

Supporting Information

Angucycline Glycosides from Mangrove-Derived *Streptomyces diastaticus* subsp. SCSIO GJ056

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Table of Contents

		Page
Table S1.	Gibbs free energies ^a and equilibrium populations ^b of low-energy conformers of <i>5S</i> , <i>6S-6</i> .	S2
Table S2.	Cartesian coordinates for the low-energy reoptimized MMFF conformers of <i>5S</i> , <i>6S-6</i> at B3LYP/6-311+G (d, p) level of theory in methanol.	S2
Table S3.	Gibbs free energies ^a and equilibrium populations ^b of low-energy conformers of <i>5R</i> , <i>6R-7</i> .	S10
Table S4.	Cartesian coordinates for the low-energy reoptimized MMFF conformers of <i>5R</i> , <i>6R-7</i> at B3LYP/6-311+G (d, p) level of theory in methanol.	S11
Figure S1-S7.	1D and 2D NMR spectrum of compound 1 .	S20-26
Figure S8-S14.	1D and 2D NMR spectrum of compound 2 .	S27-33
Figure S15-S21.	1D and 2D NMR spectrum of compound 3 .	S34-40
Figure S22-S28.	1D and 2D NMR spectrum of compound 4 .	S41-47
Figure S29-S35.	1D and 2D NMR spectrum of compound 5 .	S48-54
Figure S36-S42.	1D and 2D NMR spectrum of compound 6 .	S55-61
Figure S43-S49.	1D and 2D NMR spectrum of compound 7 .	S62-68
Figure S50-S56.	1D and 2D NMR spectrum of compound 8 .	S69-75
Figure S57-S63.	1D and 2D NMR spectrum of compound 9 .	S76-82

Table S1. Gibbs free energies^a and equilibrium populations^b of low-energy conformers of 5S, 6S-6.

Conformers	In methanol	
	ΔG	P (%)
6a	0.19	21.41
6b	0	33.99
6c	1.26	9.02
6d	1.26	9.02
6e	0.17	26.56

^aB3LYP/6-31+G(d,p), in kcal/mol. ^bFrom ΔG values at 298.15K.

Table S2. Cartesian coordinates for the low-energy reoptimized MMFF conformers of 5S, 6S-6 at B3LYP/6-311+G (d, p) level of theory in methanol.

6a		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
1.	6.	0.	-2.489164	-1.692739	0.132580
2.	6.	0.	-2.876234	-0.361024	0.234076
3.	6.	0.	-1.876124	0.641492	0.218574
4.	6.	0.	-0.515890	0.280471	0.111762
5.	6.	0.	-0.156760	-1.076871	0.003965
6.	6.	0.	-1.142438	-2.058928	0.012506
7.	6.	0.	0.530855	1.297727	0.116096
8.	6.	0.	1.940794	0.886720	0.019297
9.	6.	0.	2.337380	-0.417624	-0.160880
10.	6.	0.	1.266138	-1.472384	-0.132134
11.	6.	0.	2.971484	1.994657	0.159700
12.	6.	0.	4.145420	1.454256	0.966901
13.	6.	0.	4.697863	0.220798	0.283343
14.	6.	0.	3.785759	-0.741381	-0.250233
15.	8.	0.	0.241656	2.513150	0.198068
16.	8.	0.	1.531194	-2.679755	-0.185030
17.	8.	0.	3.632901	1.197290	2.272552
18.	8.	0.	-2.264713	1.923895	0.315290
19.	6.	0.	6.067575	0.077473	0.174339
20.	6.	0.	6.637351	-1.023209	-0.494815
21.	6.	0.	5.775200	-1.961989	-1.029387
22.	6.	0.	4.373552	-1.856642	-0.916510
23.	8.	0.	3.705231	-2.851187	-1.527338
24.	6.	0.	-7.124481	-0.296717	-0.266691
25.	6.	0.	-6.379021	0.933454	-0.777723
26.	6.	0.	-4.891149	0.626007	-0.957172
27.	6.	0.	-4.328056	0.044119	0.358214

28.	8.	0.	-5.077768	-1.099520	0.752090
29.	6.	0.	-6.458545	-0.825030	1.011569
30.	8.	0.	-8.477098	0.017516	0.022956
31.	6.	0.	-7.091811	-2.108590	1.523239
32.	8.	0.	-7.029144	1.306699	-1.996550
33.	6.	0.	4.622973	0.896339	3.238085
34.	8.	0.	3.503245	2.422493	-1.089159
35.	6.	0.	2.648593	3.259507	-1.850331
36.	6.	0.	8.133925	-1.161369	-0.617603
37.	1.	0.	6.713851	0.845359	0.593562
38.	1.	0.	-3.260408	-2.453792	0.161329
39.	1.	0.	-0.853285	-3.100147	-0.069352
40.	1.	0.	2.518479	2.836356	0.694159
41.	1.	0.	4.927060	2.226721	1.013108
42.	1.	0.	-1.429290	2.469612	0.302340
43.	1.	0.	6.151182	-2.834104	-1.555688
44.	1.	0.	2.819635	-2.940773	-1.098527
45.	1.	0.	-7.059764	-1.080490	-1.040525
46.	1.	0.	-6.504558	1.732787	-0.028792
47.	1.	0.	-4.334725	1.529535	-1.230909
48.	1.	0.	-4.766586	-0.109737	-1.760365
49.	1.	0.	-4.405692	0.818826	1.139278
50.	1.	0.	-6.532613	-0.040675	1.783765
51.	1.	0.	-8.801049	0.504479	-0.753621
52.	1.	0.	-6.594592	-2.438161	2.440664
53.	1.	0.	-8.152634	-1.943474	1.728807
54.	1.	0.	-6.999499	-2.902818	0.774041
55.	1.	0.	-6.710138	2.185116	-2.254672
56.	1.	0.	4.100863	0.767209	4.189549
57.	1.	0.	5.168971	-0.026390	2.999327
58.	1.	0.	5.350313	1.718063	3.337947
59.	1.	0.	3.231331	3.581765	-2.717267
60.	1.	0.	1.751253	2.732120	-2.201274
61.	1.	0.	2.329141	4.140682	-1.276428
62.	1.	0.	8.570530	-0.289041	-1.119780
63.	1.	0.	8.607617	-1.231701	0.369771
64.	1.	0.	8.409433	-2.053113	-1.188091

6b		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
1.	6.	0.	-2.543703	-1.684707	0.292404
2.	6.	0.	-2.914804	-0.344518	0.300667
3.	6.	0.	-1.900163	0.642871	0.266055
4.	6.	0.	-0.543436	0.258947	0.221859
5.	6.	0.	-0.199953	-1.106748	0.206905
6.	6.	0.	-1.198852	-2.074349	0.245036
7.	6.	0.	0.518253	1.259930	0.207018
8.	6.	0.	1.922331	0.819760	0.144358
9.	6.	0.	2.301266	-0.491728	-0.005502
10.	6.	0.	1.221101	-1.526335	0.145658
11.	6.	0.	2.937757	1.935422	0.193604
12.	6.	0.	4.234322	1.429634	0.819019
13.	6.	0.	4.697118	0.168544	0.123792
14.	6.	0.	3.734004	-0.832831	-0.207728
15.	8.	0.	0.252114	2.481603	0.241793
16.	8.	0.	1.480673	-2.730636	0.259663
17.	8.	0.	3.927317	1.226634	2.198679
18.	8.	0.	-2.271433	1.934125	0.283302
19.	6.	0.	6.040529	0.025994	-0.169915
20.	6.	0.	6.529232	-1.120310	-0.824816
21.	6.	0.	5.617632	-2.108961	-1.145602
22.	6.	0.	4.244463	-2.002101	-0.845510
23.	8.	0.	3.517101	-3.055287	-1.260660
24.	6.	0.	-7.135323	-0.254413	-0.389793
25.	6.	0.	-6.349942	0.936133	-0.933433
26.	6.	0.	-4.860379	0.600988	-1.028014
27.	6.	0.	-4.364239	0.085616	0.341024
28.	8.	0.	-5.147943	-1.024643	0.763169
29.	6.	0.	-6.534615	-0.719142	0.944382
30.	8.	0.	-8.494795	0.092011	-0.179142
31.	6.	0.	-7.208932	-1.964374	1.496641
32.	8.	0.	-6.939567	1.248564	-2.199202
33.	6.	0.	5.047151	0.945659	3.017544
34.	8.	0.	3.151575	2.407034	-1.134381
35.	6.	0.	3.239825	3.819396	-1.232550
36.	6.	0.	7.994670	-1.256548	-1.153975
37.	1.	0.	6.727593	0.824902	0.100627
38.	1.	0.	-3.326518	-2.433094	0.336143
39.	1.	0.	-0.922256	-3.122217	0.238912
40.	1.	0.	2.537876	2.733839	0.826293

41.	1.	0.	5.010951	2.204414	0.721060
42.	1.	0.	-1.427977	2.466912	0.275359
43.	1.	0.	5.931794	-3.022283	-1.641718
44.	1.	0.	2.699487	-3.109001	-0.709430
45.	1.	0.	-7.048231	-1.080537	-1.115920
46.	1.	0.	-6.497173	1.777409	-0.236141
47.	1.	0.	-4.279006	1.480904	-1.325684
48.	1.	0.	-4.710757	-0.180129	-1.782555
49.	1.	0.	-4.463115	0.903019	1.074742
50.	1.	0.	-6.631428	0.107721	1.668270
51.	1.	0.	-8.776811	0.538693	-0.995275
52.	1.	0.	-6.758766	-2.247906	2.452942
53.	1.	0.	-8.275502	-1.775408	1.643527
54.	1.	0.	-7.094010	-2.800421	0.797776
55.	1.	0.	-6.593919	2.105639	-2.492444
56.	1.	0.	4.671575	0.865801	4.040886
57.	1.	0.	5.539214	0.003759	2.740464
58.	1.	0.	5.791927	1.756716	2.972447
59.	1.	0.	3.418019	4.047663	-2.286647
60.	1.	0.	2.305500	4.298422	-0.909527
61.	1.	0.	4.073255	4.224856	-0.638510
62.	1.	0.	8.323798	-0.453534	-1.825538
63.	1.	0.	8.612523	-1.190203	-0.249728
64.	1.	0.	8.209724	-2.212166	-1.640870

6c		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
1.	6.	0.	-2.467909	-1.708636	0.267512
2.	6.	0.	-2.847310	-0.370838	0.262877
3.	6.	0.	-1.841259	0.621393	0.169951
4.	6.	0.	-0.483251	0.245230	0.089595
5.	6.	0.	-0.131904	-1.118334	0.089847
6.	6.	0.	-1.123311	-2.090747	0.177397
7.	6.	0.	0.569483	1.252831	0.009369
8.	6.	0.	1.975337	0.827997	-0.065217
9.	6.	0.	2.368262	-0.489513	-0.123798
10.	6.	0.	1.288575	-1.532729	-0.015460

11.	6.	0.	3.009993	1.937538	-0.039286
12.	6.	0.	4.184035	1.481513	0.828988
13.	6.	0.	4.724558	0.177081	0.291774
14.	6.	0.	3.814504	-0.824516	-0.167128
15.	8.	0.	0.286252	2.473714	0.003410
16.	8.	0.	1.541952	-2.742712	0.018981
17.	8.	0.	3.784014	1.280920	2.183419
18.	8.	0.	-2.222091	1.910009	0.166790
19.	6.	0.	6.093882	0.006803	0.248194
20.	6.	0.	6.668167	-1.162473	-0.284930
21.	6.	0.	5.810446	-2.138232	-0.757773
22.	6.	0.	4.408503	-2.007263	-0.702523
23.	8.	0.	3.747356	-3.049224	-1.236893
24.	6.	0.	-7.091661	-0.313254	-0.270193
25.	6.	0.	-6.333661	0.872674	-0.860011
26.	6.	0.	-4.847876	0.541381	-1.008003
27.	6.	0.	-4.297112	0.051671	0.349373
28.	8.	0.	-5.057206	-1.055864	0.819300
29.	6.	0.	-6.438678	-0.756758	1.046955
30.	8.	0.	-8.443758	0.029826	-0.012631
31.	6.	0.	-7.083687	-1.998917	1.639491
32.	8.	0.	-6.973421	1.164896	-2.106138
33.	6.	0.	3.678080	2.469607	2.946520
34.	8.	0.	3.555915	2.226065	-1.322948
35.	6.	0.	2.701384	2.956045	-2.187020
36.	6.	0.	8.165425	-1.332944	-0.334294
37.	1.	0.	6.736624	0.801395	0.619070
38.	1.	0.	-3.243331	-2.460757	0.355796
39.	1.	0.	-0.840236	-3.136815	0.179498
40.	1.	0.	2.547687	2.839206	0.376553
41.	1.	0.	4.968794	2.249326	0.775771
42.	1.	0.	-1.382849	2.447279	0.110272
43.	1.	0.	6.190830	-3.061819	-1.183410
44.	1.	0.	2.847091	-3.089275	-0.832101
45.	1.	0.	-7.027867	-1.149168	-0.987514
46.	1.	0.	-6.457290	1.723078	-0.169312
47.	1.	0.	-4.282199	1.417973	-1.343059
48.	1.	0.	-4.725369	-0.252276	-1.754323
49.	1.	0.	-4.373570	0.881012	1.072423
50.	1.	0.	-6.514793	0.078776	1.763325
51.	1.	0.	-8.759114	0.463352	-0.823646
52.	1.	0.	-6.989059	-2.843163	0.947505
53.	1.	0.	-6.596548	-2.267188	2.581973
54.	1.	0.	-8.145301	-1.814659	1.823526

55.	1.	0.	-6.645709	2.020548	-2.423143
56.	1.	0.	3.474039	2.161483	3.975251
57.	1.	0.	4.616269	3.045954	2.925781
58.	1.	0.	2.860738	3.123409	2.608351
59.	1.	0.	3.290465	3.183461	-3.079373
60.	1.	0.	1.815816	2.377689	-2.484447
61.	1.	0.	2.362829	3.894118	-1.724465
62.	1.	0.	8.637881	-0.514870	-0.892163
63.	1.	0.	8.597018	-1.323005	0.674571
64.	1.	0.	8.446962	-2.275754	-0.812260

6d		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
1.	6.	0.	-2.467904	-1.708579	0.267506
2.	6.	0.	-2.847302	-0.370779	0.262818
3.	6.	0.	-1.841247	0.621453	0.169923
4.	6.	0.	-0.483224	0.245283	0.089651
5.	6.	0.	-0.131891	-1.118280	0.089980
6.	6.	0.	-1.123306	-2.090692	0.177486
7.	6.	0.	0.569517	1.252887	0.009494
8.	6.	0.	1.975375	0.828024	-0.065144
9.	6.	0.	2.368281	-0.489486	-0.123650
10.	6.	0.	1.288597	-1.532693	-0.015137
11.	6.	0.	3.010053	1.937547	-0.039274
12.	6.	0.	4.184119	1.481537	0.828995
13.	6.	0.	4.724602	0.177087	0.291774
14.	6.	0.	3.814515	-0.824505	-0.167050
15.	8.	0.	0.286319	2.473771	0.003613
16.	8.	0.	1.542002	-2.742656	0.019655
17.	8.	0.	3.784202	1.280972	2.183432
18.	8.	0.	-2.222068	1.910061	0.166741
19.	6.	0.	6.093927	0.006796	0.248071
20.	6.	0.	6.668148	-1.162464	-0.285139
21.	6.	0.	5.810376	-2.138211	-0.757935
22.	6.	0.	4.408449	-2.007244	-0.702521
23.	8.	0.	3.747216	-3.049177	-1.236854
24.	6.	0.	-7.091661	-0.313305	-0.270242

25.	6.	0.	-6.333687	0.872585	-0.860157
26.	6.	0.	-4.847907	0.541282	-1.008158
27.	6.	0.	-4.297109	0.051731	0.349261
28.	8.	0.	-5.057182	-1.055774	0.819324
29.	6.	0.	-6.438660	-0.756680	1.046942
30.	8.	0.	-8.443769	0.029765	-0.012684
31.	6.	0.	-7.083635	-1.998808	1.639585
32.	8.	0.	-6.973494	1.164727	-2.106283
33.	6.	0.	3.677894	2.469691	2.946436
34.	8.	0.	3.555991	2.226053	-1.322937
35.	6.	0.	2.701229	2.955557	-2.187180
36.	6.	0.	8.165397	-1.332985	-0.334611
37.	1.	0.	6.736708	0.801373	0.618911
38.	1.	0.	-3.243347	-2.460683	0.355765
39.	1.	0.	-0.840211	-3.136755	0.179659
40.	1.	0.	2.547757	2.839236	0.376526
41.	1.	0.	4.968877	2.249355	0.775701
42.	1.	0.	-1.382807	2.447308	0.110314
43.	1.	0.	6.190720	-3.061780	-1.183647
44.	1.	0.	2.847081	-3.089280	-0.831825
45.	1.	0.	-7.027867	-1.149275	-0.987494
46.	1.	0.	-6.457297	1.723042	-0.169520
47.	1.	0.	-4.282242	1.417838	-1.343326
48.	1.	0.	-4.725412	-0.252463	-1.754386
49.	1.	0.	-4.373579	0.881139	1.072231
50.	1.	0.	-6.514808	0.078915	1.763238
51.	1.	0.	-8.759125	0.463321	-0.823684
52.	1.	0.	-8.145233	-1.814532	1.823697
53.	1.	0.	-6.989071	-2.843089	0.947635
54.	1.	0.	-6.596417	-2.267023	2.582041
55.	1.	0.	-6.645559	2.020216	-2.423501
56.	1.	0.	3.474503	2.161567	3.975295
57.	1.	0.	4.615724	3.046602	2.925200
58.	1.	0.	2.860004	3.122952	2.608546
59.	1.	0.	3.290193	3.182843	-3.079642
60.	1.	0.	1.815803	2.376864	-2.484389
61.	1.	0.	2.362458	3.893685	-1.724893
62.	1.	0.	8.596973	-1.323705	0.674268
63.	1.	0.	8.446876	-2.275510	-0.813171
64.	1.	0.	8.637915	-0.514587	-0.891954

6e		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
1.	6.	0.	-2.493451	-1.680644	0.146493
2.	6.	0.	-2.877764	-0.347987	0.243227
3.	6.	0.	-1.874836	0.652187	0.230054
4.	6.	0.	-0.515270	0.287043	0.126141
5.	6.	0.	-0.159279	-1.071424	0.023123
6.	6.	0.	-1.147289	-2.051030	0.032704
7.	6.	0.	0.533940	1.301696	0.126301
8.	6.	0.	1.942941	0.886825	0.023949
9.	6.	0.	2.336031	-0.419244	-0.149871
10.	6.	0.	1.262946	-1.471275	-0.107728
11.	6.	0.	2.976098	1.994219	0.148955
12.	6.	0.	4.155856	1.458471	0.950524
13.	6.	0.	4.700966	0.218427	0.273041
14.	6.	0.	3.783481	-0.746490	-0.245846
15.	8.	0.	0.248670	2.517633	0.207659
16.	8.	0.	1.525896	-2.679820	-0.145589
17.	8.	0.	3.654363	1.212761	2.262792
18.	8.	0.	-2.261083	1.934035	0.326241
19.	6.	0.	6.069721	0.071743	0.155389
20.	6.	0.	6.632738	-1.035593	-0.508191
21.	6.	0.	5.765088	-1.977679	-1.028022
22.	6.	0.	4.364527	-1.868641	-0.906121
23.	8.	0.	3.689835	-2.867675	-1.502991
24.	6.	0.	-7.112078	-0.293353	-0.283222
25.	6.	0.	-6.371327	0.929103	-0.821677
26.	6.	0.	-4.884613	0.619080	-0.971317
27.	6.	0.	-4.328759	0.063492	0.355458
28.	8.	0.	-5.080612	-1.074817	0.776847
29.	6.	0.	-6.459413	-0.788134	1.019605
30.	8.	0.	-8.470445	0.115454	-0.090178
31.	6.	0.	-7.091526	-2.057313	1.572100
32.	8.	0.	-6.891679	1.324315	-2.080288
33.	6.	0.	4.653016	0.922648	3.222613
34.	8.	0.	3.498314	2.412160	-1.107213
35.	6.	0.	2.638062	3.243990	-1.868344
36.	6.	0.	8.128162	-1.177115	-0.641314
37.	1.	0.	6.720229	0.842222	0.563148
38.	1.	0.	-3.266153	-2.440369	0.172928
39.	1.	0.	-0.860448	-3.093189	-0.045180
40.	1.	0.	2.528220	2.840272	0.680801

41.	1.	0.	4.938868	2.230189	0.983846
42.	1.	0.	-1.426769	2.480362	0.309756
43.	1.	0.	6.135789	-2.855103	-1.549237
44.	1.	0.	2.807801	-2.952033	-1.066050
45.	1.	0.	-7.051175	-1.092543	-1.037862
46.	1.	0.	-6.500472	1.741625	-0.084307
47.	1.	0.	-4.339393	1.522079	-1.260843
48.	1.	0.	-4.749394	-0.128405	-1.762196
49.	1.	0.	-4.407458	0.851099	1.122478
50.	1.	0.	-6.539323	0.018896	1.767719
51.	1.	0.	-9.029488	-0.675296	-0.080512
52.	1.	0.	-7.025865	-2.871375	0.840797
53.	1.	0.	-6.573904	-2.373114	2.482643
54.	1.	0.	-8.144171	-1.885366	1.820892
55.	1.	0.	-7.854056	1.383070	-1.954112
56.	1.	0.	4.139305	0.801496	4.179714
57.	1.	0.	5.198859	-0.001270	2.987960
58.	1.	0.	5.379635	1.746596	3.308590
59.	1.	0.	3.214820	3.560237	-2.741447
60.	1.	0.	1.738542	2.714111	-2.209585
61.	1.	0.	2.322543	4.128990	-1.298302
62.	1.	0.	8.398069	-2.077098	-1.201483
63.	1.	0.	8.561458	-0.312507	-1.159501
64.	1.	0.	8.610055	-1.233942	0.342948

Table S3. Gibbs free energies^a and equilibrium populations^b of low-energy conformers of 5R, 6R-7.

Conformers	In methanol	
	ΔG	P (%)
7a	0.21	22.58
7b	0	33.32
7c	1.38	8.87
7d	1.38	8.87
7e	0.19	26.35

^aB3LYP/6-31+G (d, p), in kcal/mol. ^bFrom ΔG values at 298.15K.

Table S4. Cartesian coordinates for the low-energy reoptimized MMFF conformers of 5*R*, 6*R*-7 at B3LYP/6-311+G (d, p) level of theory in methanol.

7a		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
1.	6.	0.	-2.493775	1.703531	0.166657
2.	6.	0.	-2.881627	0.422797	-0.211115
3.	6.	0.	-1.879183	-0.545930	-0.460590
4.	6.	0.	-0.516994	-0.206238	-0.316312
5.	6.	0.	-0.156757	1.099088	0.069889
6.	6.	0.	-1.143956	2.050007	0.309079
7.	6.	0.	0.530548	-1.191068	-0.567964
8.	6.	0.	1.941371	-0.807831	-0.396667
9.	6.	0.	2.345624	0.468502	-0.082633
10.	6.	0.	1.270255	1.478072	0.209342
11.	6.	0.	2.961277	-1.923094	-0.557553
12.	6.	0.	4.052598	-1.724273	0.486548
13.	6.	0.	4.658466	-0.345721	0.322537
14.	6.	0.	3.794081	0.764935	0.074098
15.	8.	0.	0.241548	-2.354255	-0.930144
16.	8.	0.	1.532029	2.622822	0.598964
17.	8.	0.	3.420160	-1.918332	1.750143
18.	8.	0.	-2.267996	-1.777043	-0.832335
19.	6.	0.	6.031371	-0.209824	0.393823
20.	6.	0.	6.654231	1.038811	0.201285
21.	6.	0.	5.840037	2.126509	-0.052009
22.	6.	0.	4.434721	2.025449	-0.110749
23.	8.	0.	3.820930	3.186702	-0.399791
24.	6.	0.	-7.094297	0.183686	0.485420
25.	6.	0.	-6.319374	-1.119650	0.656723
26.	6.	0.	-4.825876	-0.837209	0.823728
27.	6.	0.	-4.336674	0.034893	-0.353233
28.	8.	0.	-5.109832	1.227088	-0.438841
29.	6.	0.	-6.504109	1.000226	-0.673593
30.	8.	0.	-8.461389	-0.074330	0.208302
31.	6.	0.	-7.166321	2.358226	-0.839195
32.	8.	0.	-6.899681	-1.774422	1.788917
33.	6.	0.	4.315312	-1.995179	2.843699
34.	8.	0.	3.607813	-1.909439	-1.825153
35.	6.	0.	2.827422	-2.399738	-2.902696
36.	6.	0.	8.154676	1.171202	0.270819
37.	1.	0.	6.640449	-1.091922	0.578291

38.	1.	0.	-3.267365	2.442840	0.339226
39.	1.	0.	-0.853931	3.052498	0.601256
40.	1.	0.	2.465560	-2.884838	-0.388666
41.	1.	0.	4.831428	-2.485650	0.333359
42.	1.	0.	-1.431338	-2.303192	-0.970592
43.	1.	0.	6.258022	3.116379	-0.208126
44.	1.	0.	2.897990	3.147203	-0.049541
45.	1.	0.	-6.985127	0.769708	1.413823
46.	1.	0.	-6.483613	-1.726053	-0.249255
47.	1.	0.	-4.251953	-1.769984	0.857776
48.	1.	0.	-4.661532	-0.298601	1.764315
49.	1.	0.	-4.453367	-0.544502	-1.284278
50.	1.	0.	-6.624265	0.412557	-1.599430
51.	1.	0.	-8.738668	-0.732594	0.867840
52.	1.	0.	-6.727956	2.894491	-1.686437
53.	1.	0.	-8.238262	2.230137	-1.010566
54.	1.	0.	-7.025197	2.962063	0.064111
55.	1.	0.	-6.558764	-2.681403	1.823206
56.	1.	0.	3.706647	-2.184031	3.731672
57.	1.	0.	5.032408	-2.822555	2.719244
58.	1.	0.	4.878833	-1.063025	2.985723
59.	1.	0.	3.491231	-2.428786	-3.770733
60.	1.	0.	2.446347	-3.410347	-2.699823
61.	1.	0.	1.973434	-1.747520	-3.130665
62.	1.	0.	8.533147	0.873788	1.256958
63.	1.	0.	8.642405	0.522425	-0.467437
64.	1.	0.	8.476491	2.199523	0.082223

7b		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
1.	6.	0.	-2.538133	1.703034	0.187635
2.	6.	0.	-2.911565	0.419766	-0.196382
3.	6.	0.	-1.899978	-0.548832	-0.406193
4.	6.	0.	-0.544326	-0.204673	-0.222194
5.	6.	0.	-0.198322	1.103000	0.169375
6.	6.	0.	-1.194290	2.052372	0.374841
7.	6.	0.	0.512332	-1.190967	-0.421534

8.	6.	0.	1.916453	-0.791893	-0.225280
9.	6.	0.	2.310999	0.497958	0.032876
10.	6.	0.	1.222921	1.483428	0.357104
11.	6.	0.	2.920173	-1.907152	-0.390637
12.	6.	0.	4.142566	-1.635848	0.481464
13.	6.	0.	4.678579	-0.246335	0.217893
14.	6.	0.	3.757896	0.836863	0.077578
15.	8.	0.	0.242265	-2.365354	-0.757112
16.	8.	0.	1.471598	2.604751	0.817009
17.	8.	0.	3.689472	-1.816755	1.823526
18.	8.	0.	-2.273023	-1.785105	-0.777549
19.	6.	0.	6.046138	-0.069716	0.117678
20.	6.	0.	6.603813	1.196608	-0.141140
21.	6.	0.	5.733038	2.262398	-0.271923
22.	6.	0.	4.335290	2.119665	-0.157674
23.	8.	0.	3.658456	3.267789	-0.341806
24.	6.	0.	-7.143158	0.170358	0.371240
25.	6.	0.	-6.370250	-1.130546	0.566820
26.	6.	0.	-4.883685	-0.843358	0.780224
27.	6.	0.	-4.360765	0.028248	-0.382505
28.	8.	0.	-5.133885	1.218441	-0.493160
29.	6.	0.	-6.519987	0.988605	-0.769362
30.	8.	0.	-8.500422	-0.091531	0.052256
31.	6.	0.	-7.179919	2.345211	-0.954223
32.	8.	0.	-6.983831	-1.786993	1.680460
33.	6.	0.	4.715009	-1.808271	2.798973
34.	8.	0.	3.274051	-1.992746	-1.768522
35.	6.	0.	3.369532	-3.322098	-2.254281
36.	6.	0.	8.096472	1.373673	-0.264451
37.	1.	0.	6.699134	-0.932841	0.227232
38.	1.	0.	-3.318208	2.441890	0.330314
39.	1.	0.	-0.916040	3.056097	0.674298
40.	1.	0.	2.455171	-2.838544	-0.053277
41.	1.	0.	4.924669	-2.376132	0.250635
42.	1.	0.	-1.431626	-2.312148	-0.876580
43.	1.	0.	6.099814	3.266428	-0.462609
44.	1.	0.	2.785407	3.194580	0.113841
45.	1.	0.	-7.064374	0.756814	1.302468
46.	1.	0.	-6.504088	-1.737679	-0.343676
47.	1.	0.	-4.308292	-1.774243	0.833912
48.	1.	0.	-4.750403	-0.302300	1.724323
49.	1.	0.	-4.447780	-0.552639	-1.315909
50.	1.	0.	-6.611384	0.401016	-1.698541
51.	1.	0.	-8.795598	-0.751316	0.702457

52.	1.	0.	-6.718060	2.882578	-1.788189
53.	1.	0.	-8.246098	2.214861	-1.156984
54.	1.	0.	-7.066658	2.949238	-0.047124
55.	1.	0.	-6.640841	-2.692705	1.725798
56.	1.	0.	4.233327	-2.014536	3.758228
57.	1.	0.	5.465452	-2.590553	2.600384
58.	1.	0.	5.227836	-0.838771	2.855305
59.	1.	0.	3.655230	-3.248776	-3.306858
60.	1.	0.	4.136513	-3.904348	-1.720756
61.	1.	0.	2.406147	-3.843941	-2.174686
62.	1.	0.	8.611568	1.052144	0.649428
63.	1.	0.	8.498219	0.768975	-1.087282
64.	1.	0.	8.362524	2.417877	-0.452499

7c		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
1.	6.	0.	2.470708	1.728892	-0.202801
2.	6.	0.	2.850937	0.453470	0.199968
3.	6.	0.	1.842895	-0.505721	0.462665
4.	6.	0.	0.482726	-0.161542	0.309202
5.	6.	0.	0.130288	1.138096	-0.102208
6.	6.	0.	1.123192	2.079234	-0.356320
7.	6.	0.	-0.571103	-1.135196	0.576937
8.	6.	0.	-1.978819	-0.745698	0.403679
9.	6.	0.	-2.377596	0.523097	0.050753
10.	6.	0.	-1.294346	1.523007	-0.252795
11.	6.	0.	-3.005036	-1.845178	0.604282
12.	6.	0.	-4.094548	-1.687113	-0.457801
13.	6.	0.	-4.683854	-0.299061	-0.366440
14.	6.	0.	-3.821951	0.816357	-0.132338
15.	8.	0.	-0.287374	-2.296745	0.952607
16.	8.	0.	-1.545603	2.664576	-0.656613
17.	8.	0.	-3.570664	-1.870714	-1.772225
18.	8.	0.	2.224182	-1.732388	0.856893
19.	6.	0.	-6.051262	-0.161265	-0.497682
20.	6.	0.	-6.674123	1.094988	-0.374654
21.	6.	0.	-5.865660	2.188130	-0.123988

