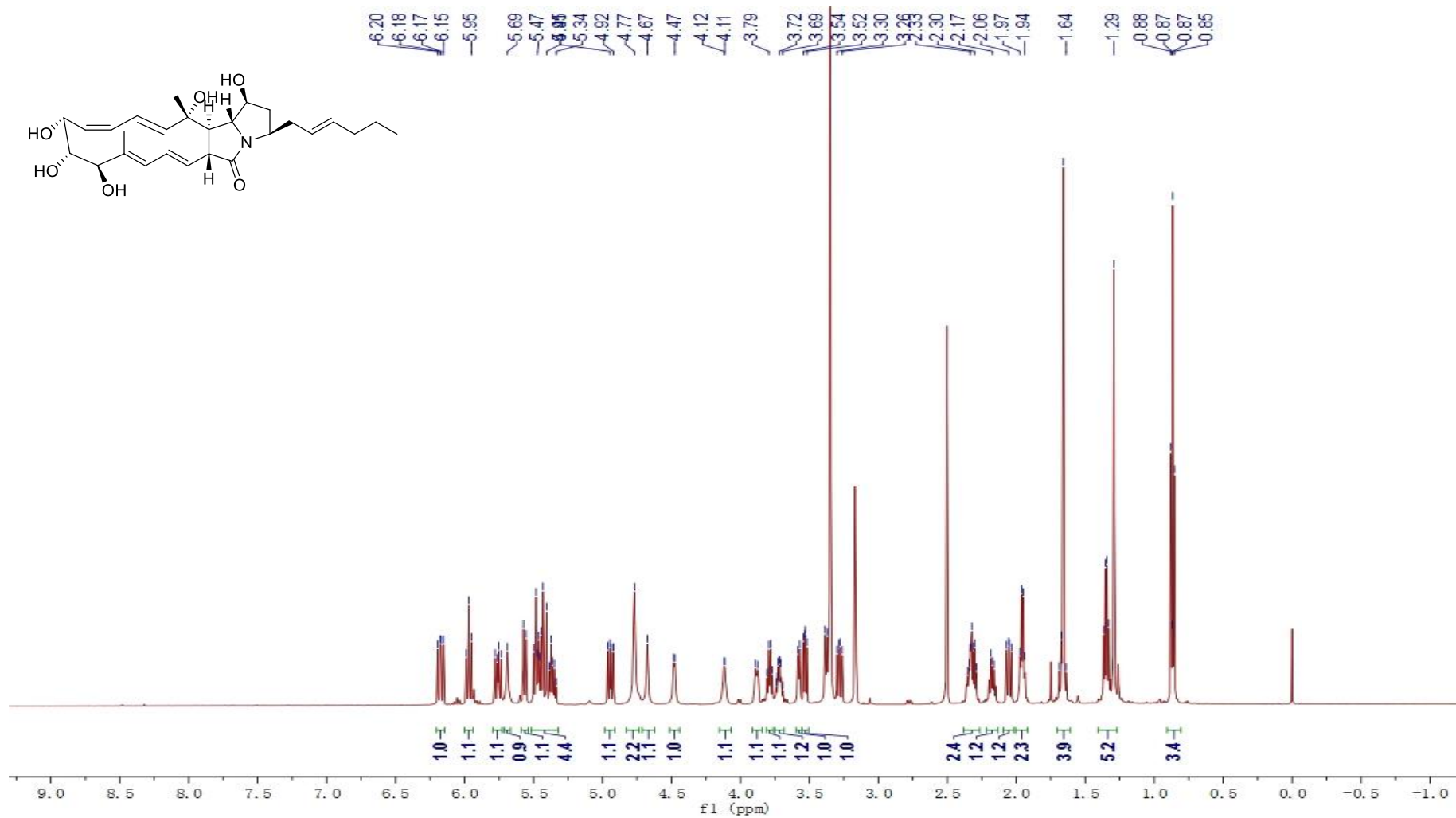


Figure S11.  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **2**



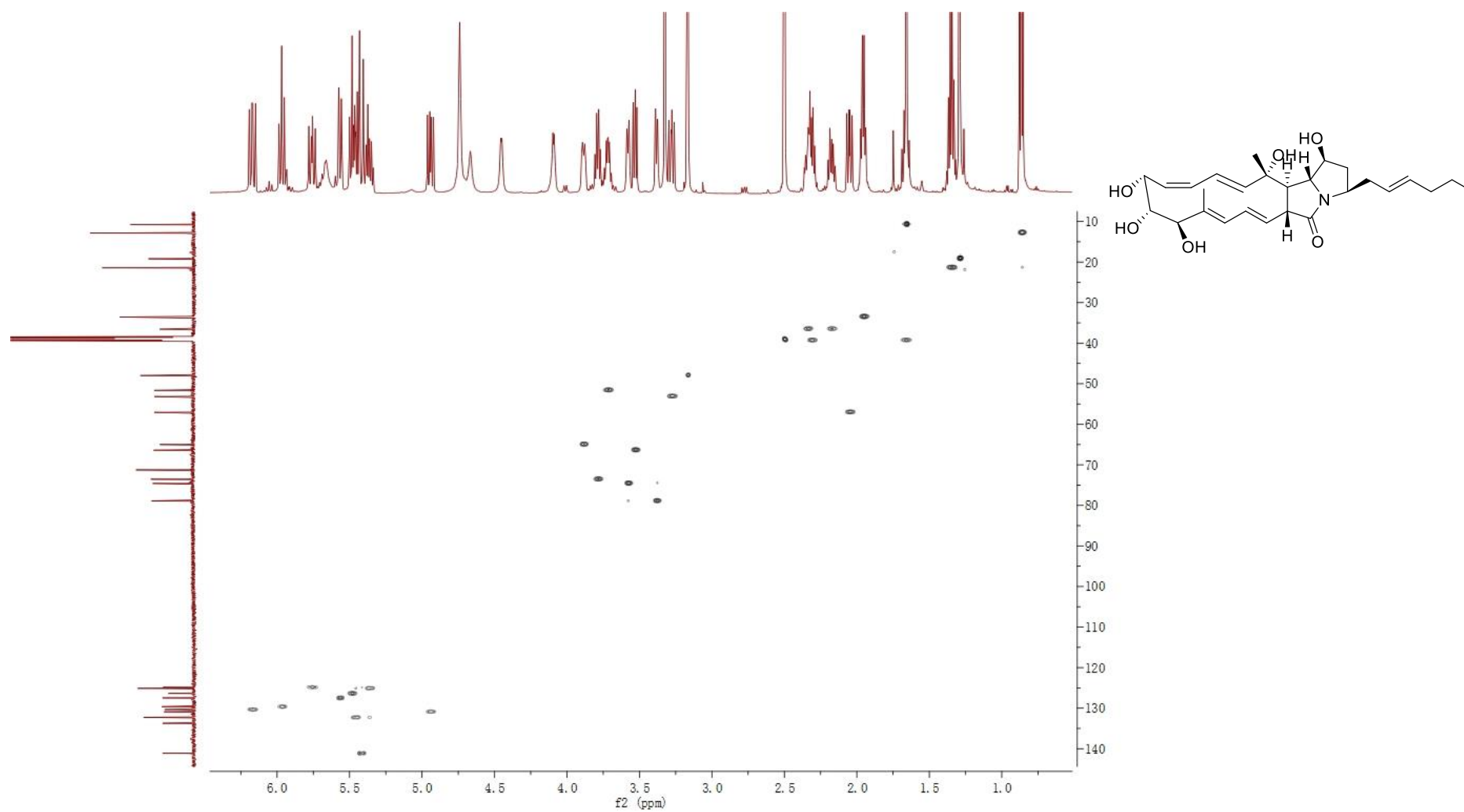


Figure S13. HSQC spectrum of compound 2

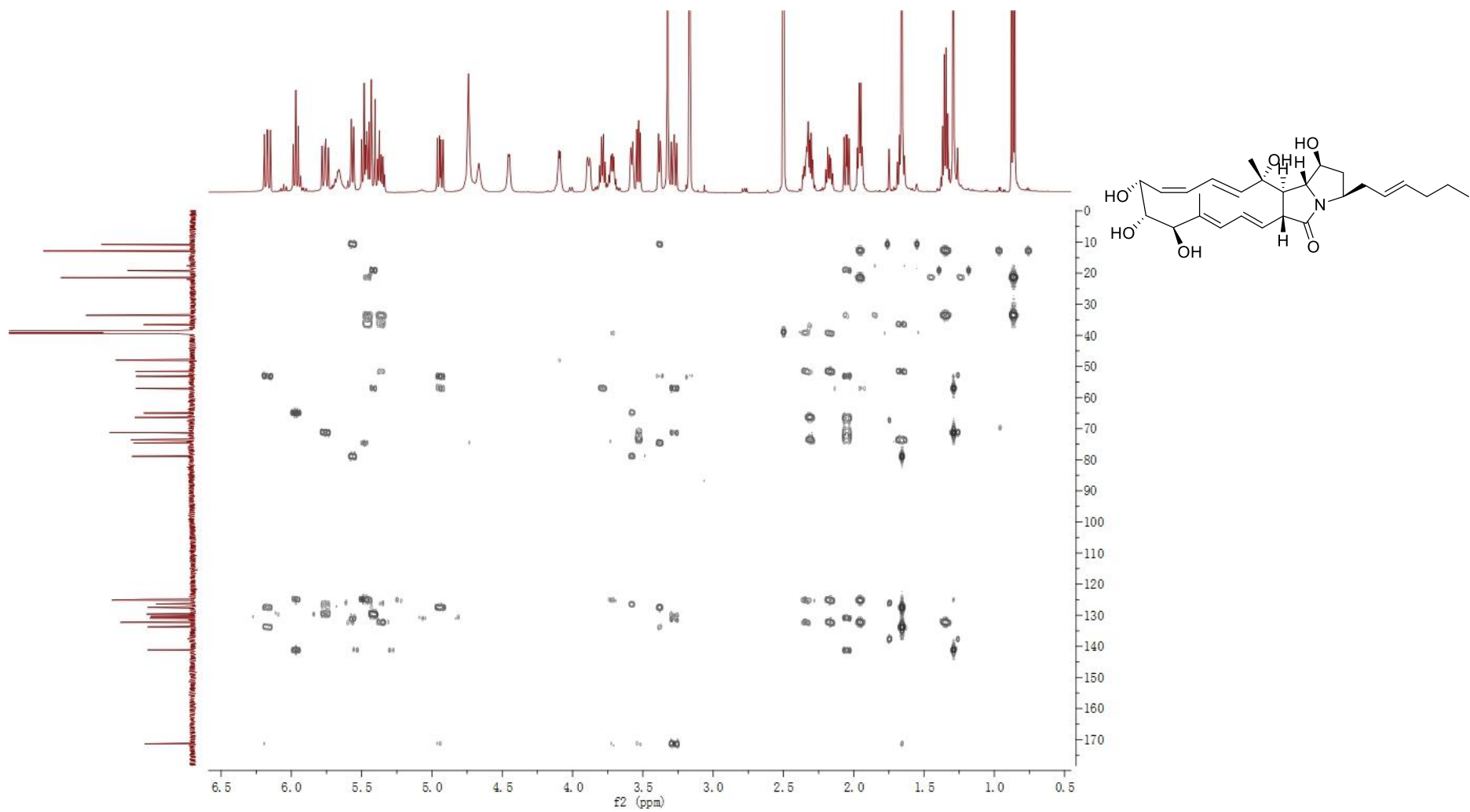


Figure S14. HMBC spectrum of compound 2



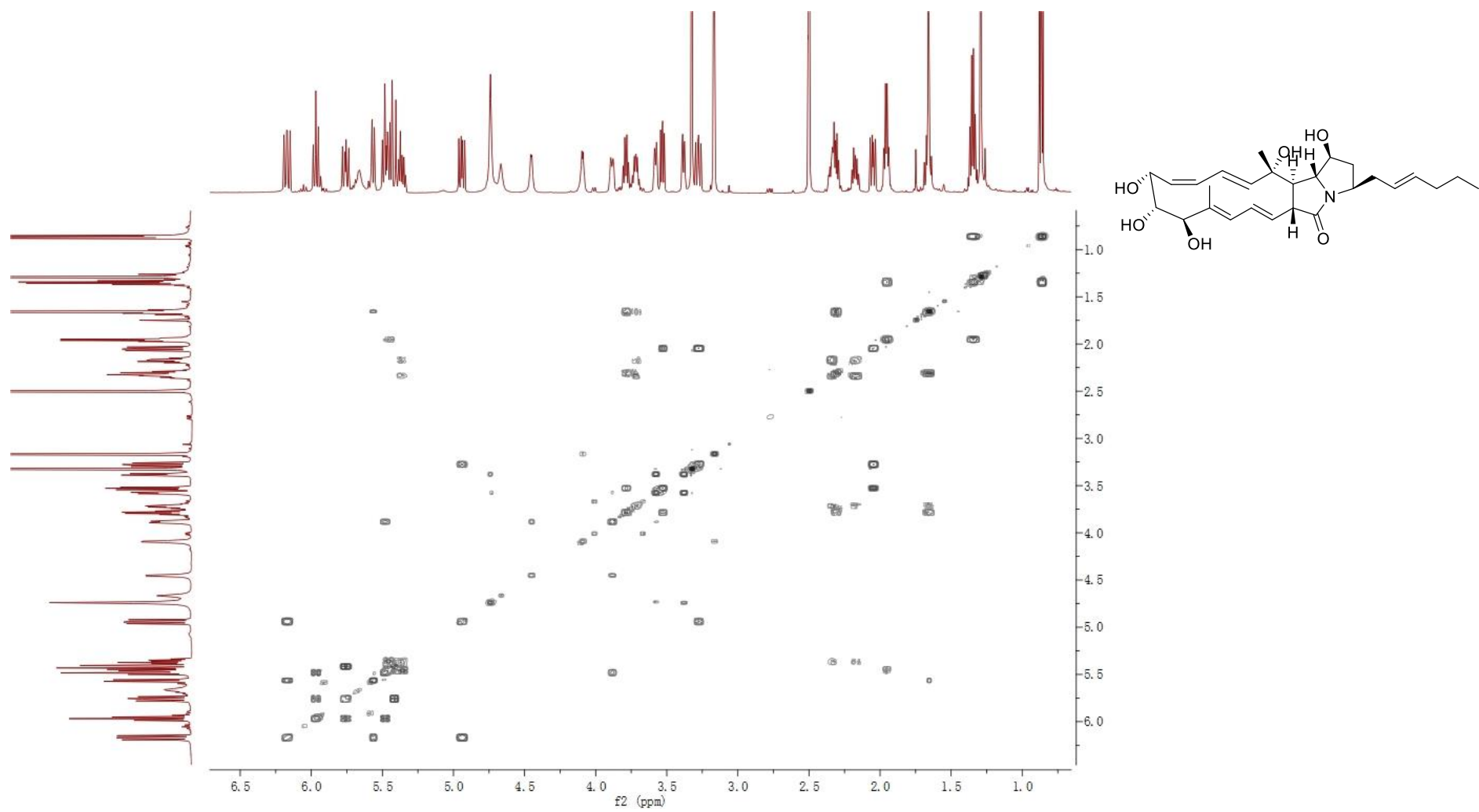


Figure S15. COSY spectrum of compound 2

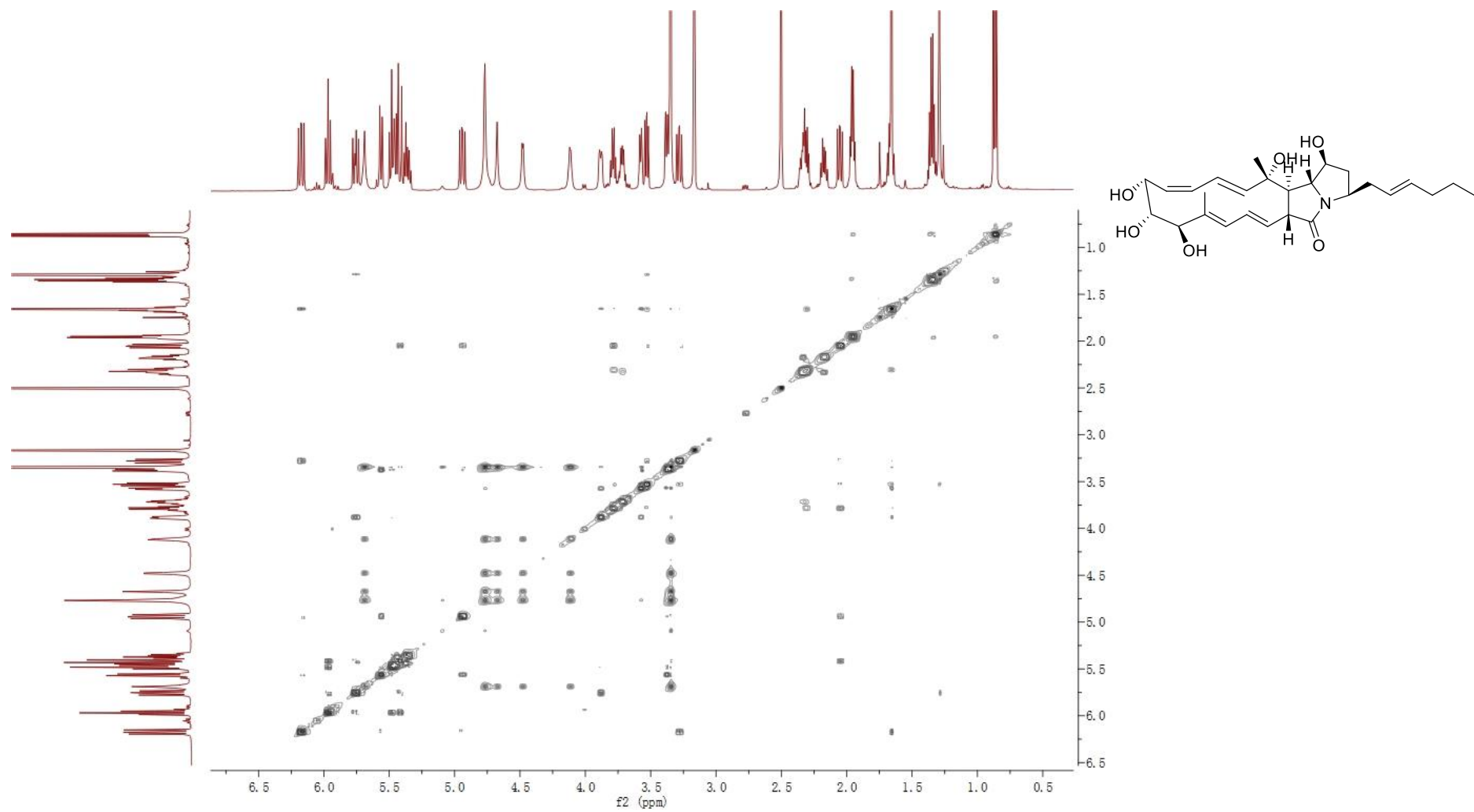


Figure S16. NOESY spectrum of compound 2

## User Spectra

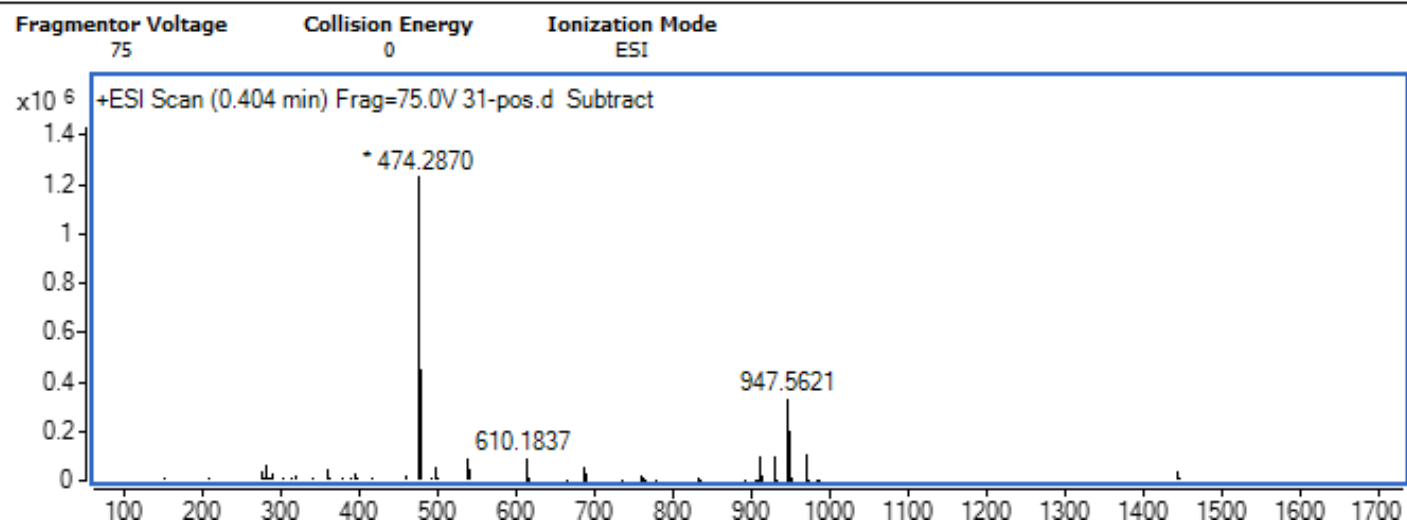


Figure S17. HRESIMS spectrum of compound **3**

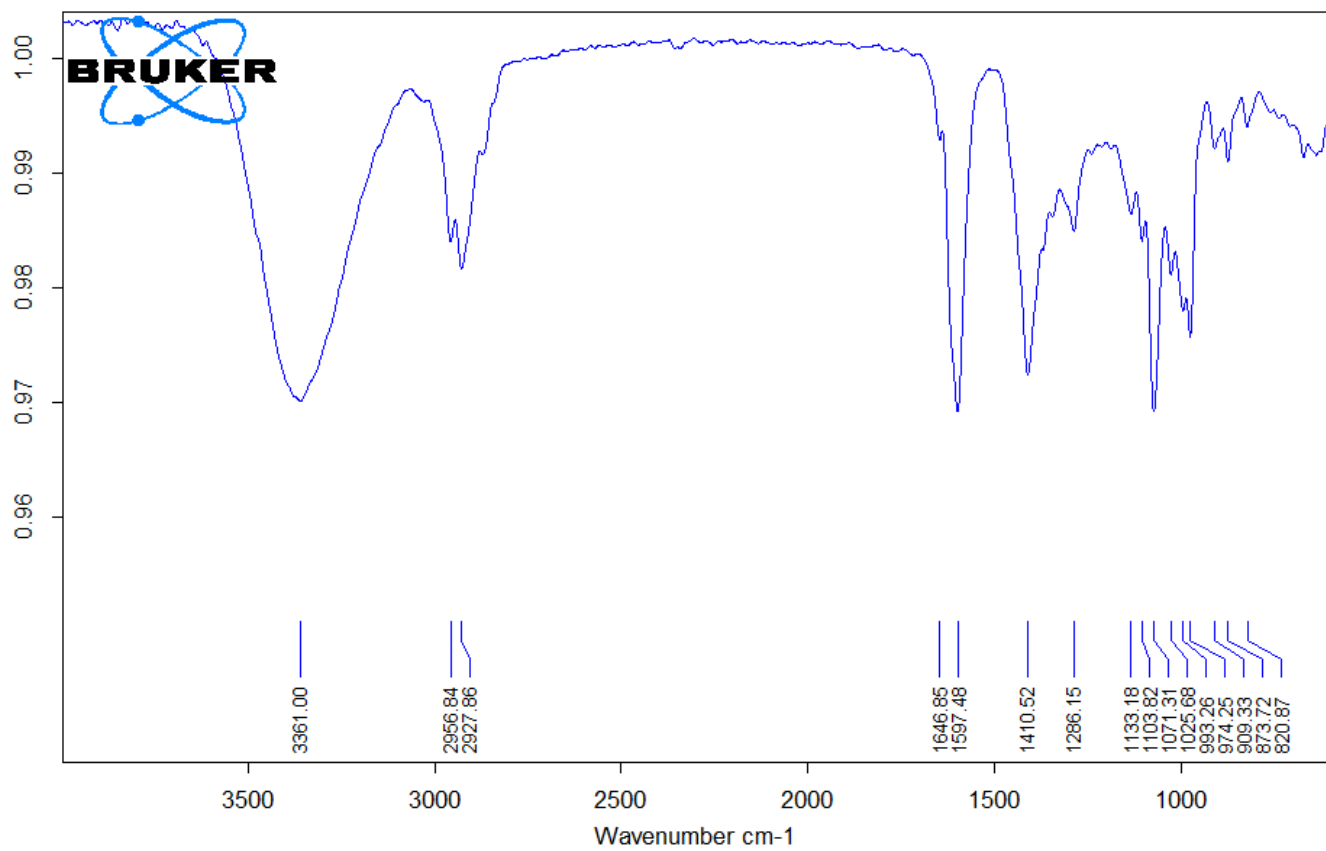


Figure S18. IR spectrum of compound 3

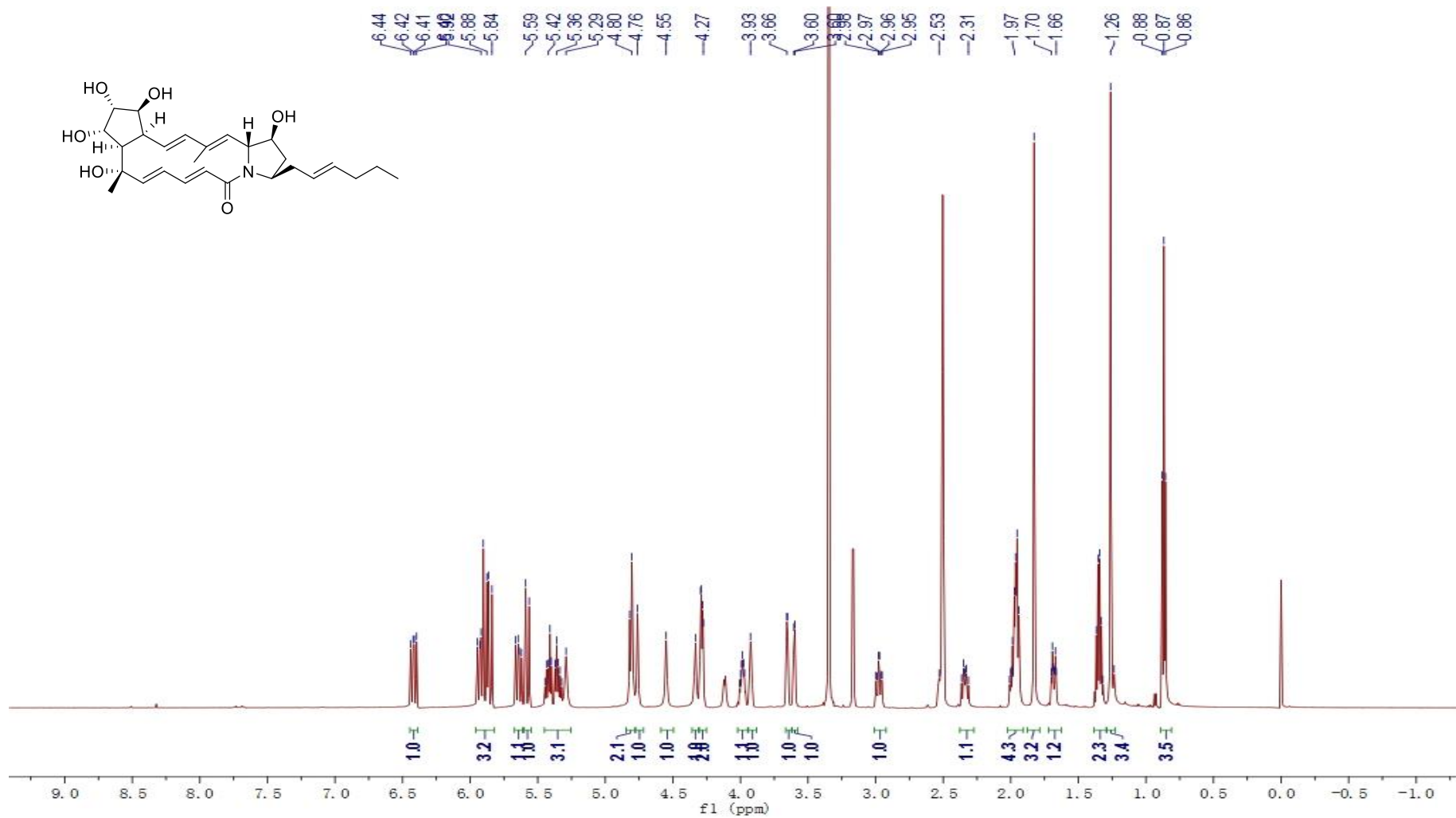


Figure S19.  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) spectrum of compound **3**