22.	6.	0.	-4.464786	2.085559	-0.012064
23.	8.	0.	-3.858040	3.254258	0.261051
24.	6.	0.	7.066336	0.187572	-0.470314
25.	6.	0.	6.287852	-1.115981	-0.623678
26.	6.	0.	4.796027	-0.831708	-0.803050
27.	6.	0.	4.303701	0.062215	0.356111
28.	8.	0.	5.080751	1.252849	0.425413
29.	6.	0.	6.472891	1.025236	0.671690
30.	8.	0.	8.431035	-0.070345	-0.181731
31.	6.	0.	7.138918	2.383580	0.818358
32.	8.	0.	6.871630	-1.791735	-1.741706
33.	6.	0.	-3.398991	-3.224810	-2.150755
34.	8.	0.	-3.666394	-1.772978	1.863651
35.	6.	0.	-2.887473	-2.186538	2.973895
36.	6.	0.	-8.169662	1.230625	-0.509913
37.	1.	0.	-6.655595	-1.045799	-0.683326
38.	1.	0.	3.248461	2.461143	-0.386310
39.	1.	0.	0.839286	3.077385	-0.668566
40.	1.	0.	-2.504901	-2.814725	0.504649
41.	1.	0.	-4.880520	-2.428797	-0.256662
42.	1.	0.	1.383790	-2.251241	1.000837
43.	1.	0.	-6.285075	3.183728	-0.015971
44.	1.	0.	-2.924153	3.203617	-0.056692
45.	1.	0.	6.963856	0.758306	-1.408918
46.	1.	0.	6.445568	-1.707396	0.293288
47.	1.	0.	4.219256	-1.763159	-0.823805
48.	1.	0.	4.638173	-0.309077	-1.753717
49.	1.	0.	4.413246	-0.501581	1.297565
50.	1.	0.	6.585871	0.452685	1.607836
51.	1.	0.	8.709784	-0.739918	-0.829150
52.	1.	0.	6.697994	2.935274	1.654281
53.	1.	0.	8.209497	2.254704	0.997448
54.	1.	0.	7.004625	2.972883	-0.095520
55.	1.	0.	6.530192	-2.698951	-1.760623
56.	1.	0.	-3.092188	-3.218069	-3.199910
57.	1.	0.	-2.624260	-3.737867	-1.562270
58.	1.	0.	-4.339007	-3.790734	-2.057131
59.	1.	0.	-3.555804	-2.172094	3.838799
60.	1.	0.	-2.491597	-3.202624	2.835160
61.	1.	0.	-2.043869	-1.509472	3.166220
62.	1.	0.	-8.508743	0.894916	-1.497980
63.	1.	0.	-8.690631	0.614123	0.233332
64.	1.	0.	-8.493028	2.267027	-0.376027

7d		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
1.	6.	0.	2.470675	1.728924	-0.202729
2.	6.	0.	2.850922	0.453507	0.200037
3.	6.	0.	1.842886	-0.505655	0.462884
4.	6.	0.	0.482708	-0.161462	0.309537
5.	6.	0.	0.130253	1.138170	-0.101876
6.	6.	0.	1.123148	2.079287	-0.356107
7.	6.	0.	-0.571111	-1.135109	0.577356
8.	6.	0.	-1.978827	-0.745635	0.404078
9.	6.	0.	-2.377629	0.523133	0.051092
10.	6.	0.	-1.294388	1.523123	-0.252288
11.	6.	0.	-3.005024	-1.845150	0.604582
12.	6.	0.	-4.094320	-1.687210	-0.457751
13.	6.	0.	-4.683733	-0.299184	-0.366622
14.	6.	0.	-3.821967	0.816297	-0.132249
15.	8.	0.	-0.287370	-2.296630	0.953087
16.	8.	0.	-1.545658	2.664784	-0.655824
17.	8.	0.	-3.570122	-1.870900	-1.772035
18.	8.	0.	2.224202	-1.732300	0.857161
19.	6.	0.	-6.051100	-0.161463	-0.498342
20.	6.	0.	-6.674078	1.094764	-0.375558
21.	6.	0.	-5.865768	2.187944	-0.124590
22.	6.	0.	-4.464929	2.085437	-0.012113
23.	8.	0.	-3.858368	3.254141	0.261410
24.	6.	0.	7.066266	0.187510	-0.470624
25.	6.	0.	6.287741	-1.116038	-0.623885
26.	6.	0.	4.795902	-0.831742	-0.803119
27.	6.	0.	4.303699	0.062233	0.356060
28.	8.	0.	5.080782	1.252845	0.425258
29.	6.	0.	6.472935	1.025201	0.671418
30.	8.	0.	8.430981	-0.070423	-0.182162
31.	6.	0.	7.139008	2.383532	0.818004
32.	8.	0.	6.871391	-1.791819	-1.741949
33.	6.	0.	-3.398436	-3.225017	-2.150468
34.	8.	0.	-3.666673	-1.772934	1.863788
35.	6.	0.	-2.887677	-2.185585	2.974304
36.	6.	0.	-8.169575	1.230283	-0.511334
37.	1.	0.	-6.655329	-1.046030	-0.684169
38.	1.	0.	3.248421	2.461155	-0.386349
39.	1.	0.	0.839226	3.077438	-0.668342
40.	1.	0.	-2.504834	-2.814691	0.505103

41.	1.	0.	-4.880299	-2.428920	-0.256731
42.	1.	0.	1.383835	-2.251139	1.001238
43.	1.	0.	-6.285274	3.183520	-0.016714
44.	1.	0.	-2.924377	3.203622	-0.056023
45.	1.	0.	6.963707	0.758220	-1.409234
46.	1.	0.	6.445532	-1.707437	0.293080
47.	1.	0.	4.219115	-1.763184	-0.823779
48.	1.	0.	4.637960	-0.309145	-1.753790
49.	1.	0.	4.413317	-0.501530	1.297525
50.	1.	0.	6.585985	0.452670	1.607567
51.	1.	0.	8.709683	-0.739971	-0.829626
52.	1.	0.	6.698134	2.935264	1.653926
53.	1.	0.	8.209593	2.254640	0.997053
54.	1.	0.	7.004694	2.972812	-0.095885
55.	1.	0.	6.529813	-2.698982	-1.760905
56.	1.	0.	-3.091568	-3.218364	-3.199606
57.	1.	0.	-2.623744	-3.738033	-1.561894
58.	1.	0.	-4.338459	-3.790931	-2.056865
59.	1.	0.	-3.556090	-2.171013	3.839141
60.	1.	0.	-2.491316	-3.201559	2.836124
61.	1.	0.	-2.044418	-1.508017	3.166389
62.	1.	0.	-8.508348	0.894145	-1.499359
63.	1.	0.	-8.690731	0.614055	0.232012
64.	1.	0.	-8.493035	2.266720	-0.377952

7e		Standard Orientation (Ångstroms)			
Center number	Atomic number	Atomic Type	X	Y	Z
1.	6.	0.	-2.496895	1.688530	0.172106
2.	6.	0.	-2.882032	0.408096	-0.208747
3.	6.	0.	-1.877177	-0.557760	-0.461359
4.	6.	0.	-0.515705	-0.214669	-0.315877
5.	6.	0.	-0.158618	1.090722	0.072854
6.	6.	0.	-1.148006	2.038631	0.314451
7.	6.	0.	0.534362	-1.196327	-0.569152
8.	6.	0.	1.944526	-0.809648	-0.395536
9.	6.	0.	2.345222	0.467586	-0.081728
10.	6.	0.	1.267500	1.473745	0.211448
11.	6.	0.	2.967191	-1.922739	-0.554514
12.	6.	0.	4.058129	-1.719494	0.489284
13.	6.	0.	4.660606	-0.339676	0.323268
14.	6.	0.	3.793253	0.768140	0.074029

15.	8.	0.	0.249450	-2.358958	-0.934760
16.	8.	0.	1.526392	2.619227	0.601302
17.	8.	0.	3.426117	-1.912882	1.753015
18.	8.	0.	-2.263845	-1.786742	-0.837847
19.	6.	0.	6.033338	-0.199902	0.393207
20.	6.	0.	6.652400	1.050090	0.198439
21.	6.	0.	5.834880	2.135270	-0.055710
22.	6.	0.	4.429935	2.030008	-0.113256
23.	8.	0.	3.811783	3.188961	-0.403762
24.	6.	0.	-7.084727	0.181717	0.487028
25.	6.	0.	-6.317580	-1.122889	0.690006
26.	6.	0.	-4.826866	-0.835579	0.839301
27.	6.	0.	-4.335761	0.014827	-0.349347
28.	8.	0.	-5.108636	1.210403	-0.464743
29.	6.	0.	-6.498996	0.972710	-0.696450
30.	8.	0.	-8.451198	-0.187434	0.271479
31.	6.	0.	-7.157069	2.328667	-0.905202
32.	8.	0.	-6.776816	-1.806851	1.844157
33.	6.	0.	4.321137	-1.986824	2.846813
34.	8.	0.	3.613127	-1.909623	-1.822492
35.	6.	0.	2.837628	-2.414380	-2.896945
36.	6.	0.	8.152553	1.187016	0.266870
37.	1.	0.	6.644968	-1.080094	0.578380
38.	1.	0.	-3.271567	2.426021	0.347832
39.	1.	0.	-0.860301	3.041115	0.608925
40.	1.	0.	2.473807	-2.885313	-0.383667
41.	1.	0.	4.838775	-2.479258	0.337207
42.	1.	0.	-1.428368	-2.314309	-0.973734
43.	1.	0.	6.250053	3.126066	-0.213585
44.	1.	0.	2.890008	3.146974	-0.050721
45.	1.	0.	-6.986125	0.784933	1.402615
46.	1.	0.	-6.480084	-1.742614	-0.210019
47.	1.	0.	-4.266350	-1.773394	0.890784
48.	1.	0.	-4.656985	-0.285521	1.772528
49.	1.	0.	-4.449096	-0.577916	-1.271576
50.	1.	0.	-6.619323	0.360668	-1.606562
51.	1.	0.	-9.010521	0.576491	0.475125
52.	1.	0.	-6.689900	2.852205	-1.744550
53.	1.	0.	-8.222245	2.207797	-1.129561
54.	1.	0.	-7.049095	2.951806	-0.009772
55.	1.	0.	-7.744387	-1.842256	1.753895
56.	1.	0.	3.712561	-2.175753	3.734801
57.	1.	0.	5.039730	-2.813074	2.723463
58.	1.	0.	4.882976	-1.053456	2.987814

59.	1.	0.	3.501537	-2.441243	-3.765014
60.	1.	0.	2.467605	-3.427875	-2.688179
61.	1.	0.	1.976400	-1.773028	-3.128225
62.	1.	0.	8.532112	0.895882	1.254486
63.	1.	0.	8.642024	0.535825	-0.468083
64.	1.	0.	8.471430	2.215282	0.072920

Figure S1. ^1H NMR (500 MHz) spectrum of compound **1** in $\text{CDCl}_3/\text{CD}_3\text{OD}$.

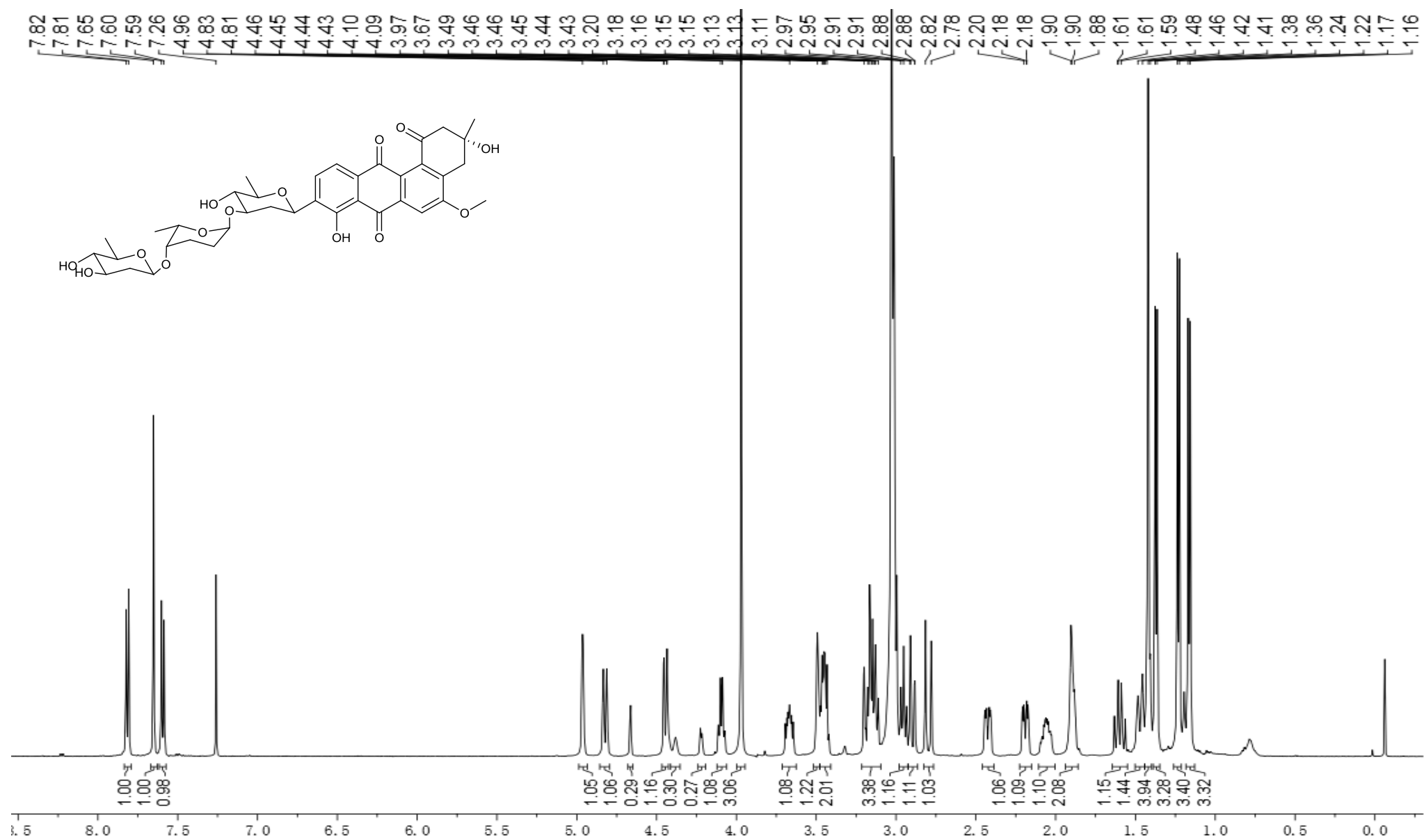


Figure S2. ^{13}C NMR (125 MHz) spectrum of compound **1** in $\text{CDCl}_3/\text{CD}_3\text{OD}$.

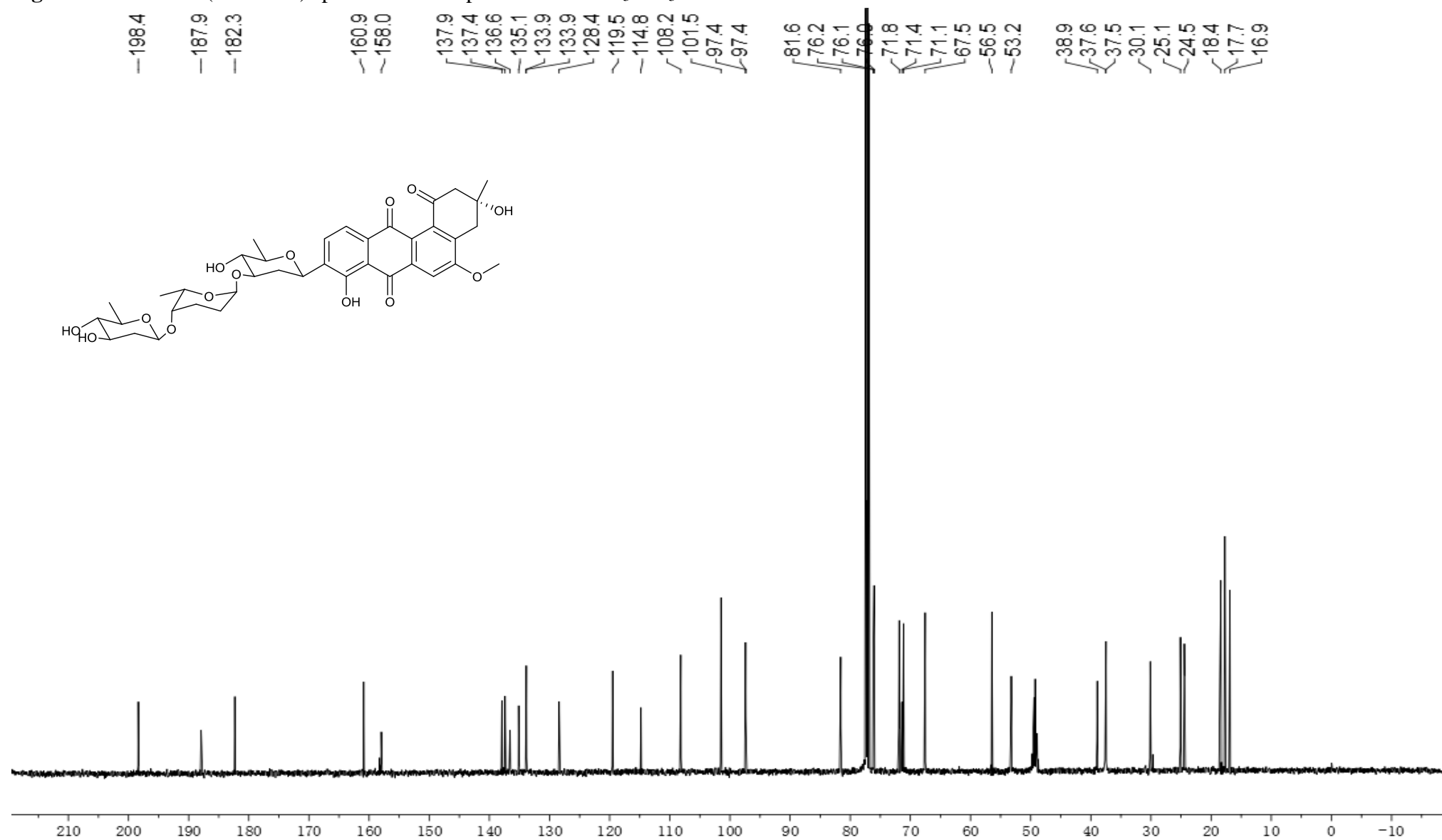


Figure S3. ^{13}C DEPT spectrum of compound **1** in $\text{CDCl}_3/\text{CD}_3\text{OD}$.

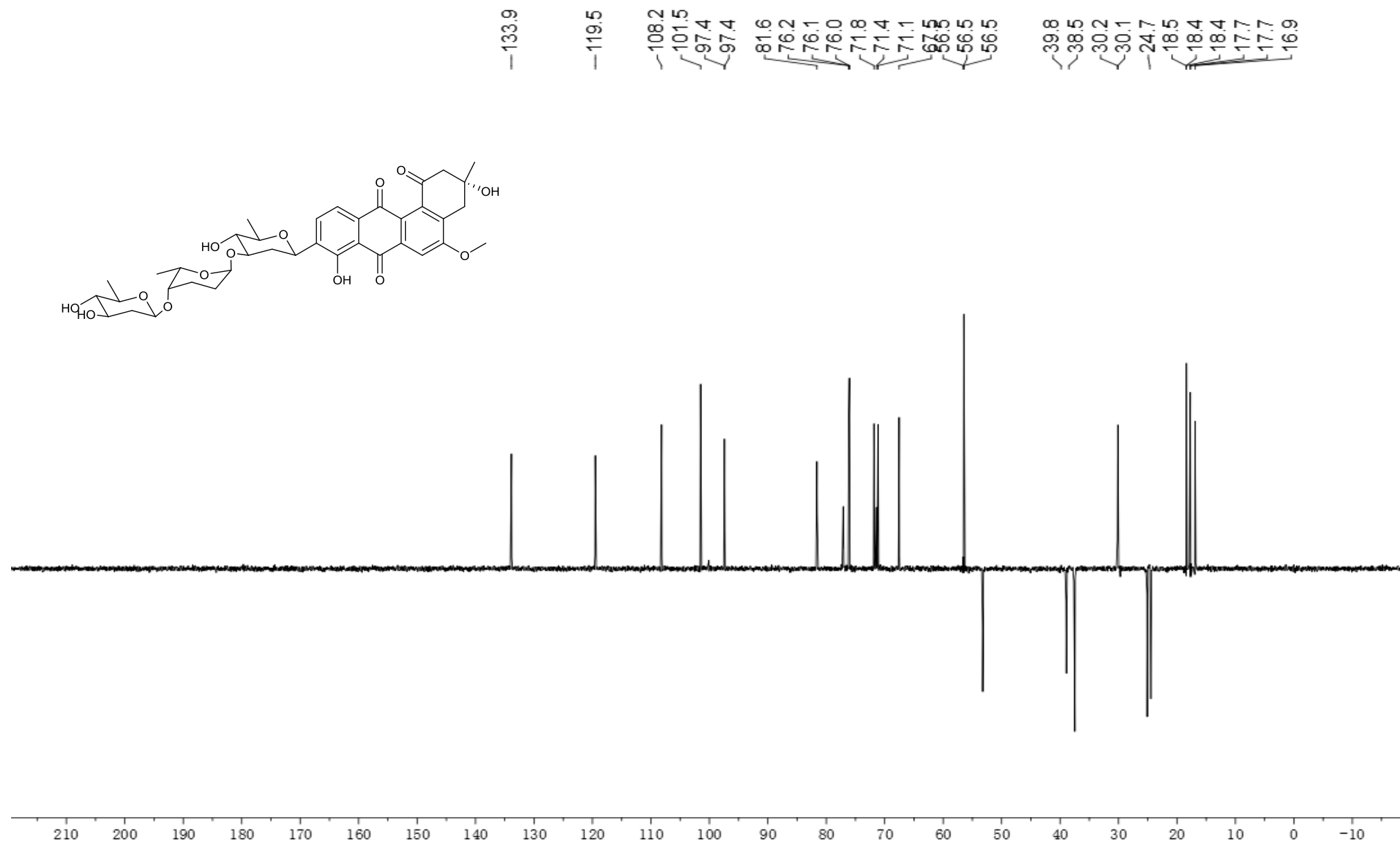


Figure S4. ^1H - ^1H COSY spectrum of compound **1** in $\text{CDCl}_3/\text{CD}_3\text{OD}$.

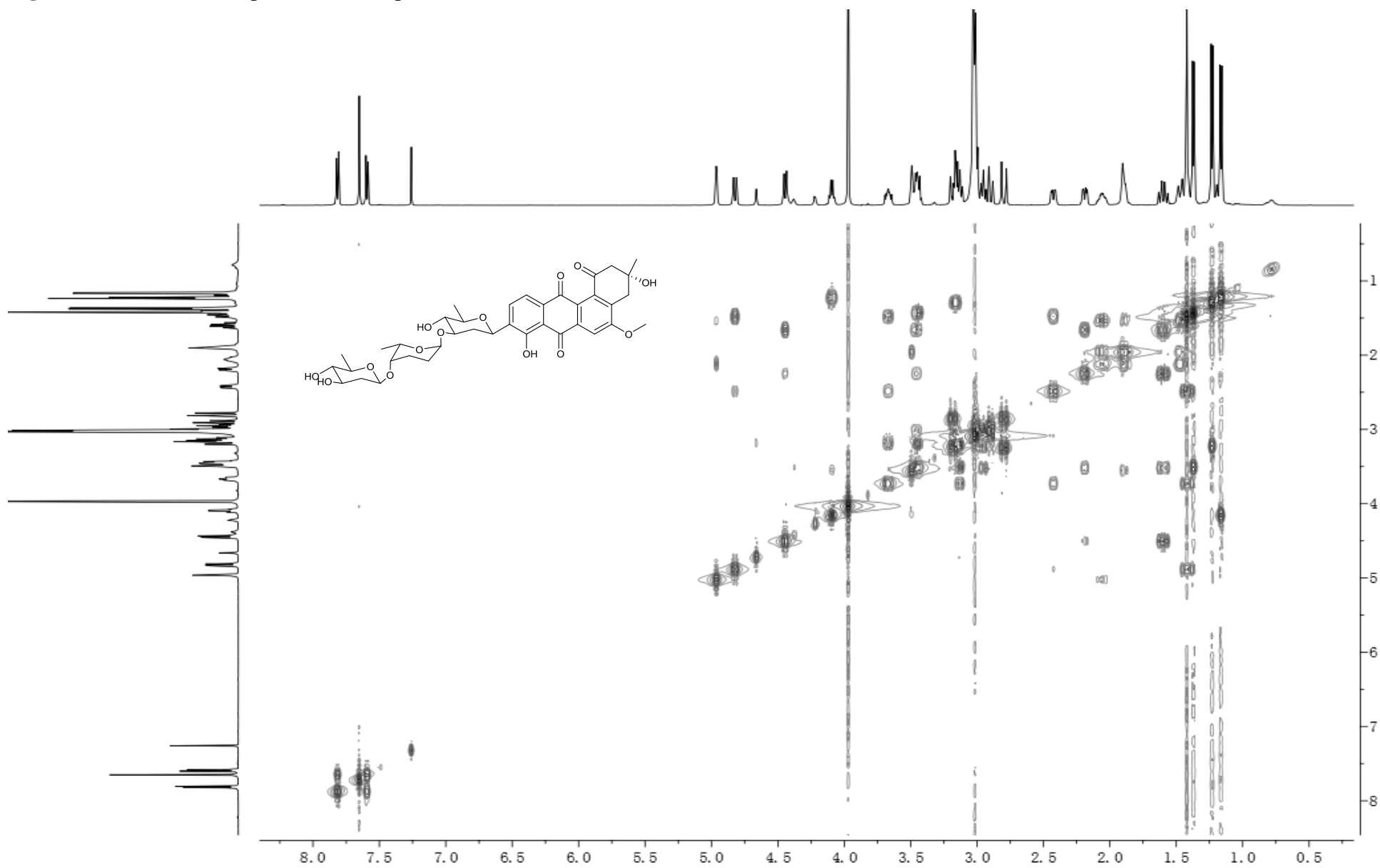


Figure S5. HSQC spectrum of compound **1** in CDCl₃/CD₃OD.

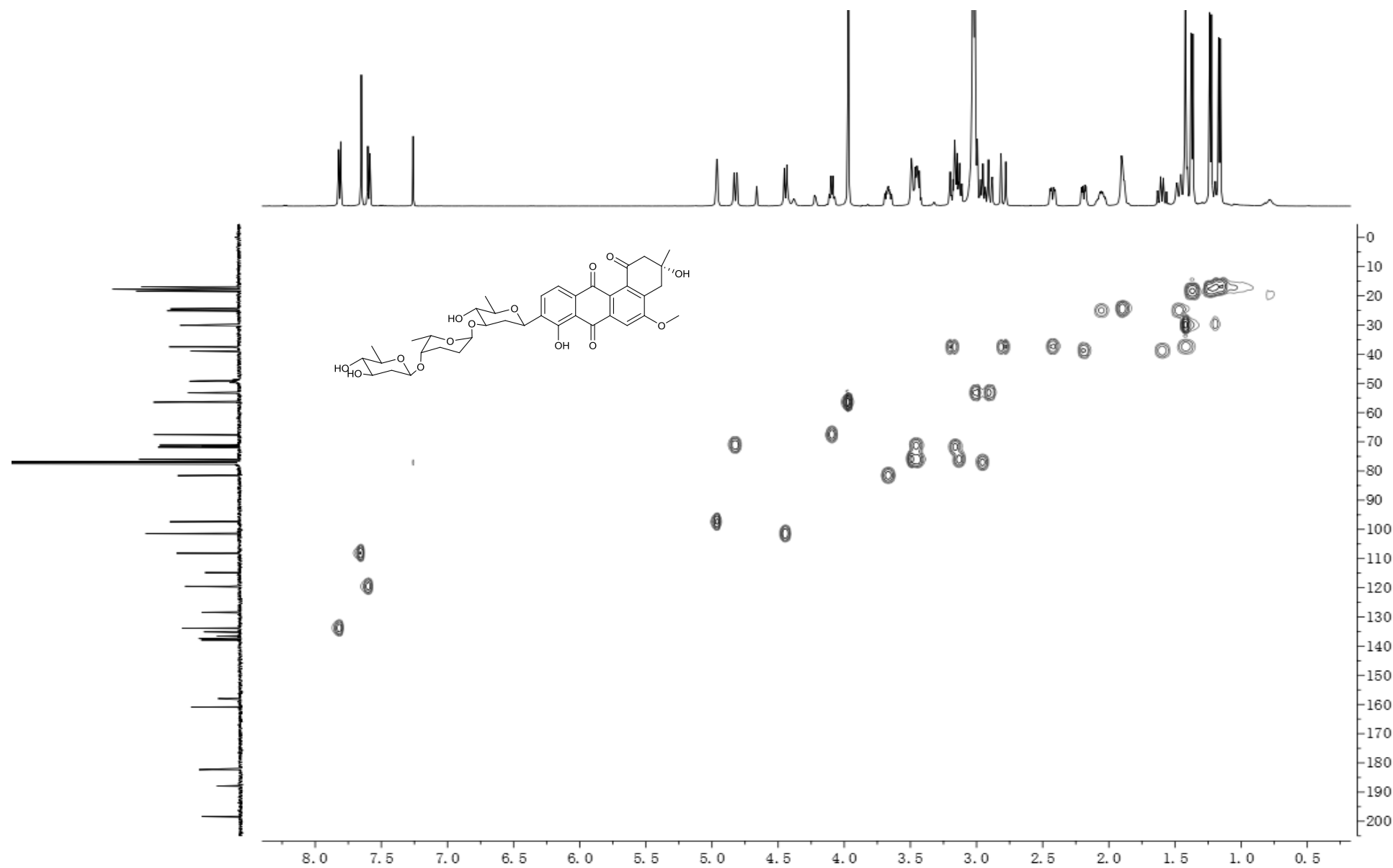


Figure S6. HMBC spectrum of compound **1** in CDCl₃/CD₃OD.

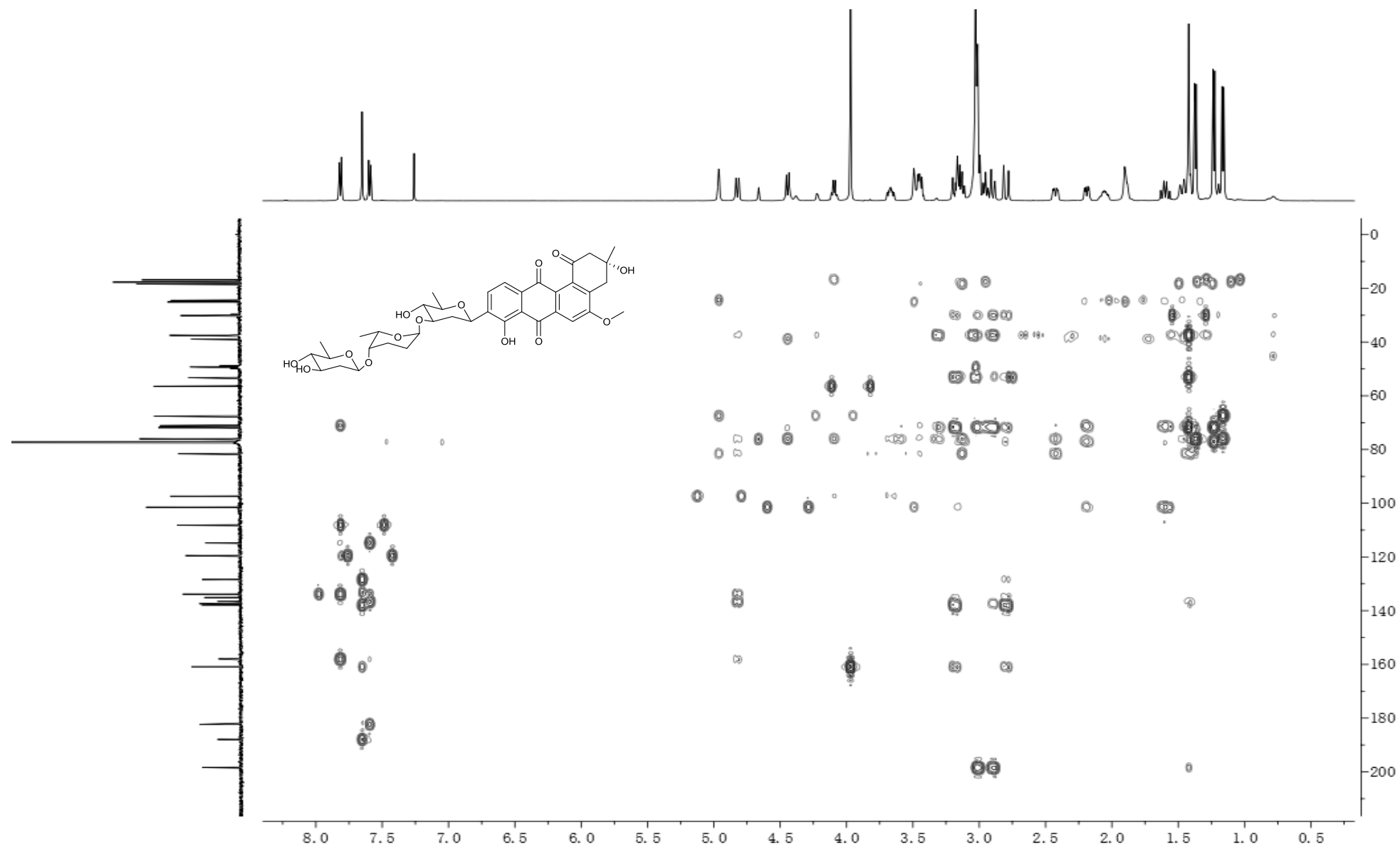


Figure S7. NOESY spectrum of compound **1** in $\text{CDCl}_3/\text{CD}_3\text{OD}$.

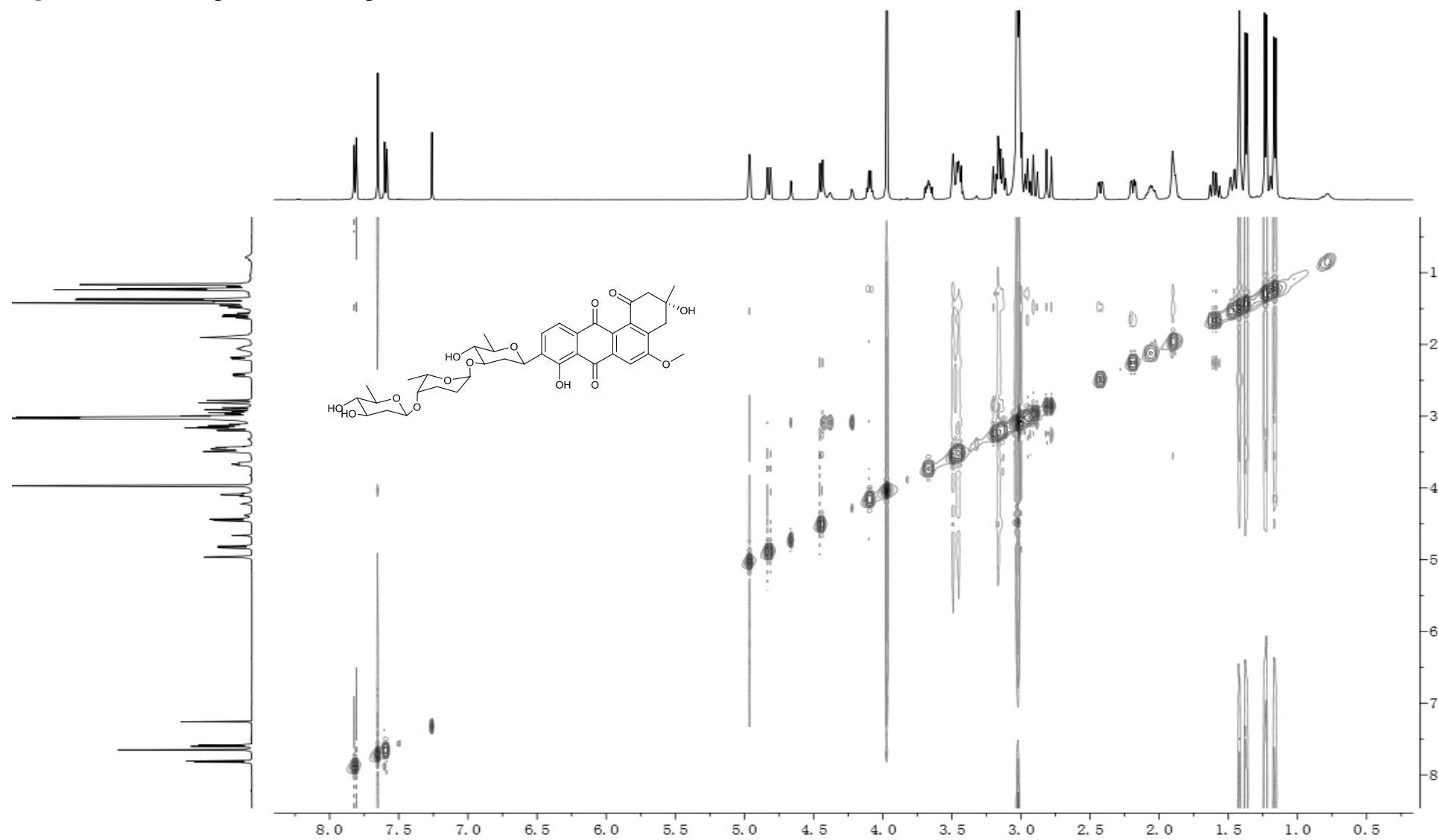


Figure S8. ^1H NMR (700 MHz) spectrum of compound **2** in $\text{DMSO-}d_6$.

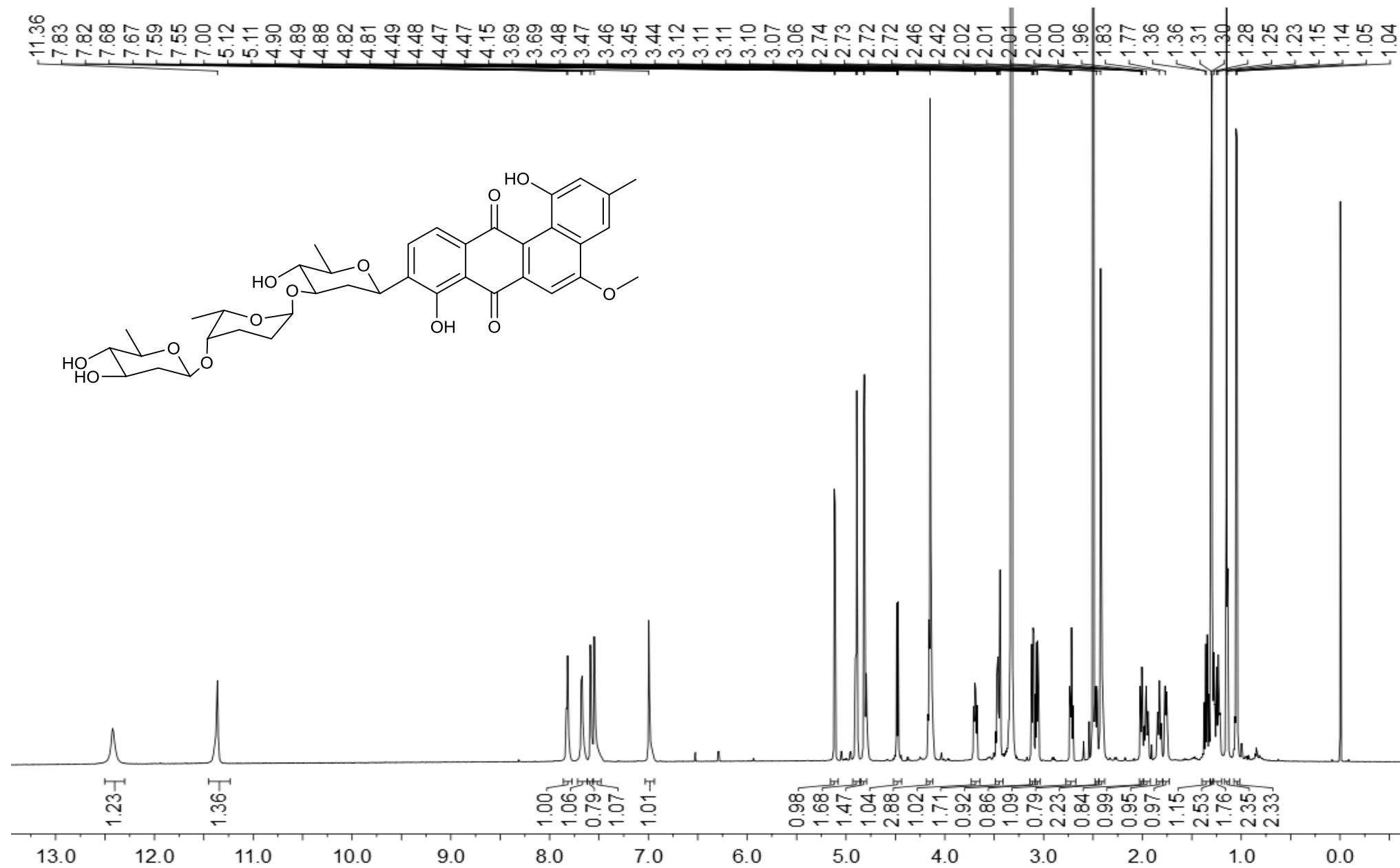


Figure S9. ^{13}C NMR (176 MHz) spectrum of compound **2** in $\text{DMSO-}d_6$.

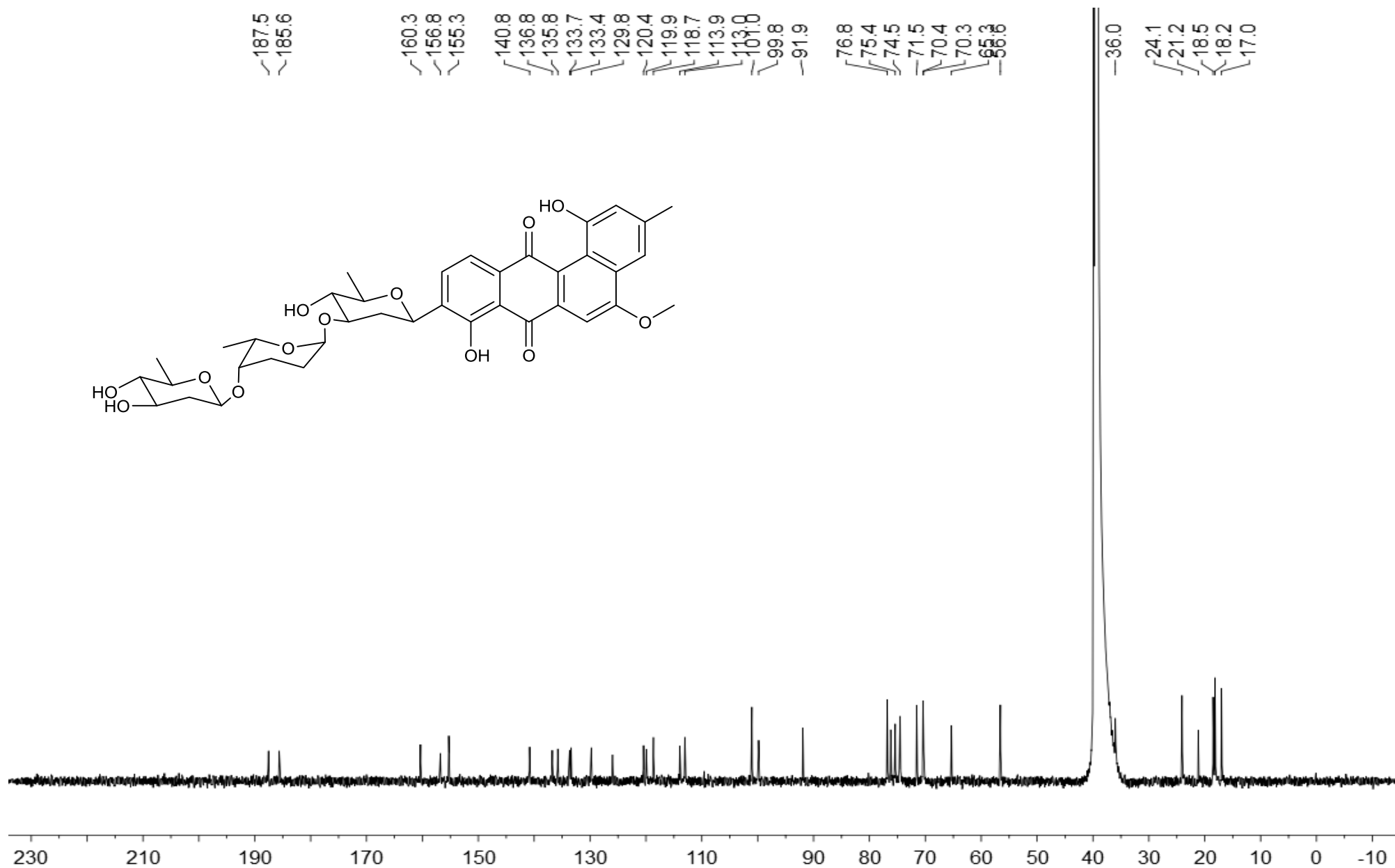


Figure S10. ^{13}C DEPT spectrum of compound **2** in $\text{DMSO-}d_6$.

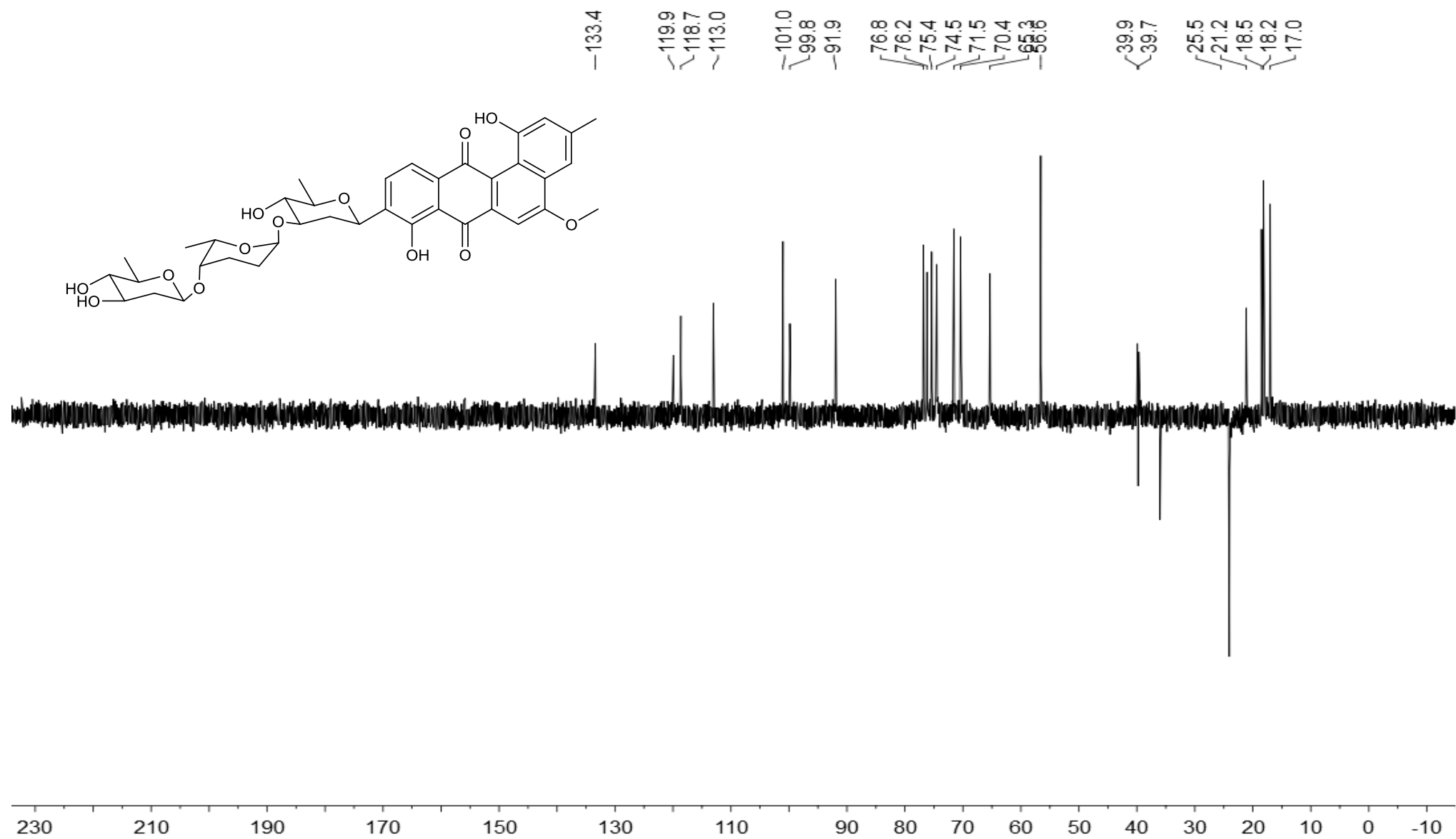


Figure S11. ^1H - ^1H COSY spectrum of compound **2** in $\text{DMSO-}d_6$.

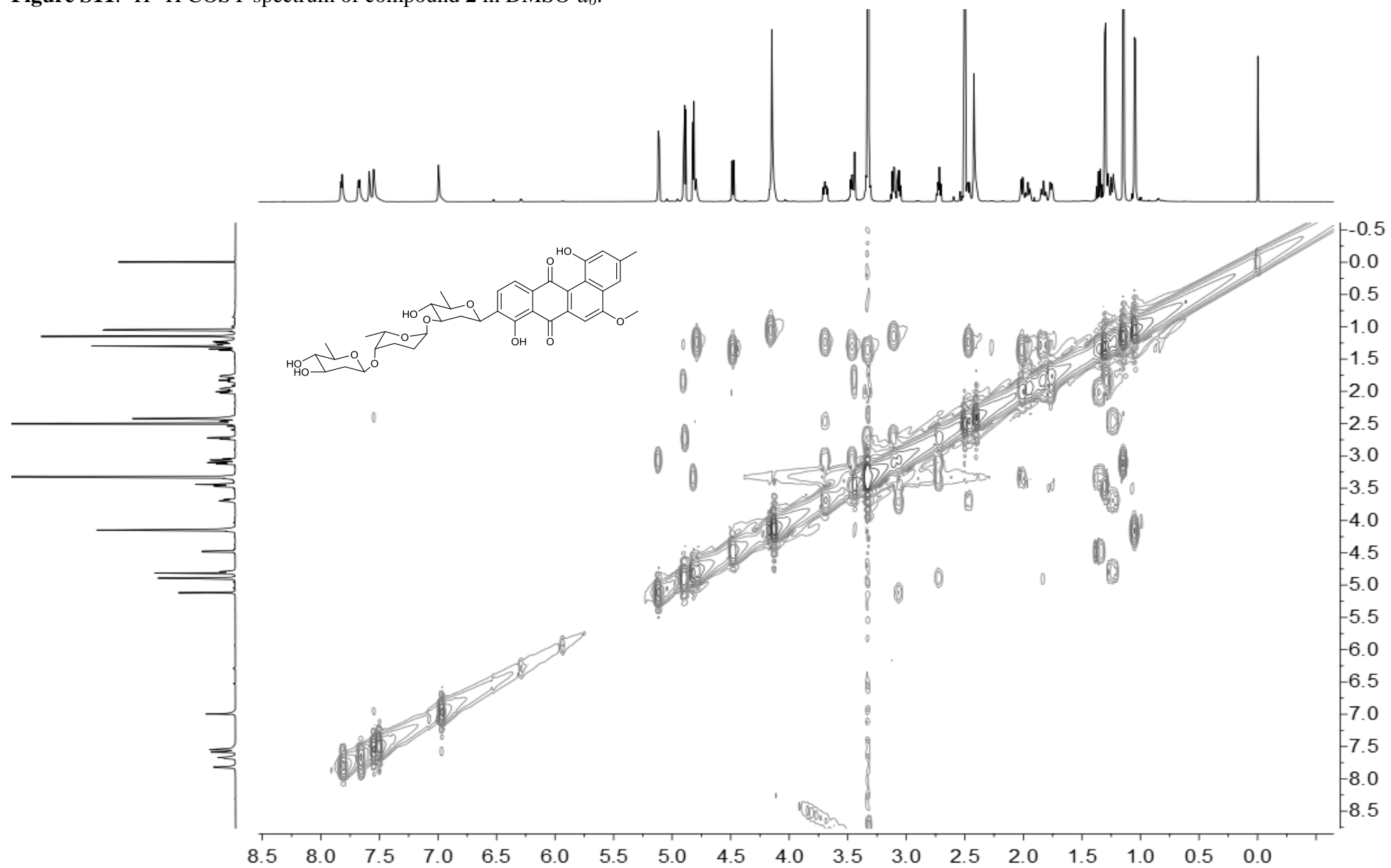


Figure S12. HSQC spectrum of compound **2** in DMSO- d_6 .

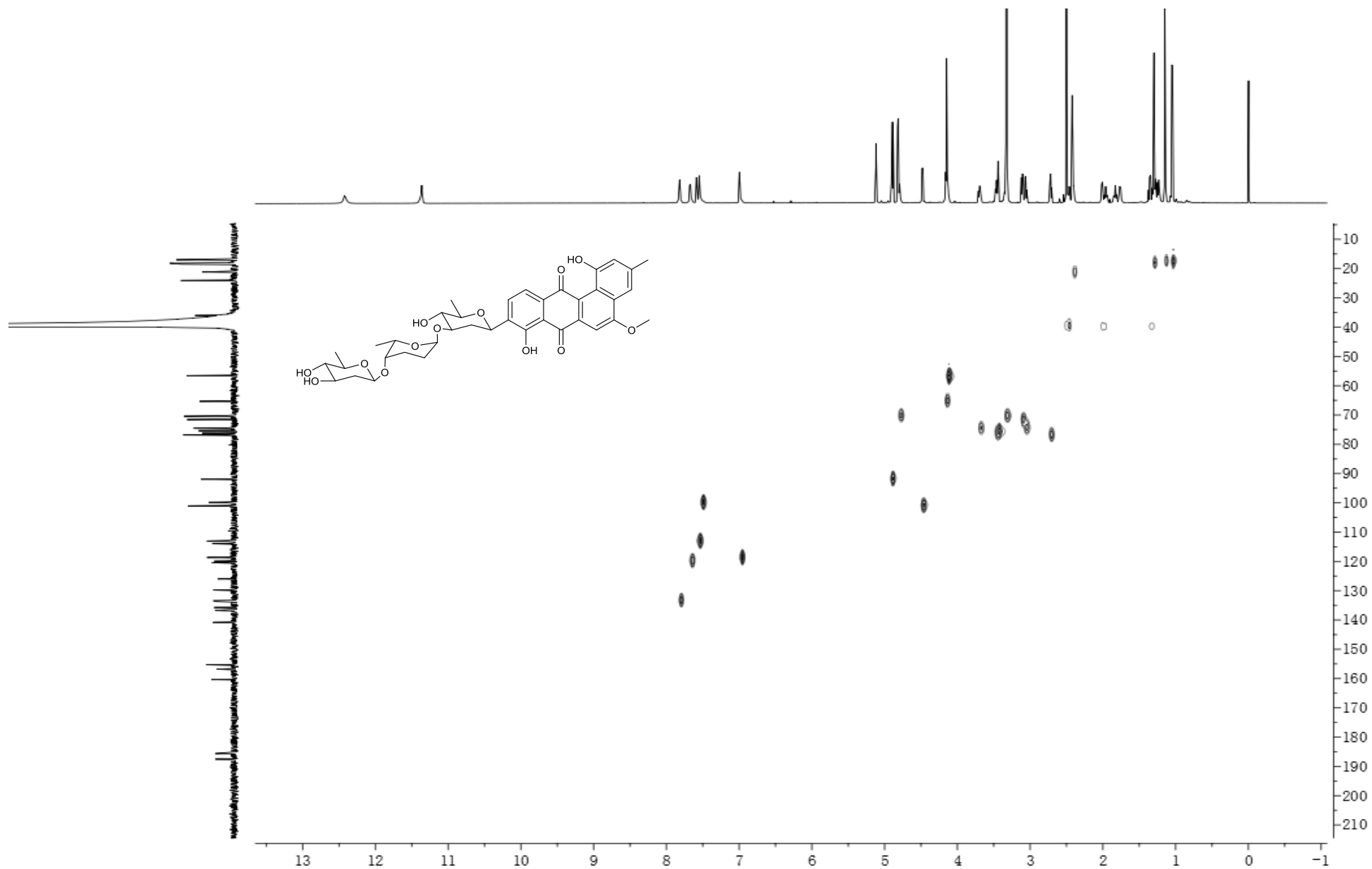


Figure S13. HMBC spectrum of compound **2** in DMSO- d_6 .

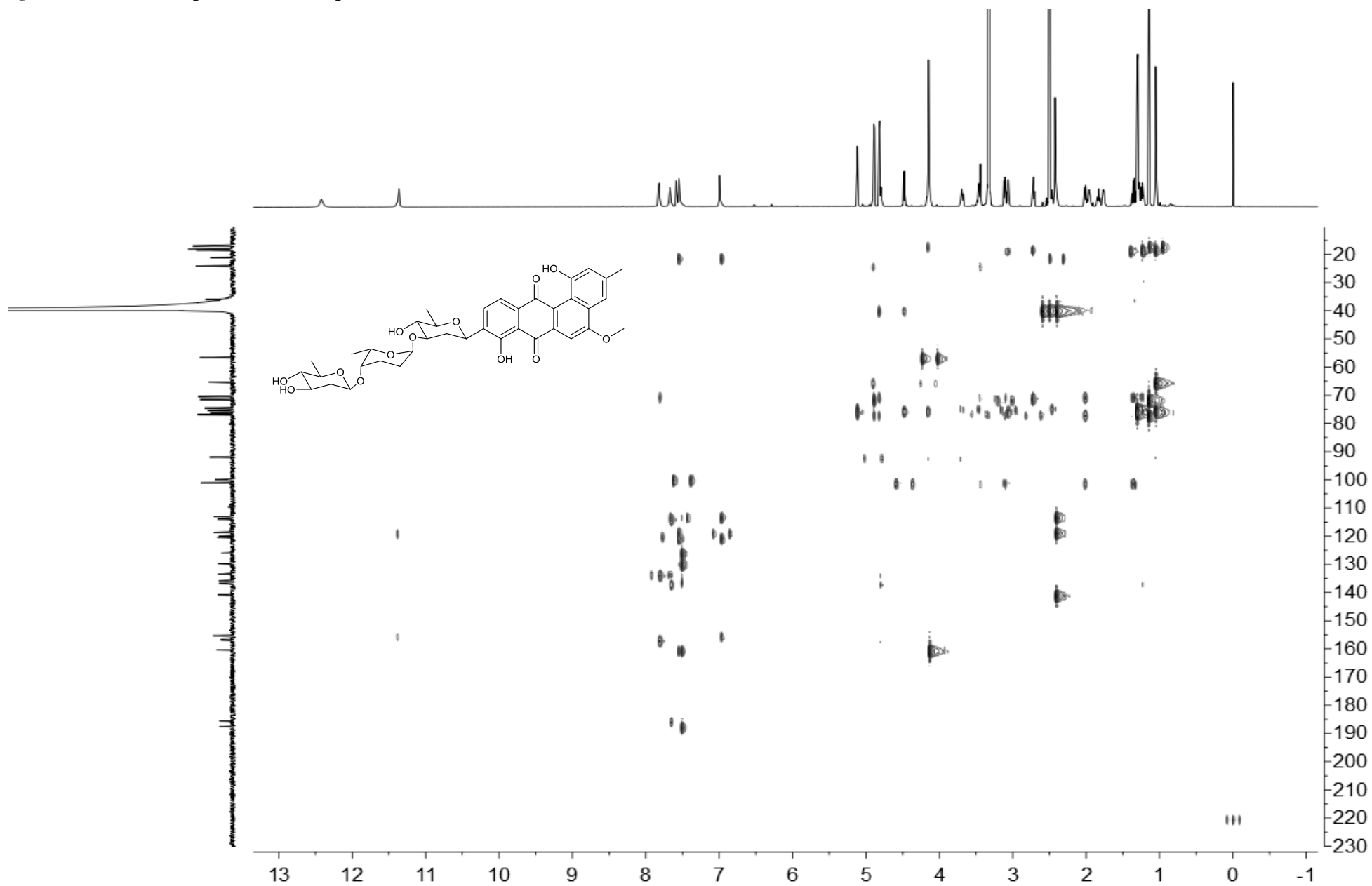


Figure S14. NOESY spectrum of compound **2** in DMSO-*d*₆.

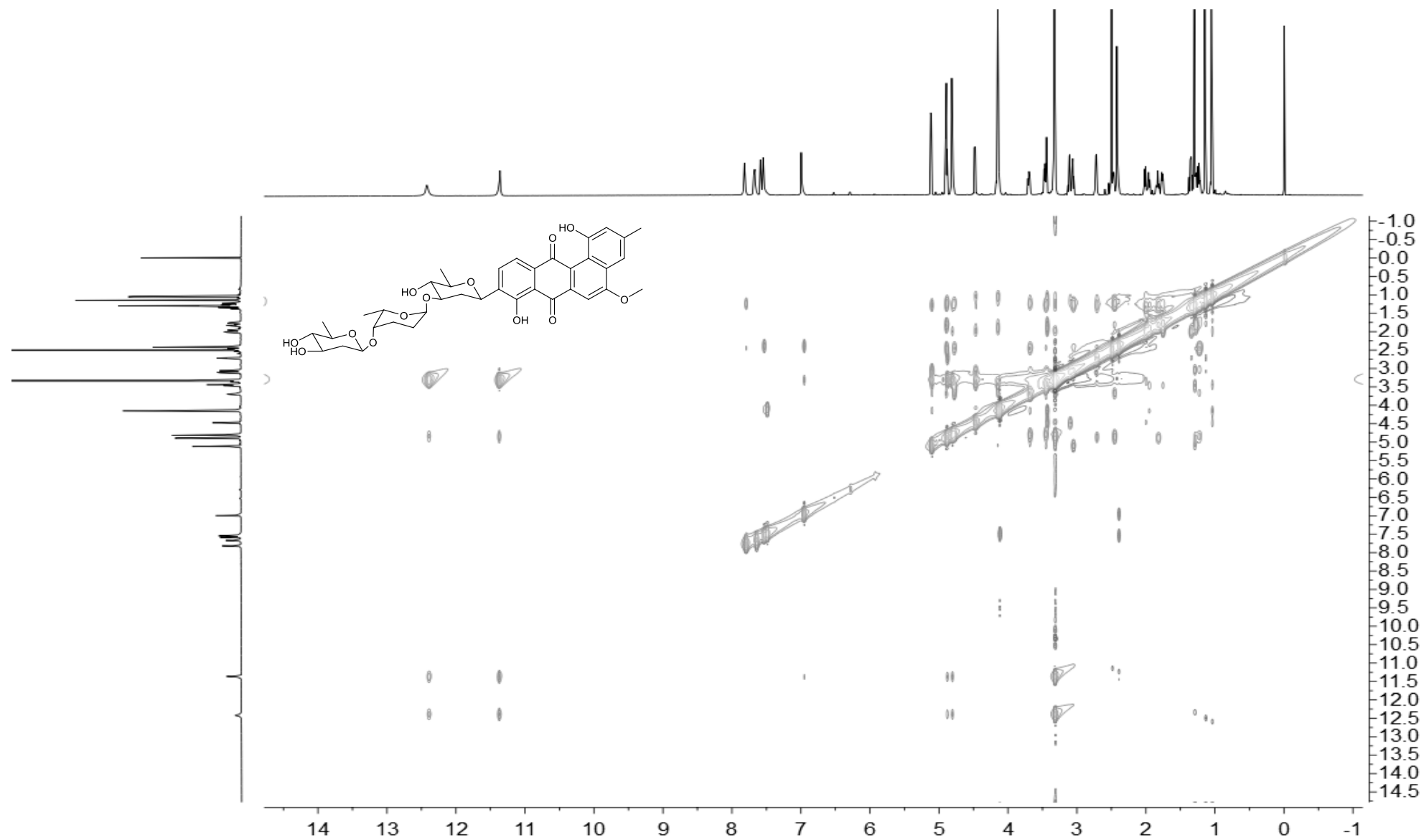


Figure S15. ^1H NMR (700 MHz) spectrum of compound **3** in $\text{DMSO-}d_6/\text{CD}_3\text{OD}$.