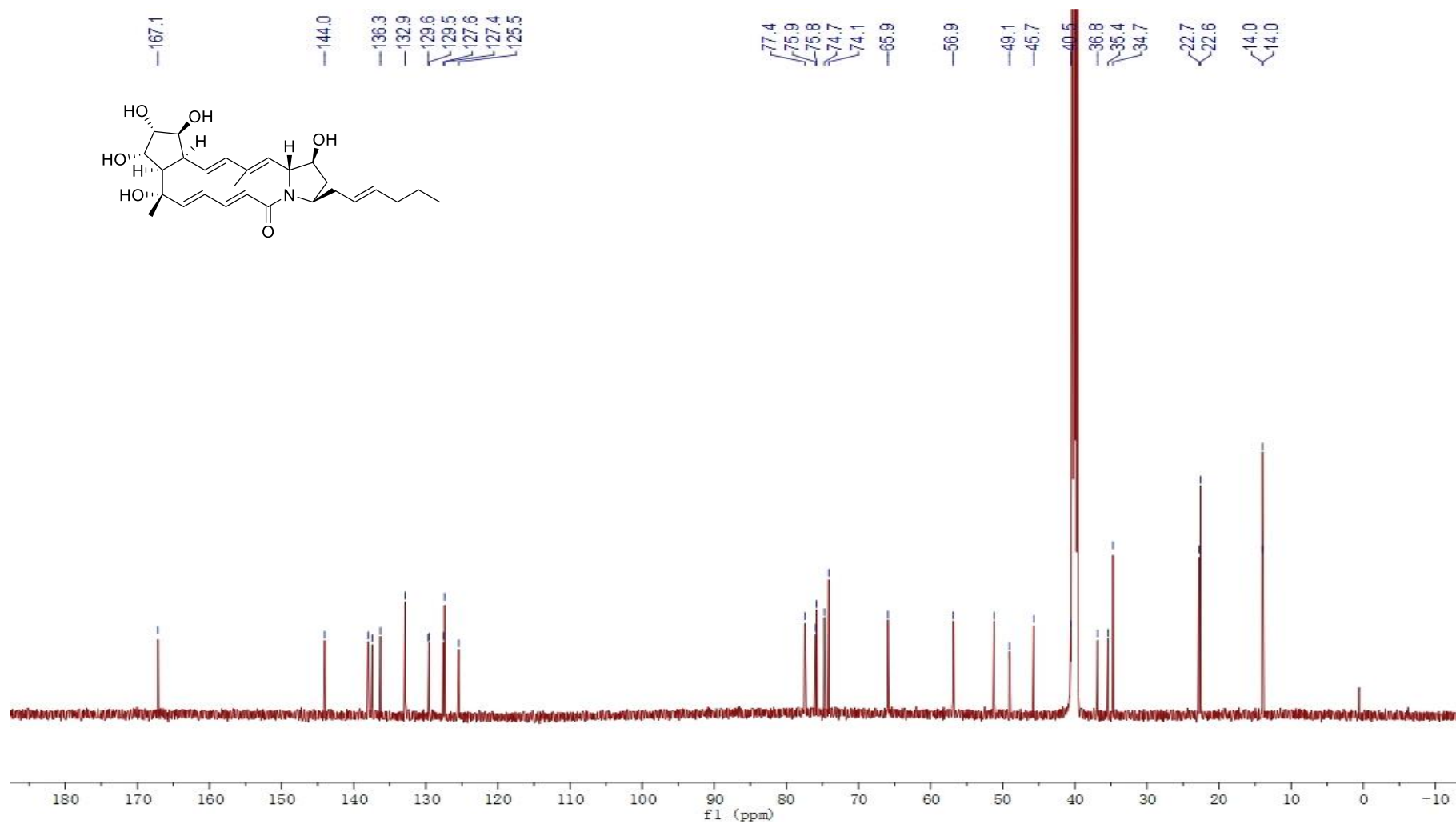


Figure S20. <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **3**

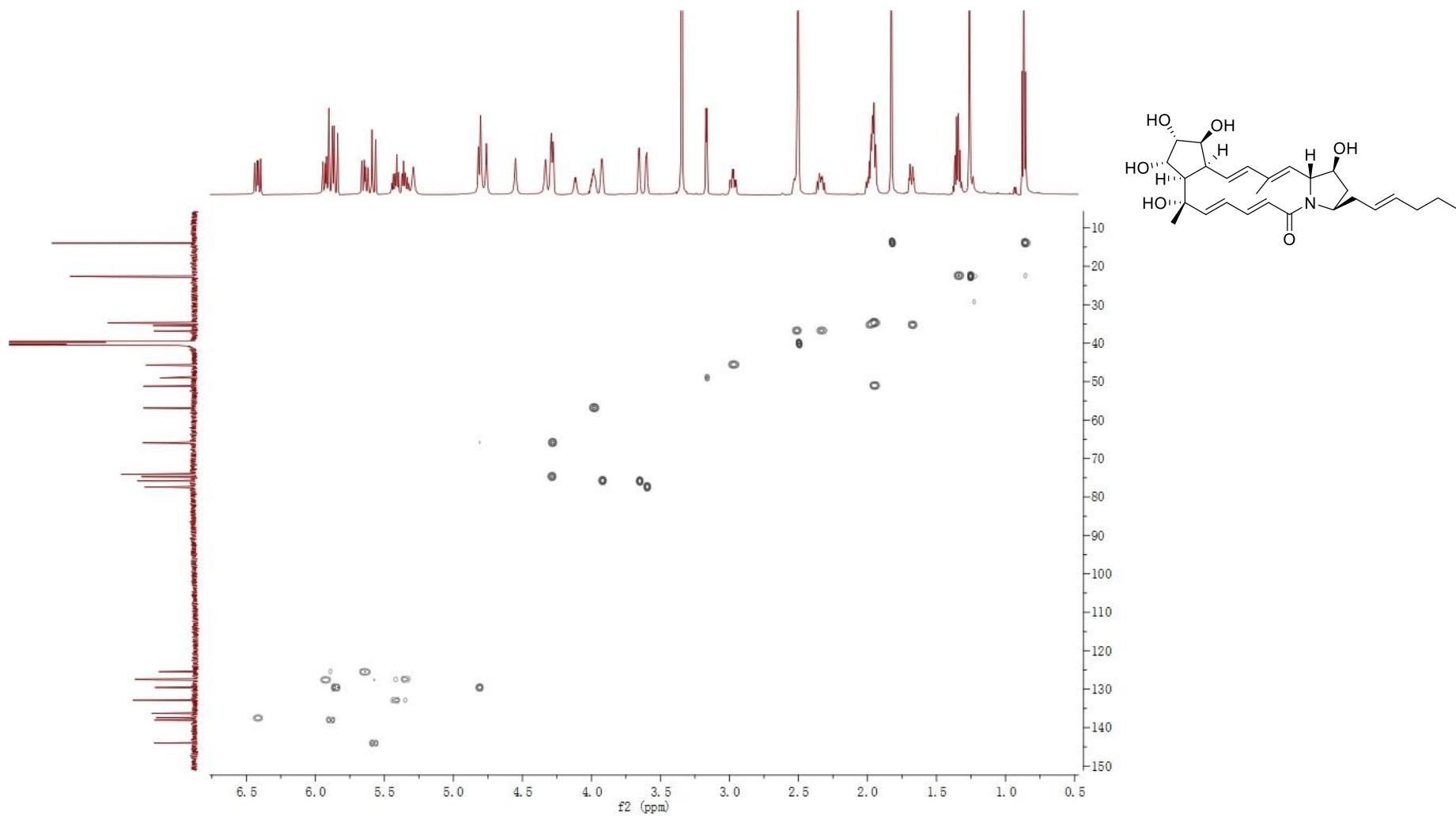


Figure S21. HSQC spectrum of compound 3

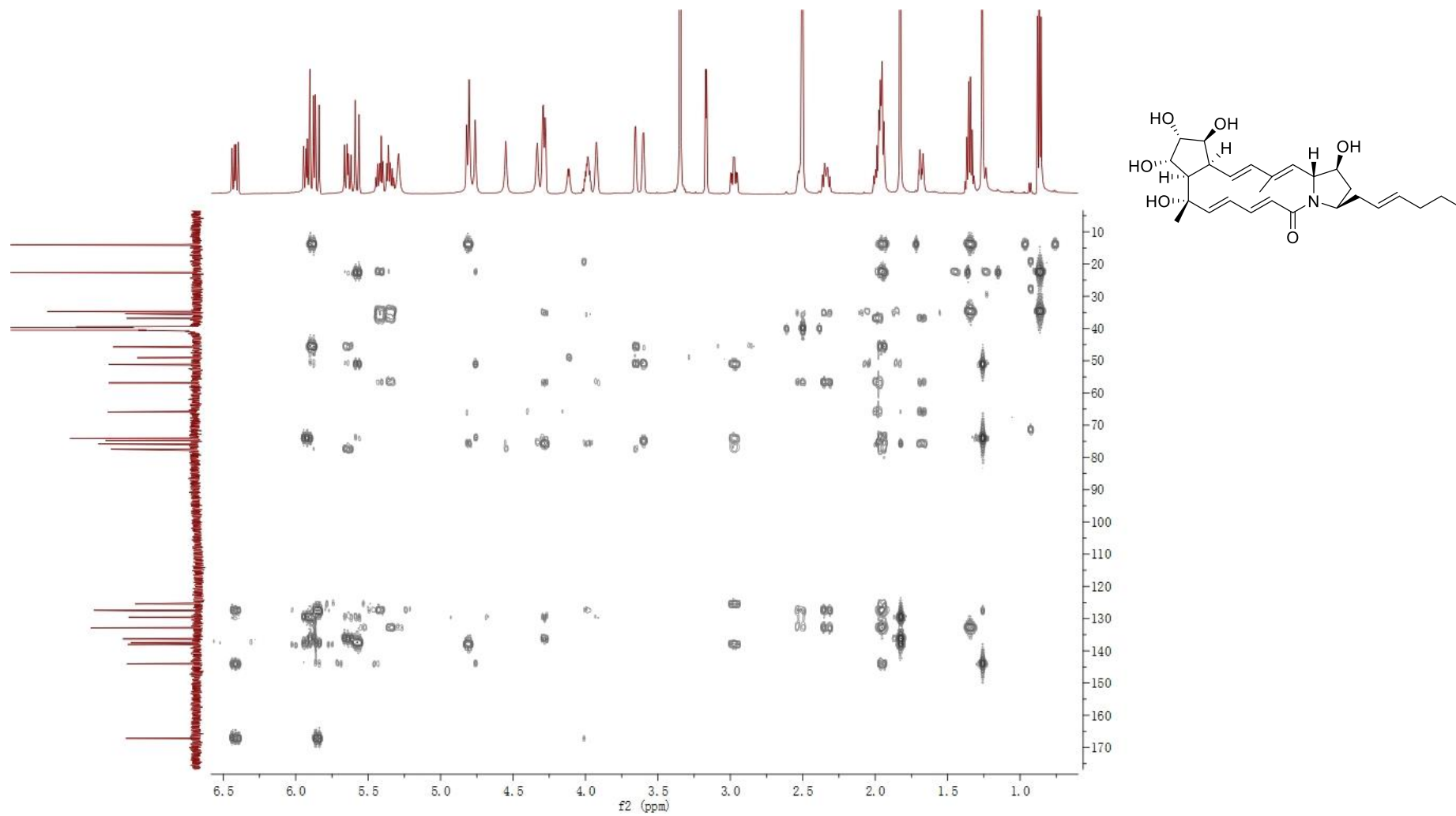


Figure S22. HMBC spectrum of compound **3**



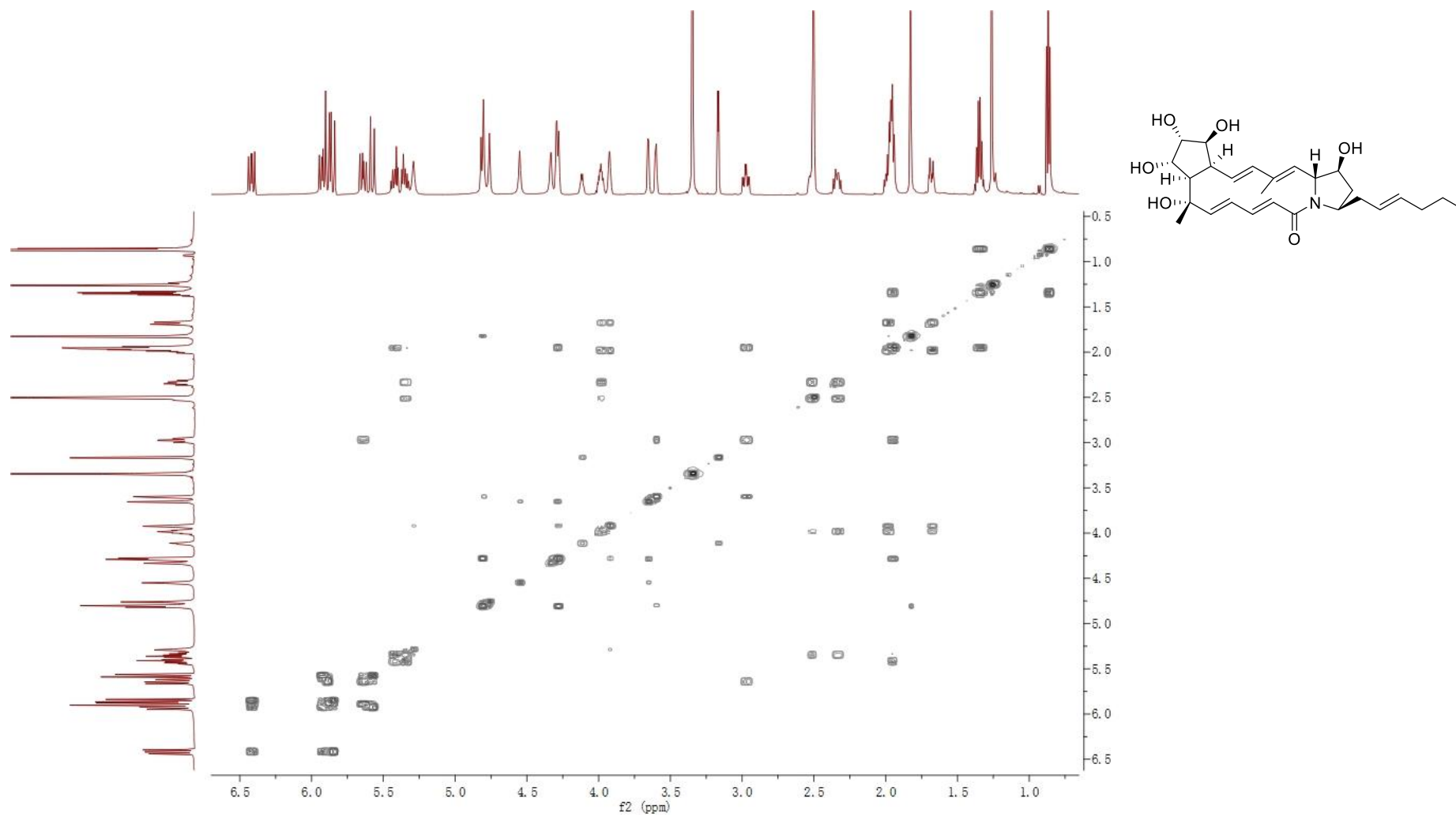


Figure S23. COSY spectrum of compound **3**

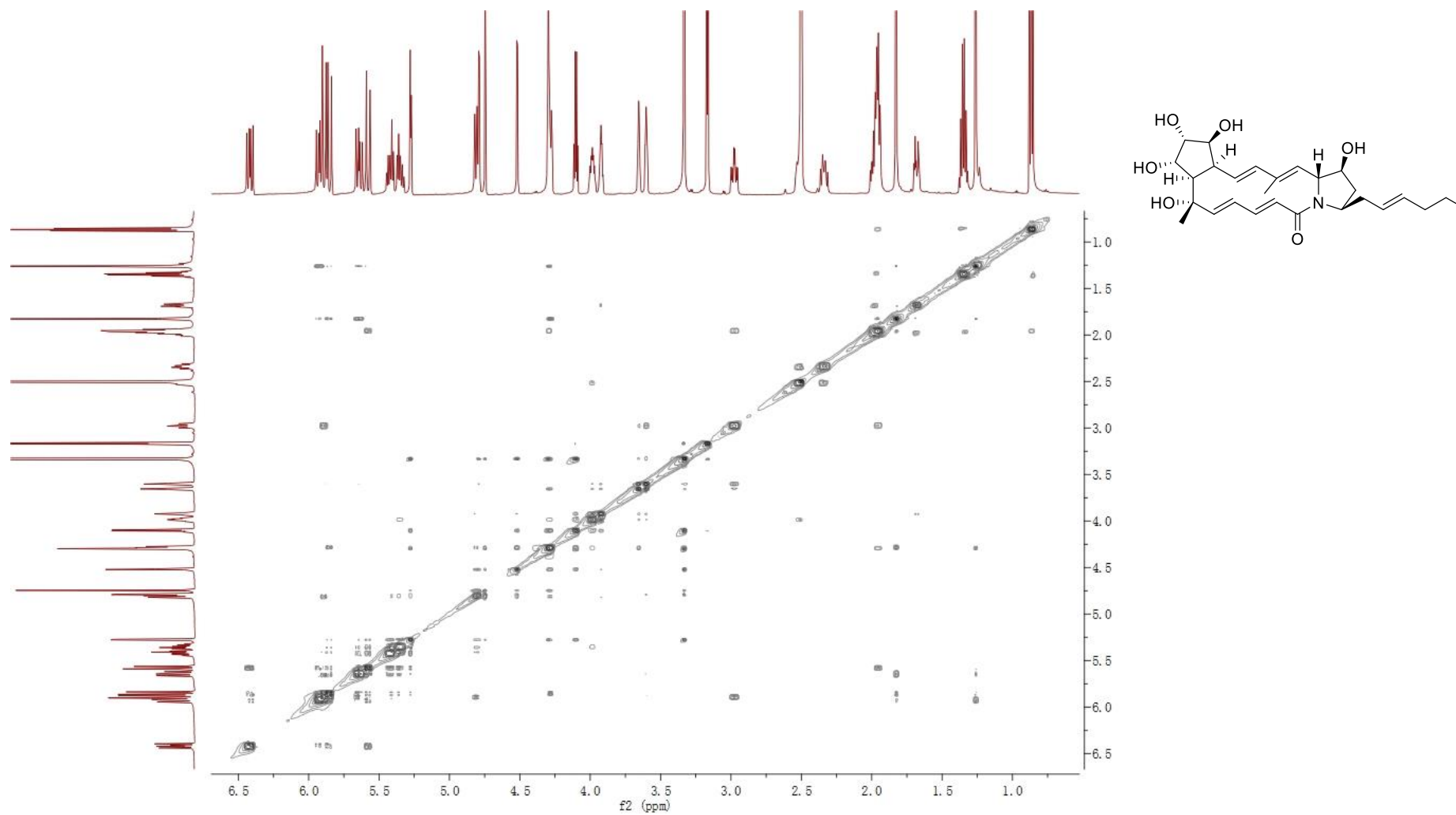


Figure S24. NOESY spectrum of compound **3**