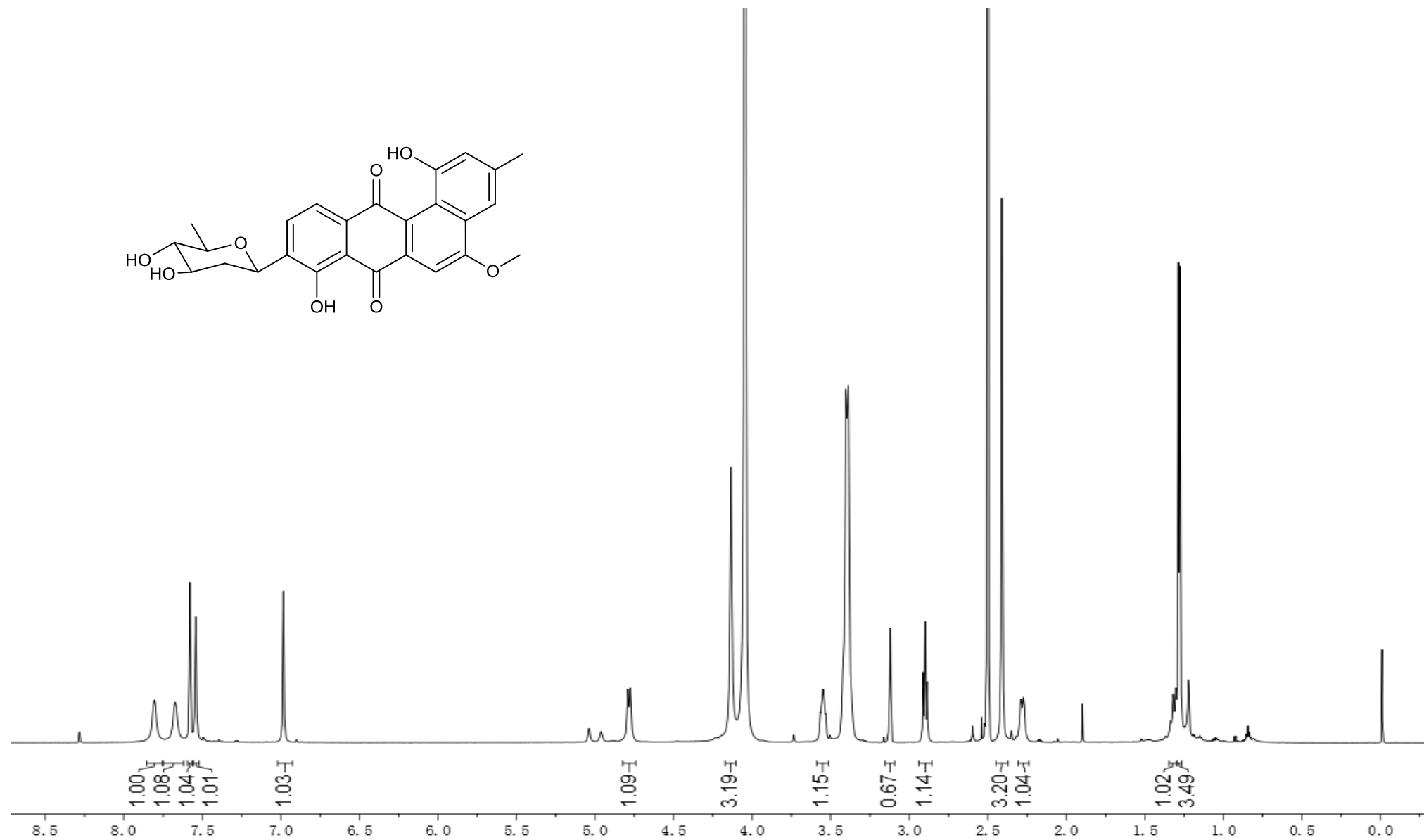


Figure S16. ^{13}C NMR (176 MHz) spectrum of compound **3** in $\text{DMSO-}d_6/\text{CD}_3\text{OD}$.

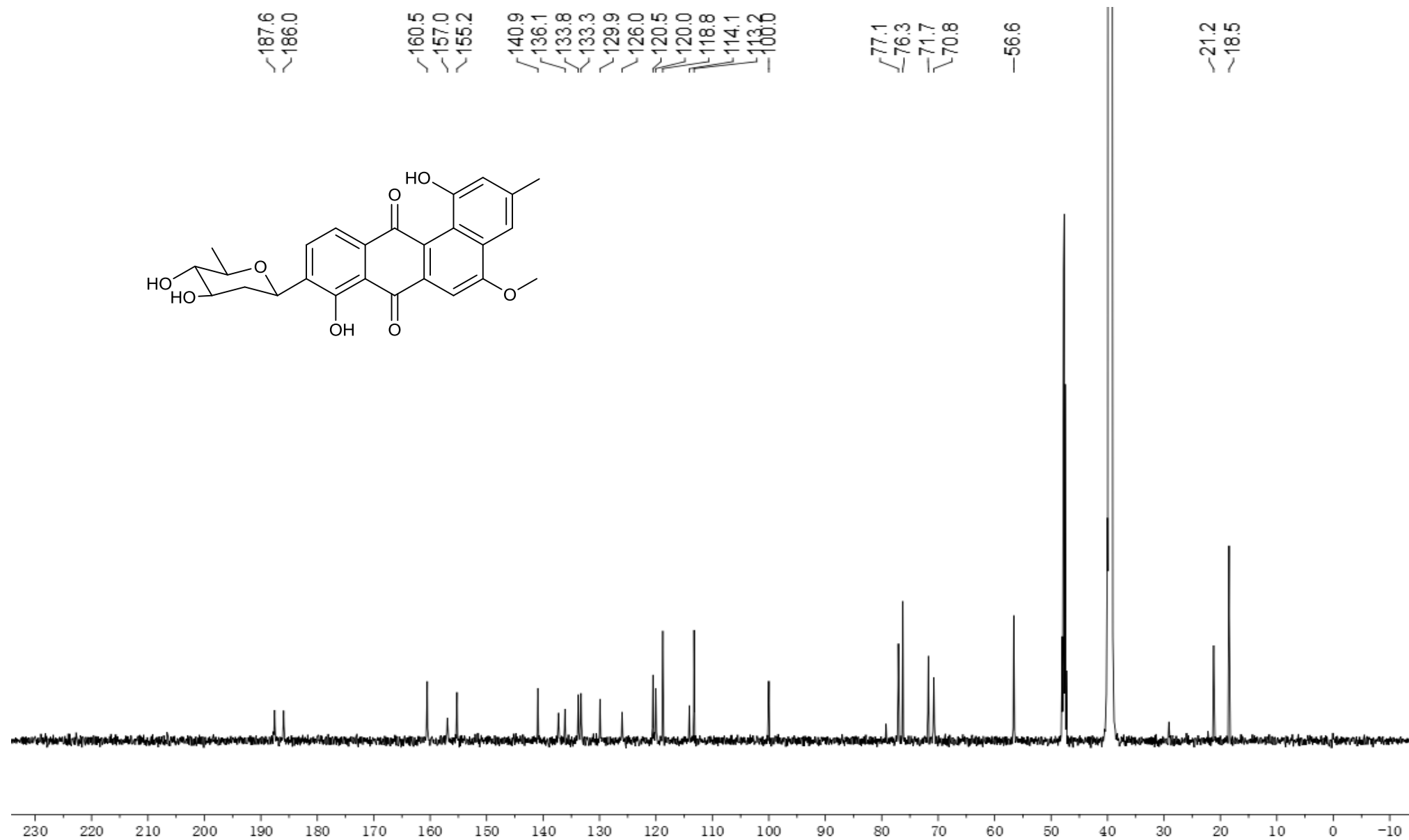


Figure S17. ^{13}C DEPT spectrum of compound **3** in $\text{DMSO-}d_6/\text{CD}_3\text{OD}$.

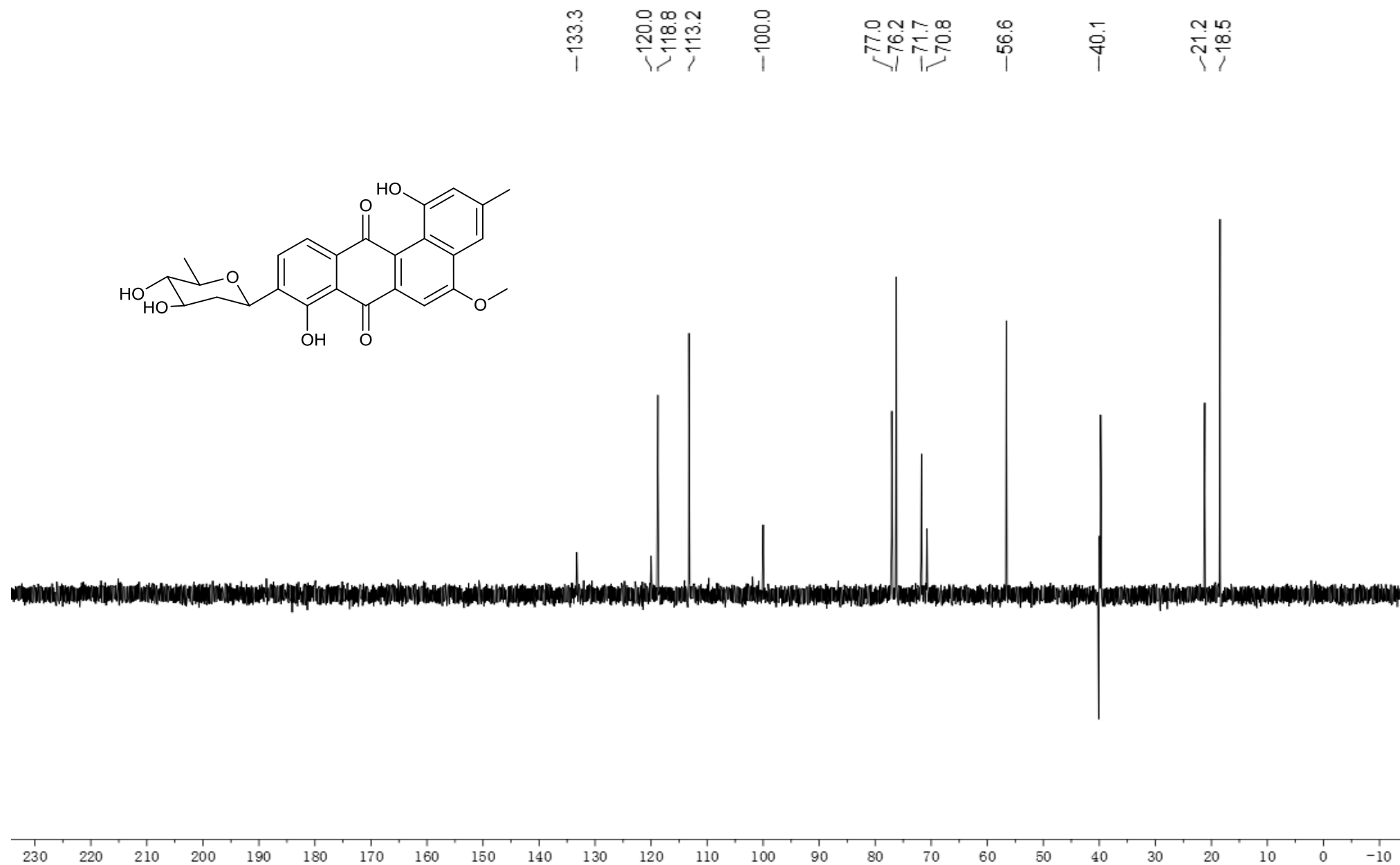


Figure S18. ^1H - ^1H COSY spectrum of compound **3** in $\text{DMSO-}d_6/\text{CD}_3\text{OD}$.

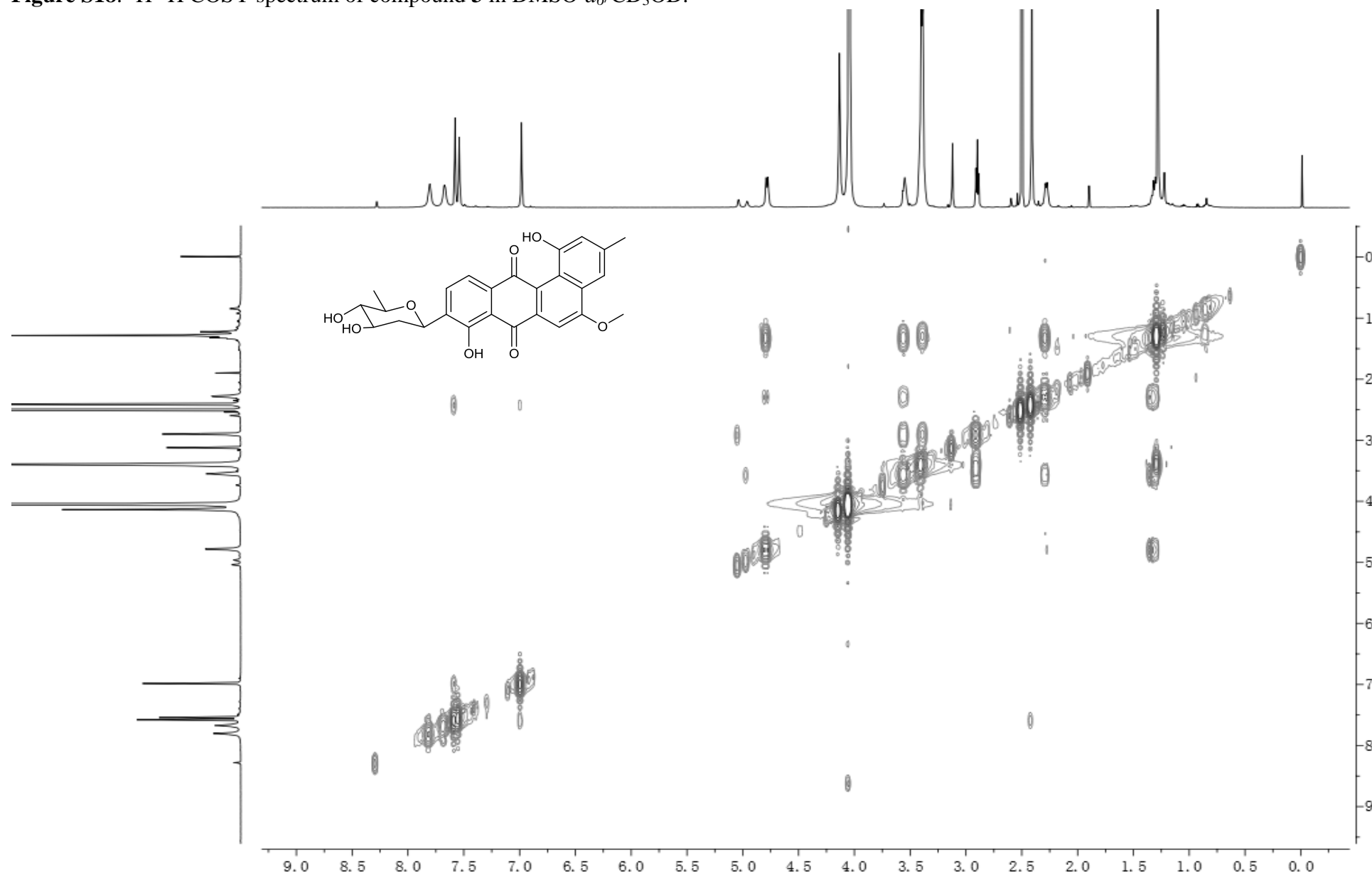


Figure S19. HSQC spectrum of compound **3** in DMSO- d_6 /CD $_3$ OD.

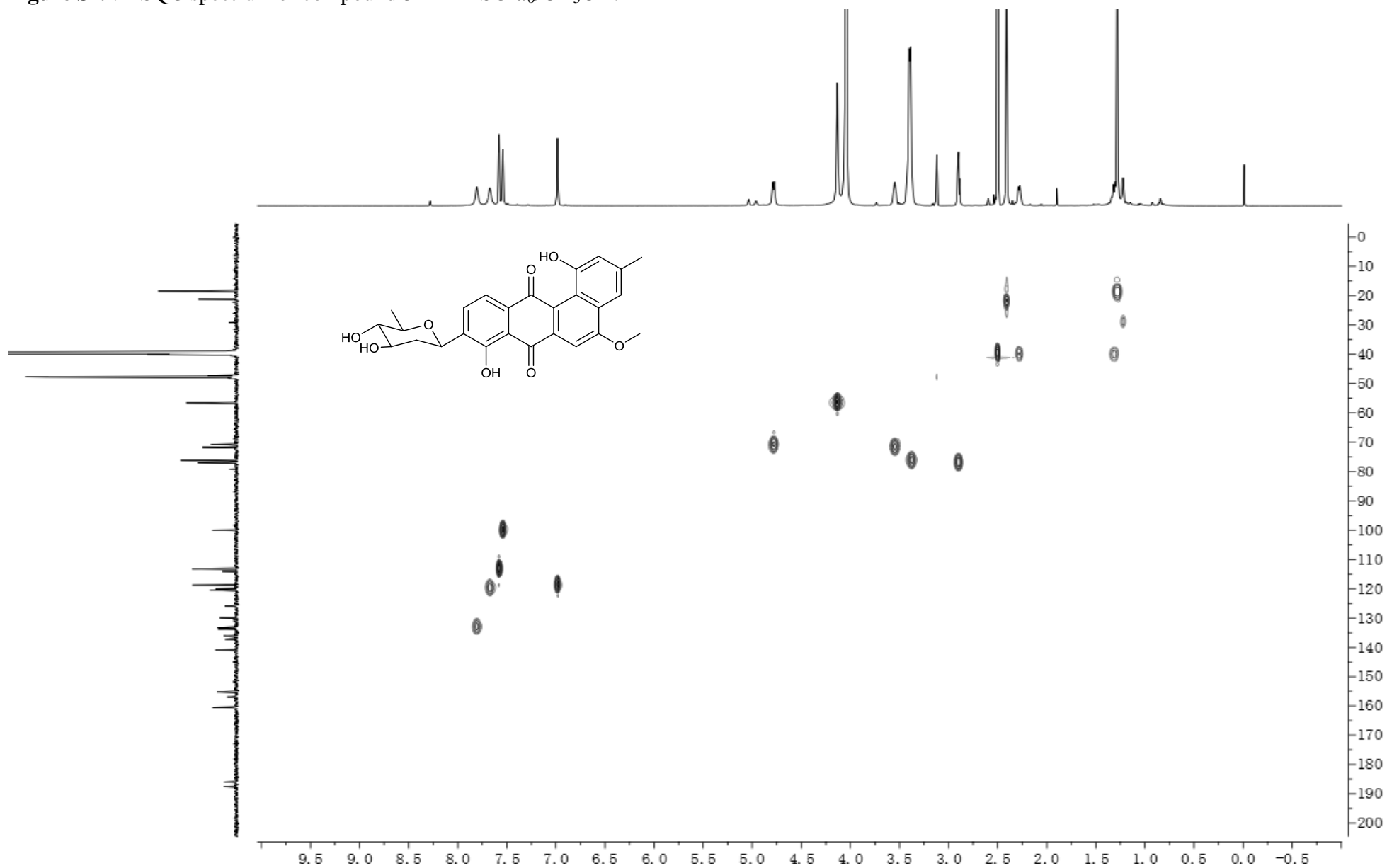


Figure S20. HMBC spectrum of compound **3** in DMSO-*d*₆/CD₃OD.

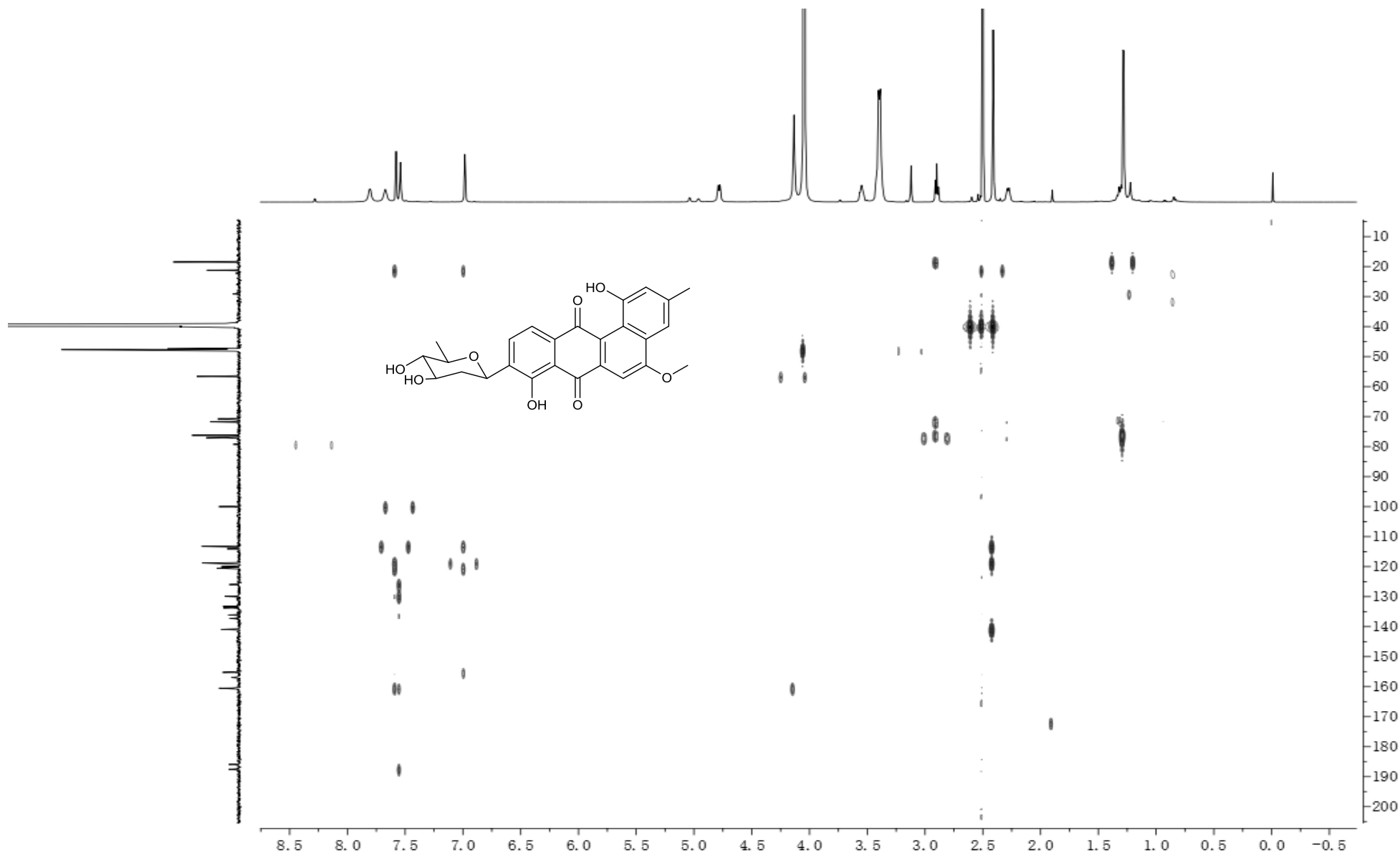


Figure S21. NOESY spectrum of compound **3** in DMSO- d_6 /CD $_3$ OD.

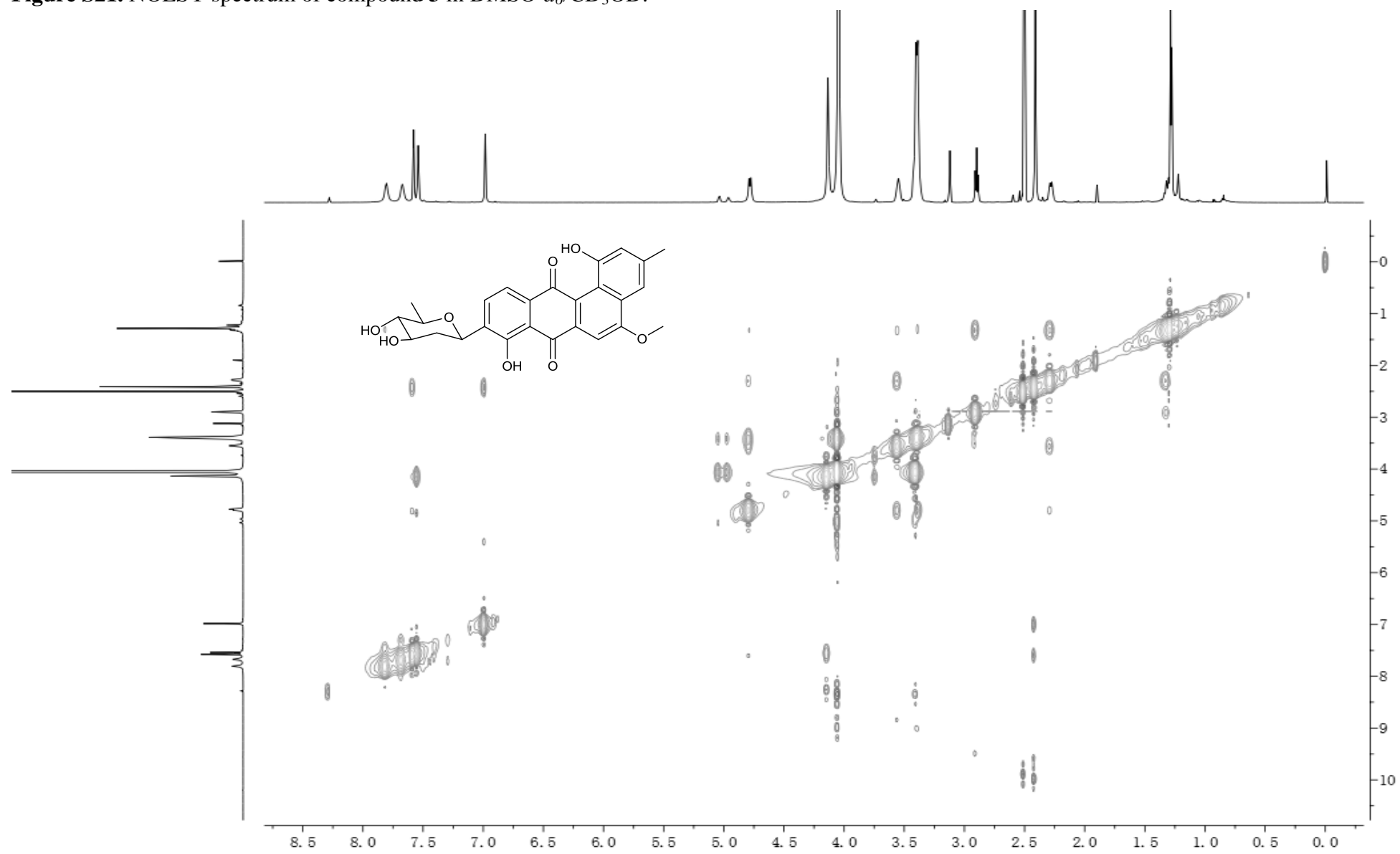


Figure S22. ^1H NMR (700 MHz) spectrum of compound **4** in $\text{DMSO-}d_6/\text{CD}_3\text{OD}$.

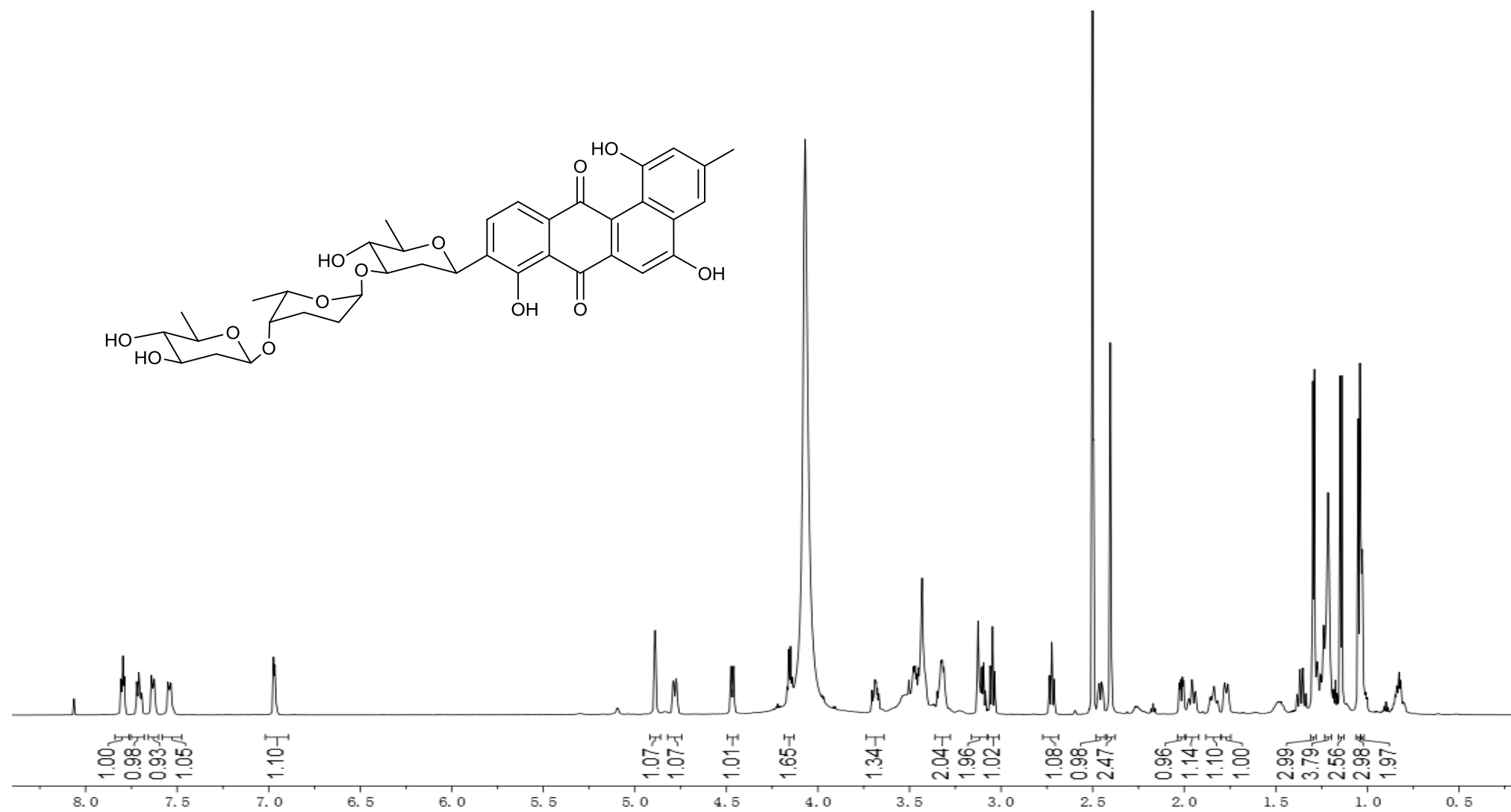


Figure S23. ^{13}C NMR (176 MHz) spectrum of compound **4** in $\text{DMSO-}d_6/\text{CD}_3\text{OD}$.

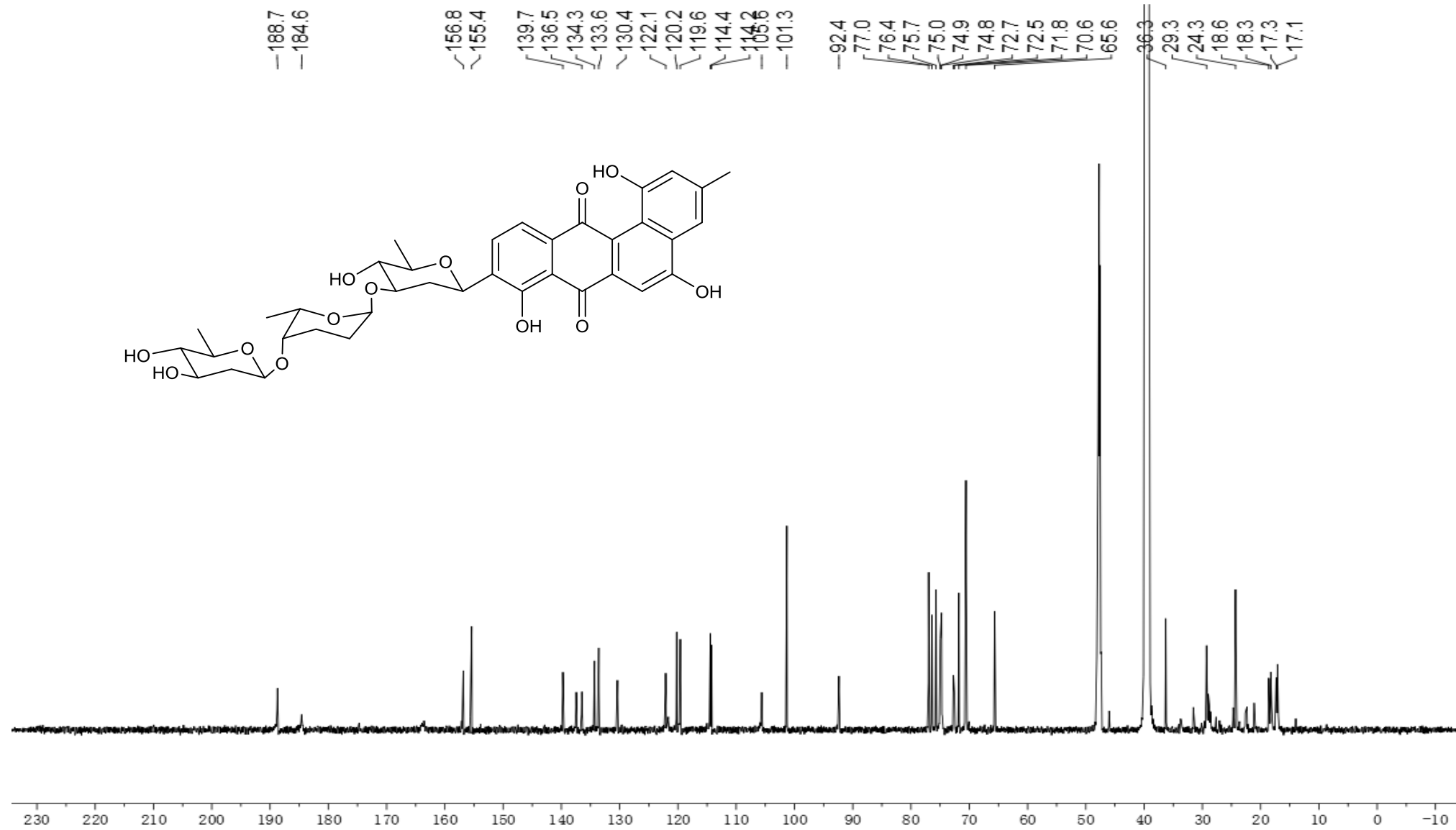


Figure S24. ^{13}C DEPT spectrum of compound **4** in $\text{DMSO-}d_6/\text{CD}_3\text{OD}$.