## User Spectra

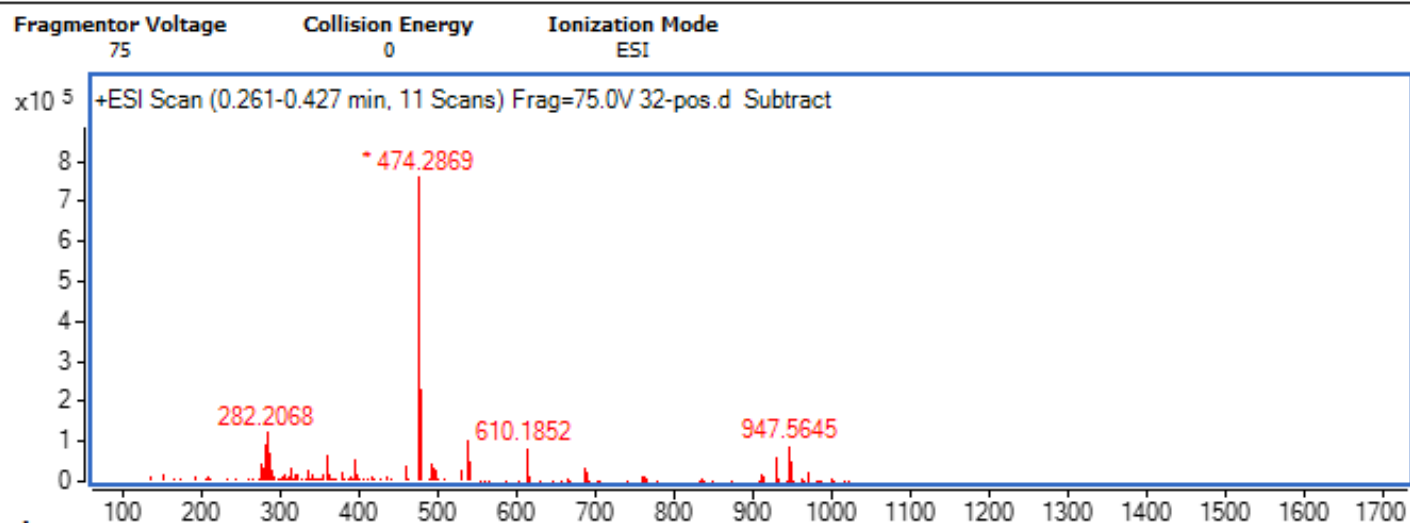


Figure S25. HRESIMS spectrum of compound **4**

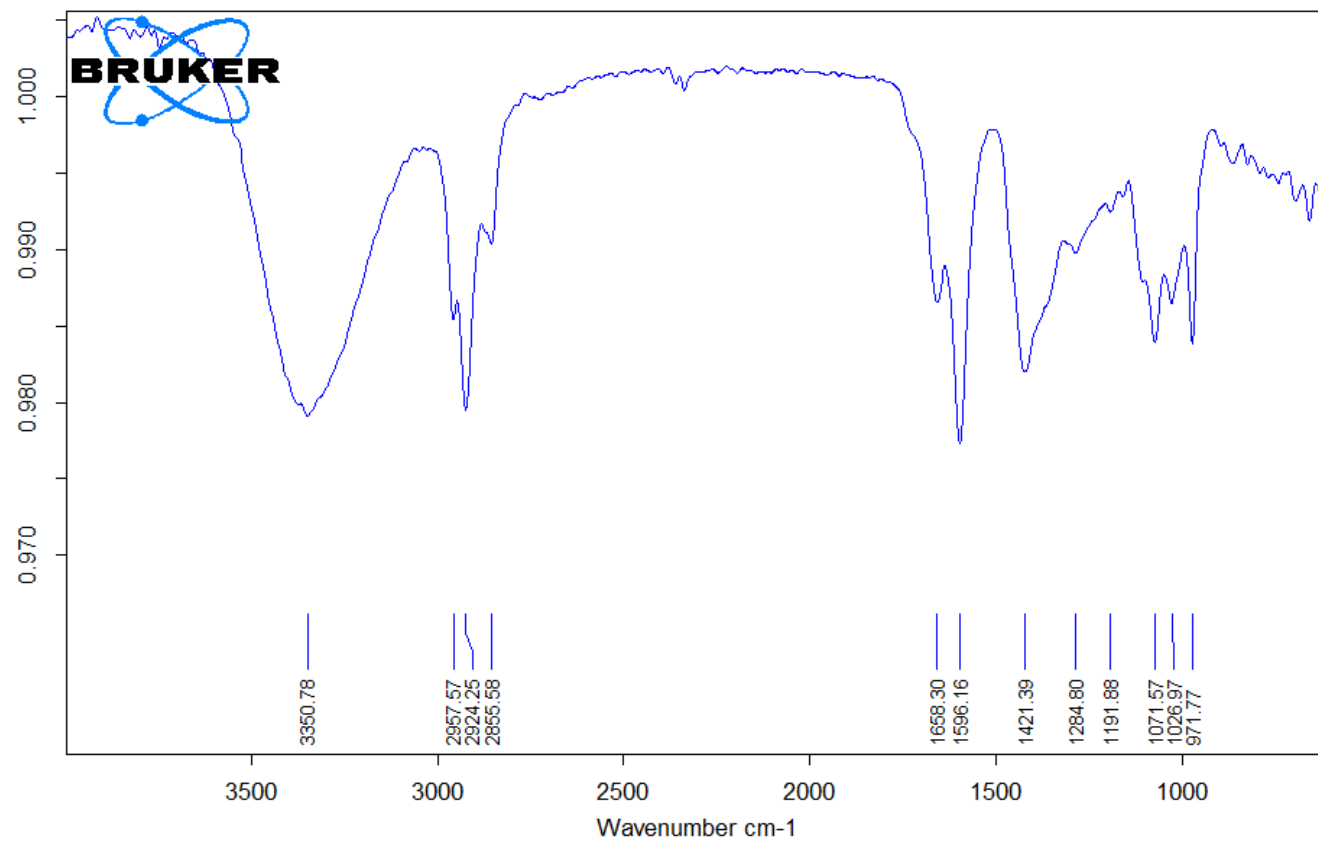


Figure S26. IR spectrum of compound 4

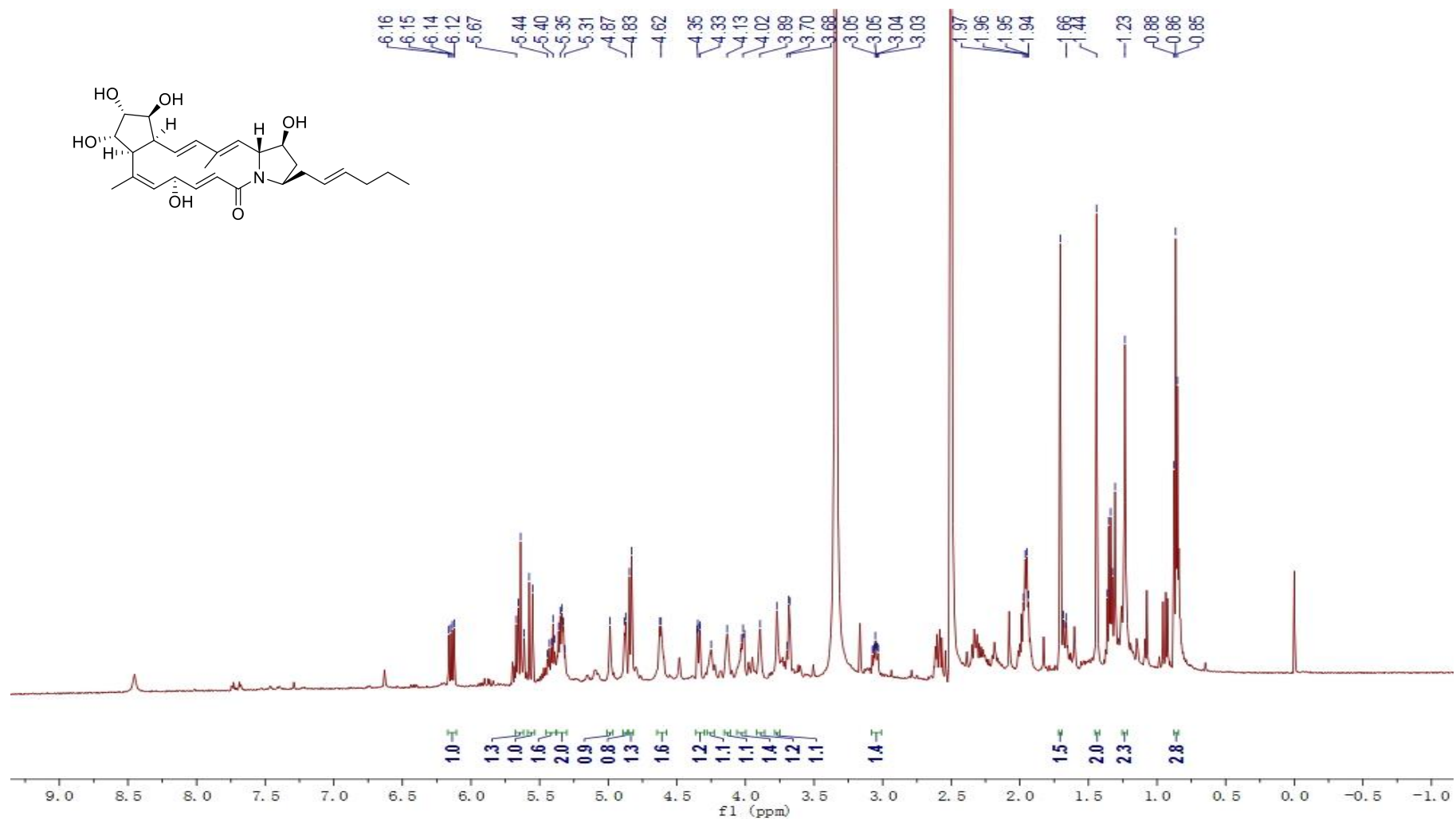


Figure S27. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **4**

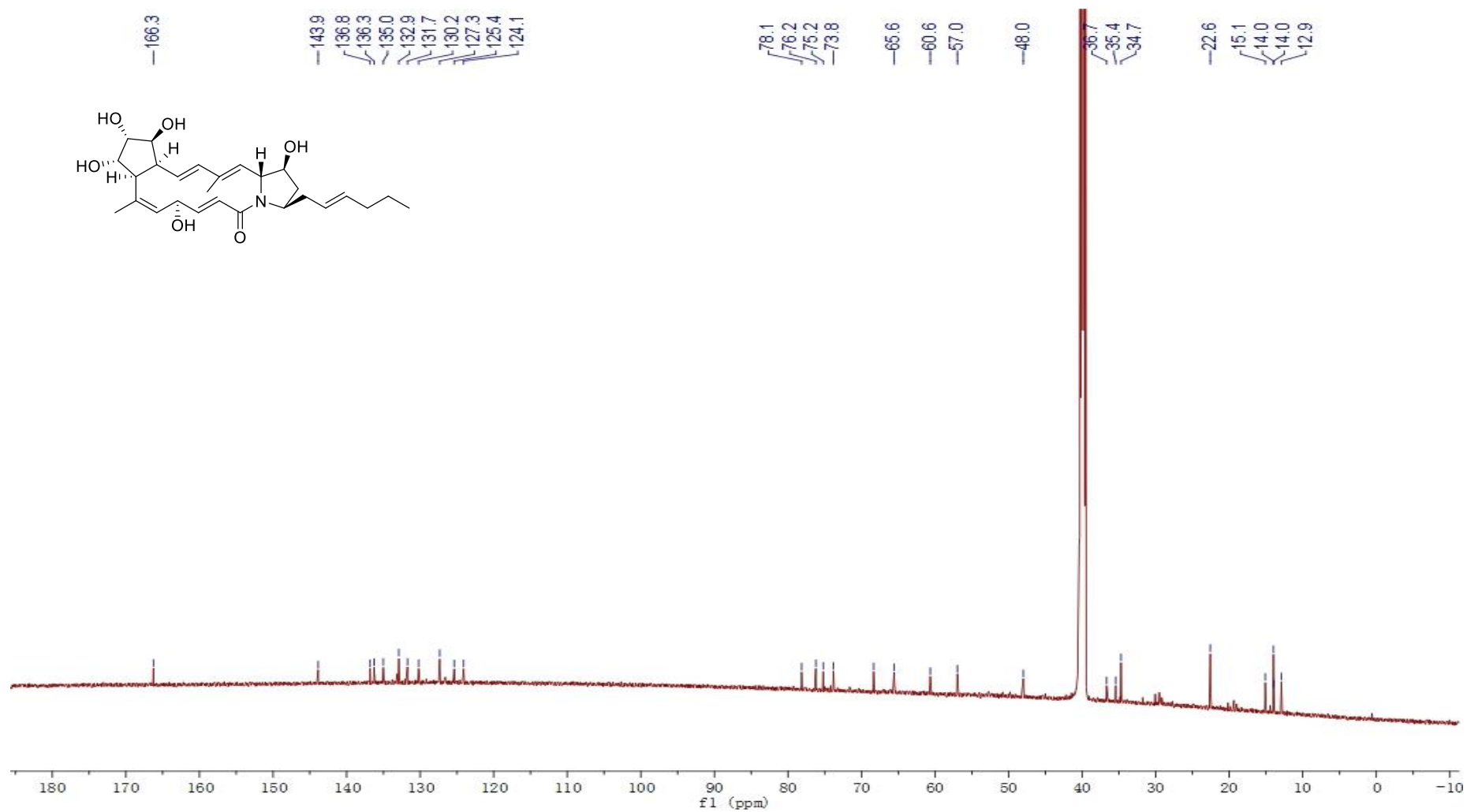


Figure S28. <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **4**

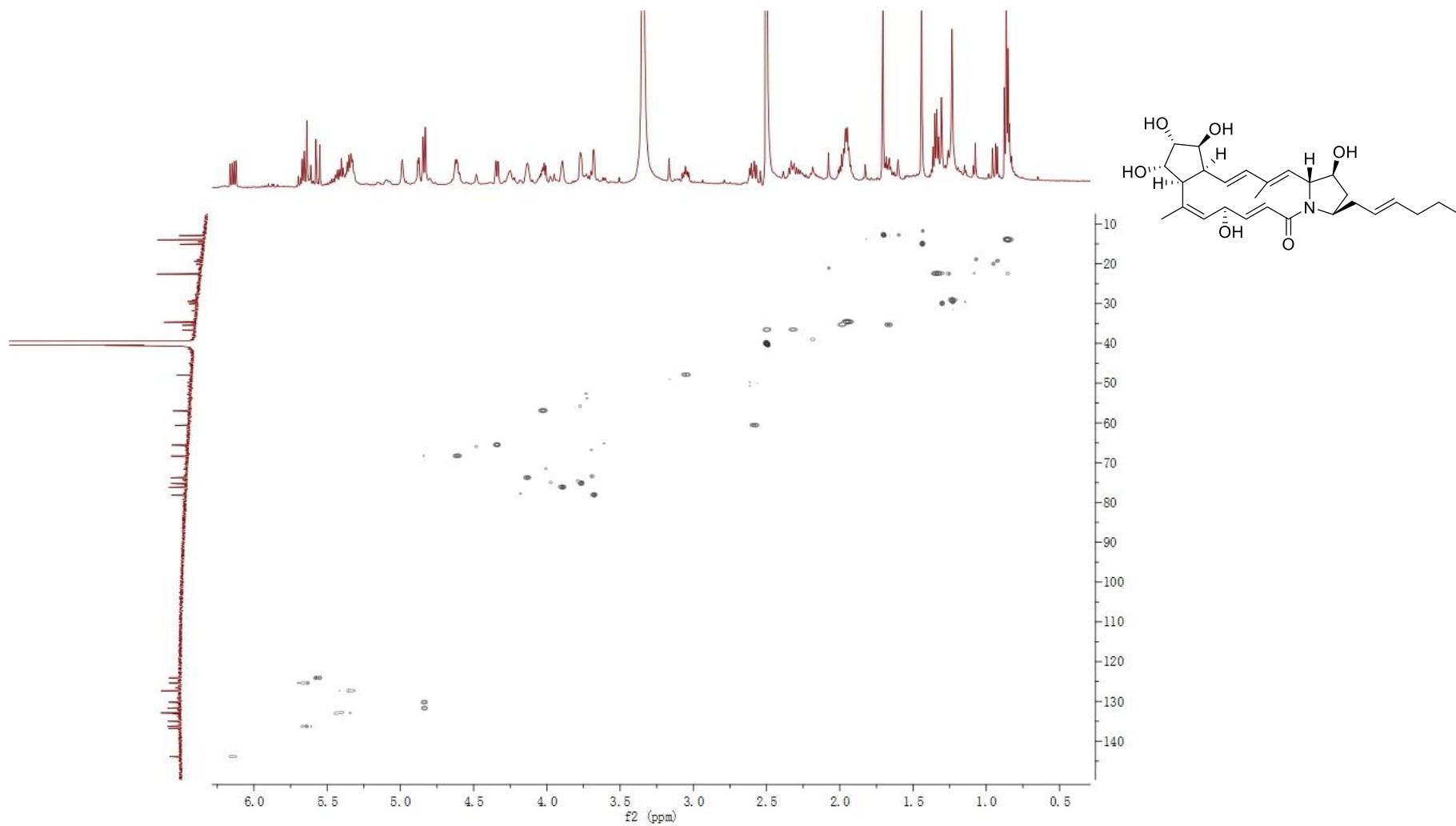


Figure S29. HSQC spectrum of compound 4

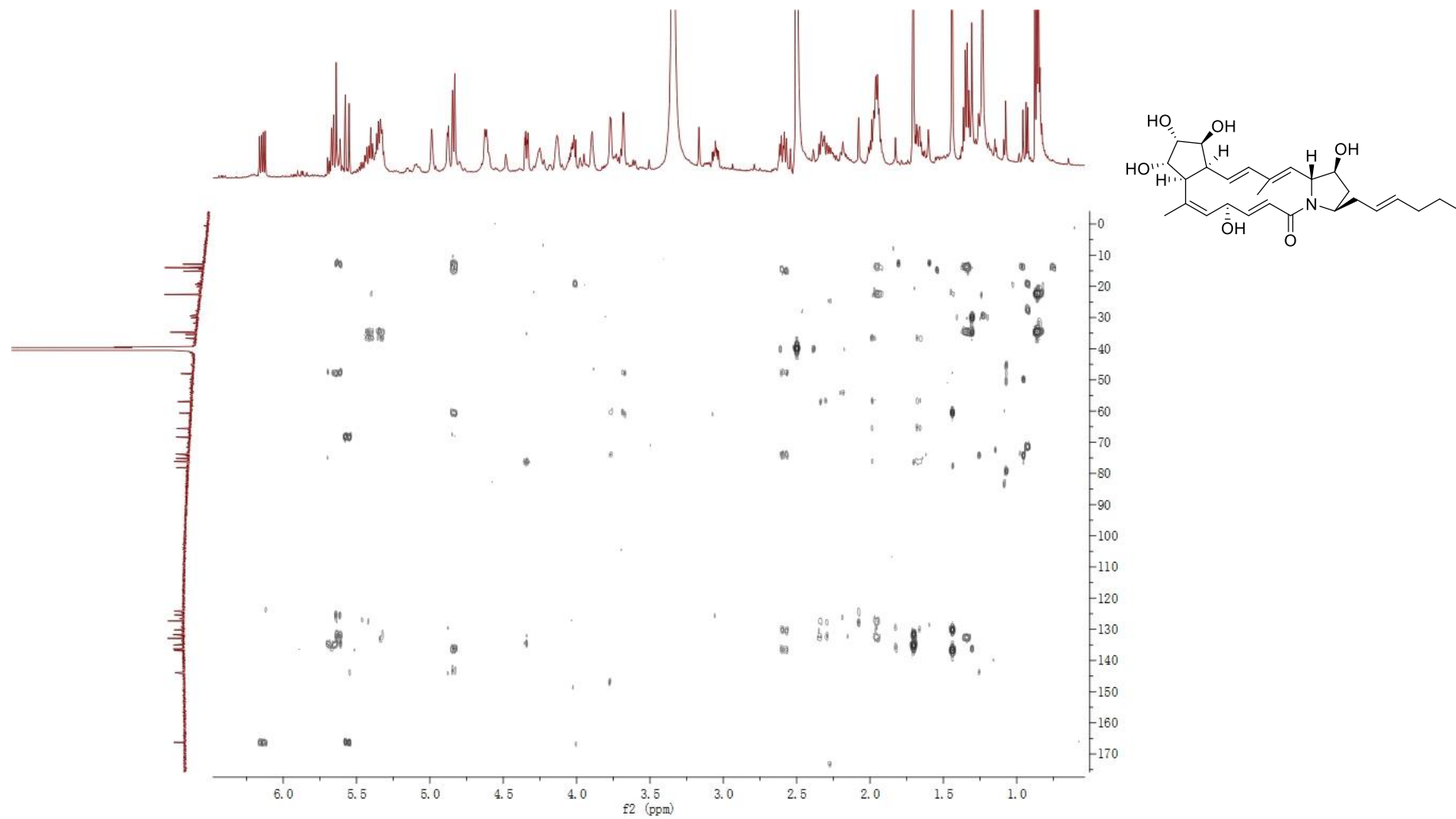


Figure S30. HMBC spectrum of compound **4**



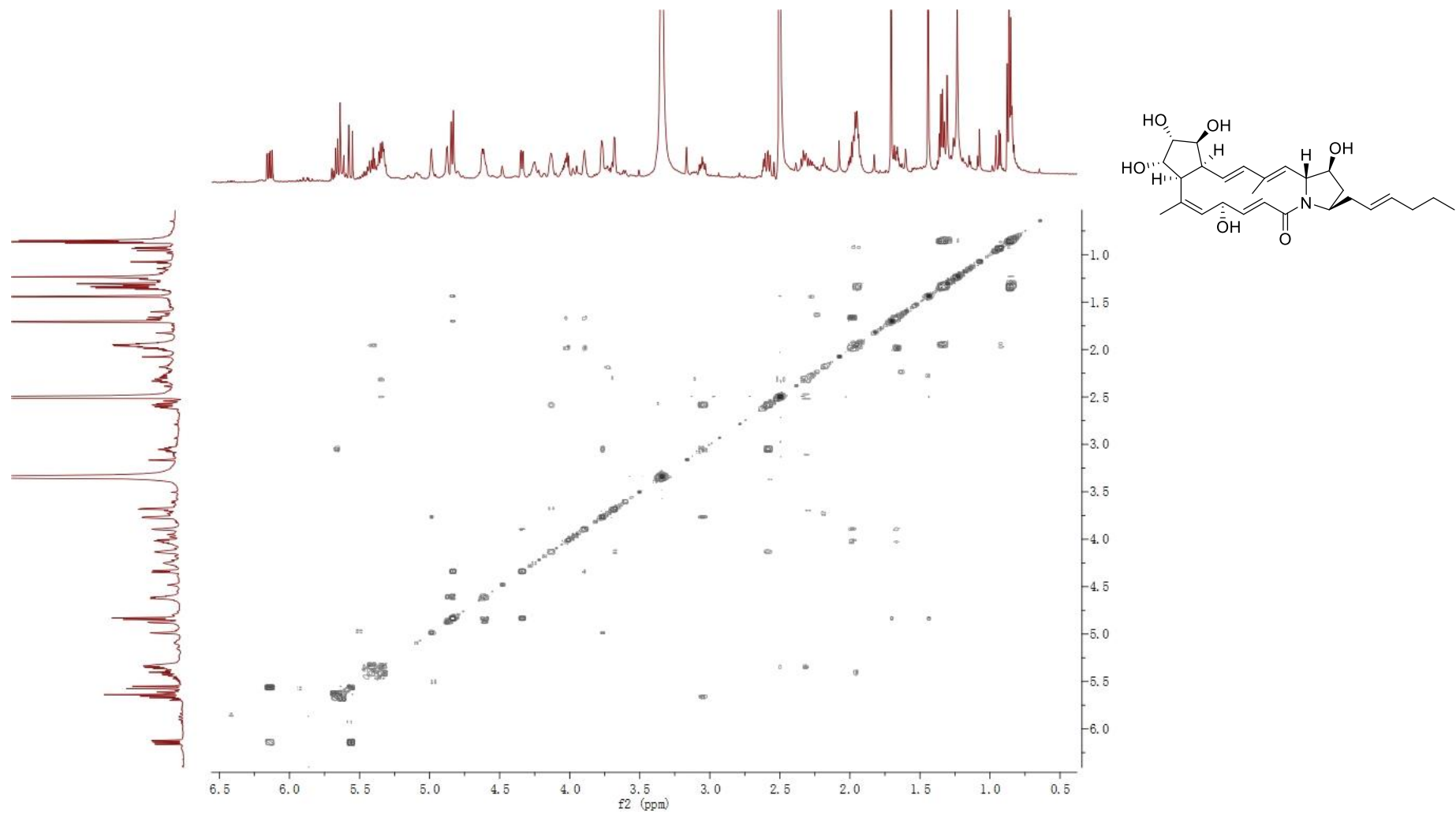


Figure S31. COSY spectrum of compound 4

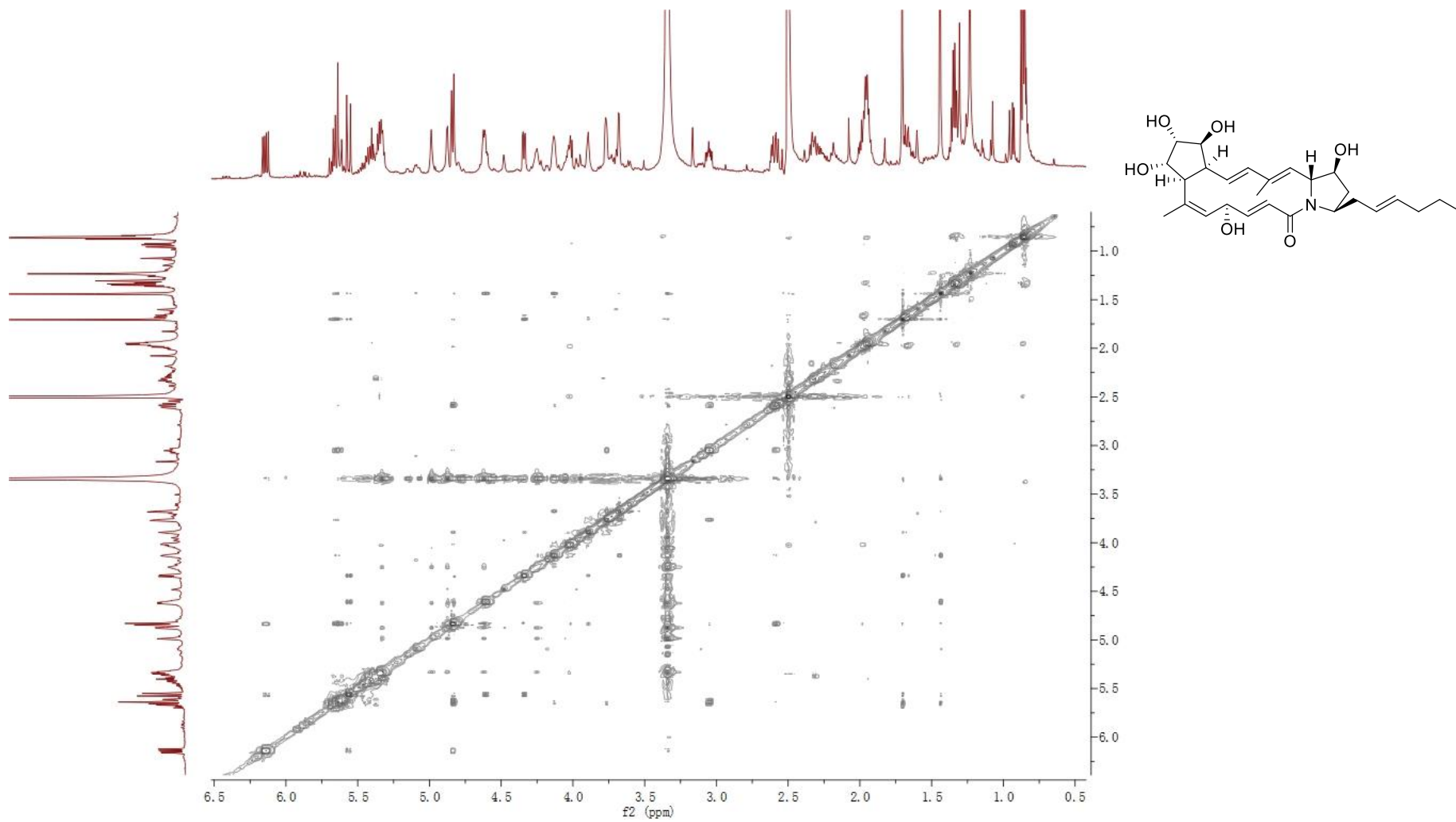


Figure S32. NOESY spectrum of compound 4

## User Spectra

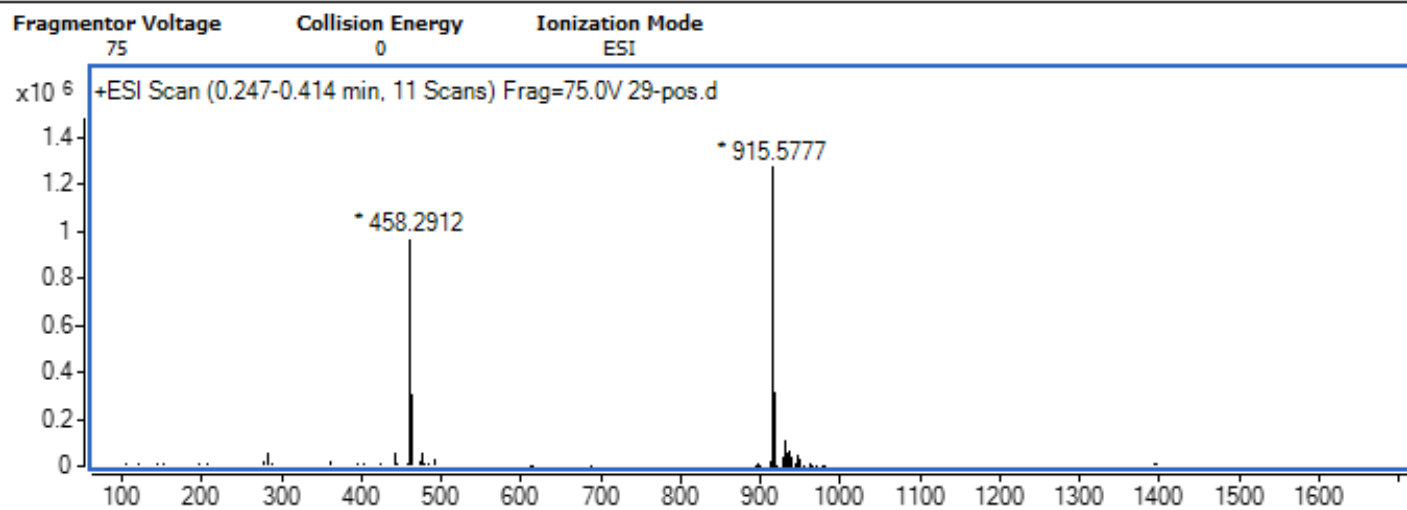


Figure S33. HRESIMS spectrum of compound **5**

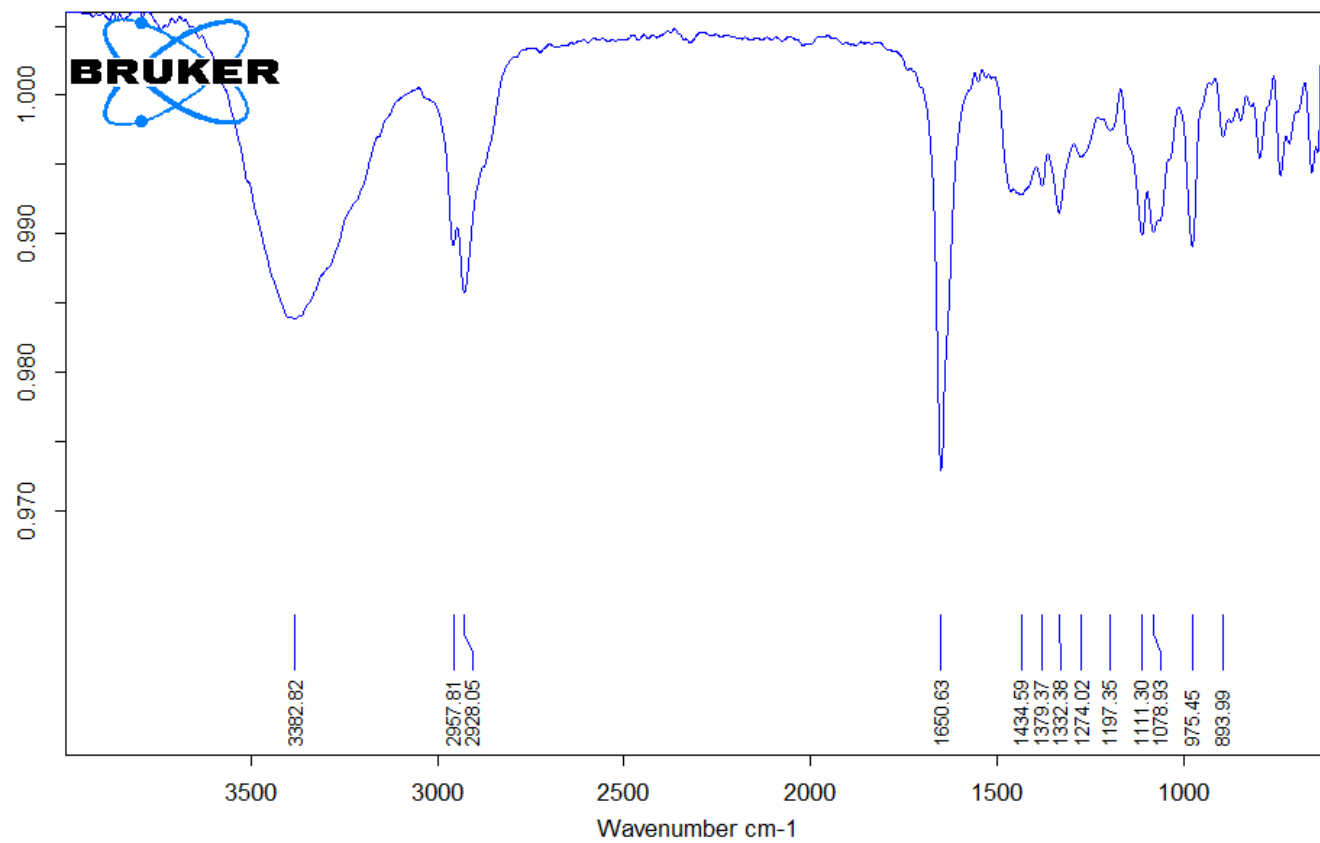


Figure S34. IR spectrum of compound **5**