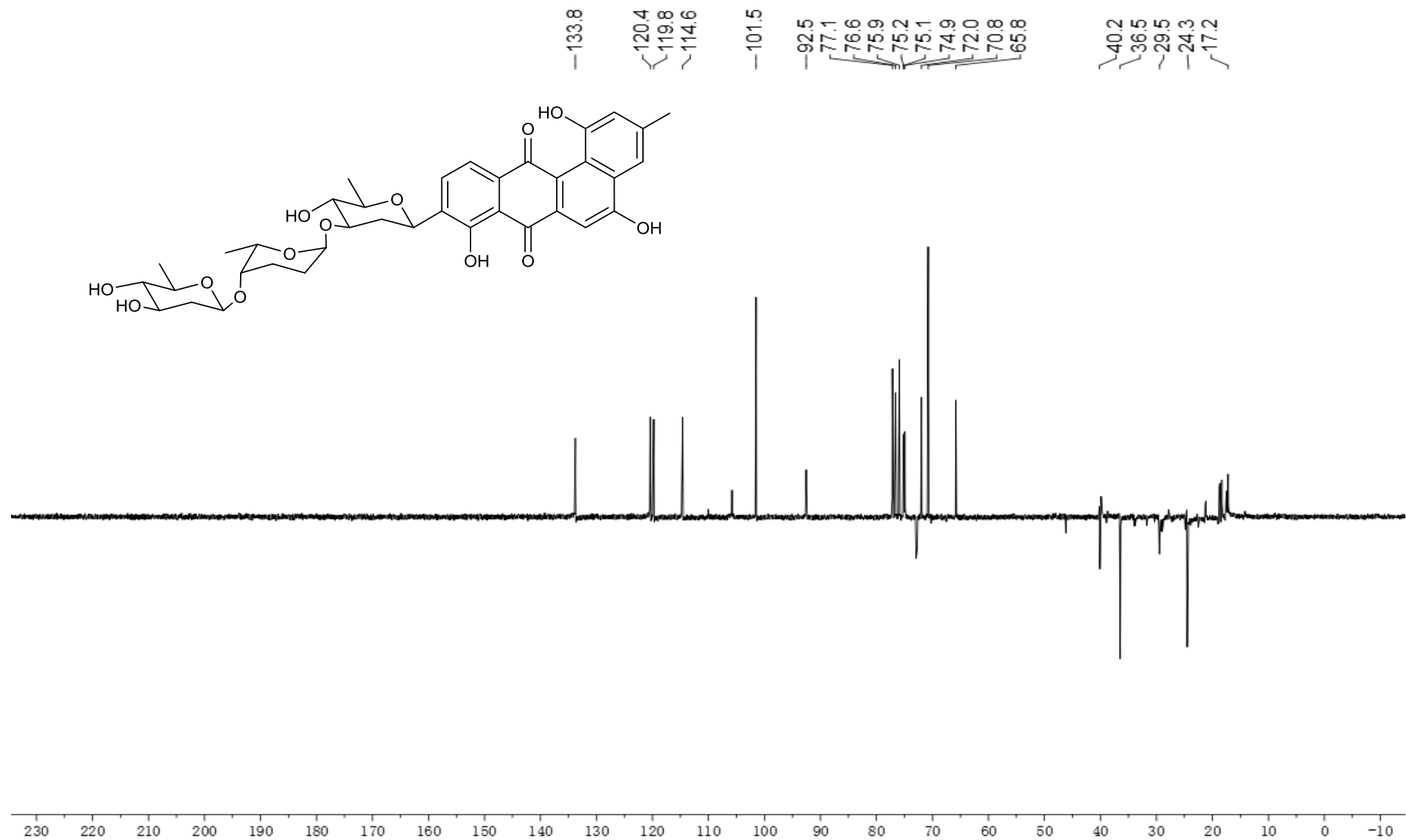


Figure S25. ^1H - ^1H COSY spectrum of compound **4** in $\text{DMSO-}d_6/\text{CD}_3\text{OD}$.

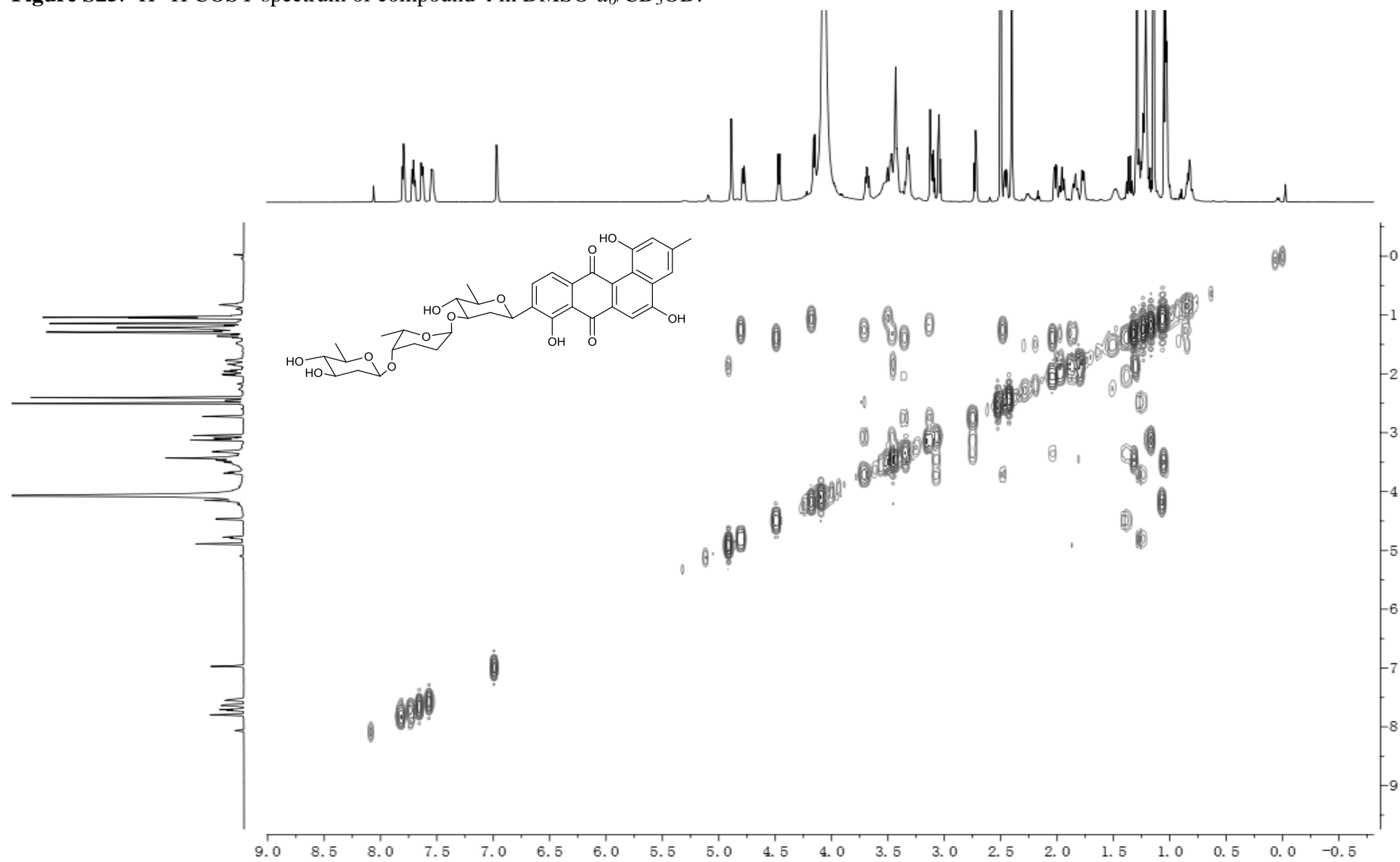


Figure S26. HSQC spectrum of compound **4** in DMSO- d_6 /CD $_3$ OD.

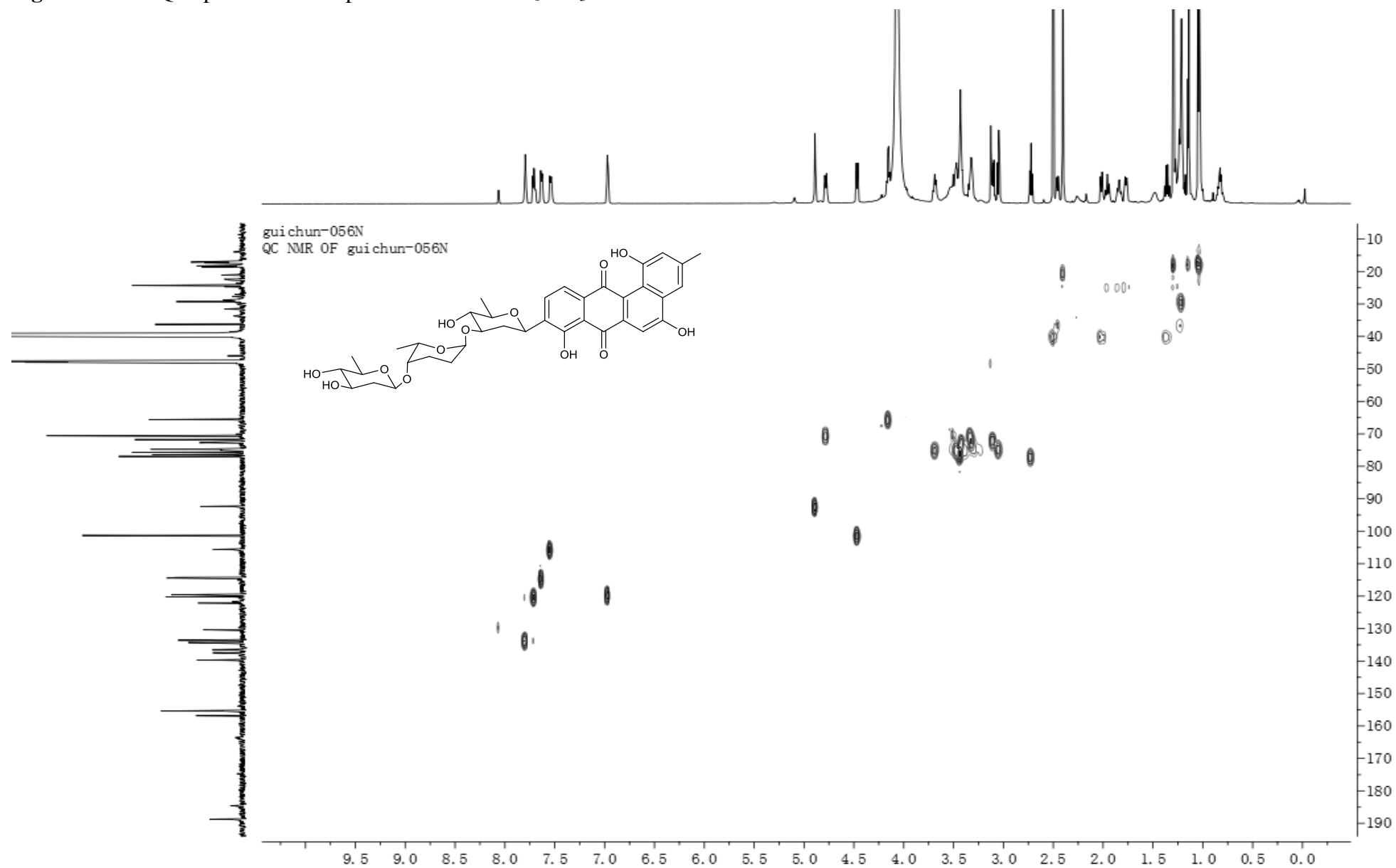


Figure S27. HMBC spectrum of compound **4** in DMSO-*d*₆/CD₃OD.

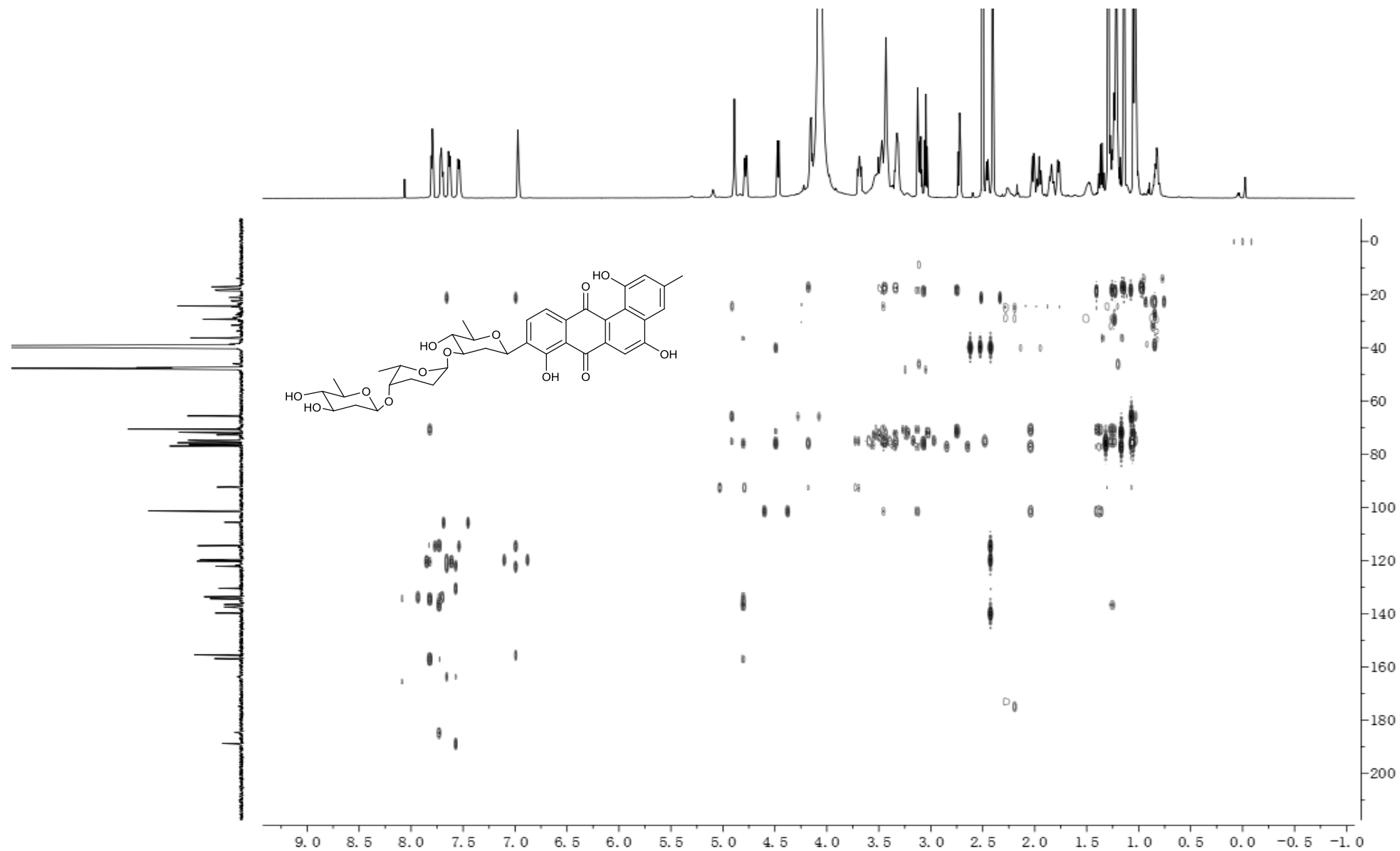


Figure S28. NOESY spectrum of compound **4** in DMSO- d_6 /CD $_3$ OD.

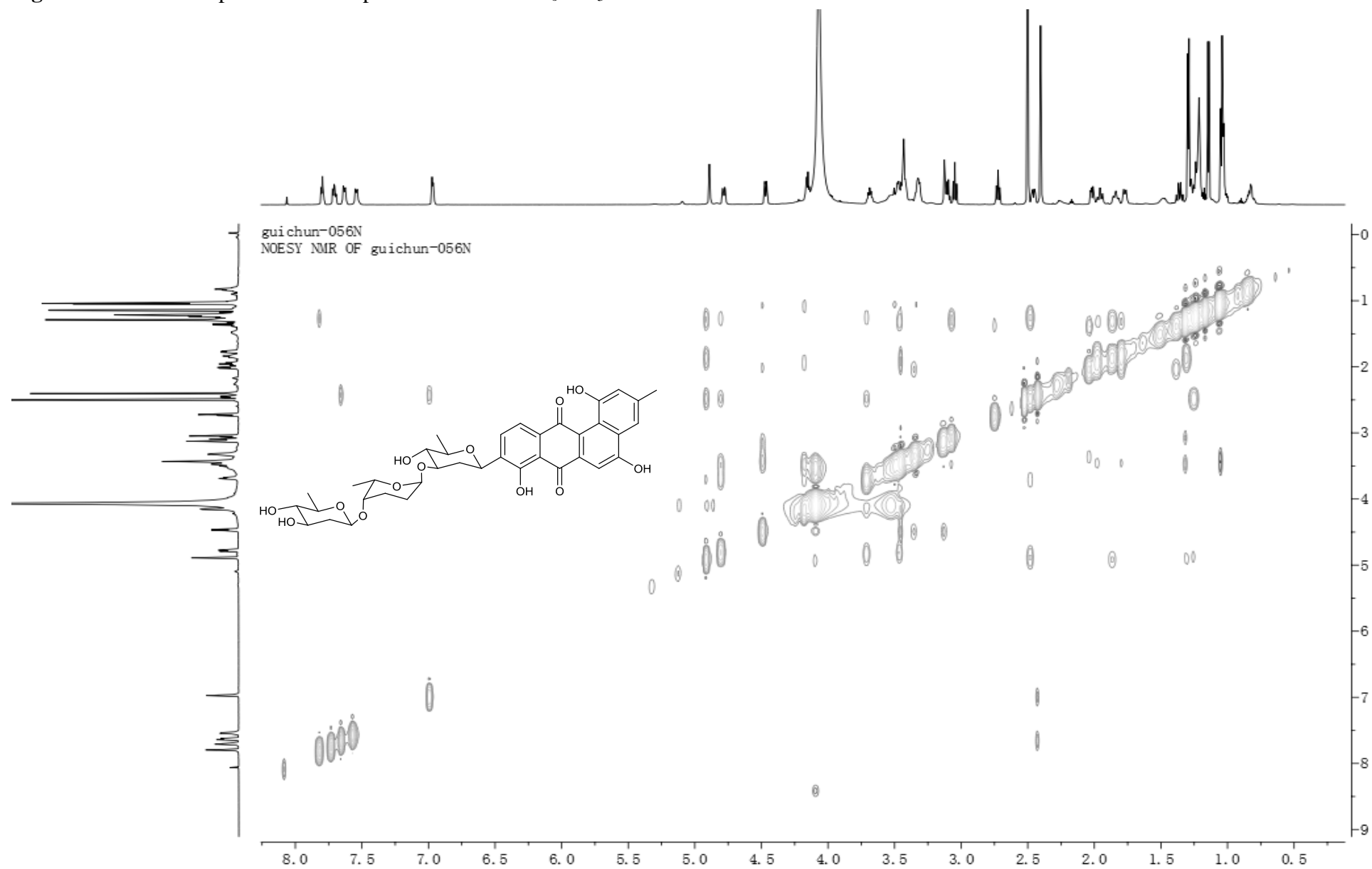


Figure S29. ^1H NMR (700 MHz) spectrum of compound **5** in $\text{DMSO-}d_6/\text{CD}_3\text{OD}$.

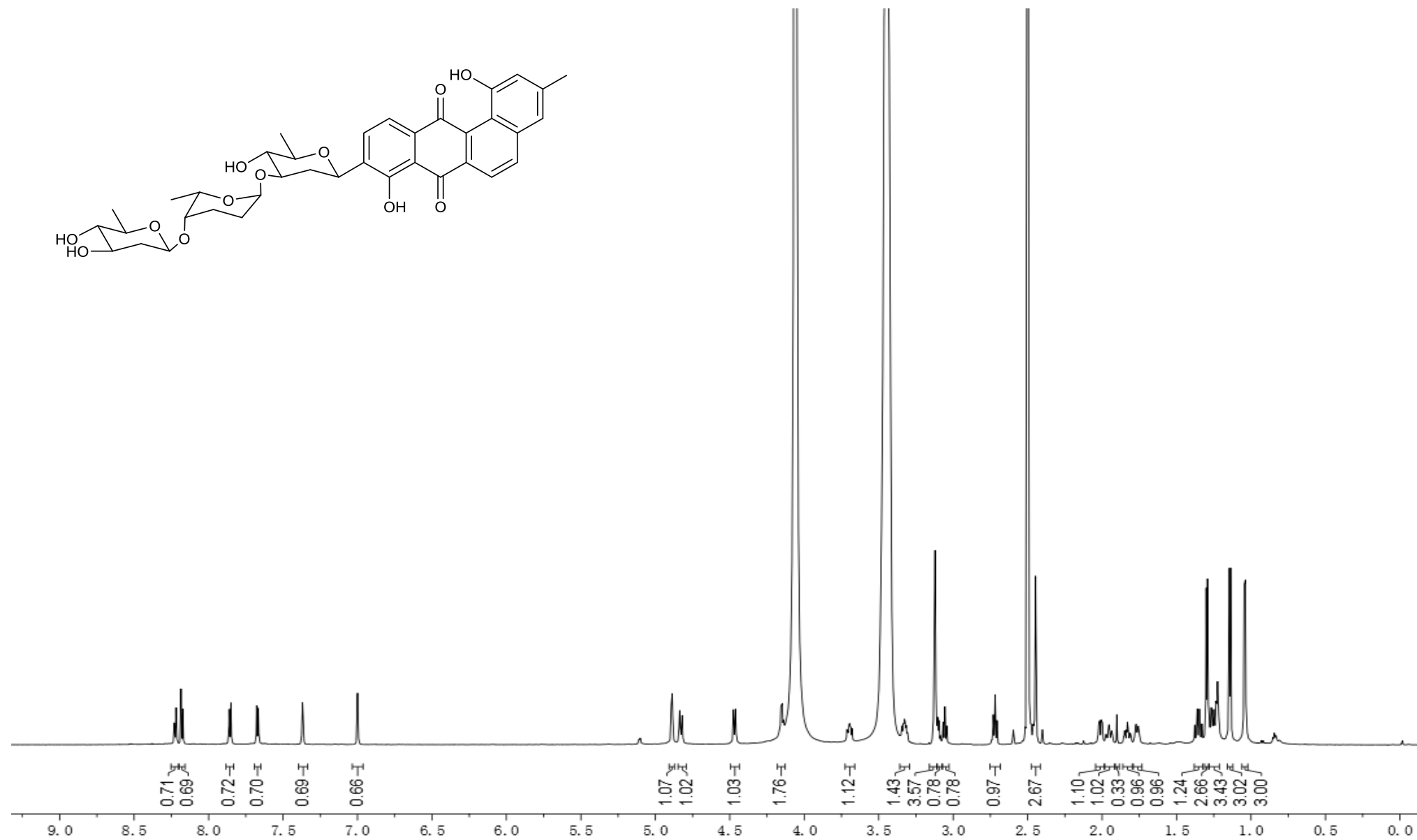


Figure S30. ^{13}C NMR (176 MHz) spectrum of compound **5** in $\text{DMSO-}d_6/\text{CD}_3\text{OD}$.

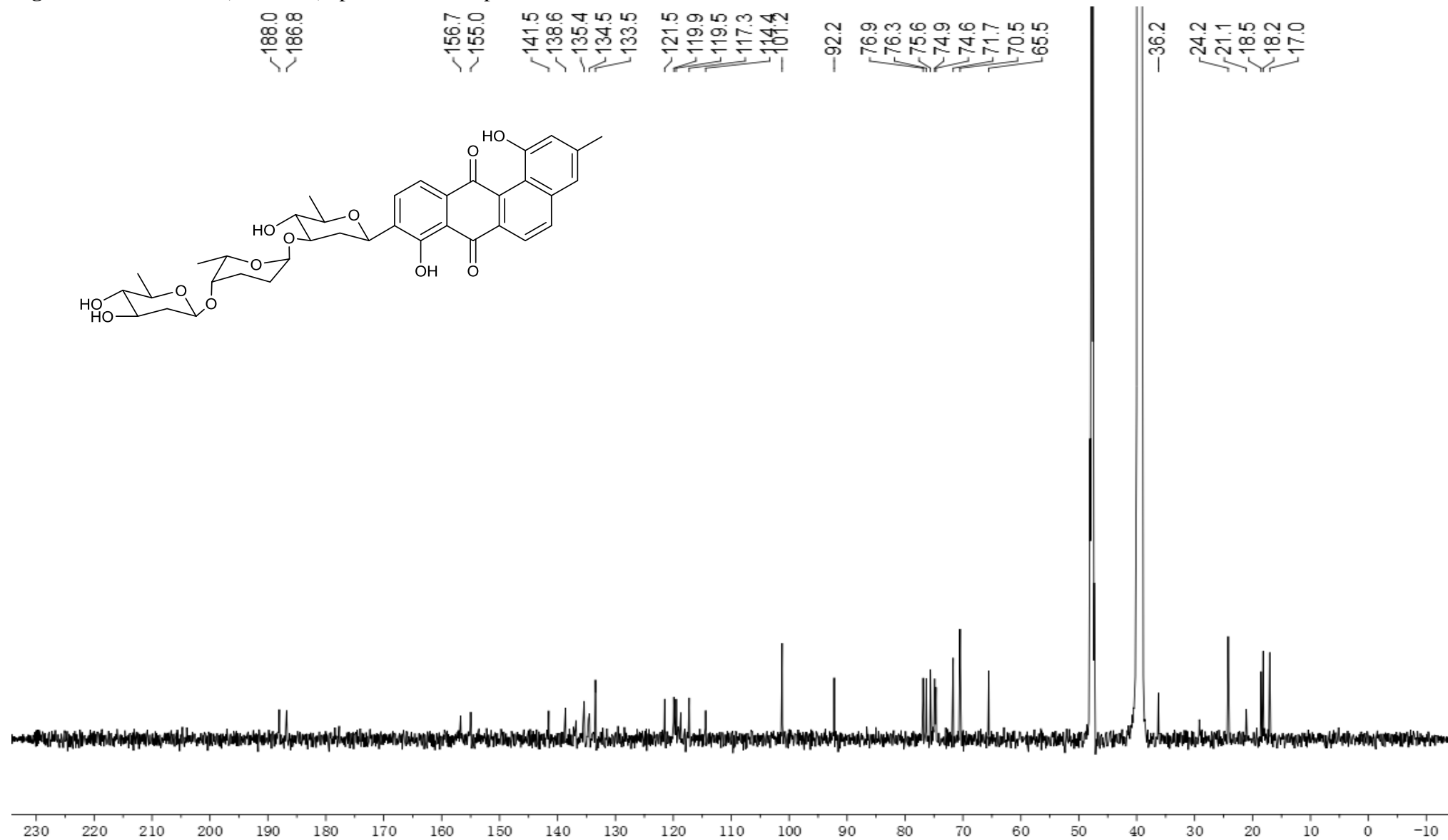


Figure S31. ^{13}C DEPT spectrum of compound **5** in $\text{DMSO-}d_6/\text{CD}_3\text{OD}$.

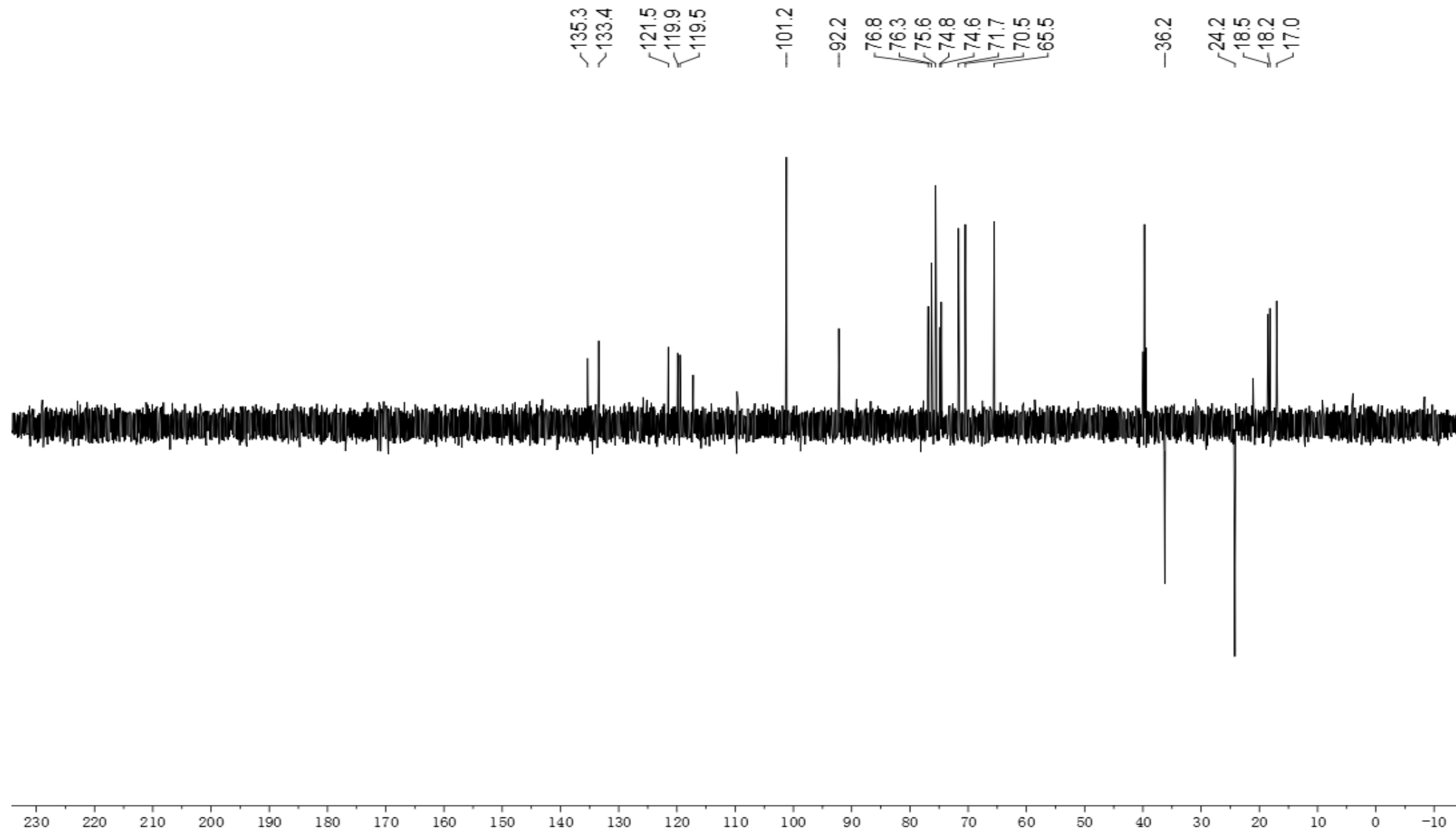


Figure S32. ^1H - ^1H COSY spectrum of compound **5** in $\text{DMSO-}d_6/\text{CD}_3\text{OD}$.