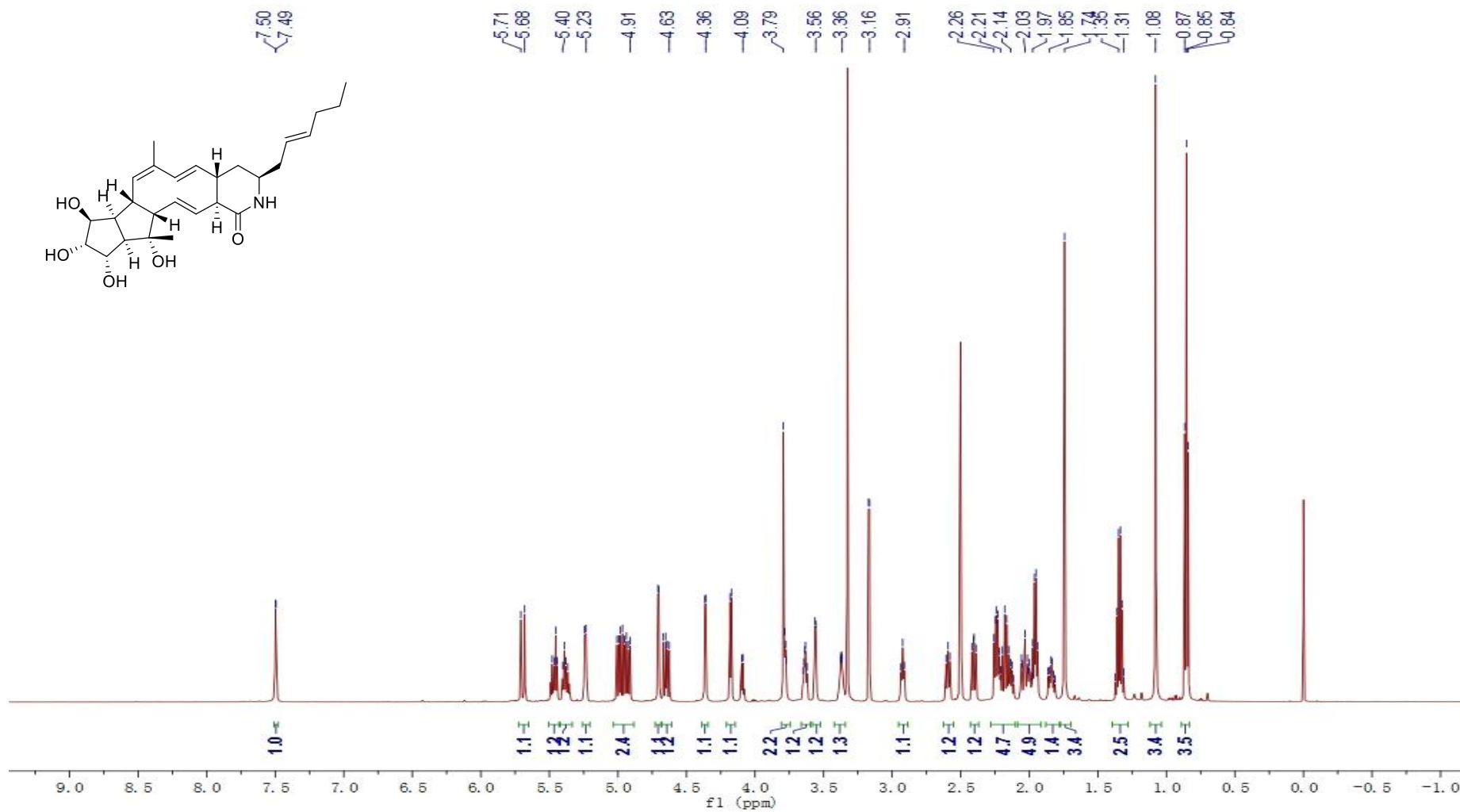


Figure S35. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **5**

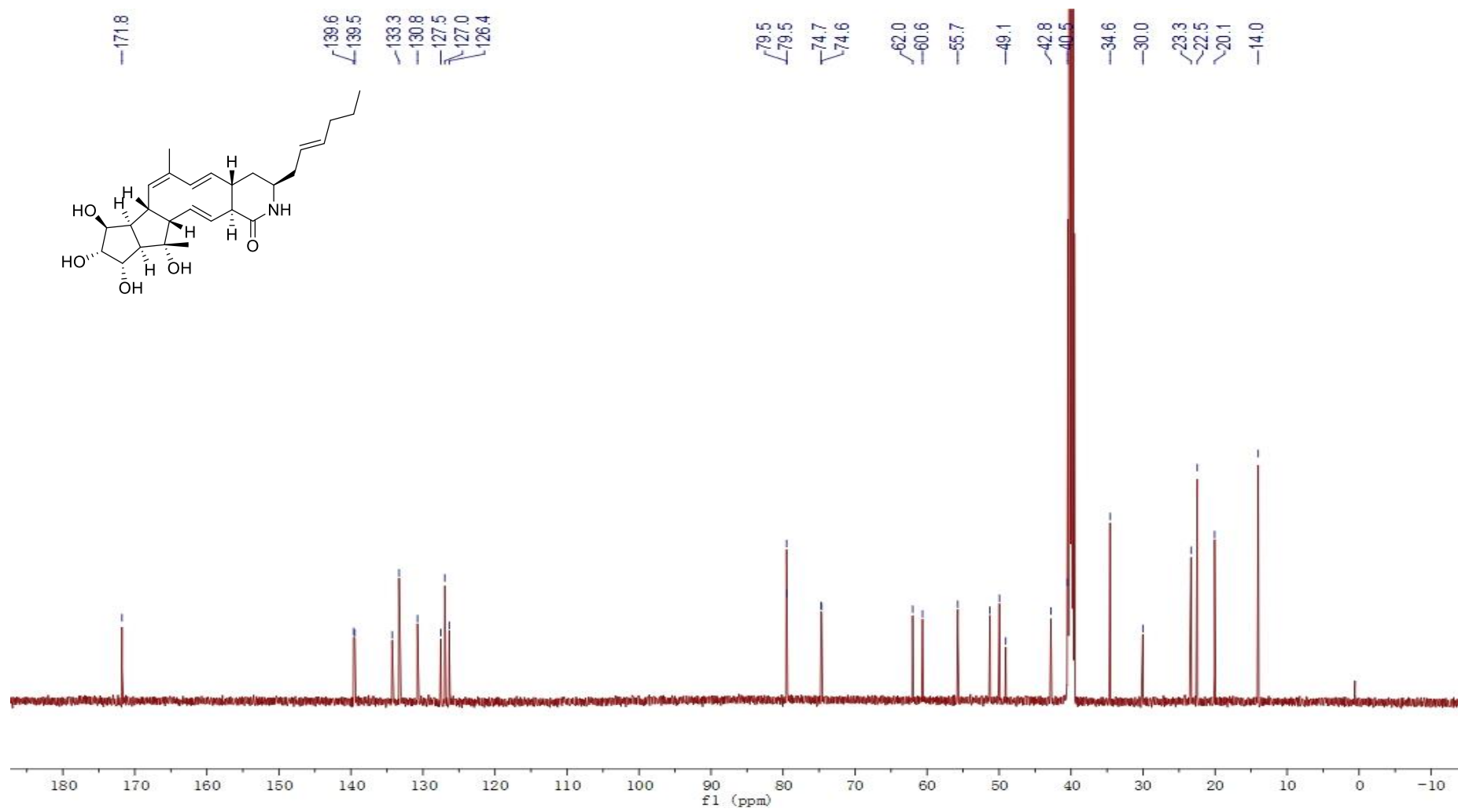


Figure S36. <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **5**

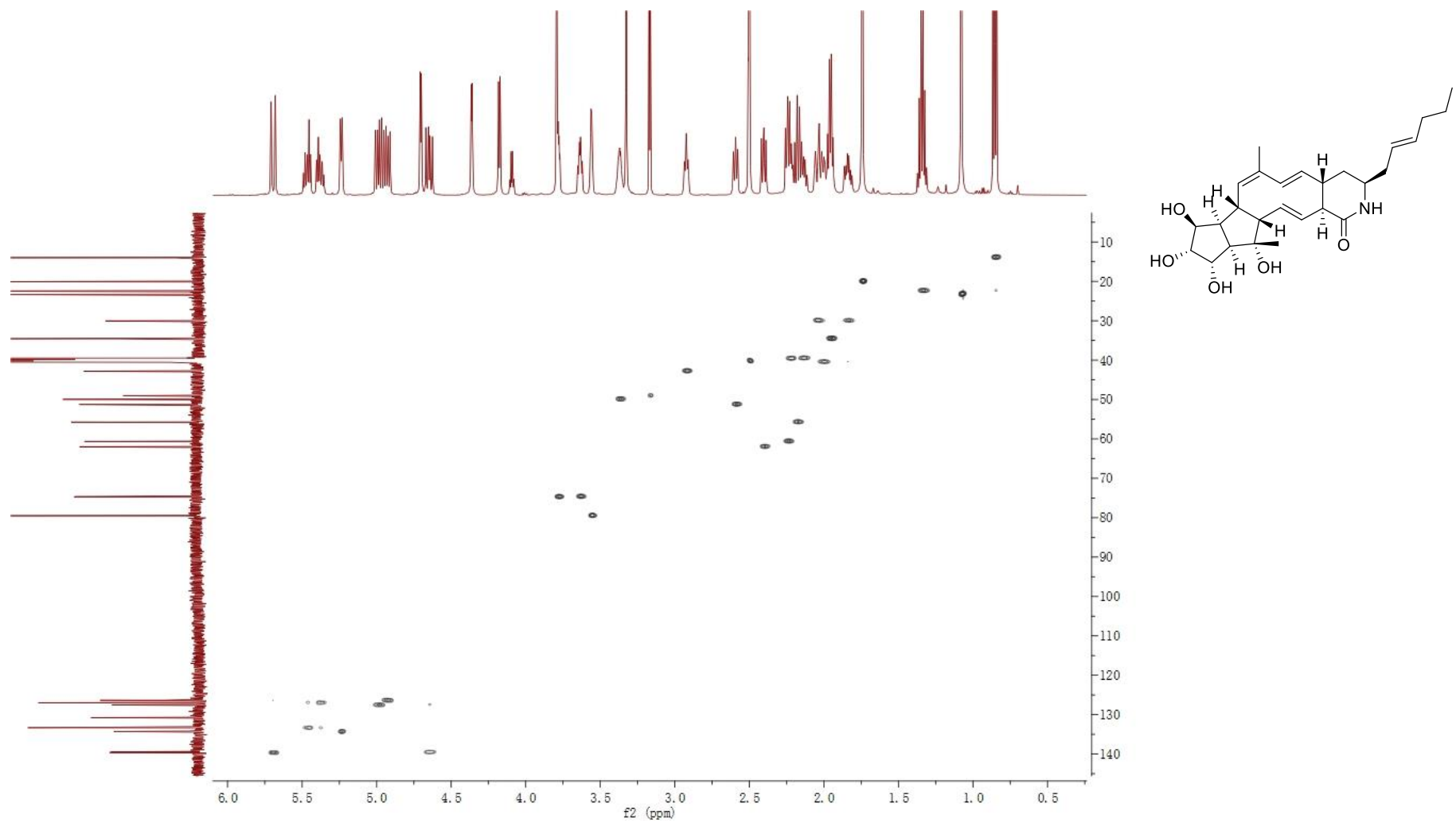


Figure S37. HSQC spectrum of compound **5**

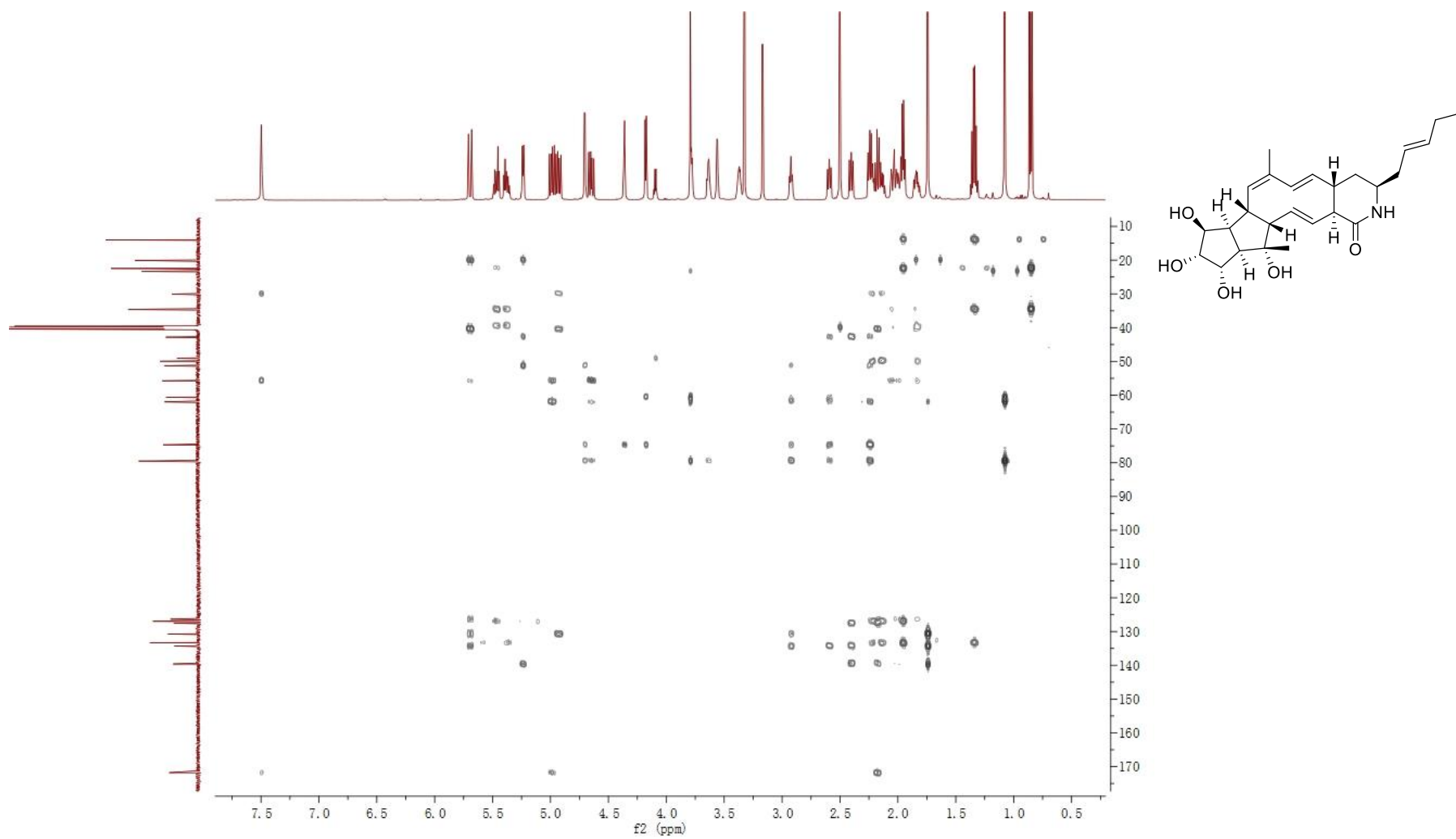


Figure S38. HMBC spectrum of compound 5



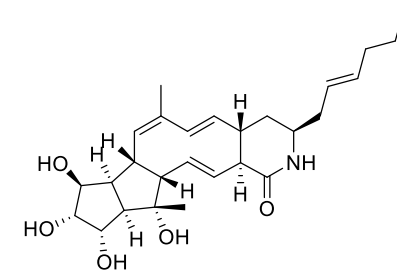
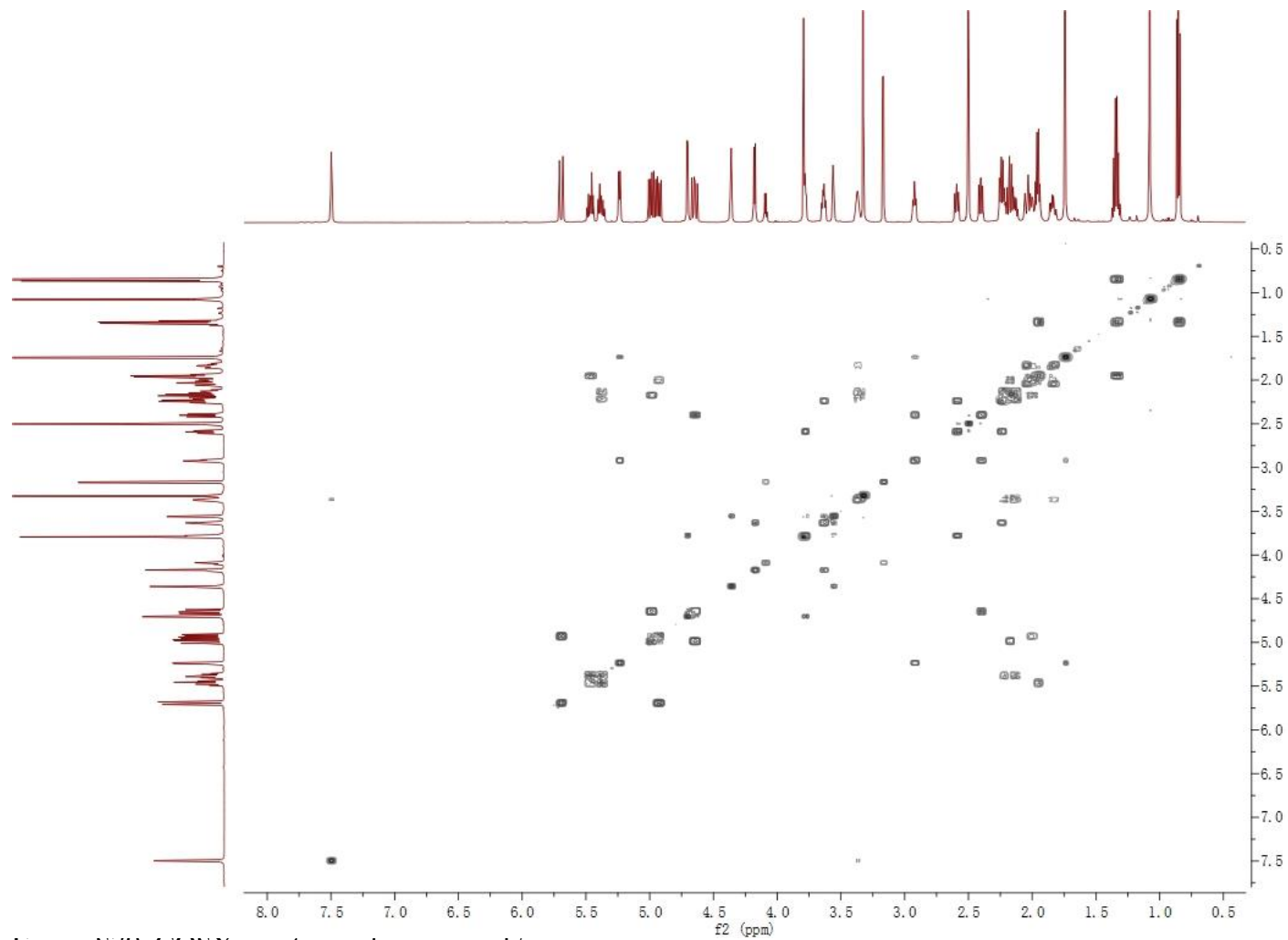


Figure S39. COSY spectrum of compound 5

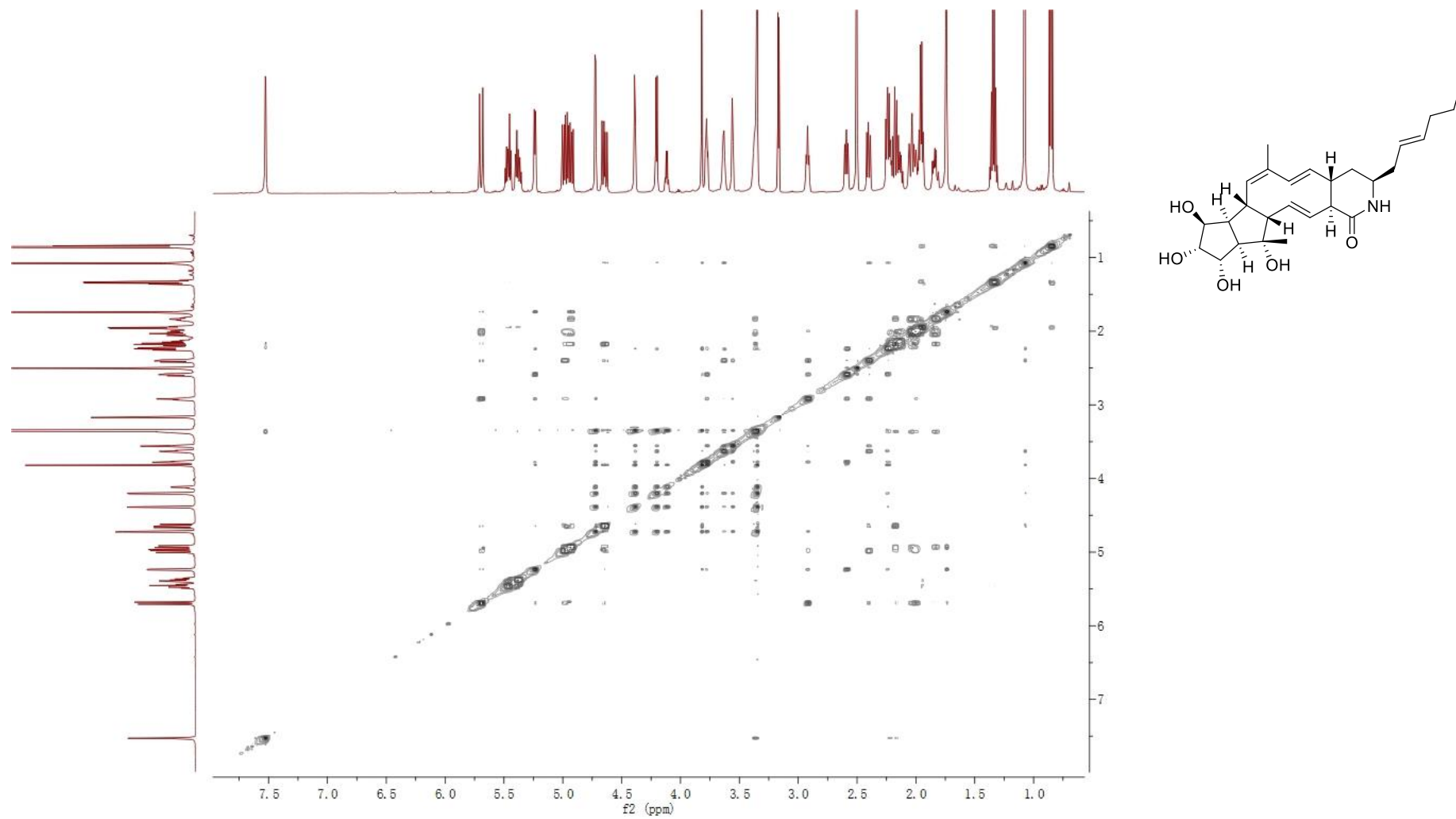


Figure S40. NOESY spectrum of compound **5**

## User Spectra

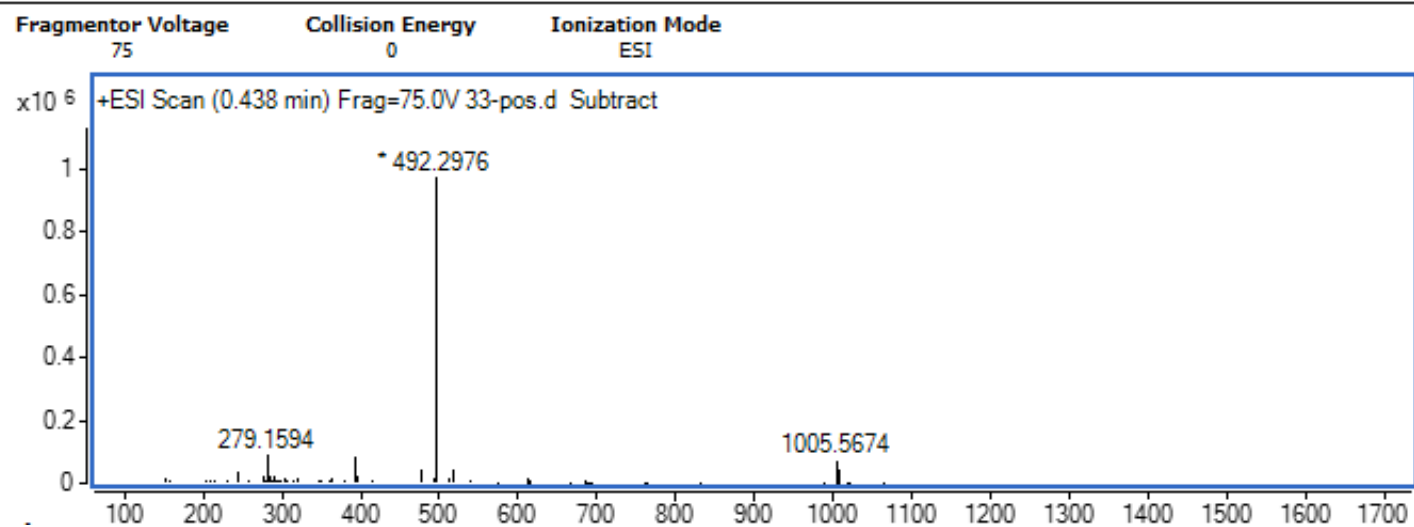


Figure S41. HRESIMS spectrum of compound **6**

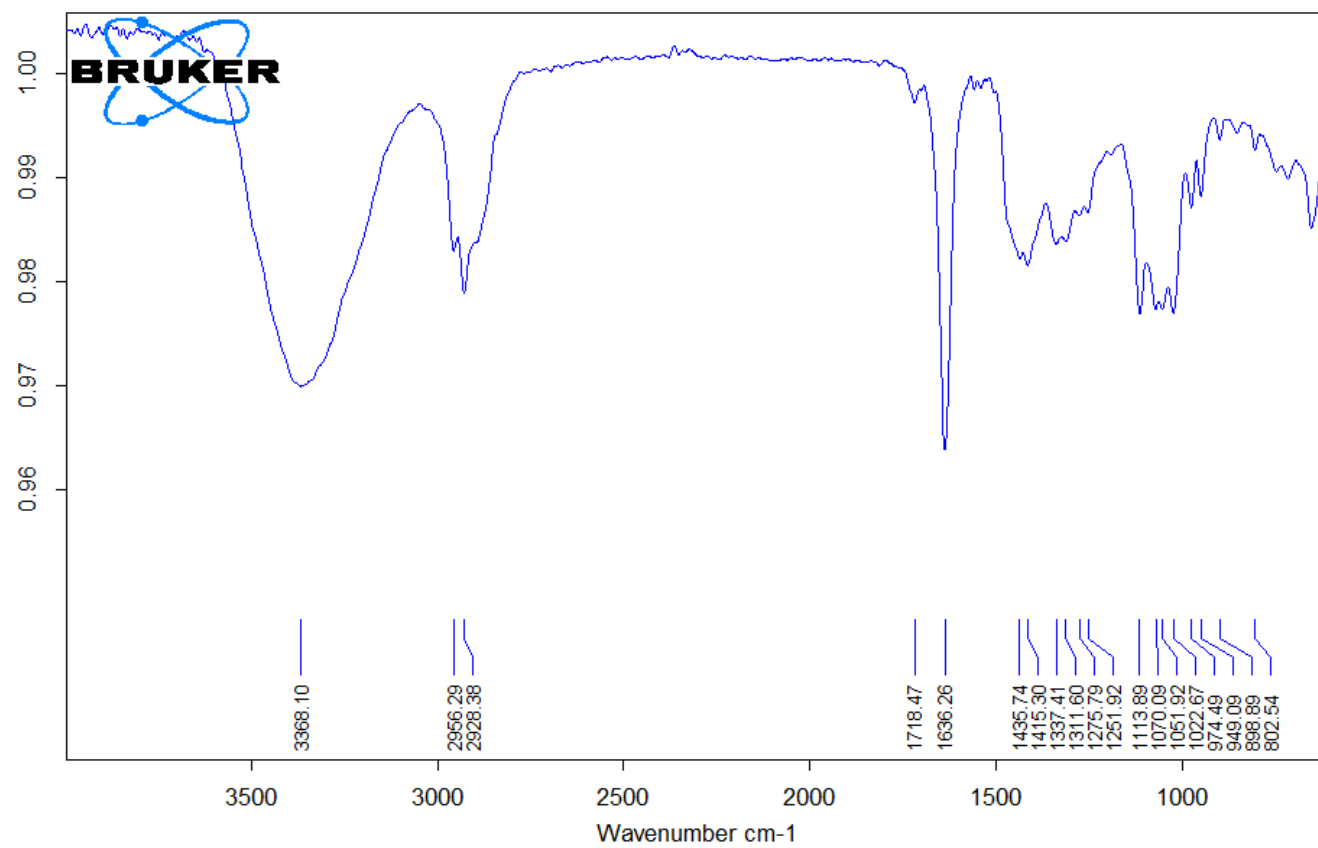


Figure S42. IR spectrum of compound **6**

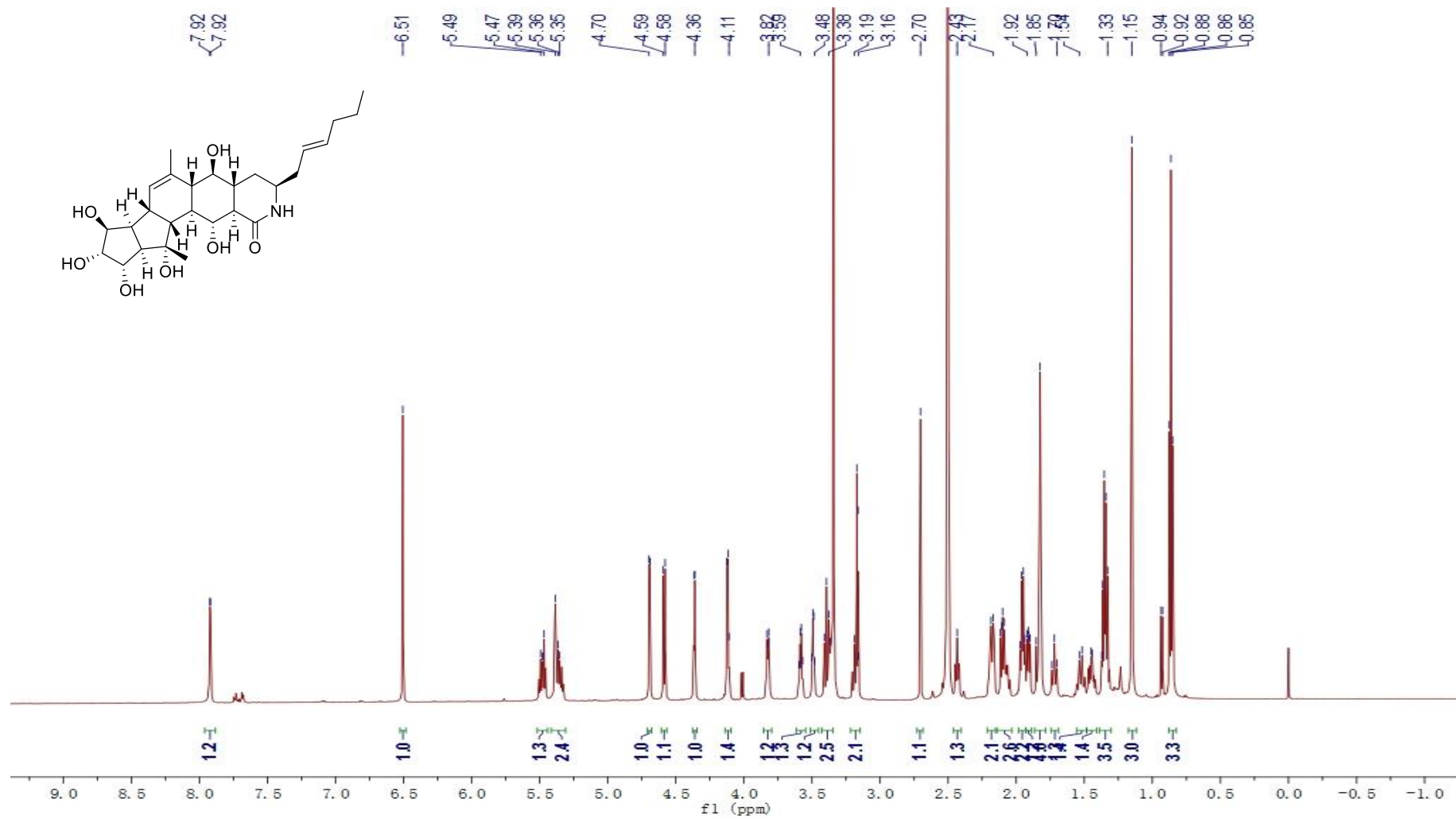


Figure S43. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 6

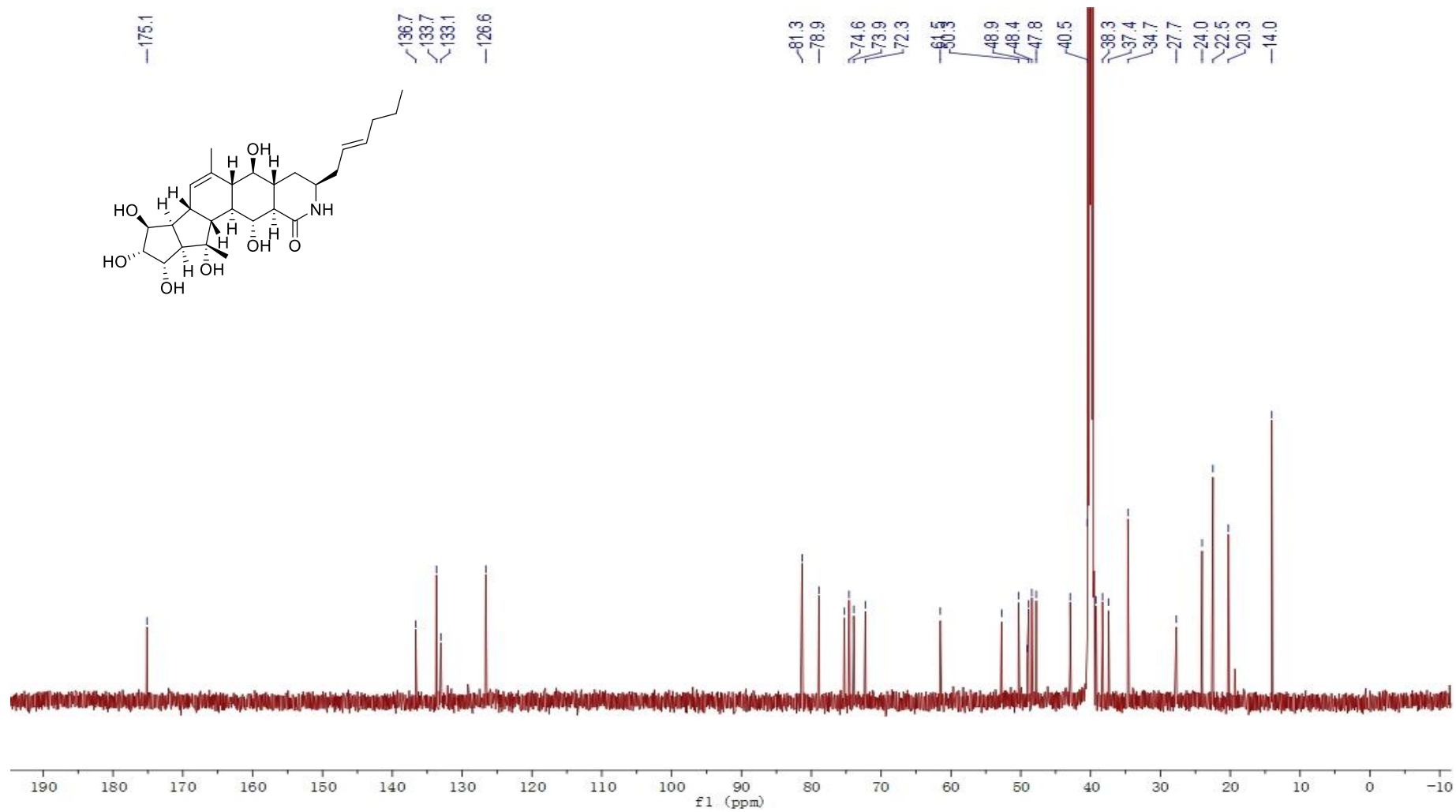


Figure S44. <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound 6