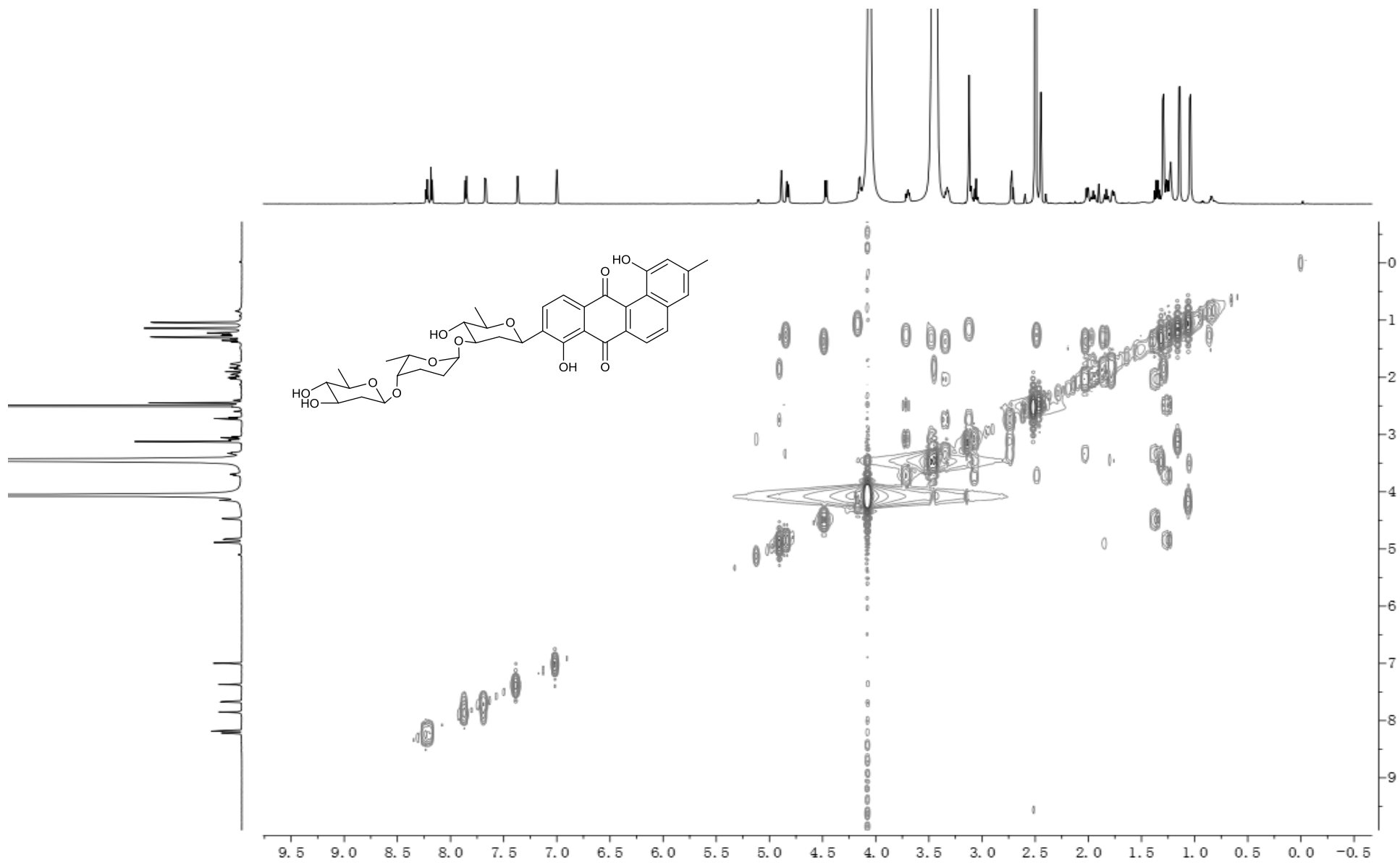


Figure S33. HSQC spectrum of compound **5** in DMSO- d_6 /CD $_3$ OD.

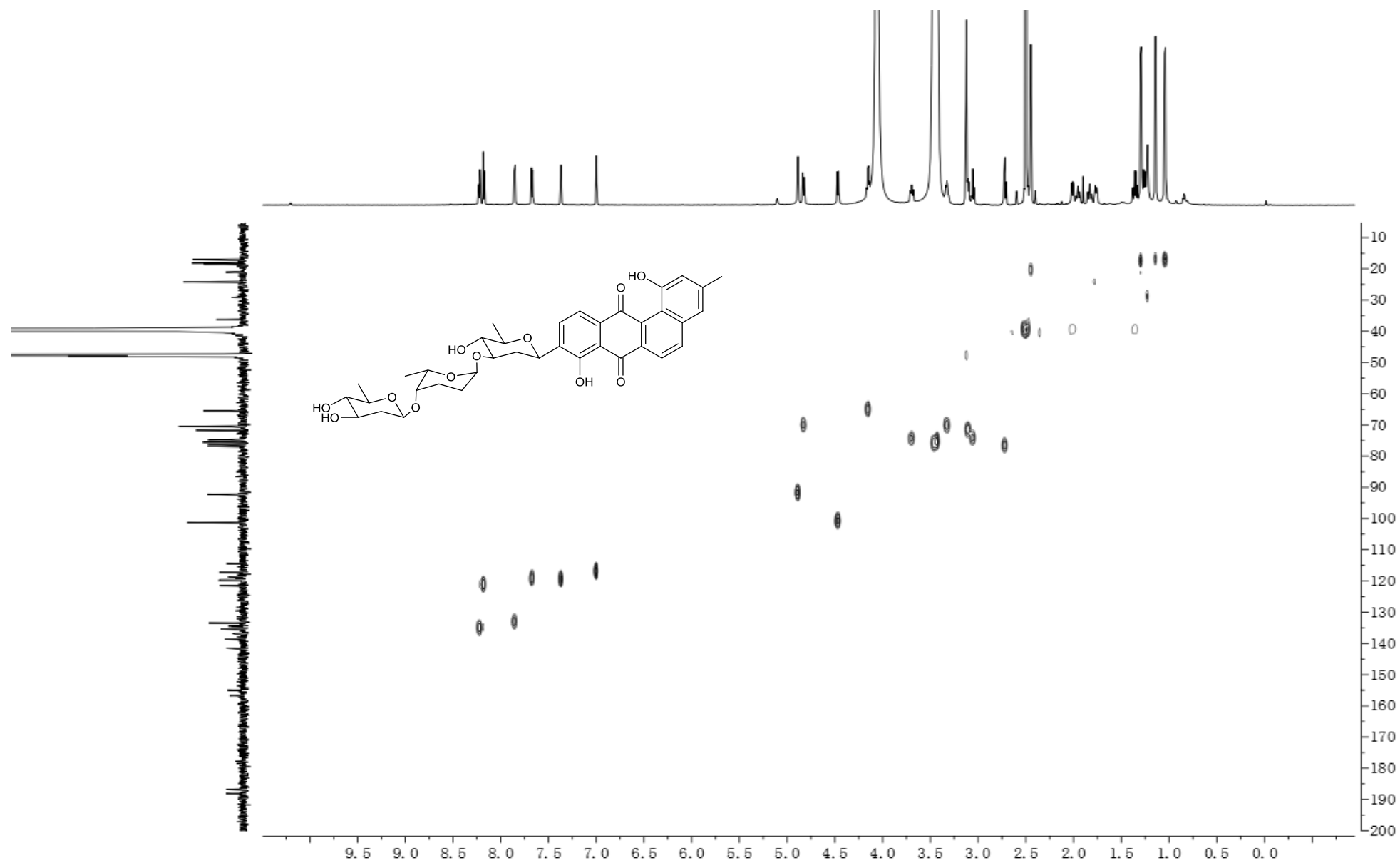


Figure S34. HMBC spectrum of compound **5** in DMSO-*d*₆/CD₃OD.

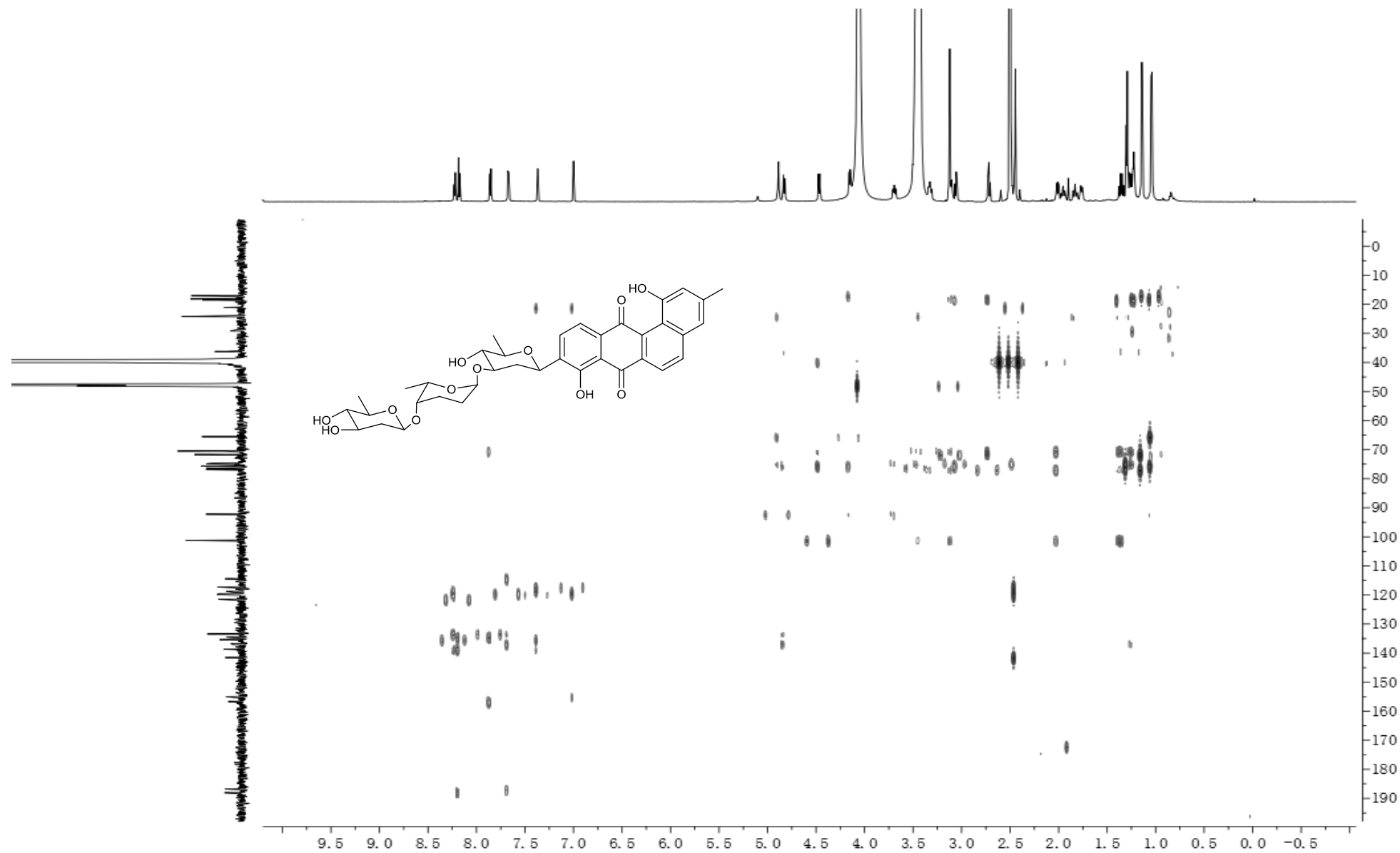


Figure S35. NOESY spectrum of compound **5** in DMSO- d_6 /CD $_3$ OD.

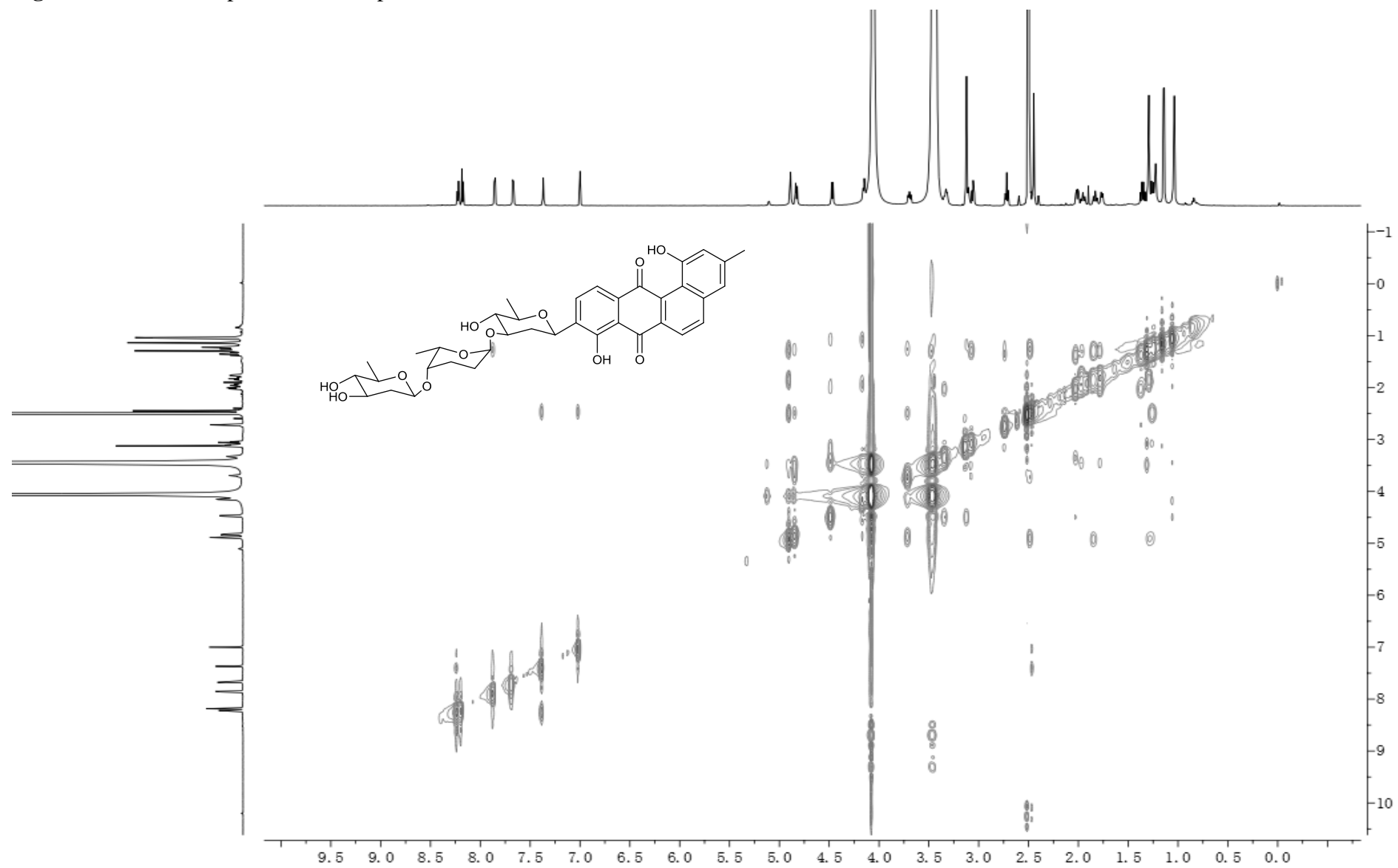


Figure S36. ^1H NMR (700 MHz) spectrum of compound **6** in CDCl_3 .

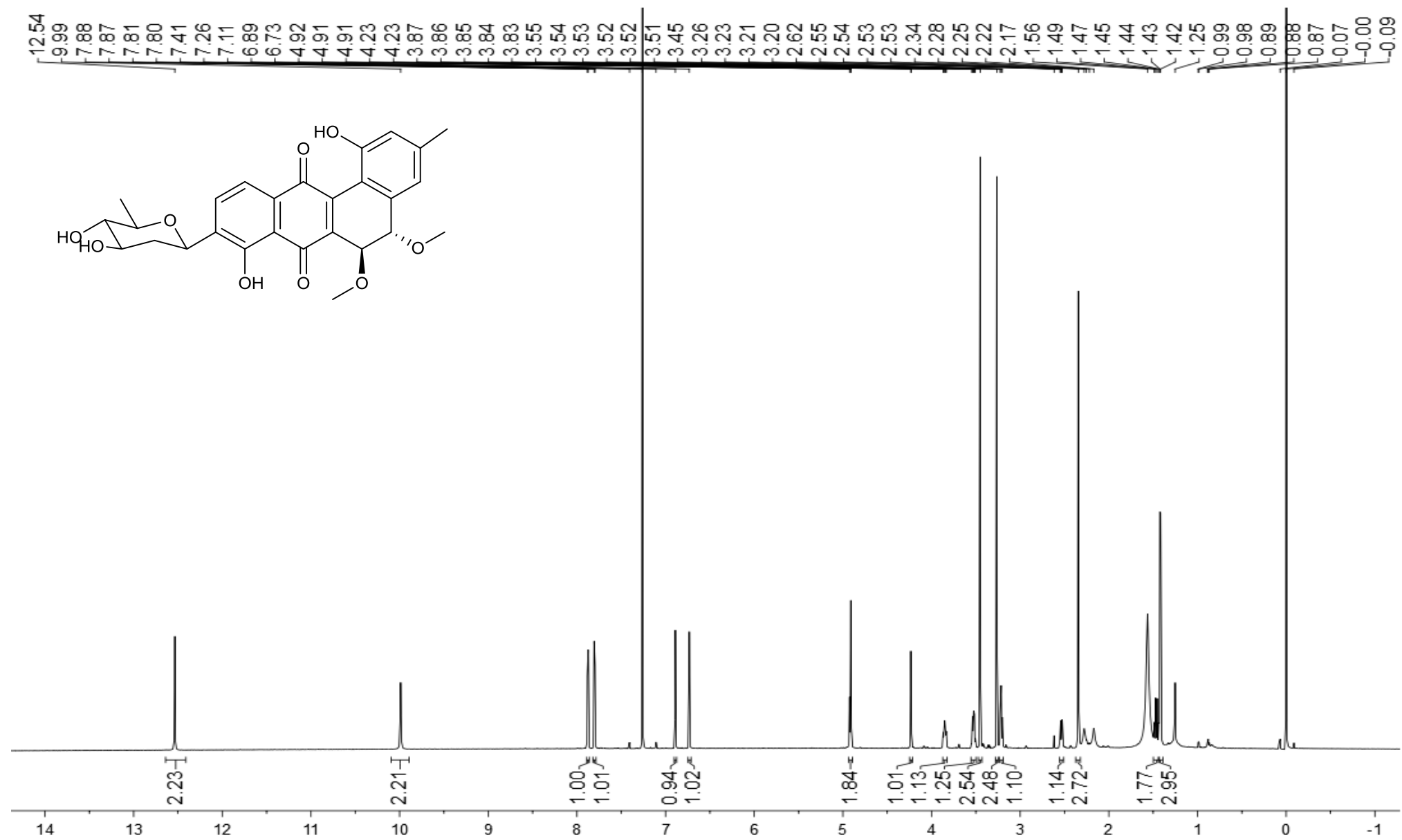


Figure S37. ^{13}C NMR (176 MHz) spectrum of compound **6** in CDCl_3 .

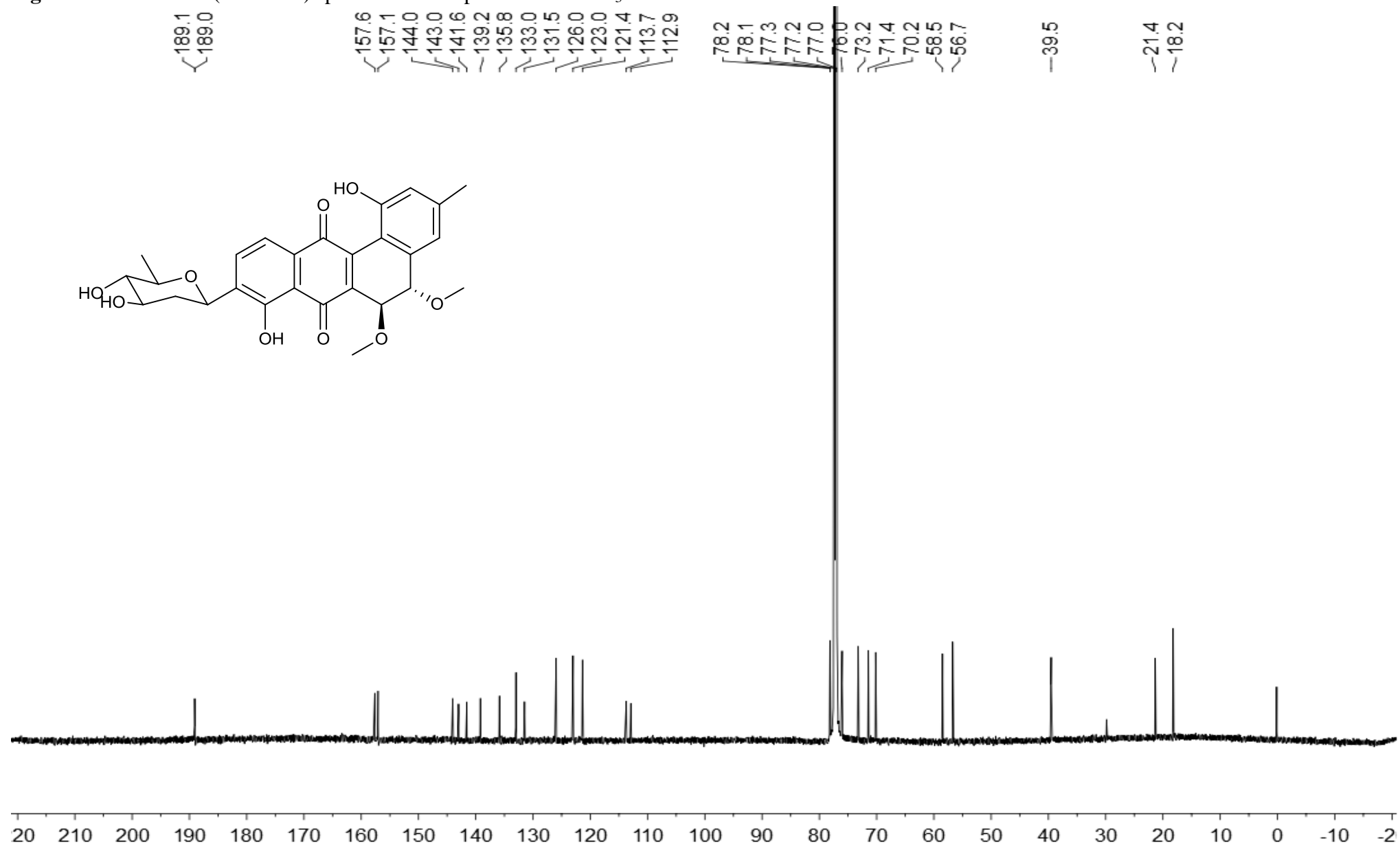


Figure S38. ^{13}C DEPT spectrum of compound **6** in CDCl_3 .

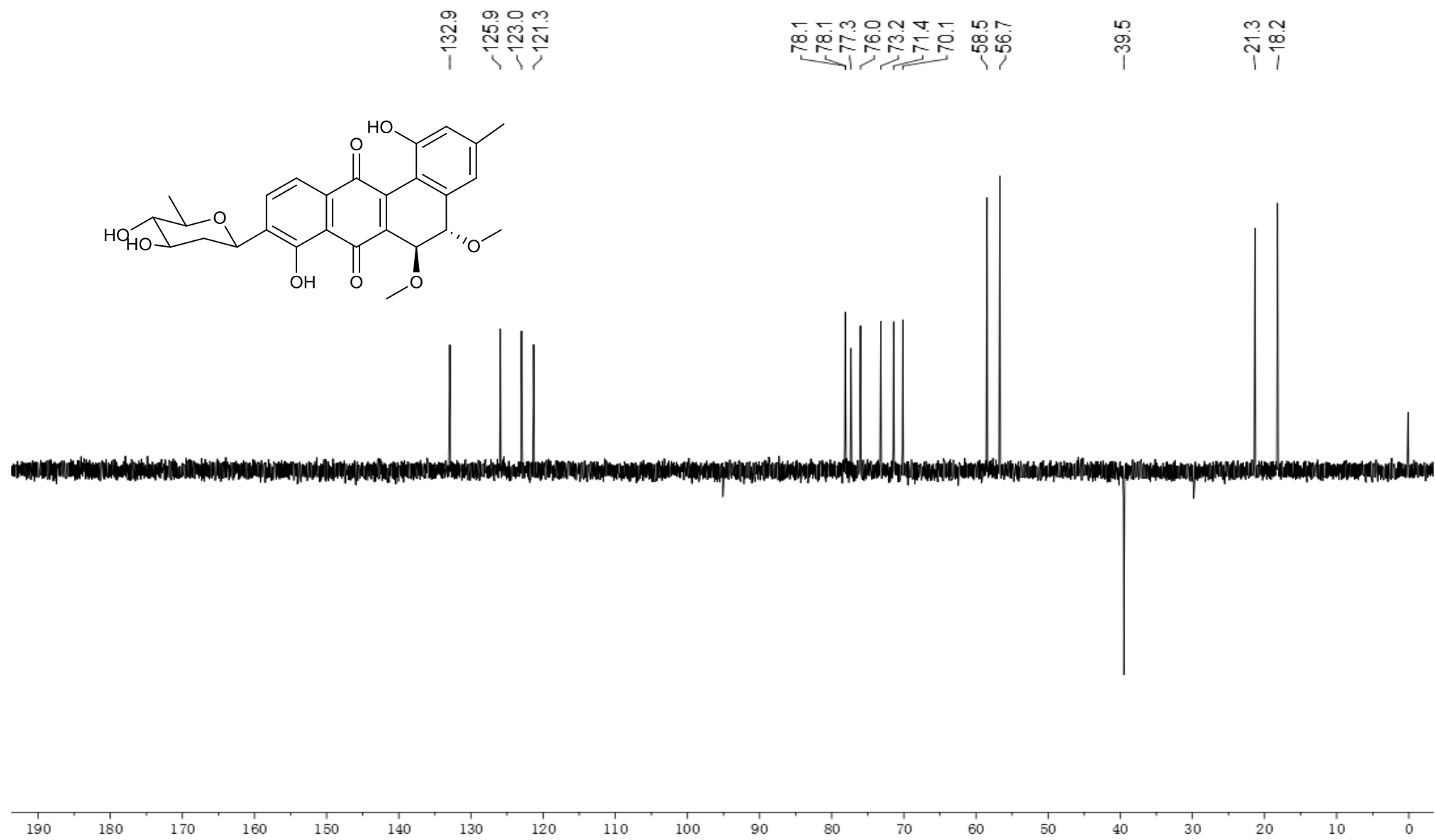


Figure S39. ^1H - ^1H COSY spectrum of compound **6** in CDCl_3 .

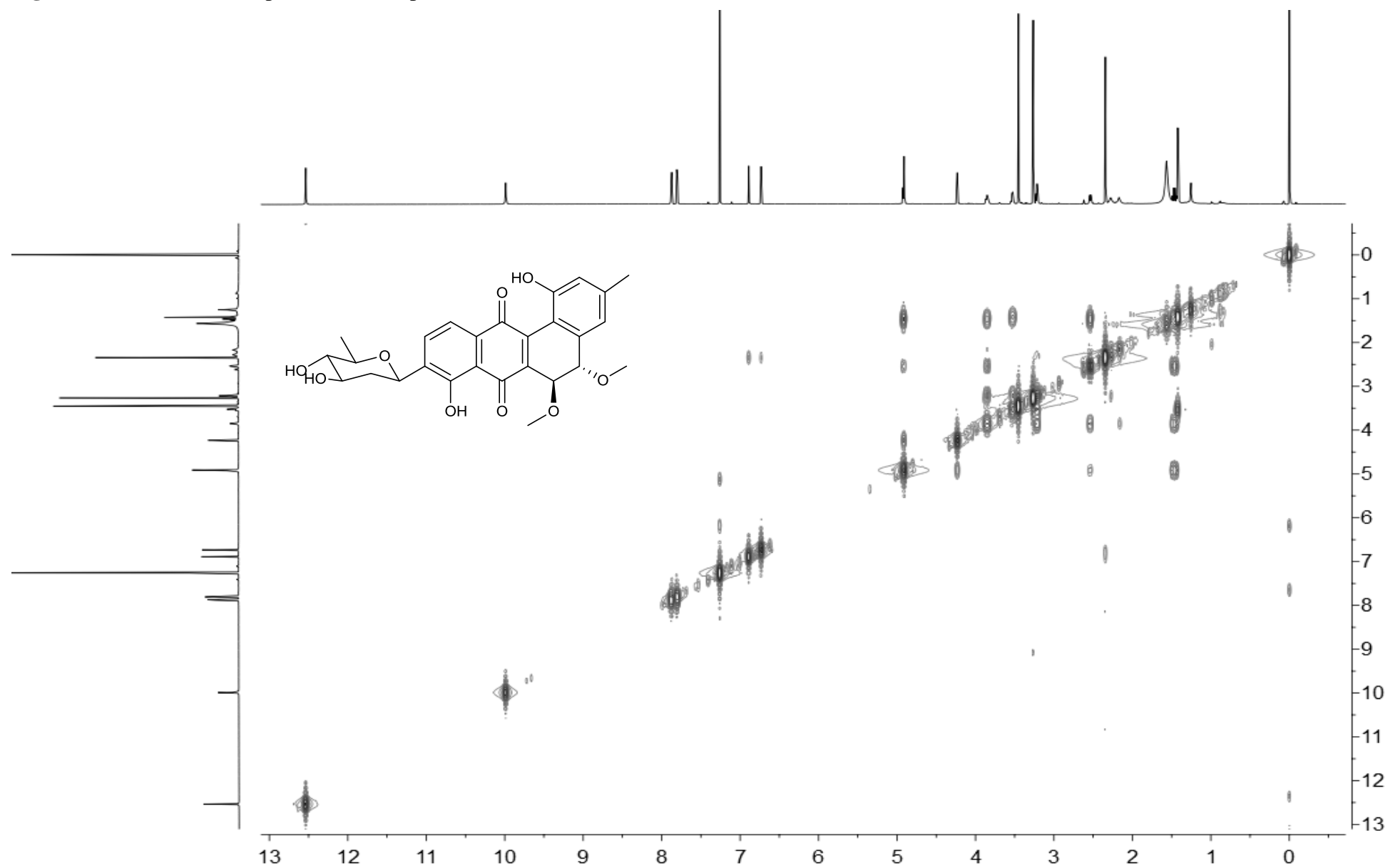


Figure S40. HSQC spectrum of compound **6** in CDCl₃.

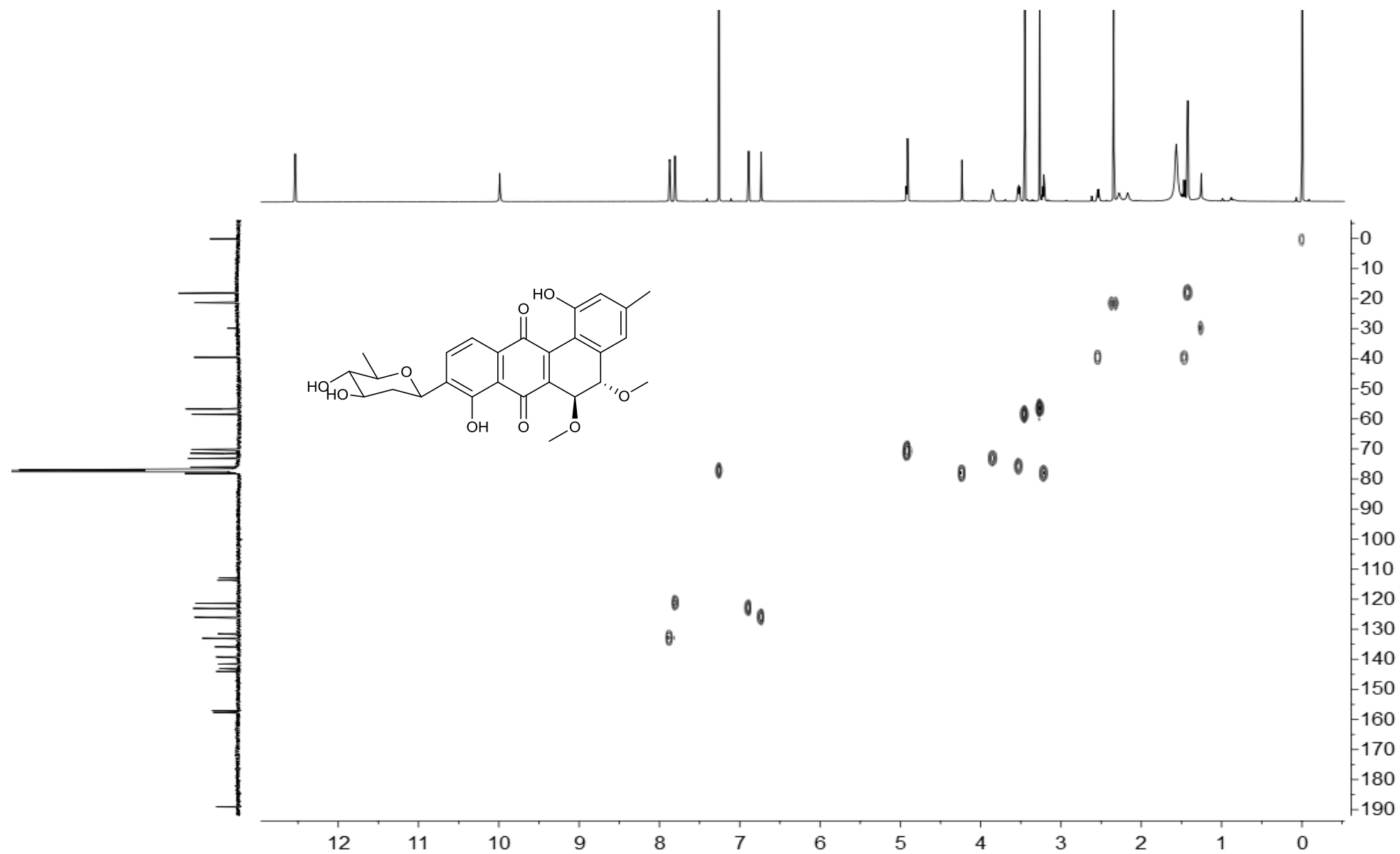


Figure S41. HMBC spectrum of compound **6** in CDCl₃.