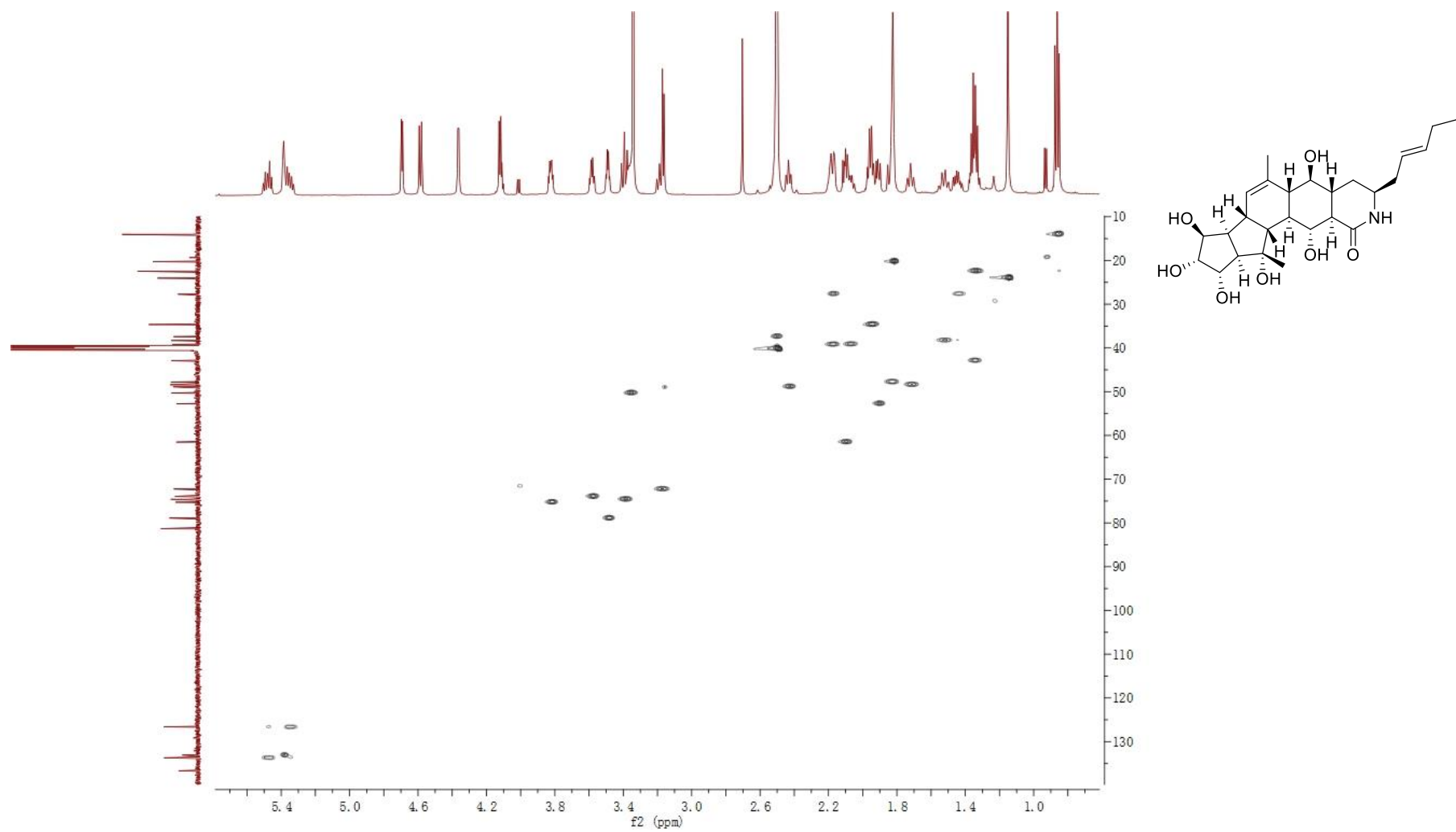


Figure S45. HSQC spectrum of compound **6**

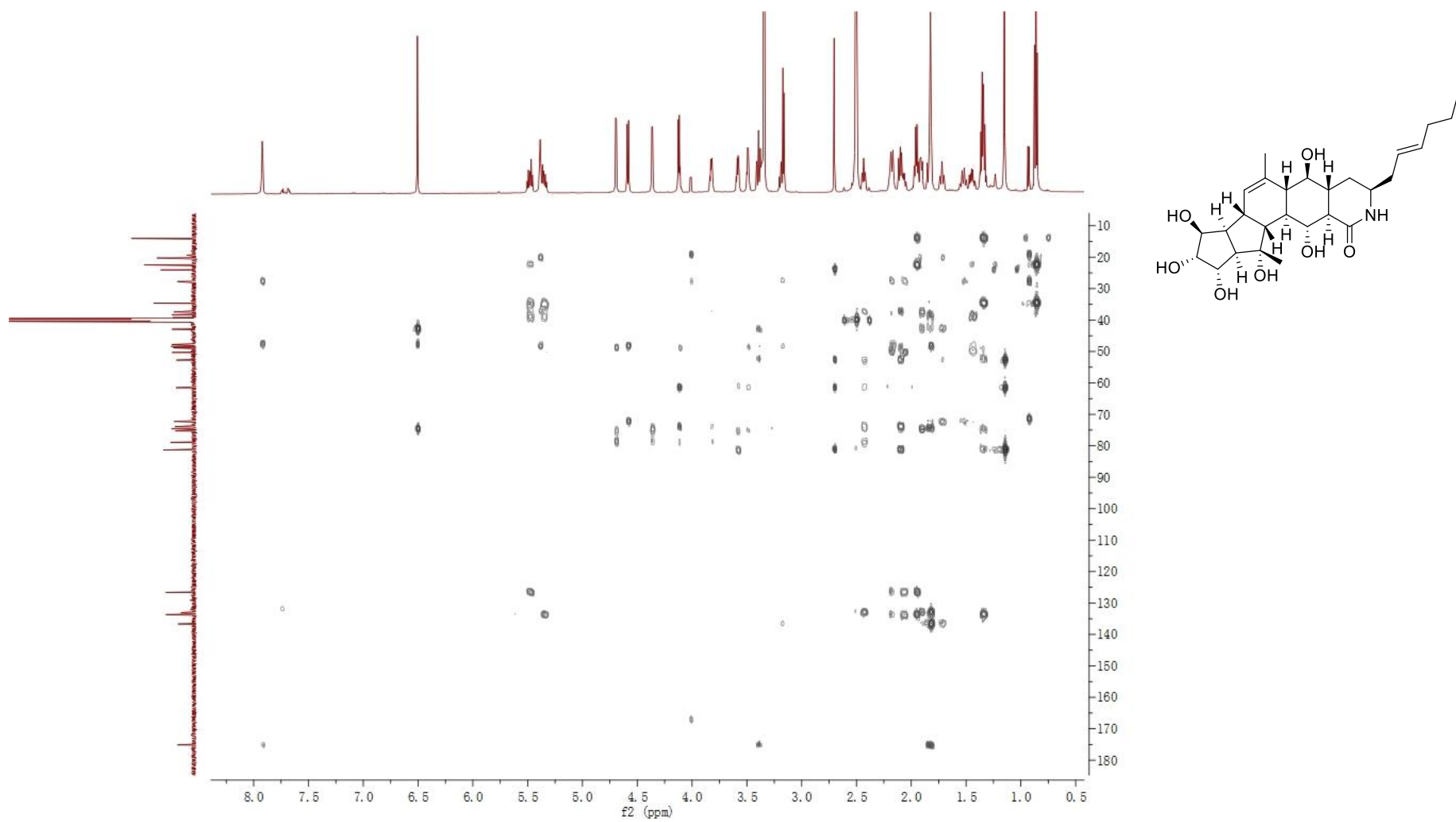


Figure S46. HMBC spectrum of compound **6**



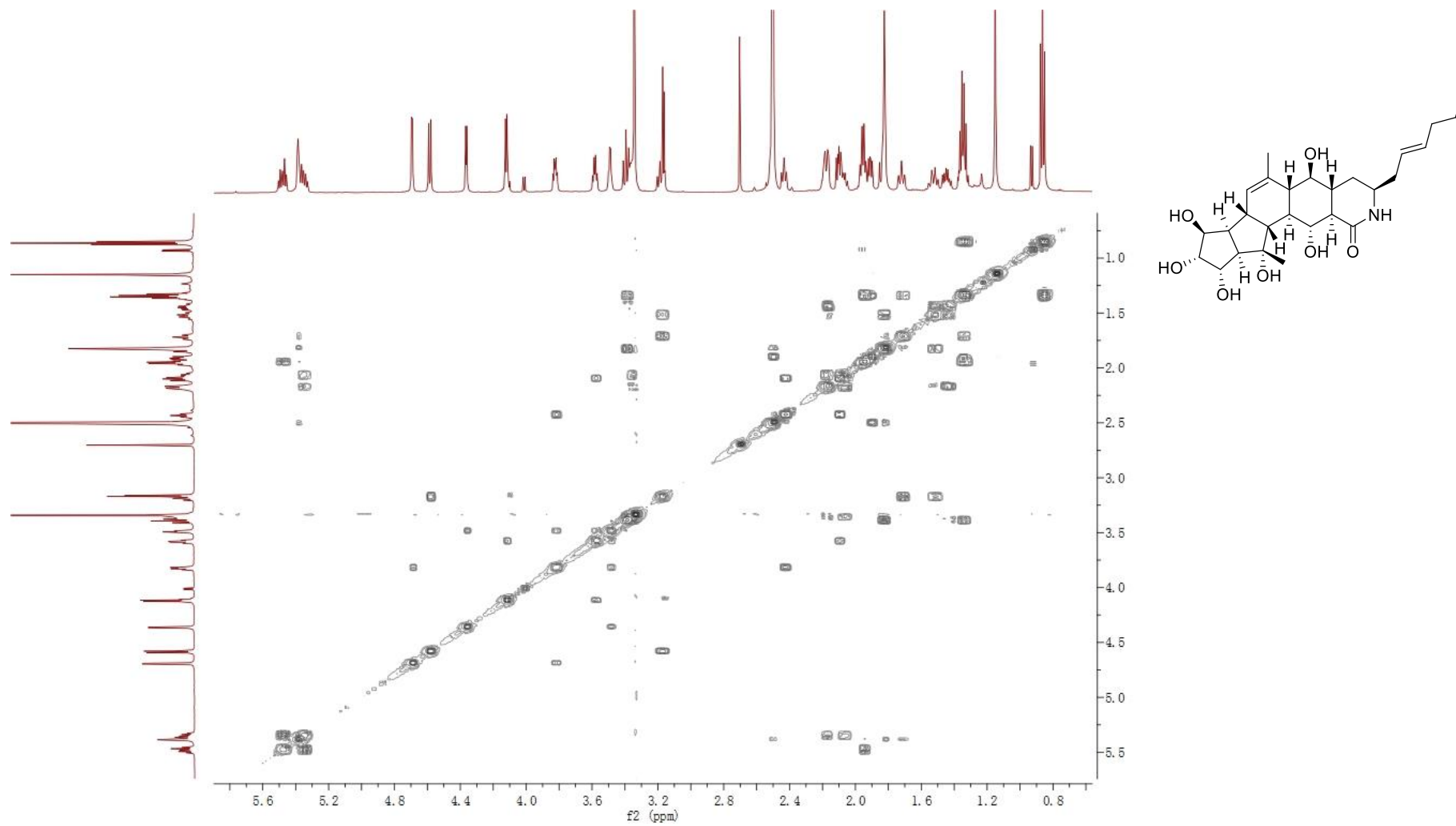


Figure S47. COSY spectrum of compound 6

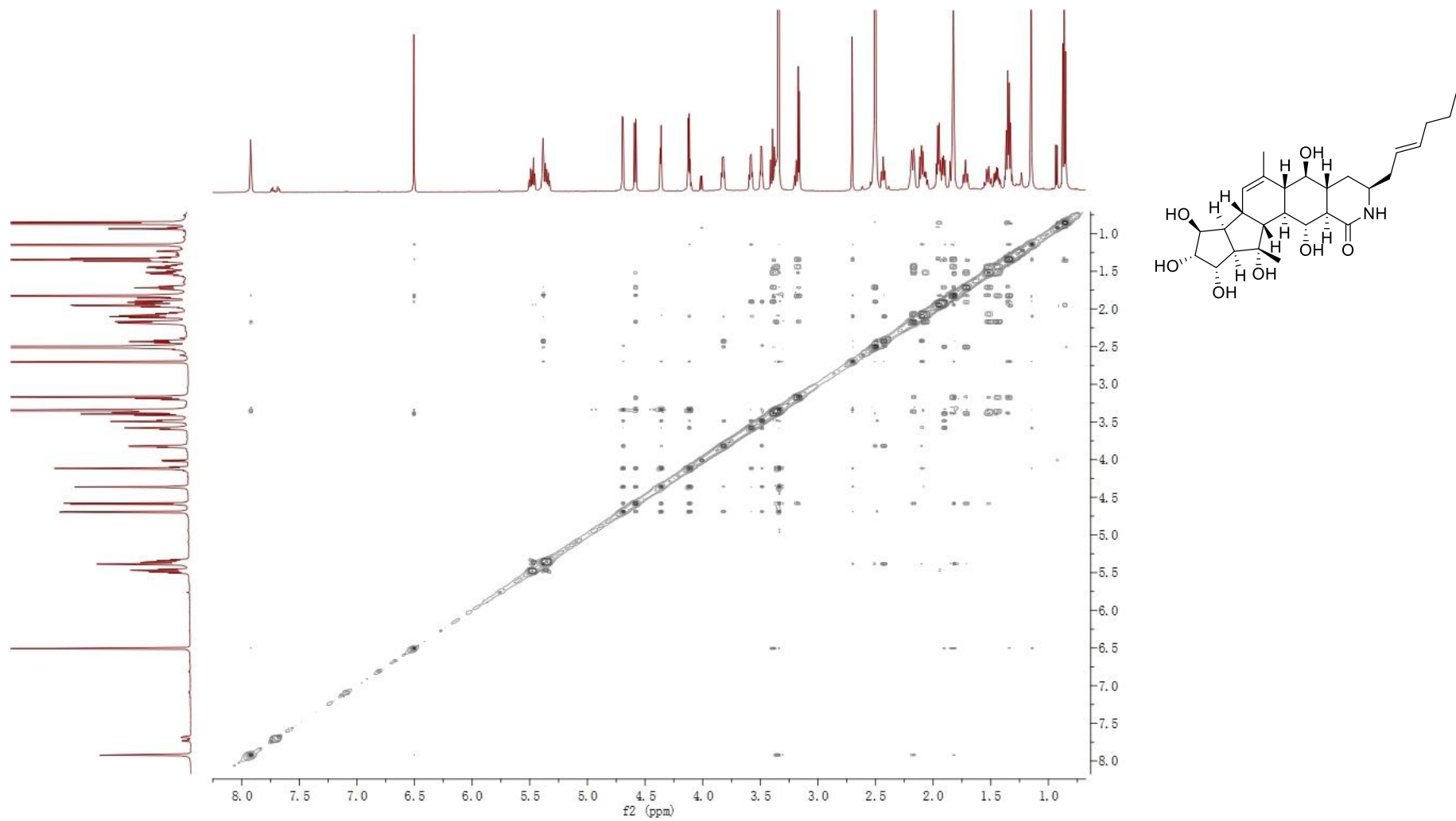


Figure S48. NOESY spectrum of compound 6

## User Spectra

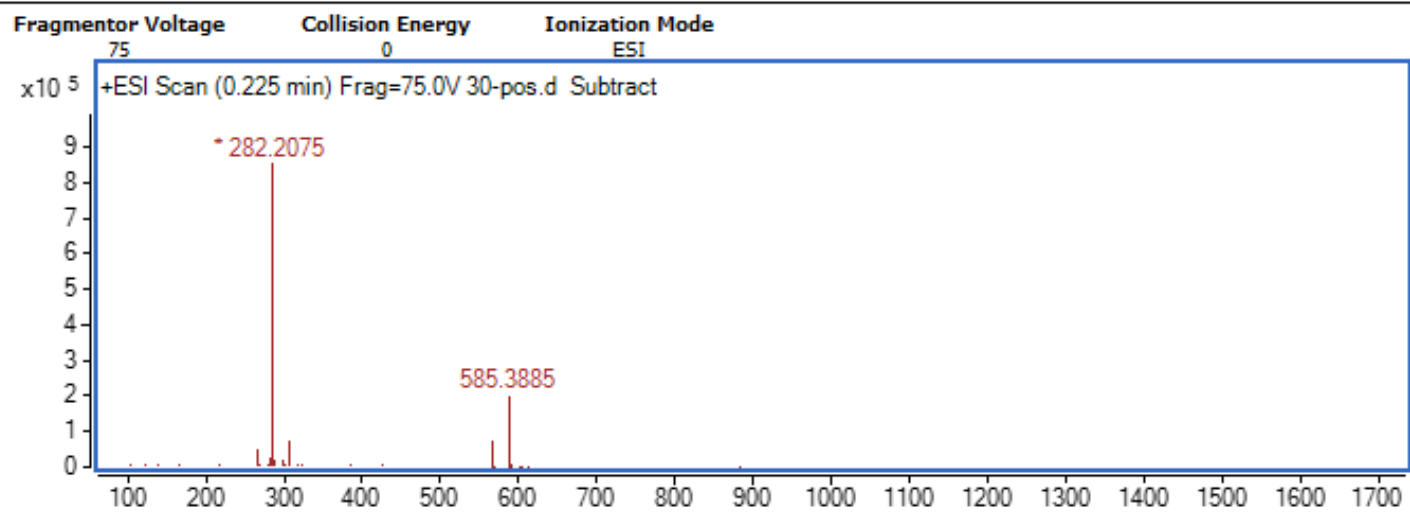


Figure S49. HRESIMS spectrum of compound **10**

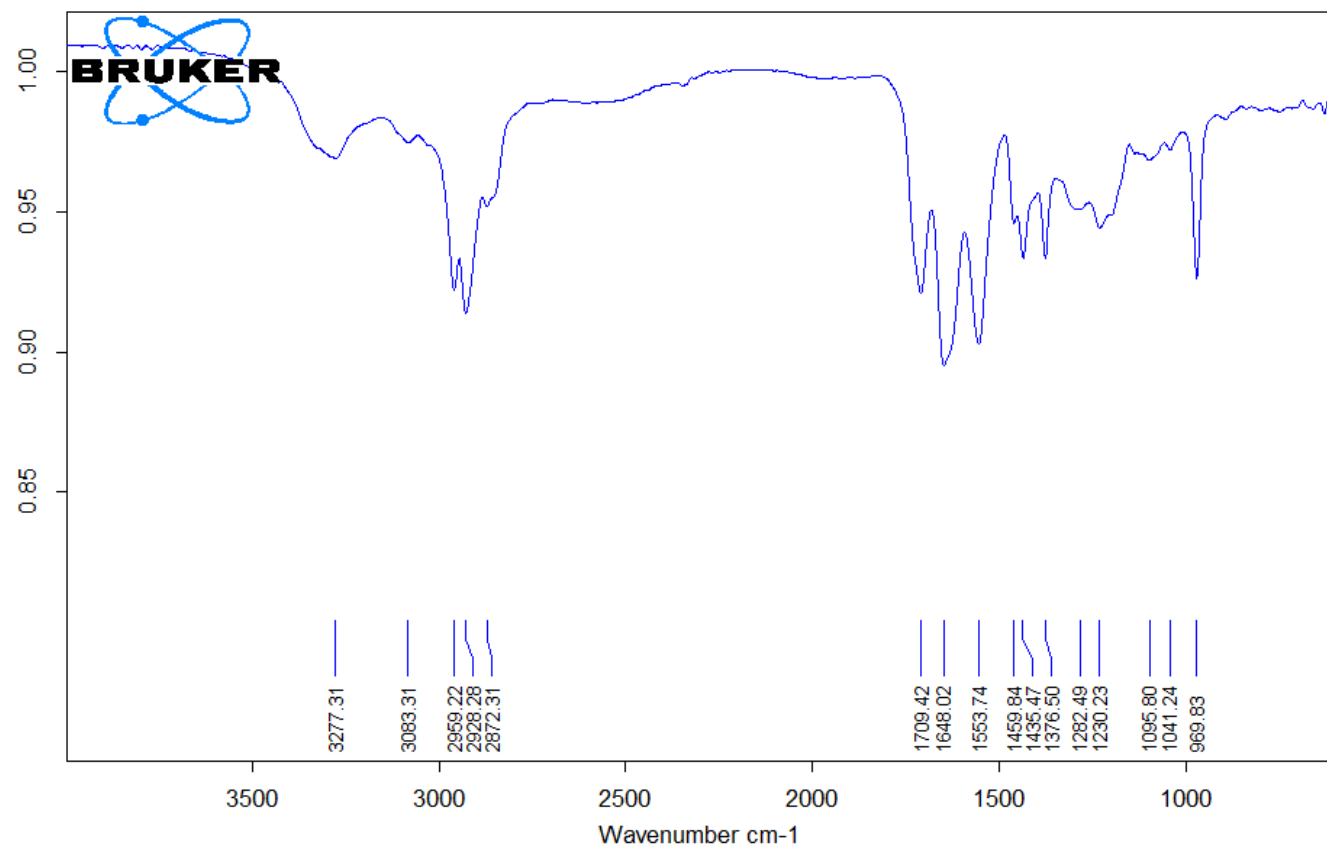


Figure S50. IR spectrum of compound **10**

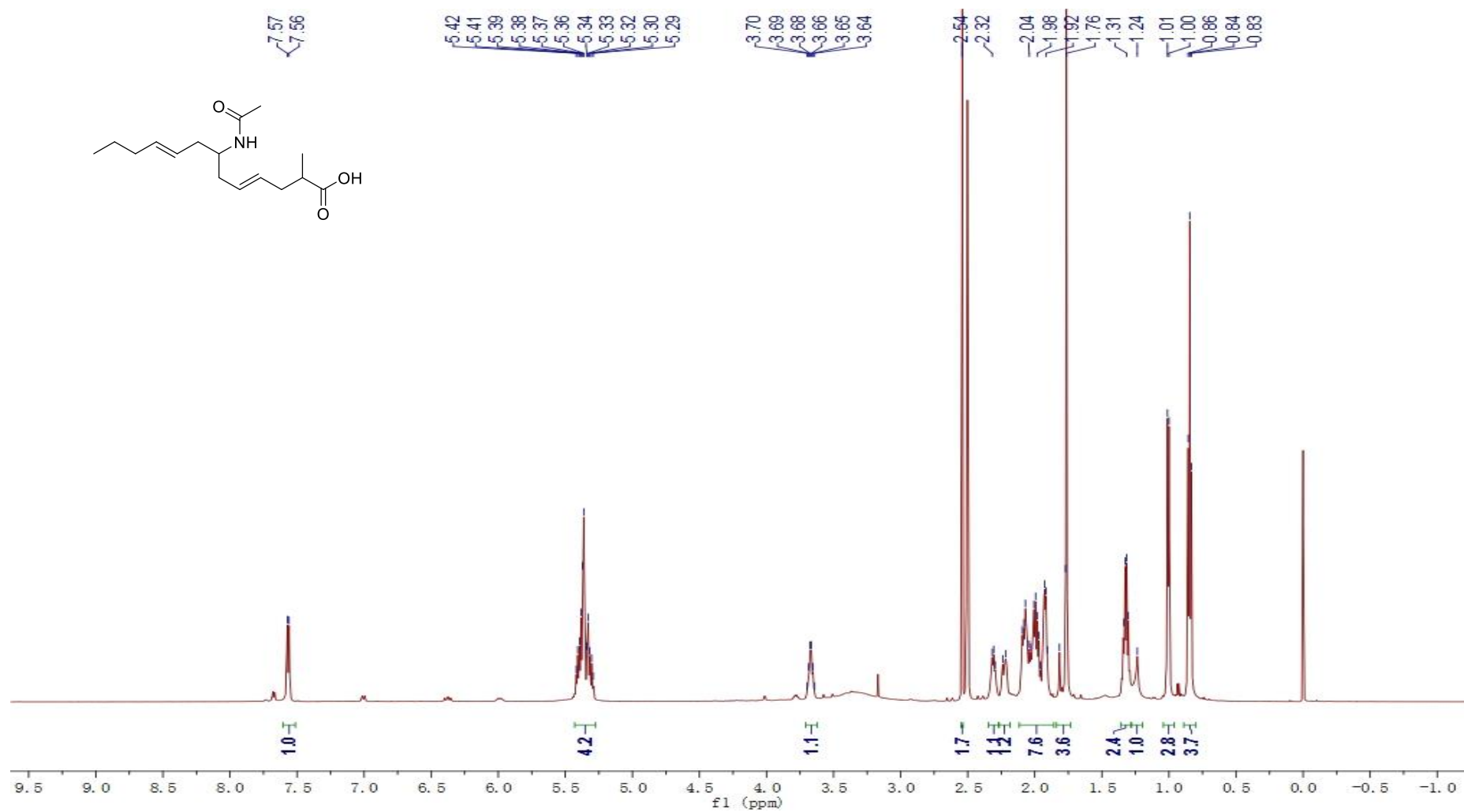


Figure S51. <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **10**

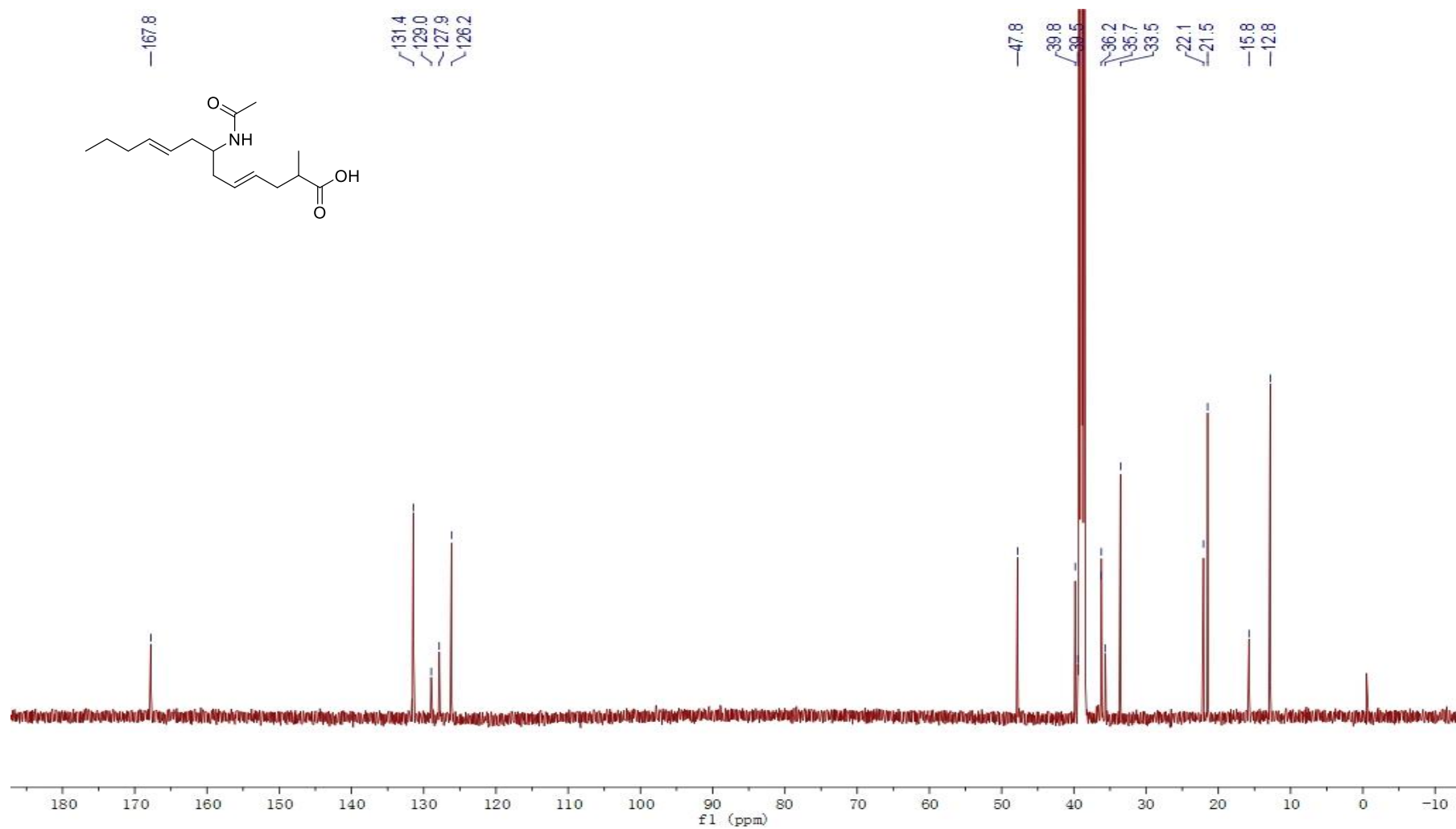


Figure S52. <sup>13</sup>C NMR (150 MHz, DMSO-*d*<sub>6</sub>) spectrum of compound **10**

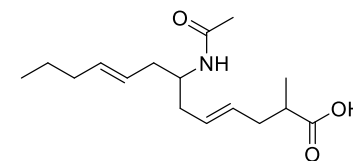
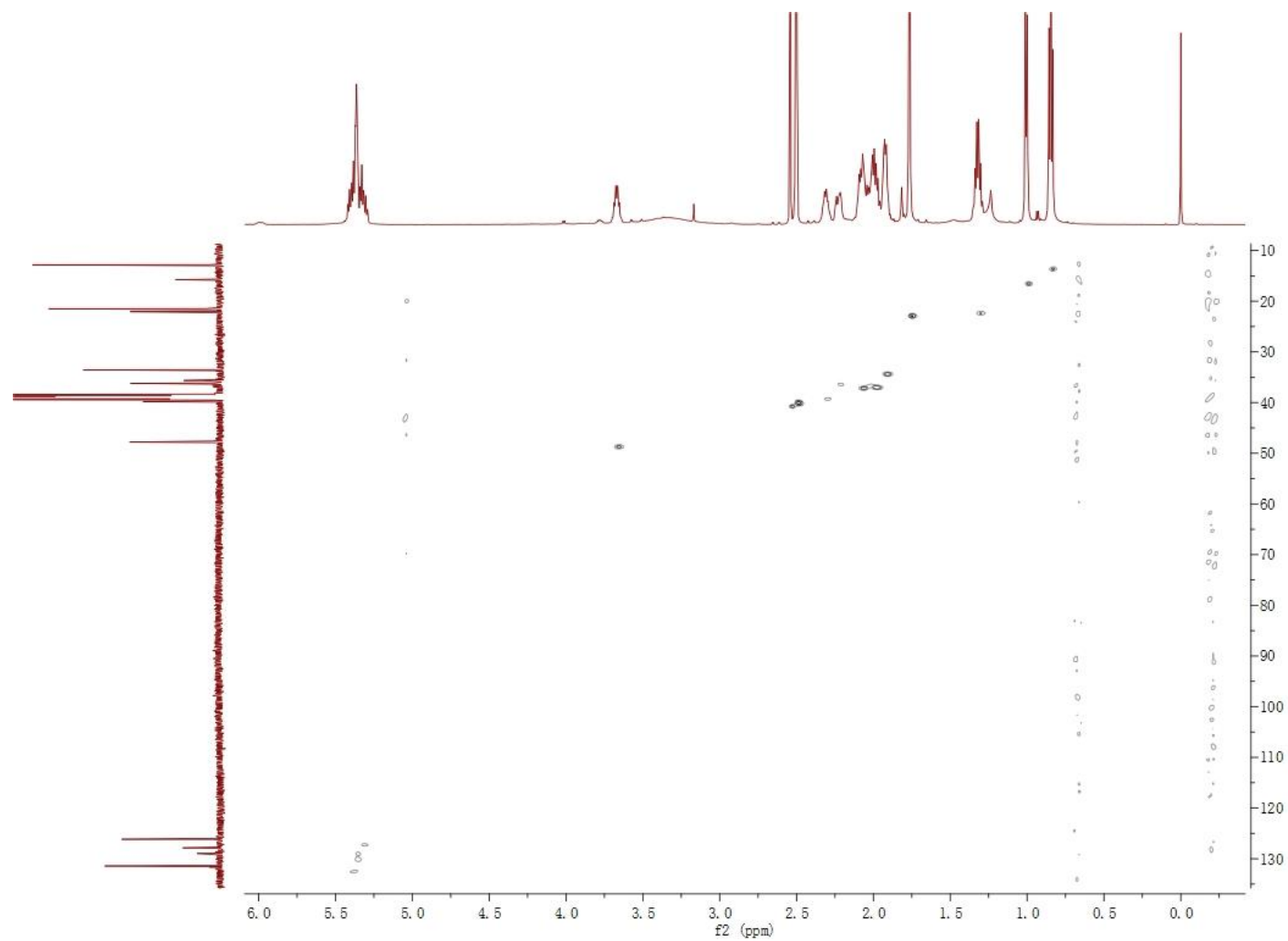


Figure S53. HSQC spectrum of compound **10**

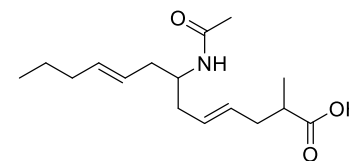
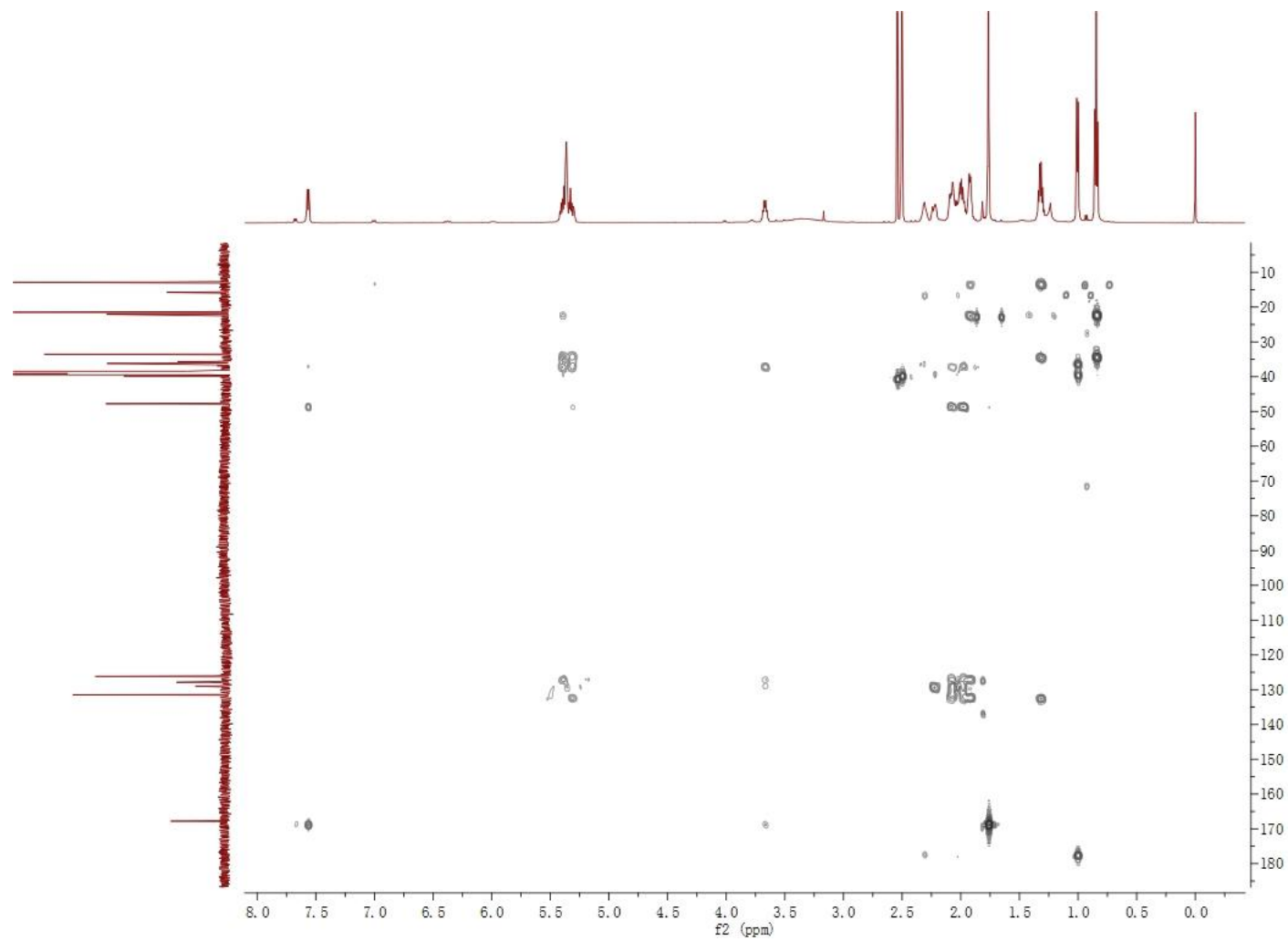


Figure S54. HMBC spectrum of compound **10**