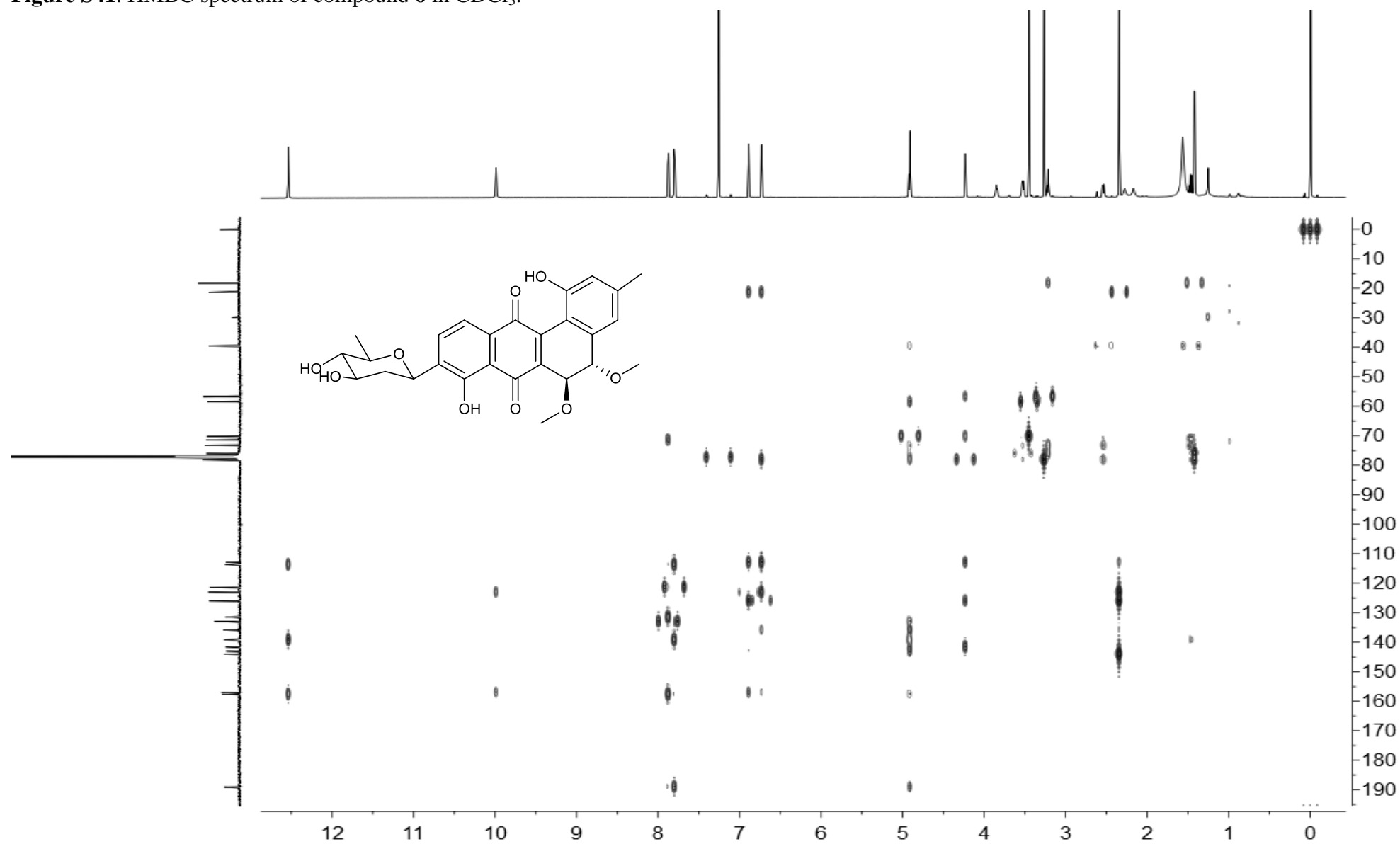


Figure S42. NOESY spectrum of compound **6** in CDCl₃.

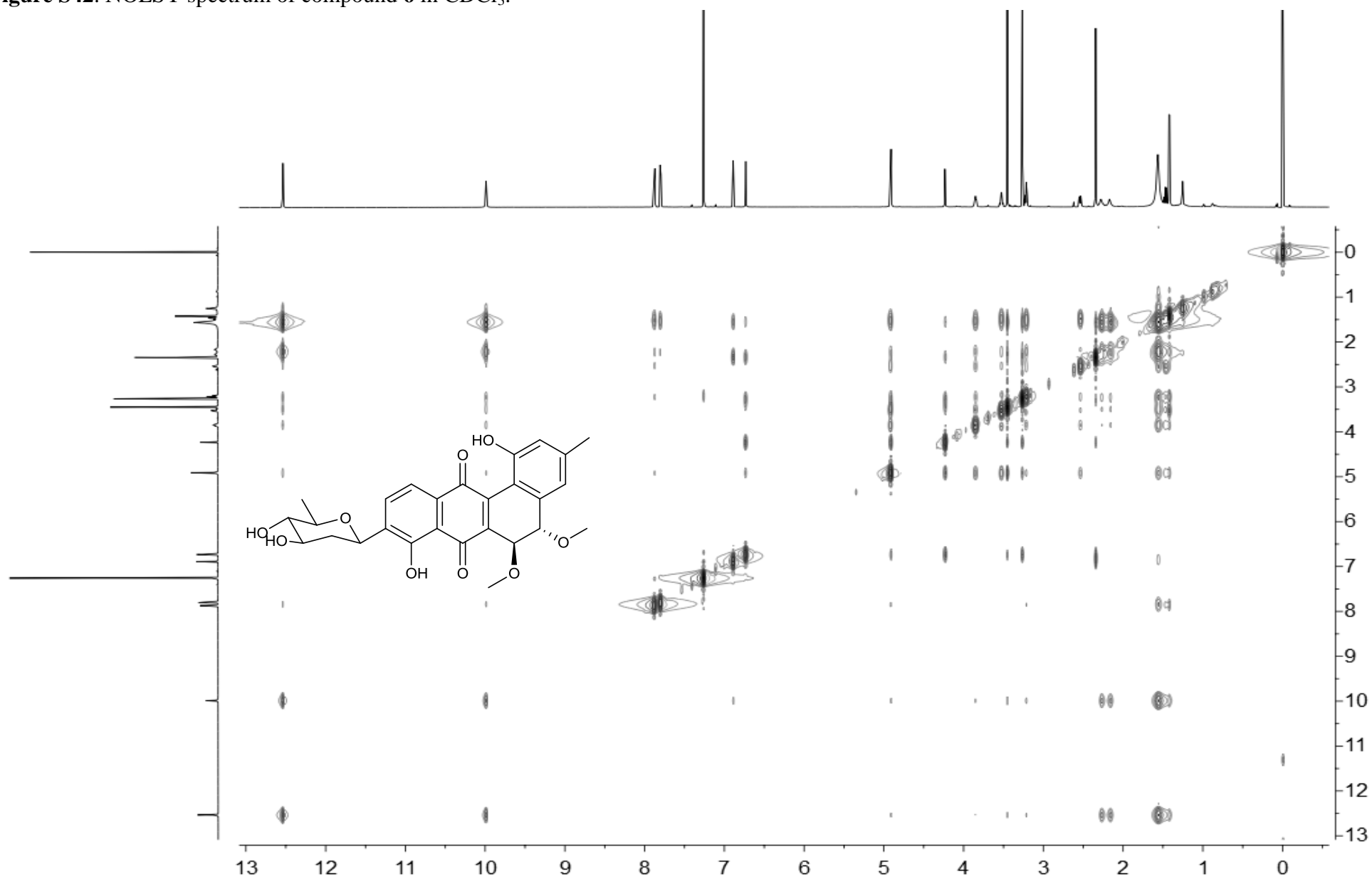


Figure S43. ^1H NMR (700 MHz) spectrum of **7** in CDCl_3 .

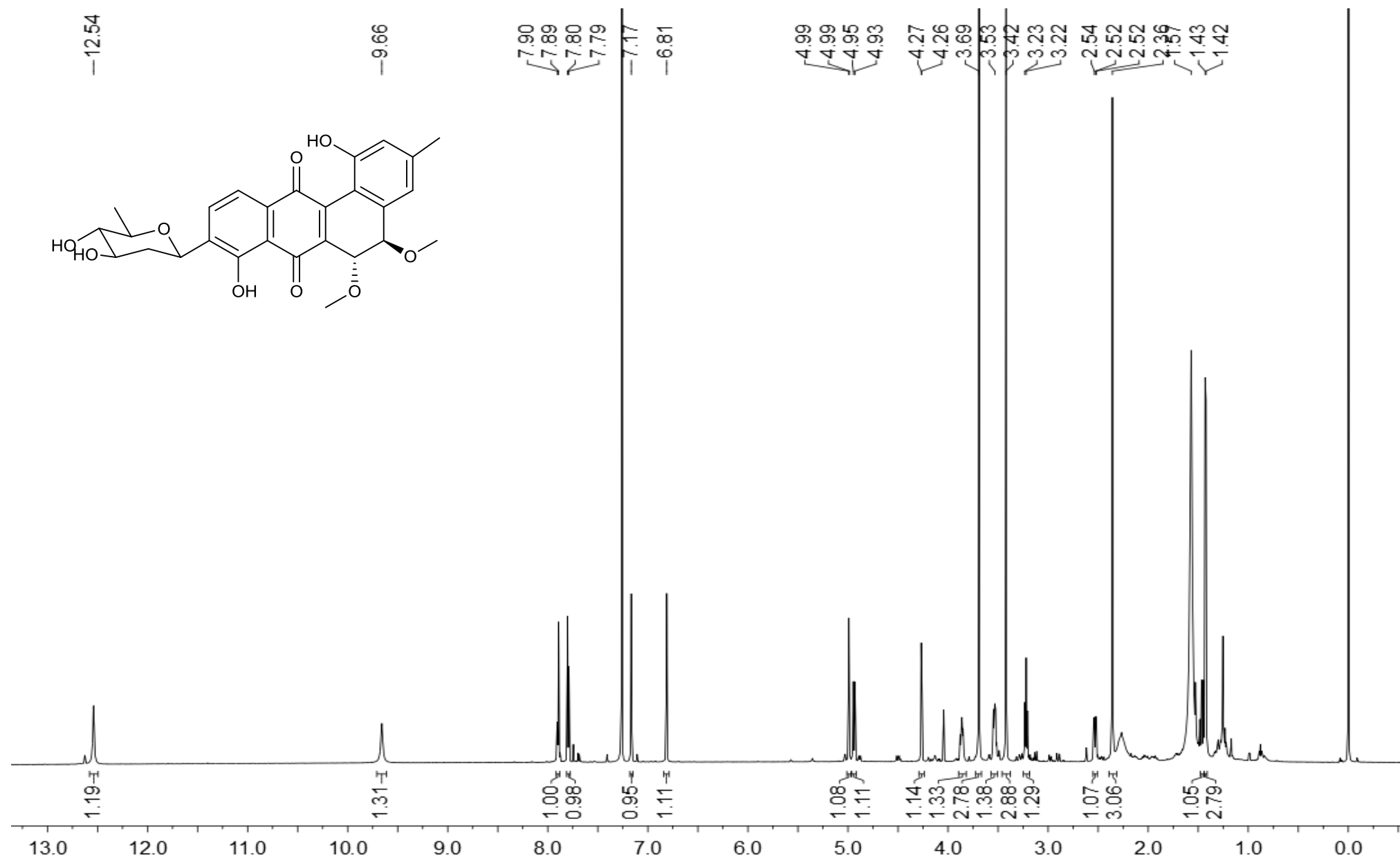


Figure S44. ^{13}C NMR (176 MHz) spectrum of compound **7** in CDCl_3 .

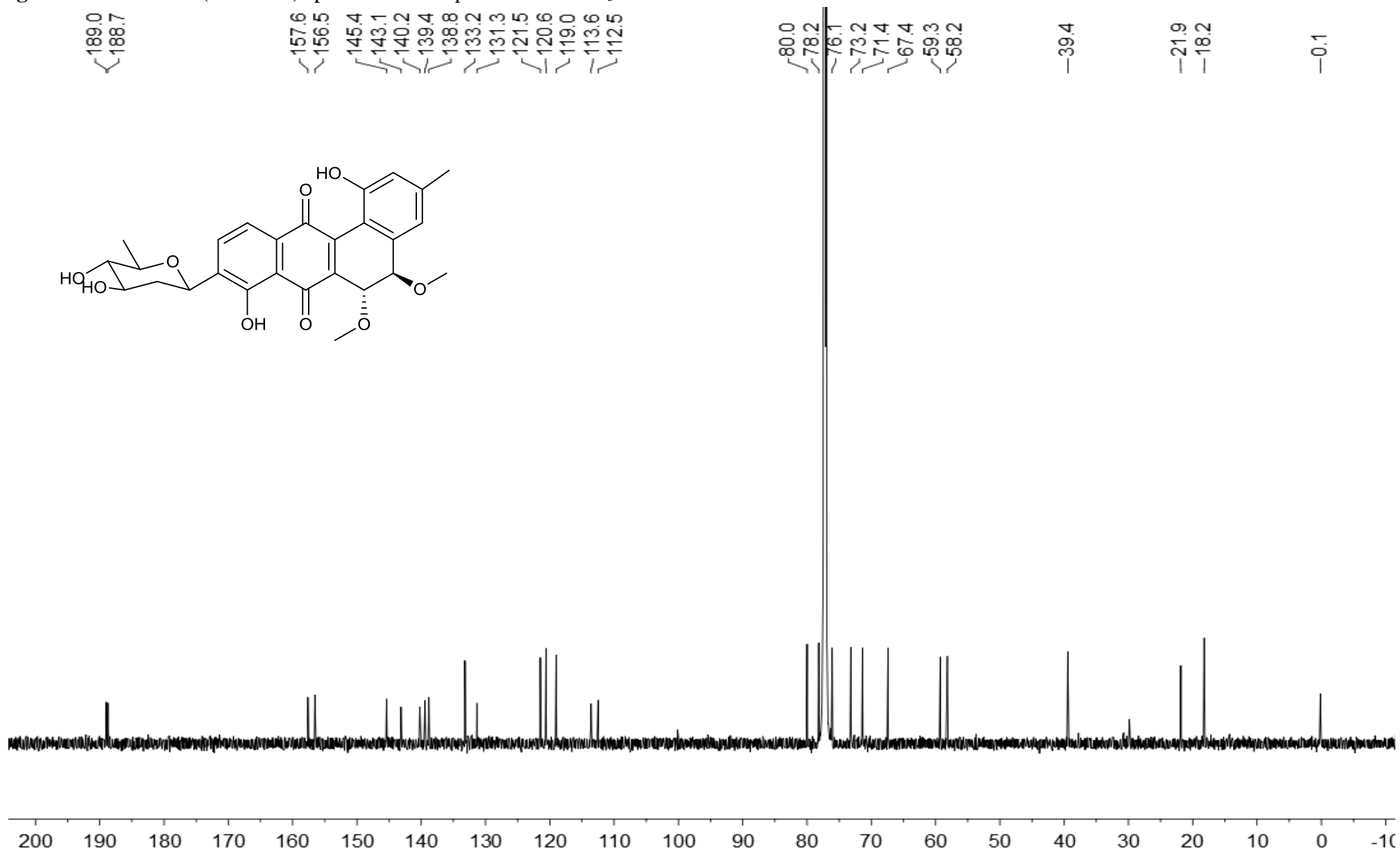


Figure S45. ^{13}C DEPT spectrum of compound **7** in CDCl_3 .

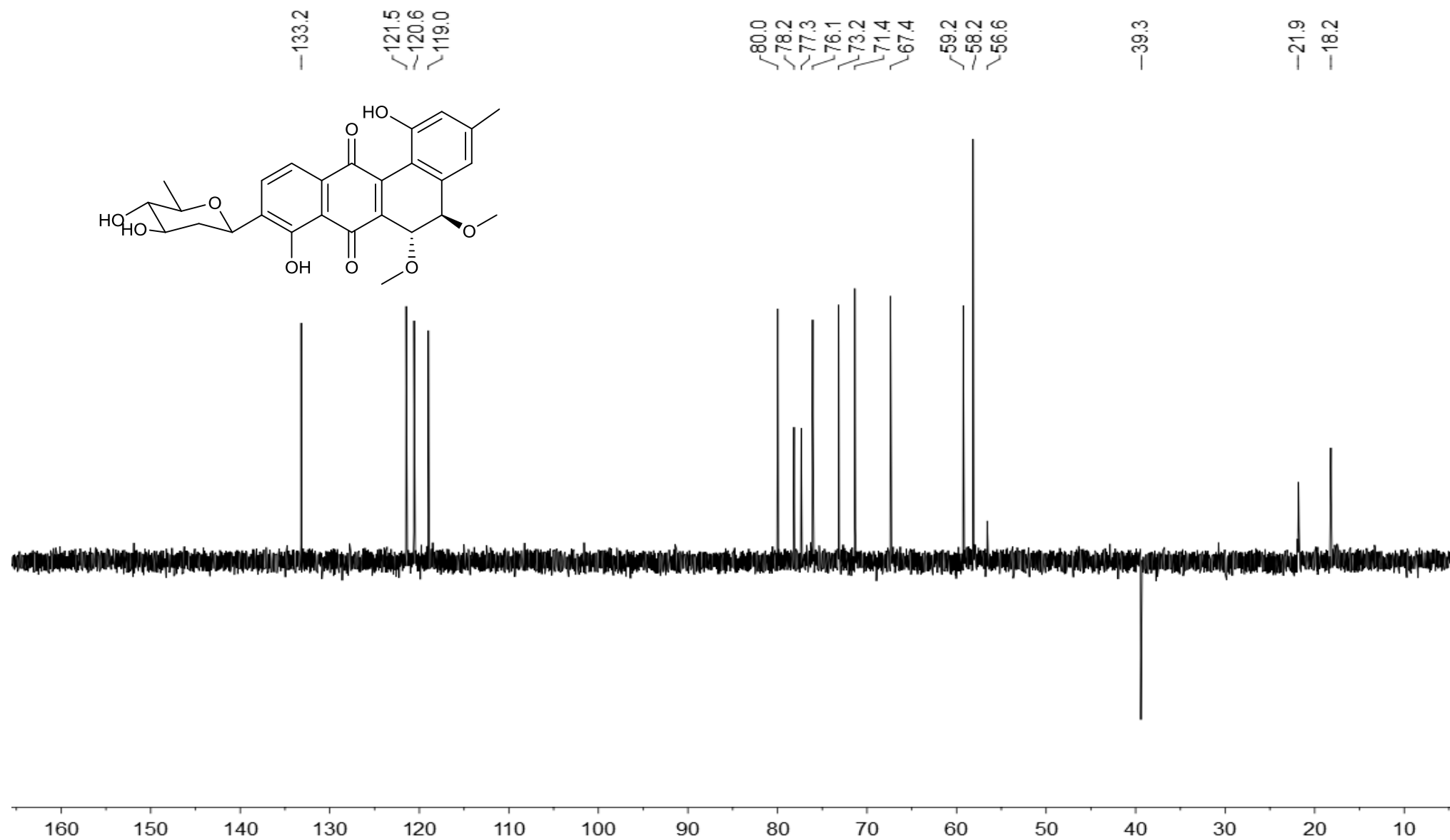


Figure S46. ^1H - ^1H COSY spectrum of compound **7** in CDCl_3 .

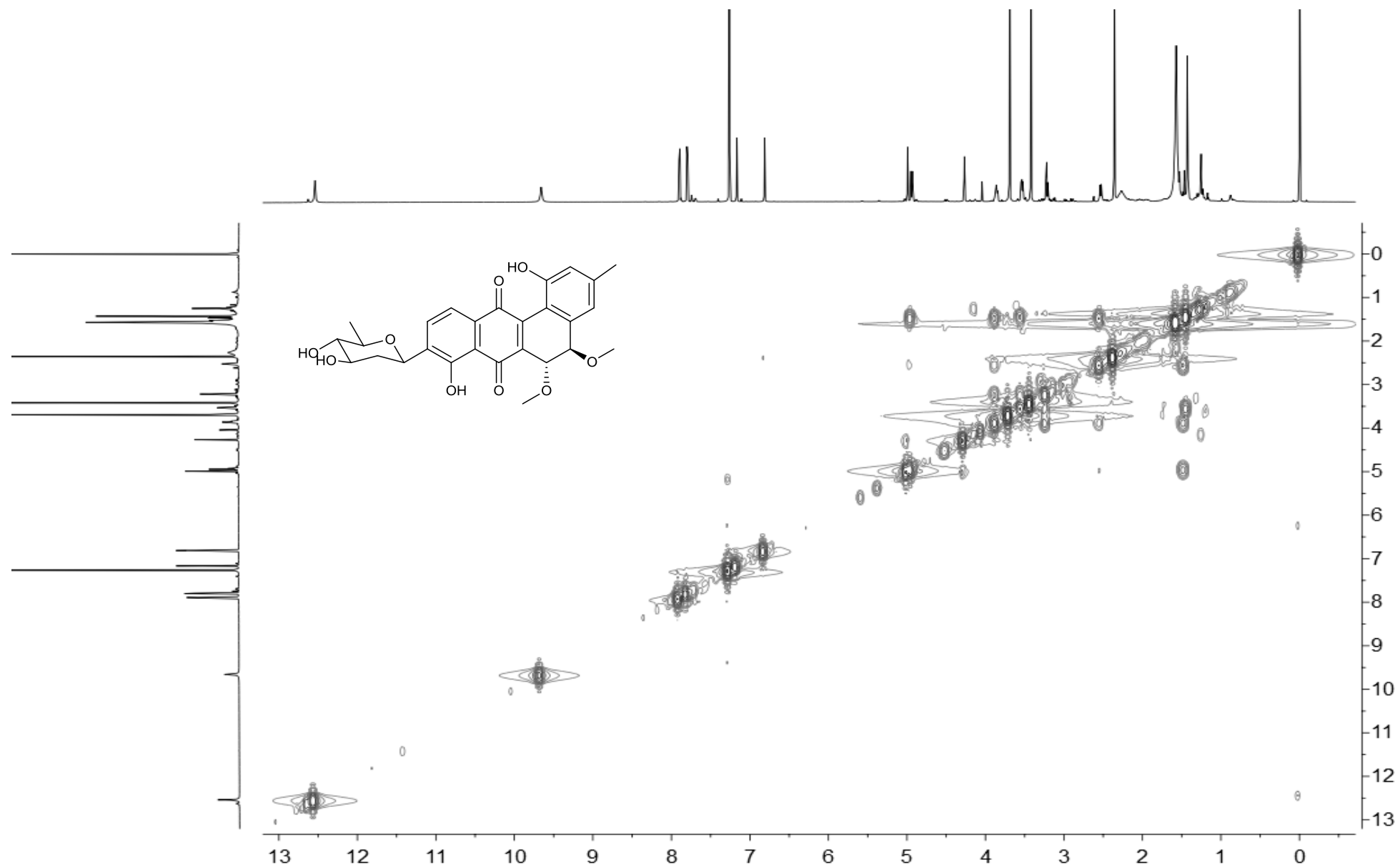


Figure S47. HSQC spectrum of compound **7** in CDCl₃.

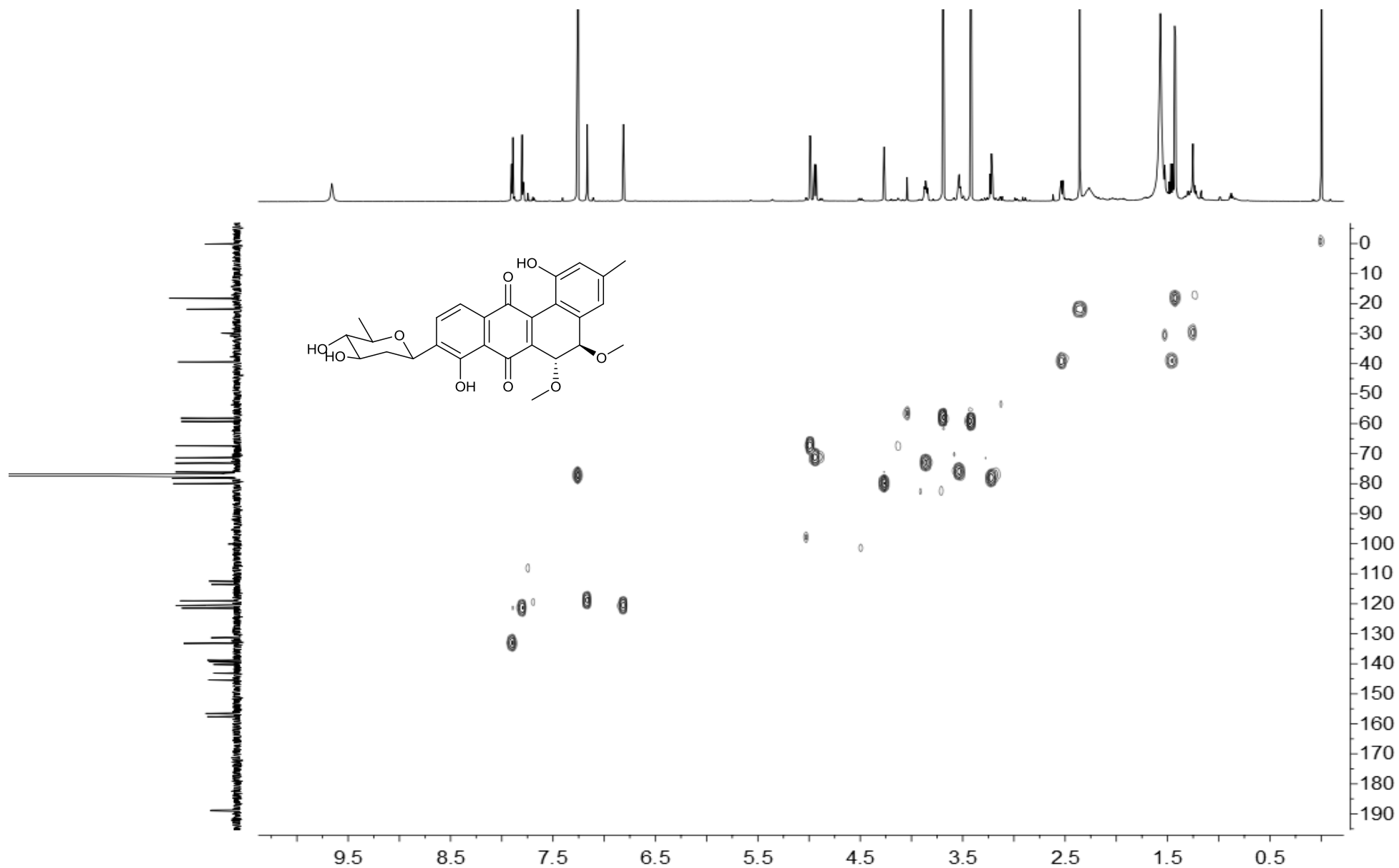


Figure S48. HMBC spectrum of compound **7** in CDCl₃.

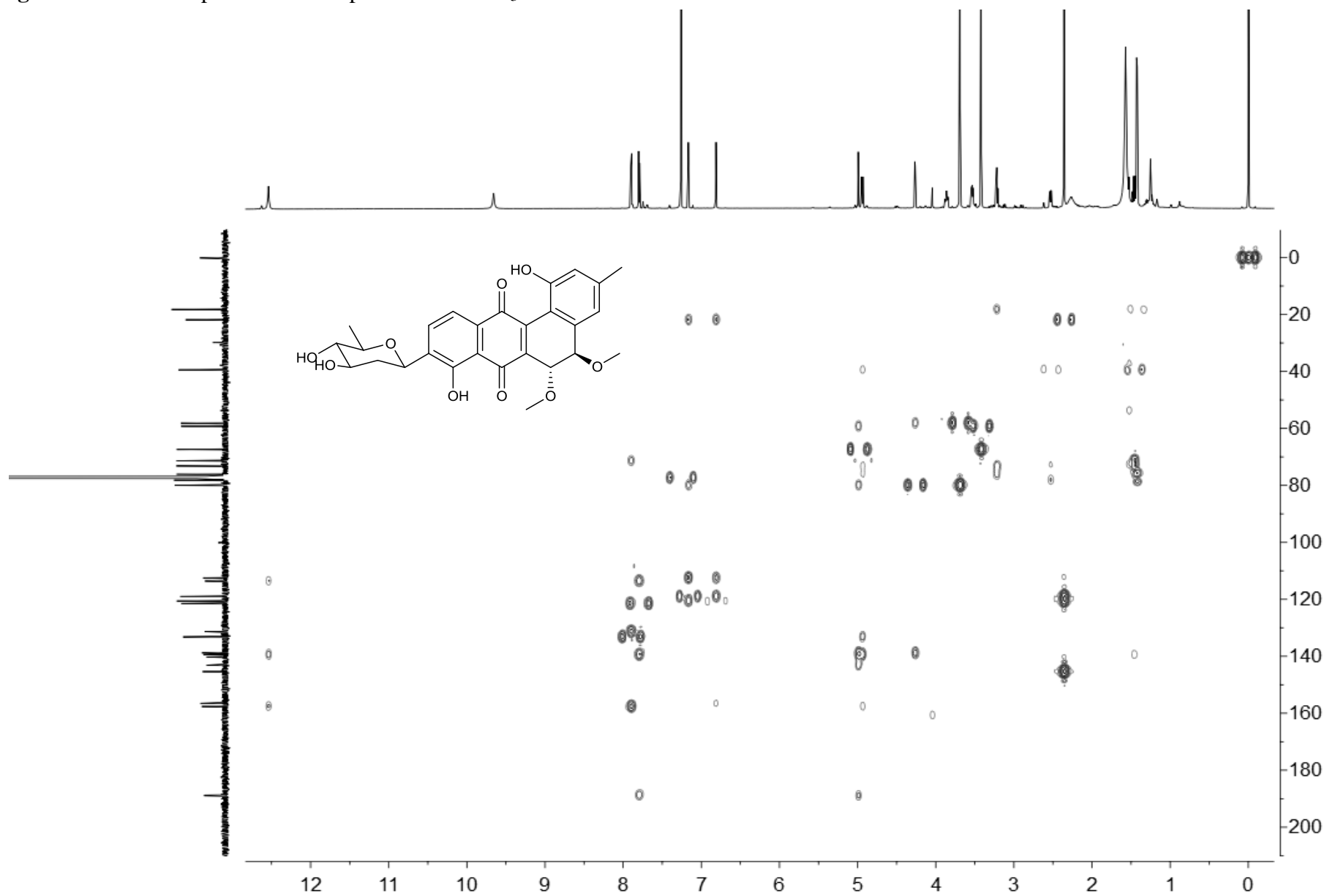


Figure S49. NOESY spectrum of compound **7** in CDCl₃.

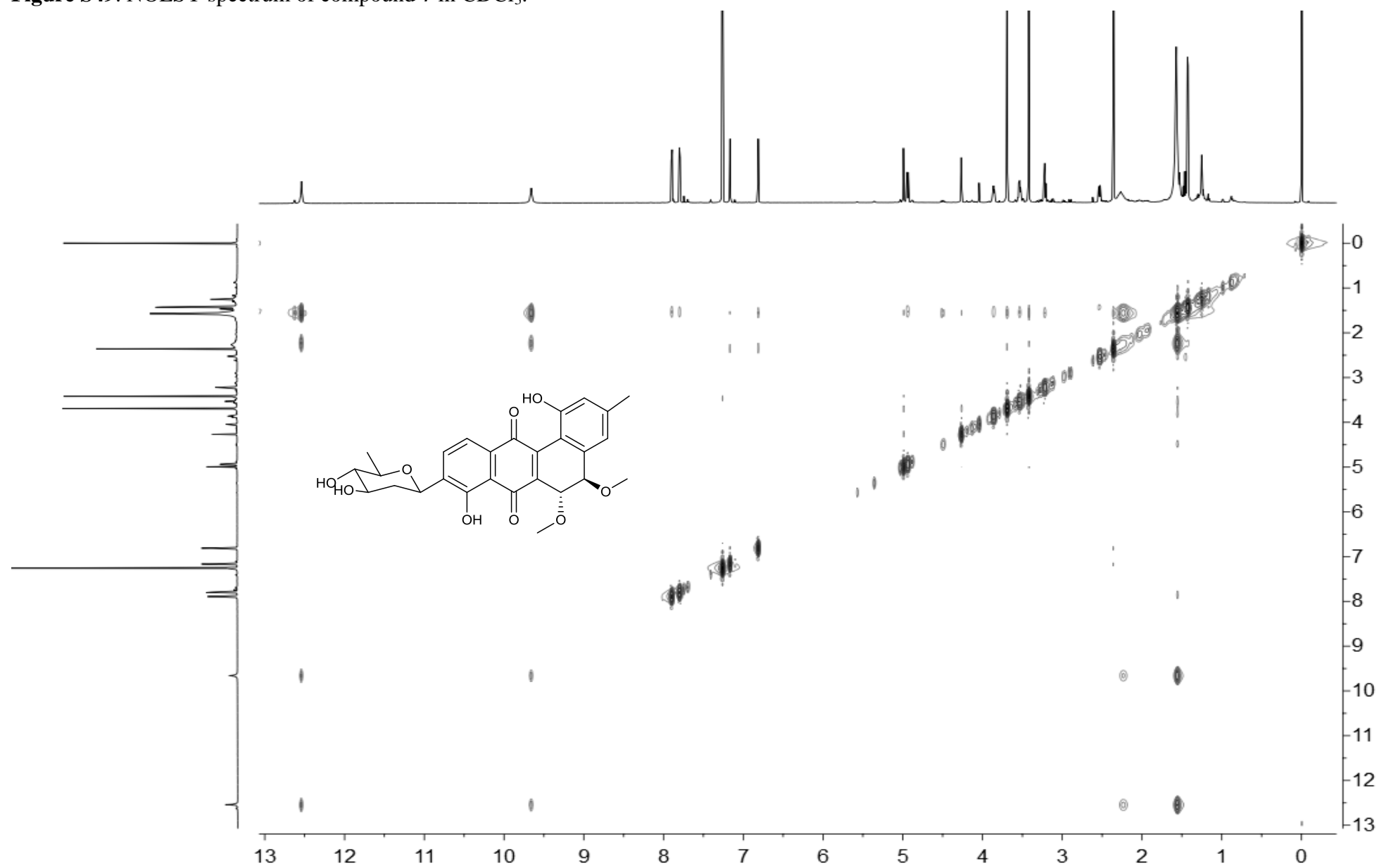


Figure S50. ^1H NMR (700 MHz) spectrum of compound **8** in CDCl_3 .

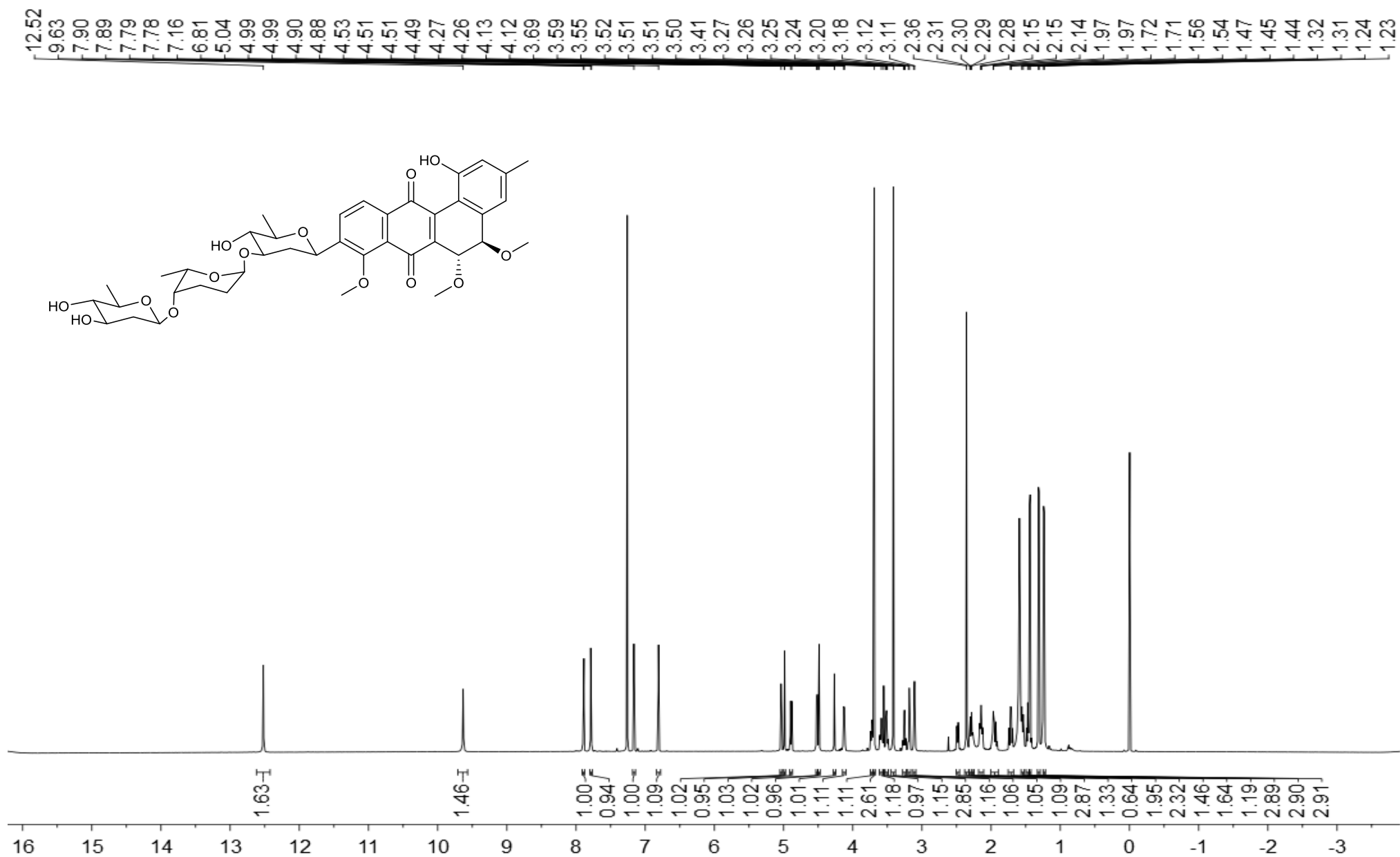


Figure S51. ^{13}C NMR (176 MHz) spectrum of compound **8** in CDCl_3 .

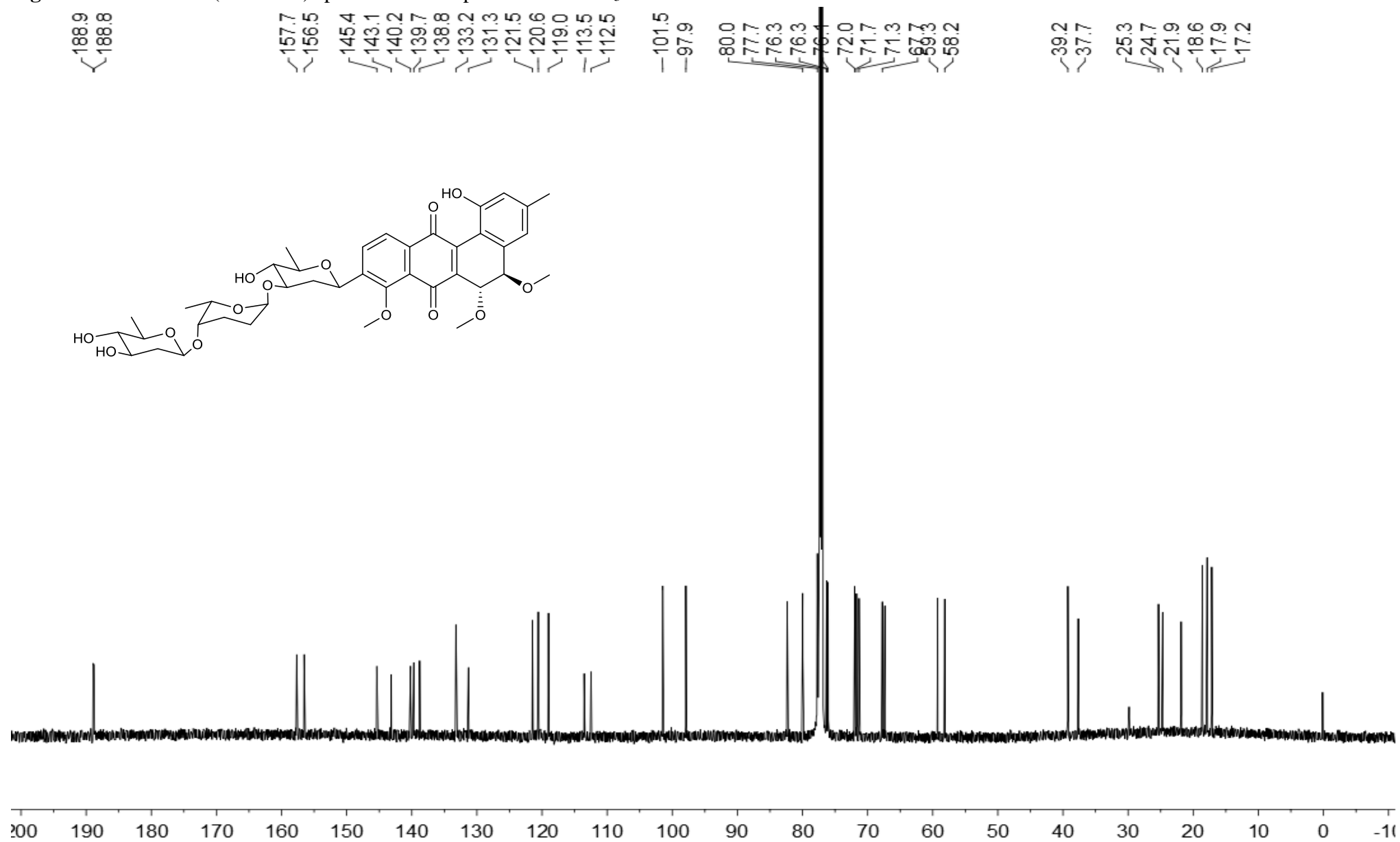


Figure S52. ^{13}C DEPT spectrum of compound **8** in CDCl_3 .

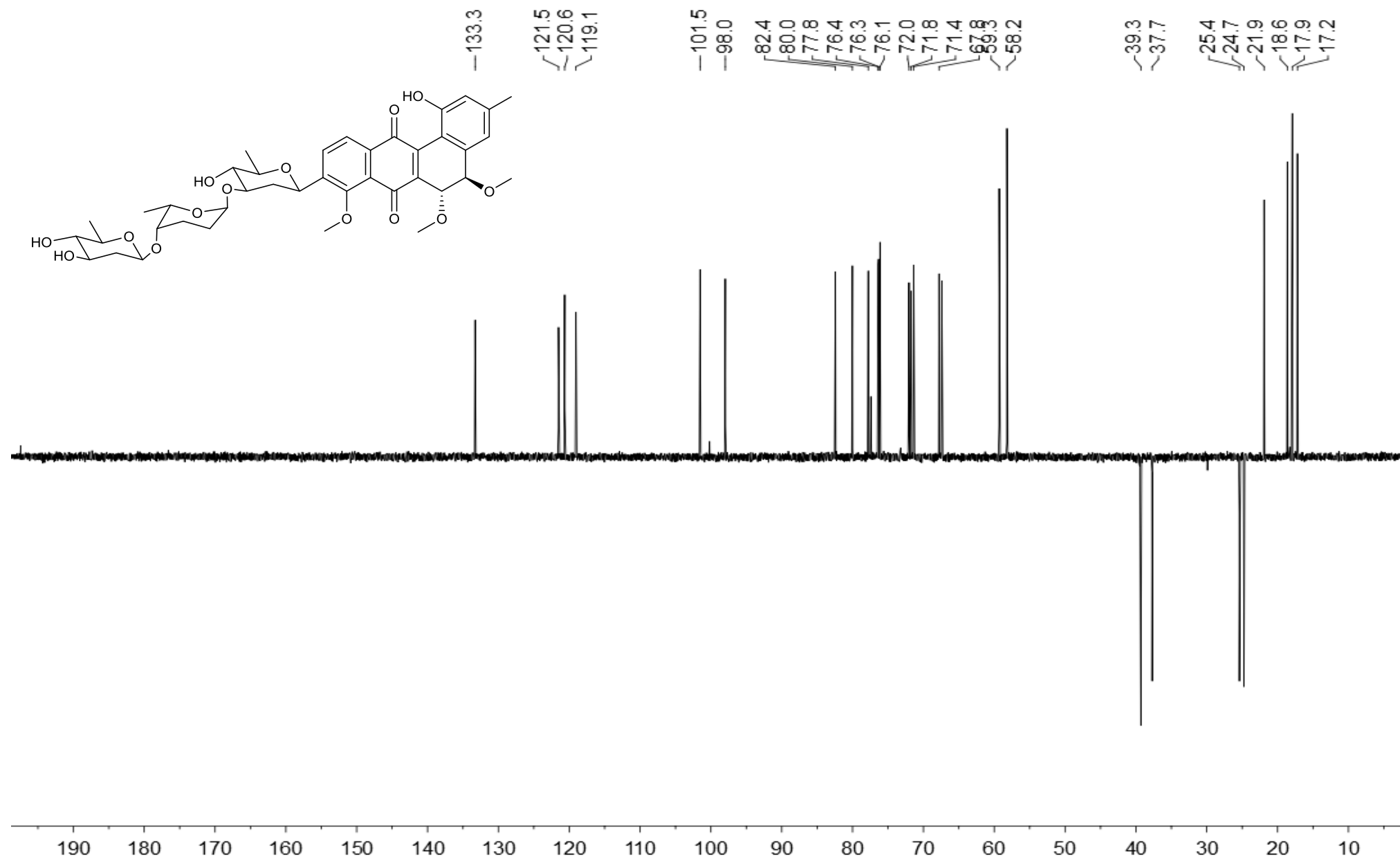


Figure S53. ^1H - ^1H COSY spectrum of compound **8** in CDCl_3 .

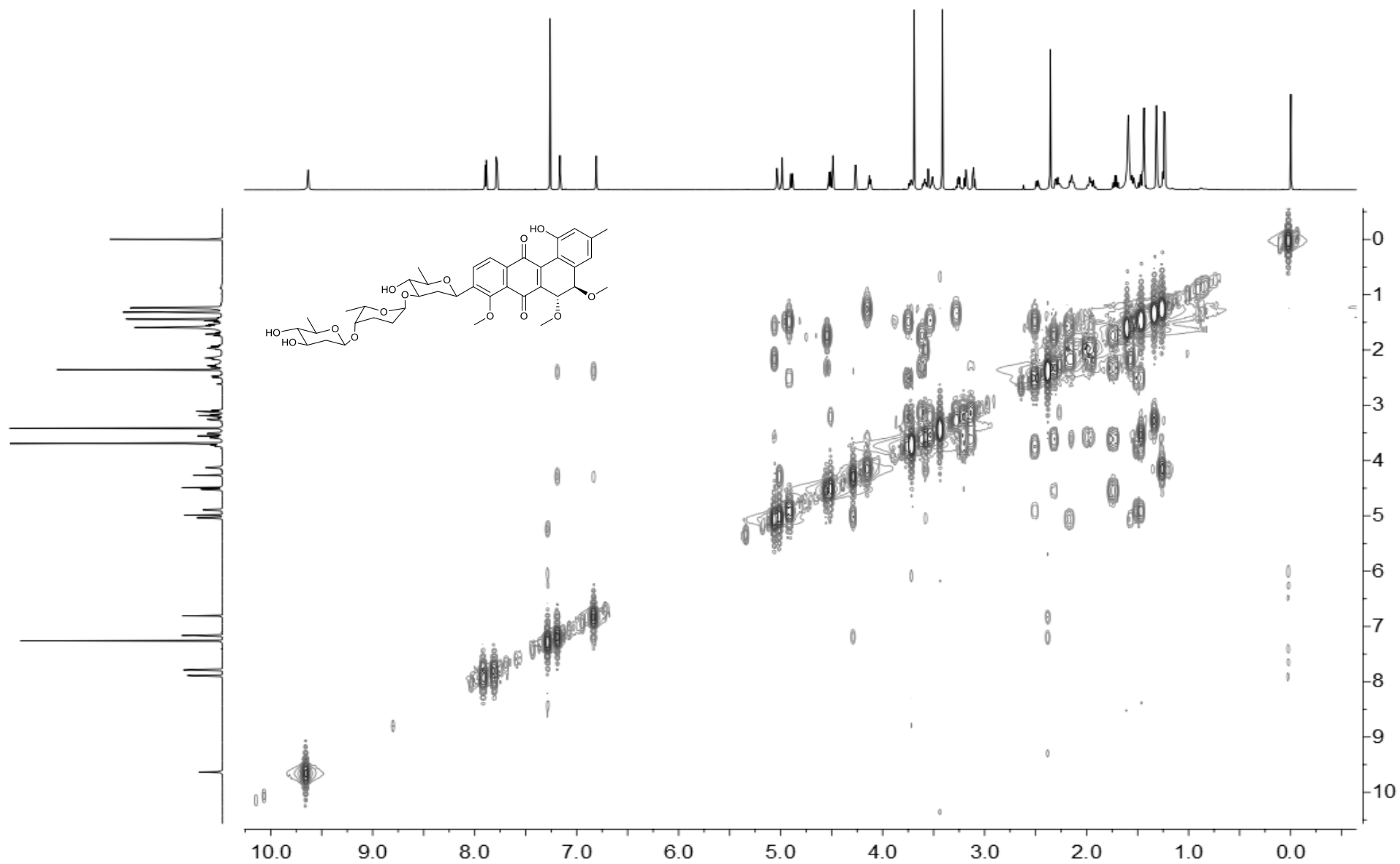


Figure S54. HSQC spectrum of compound **8** in CDCl₃.

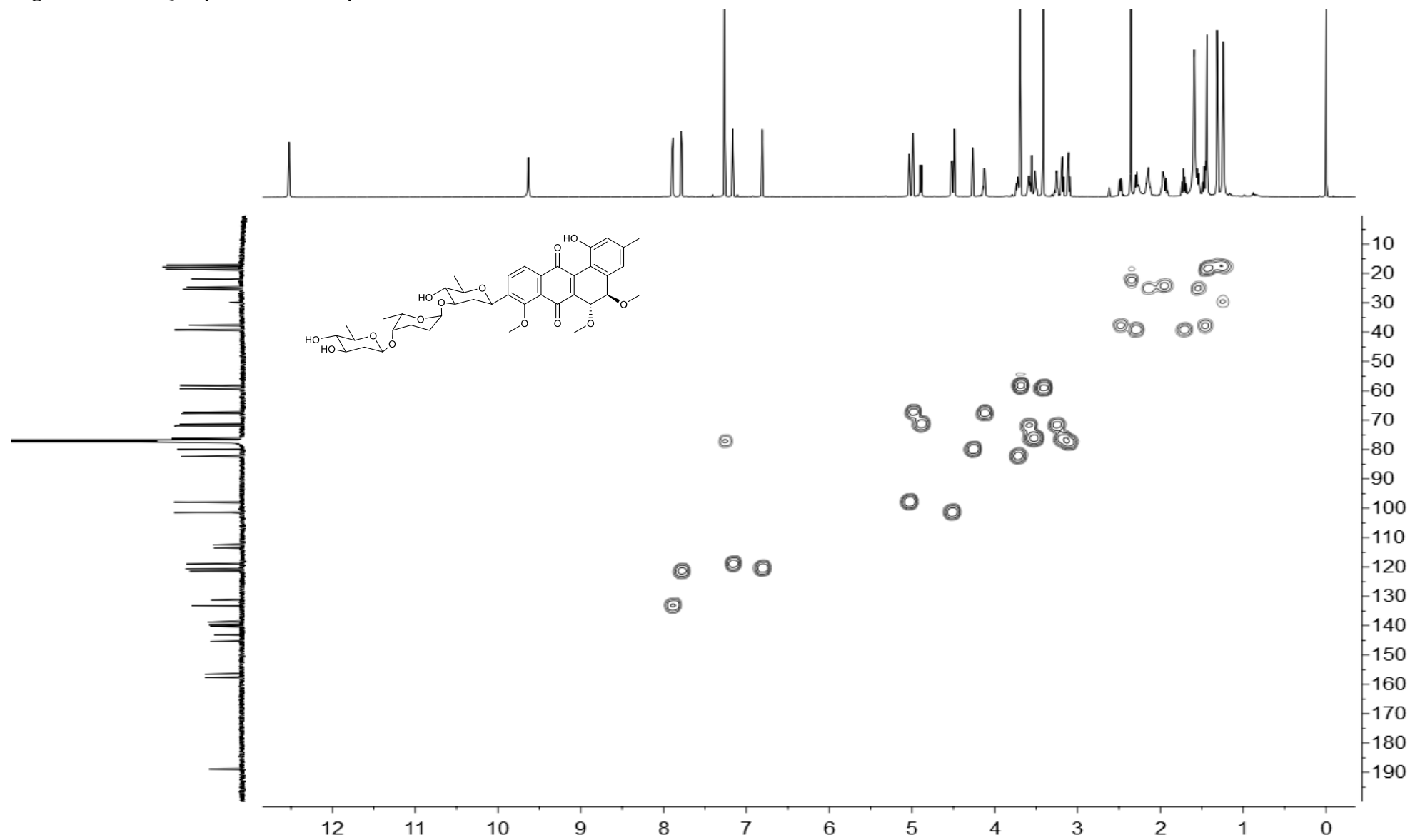


Figure S55. HMBC spectrum of compound **8** in CDCl₃.

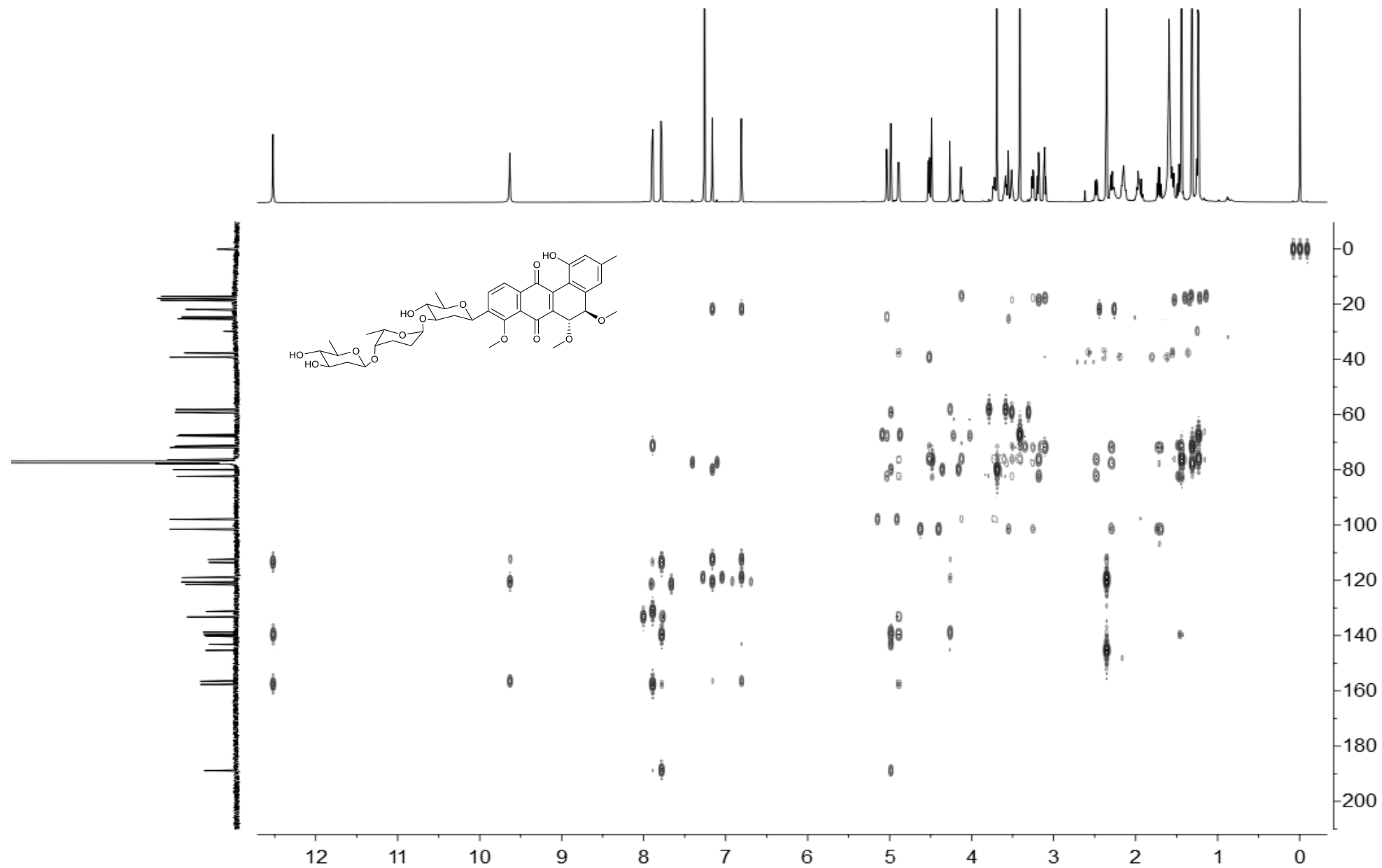


Figure S56. NOESY spectrum of compound **8** in CDCl₃.

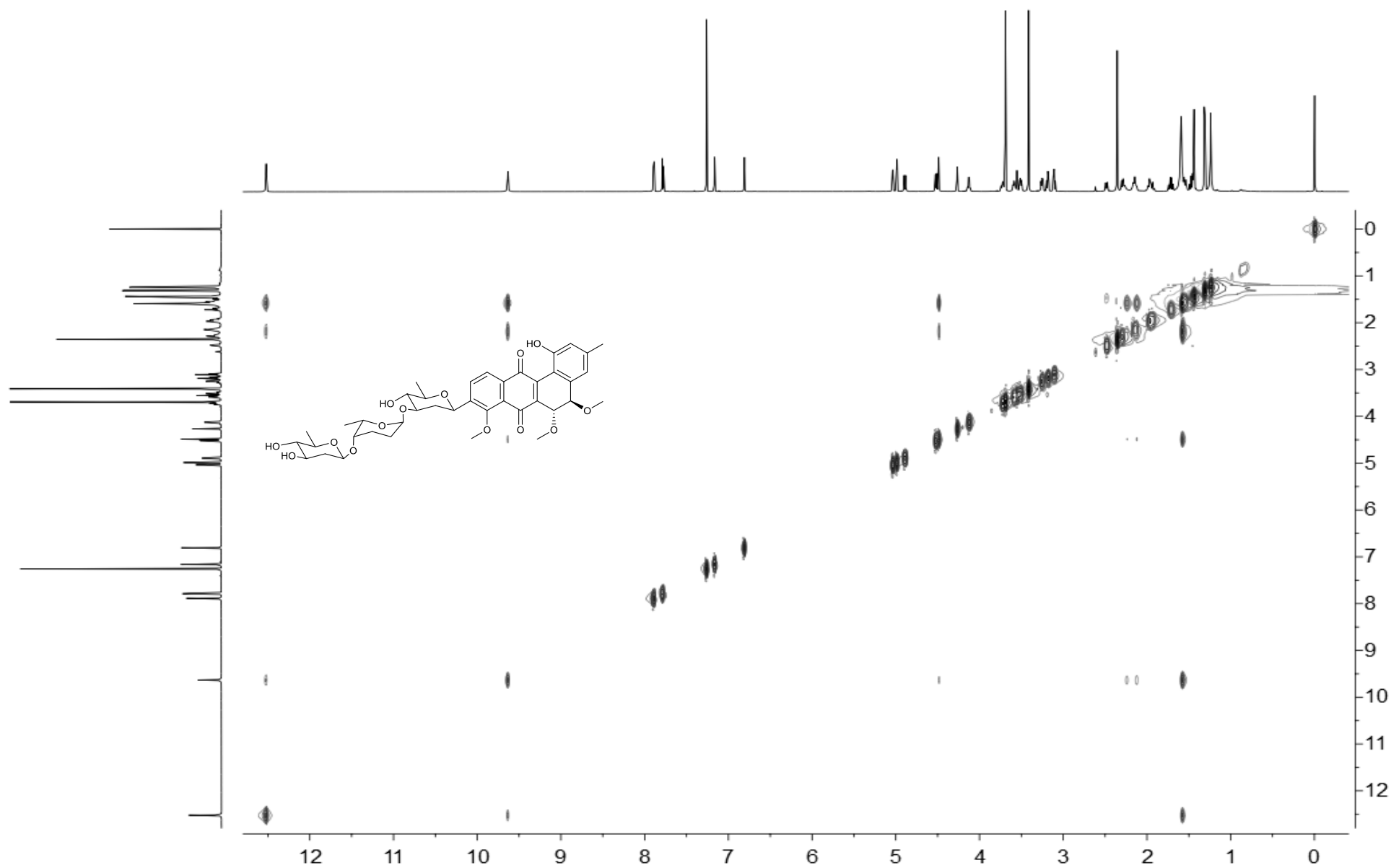


Figure S57. ^1H NMR (700 MHz) spectrum of compound **9** in CDCl_3 .

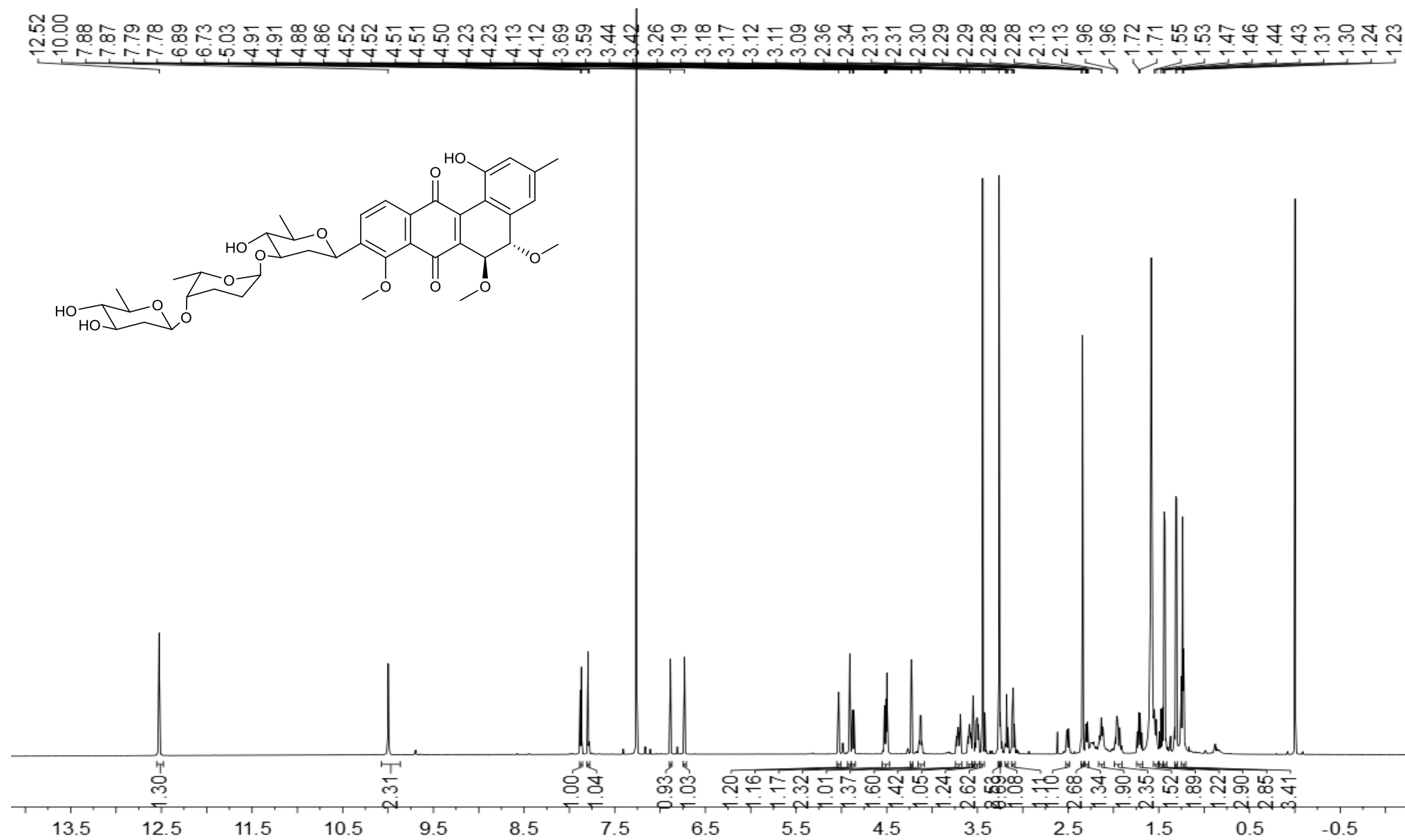


Figure S58. ^{13}C NMR (176 MHz) spectrum of compound **9** in CDCl_3 .

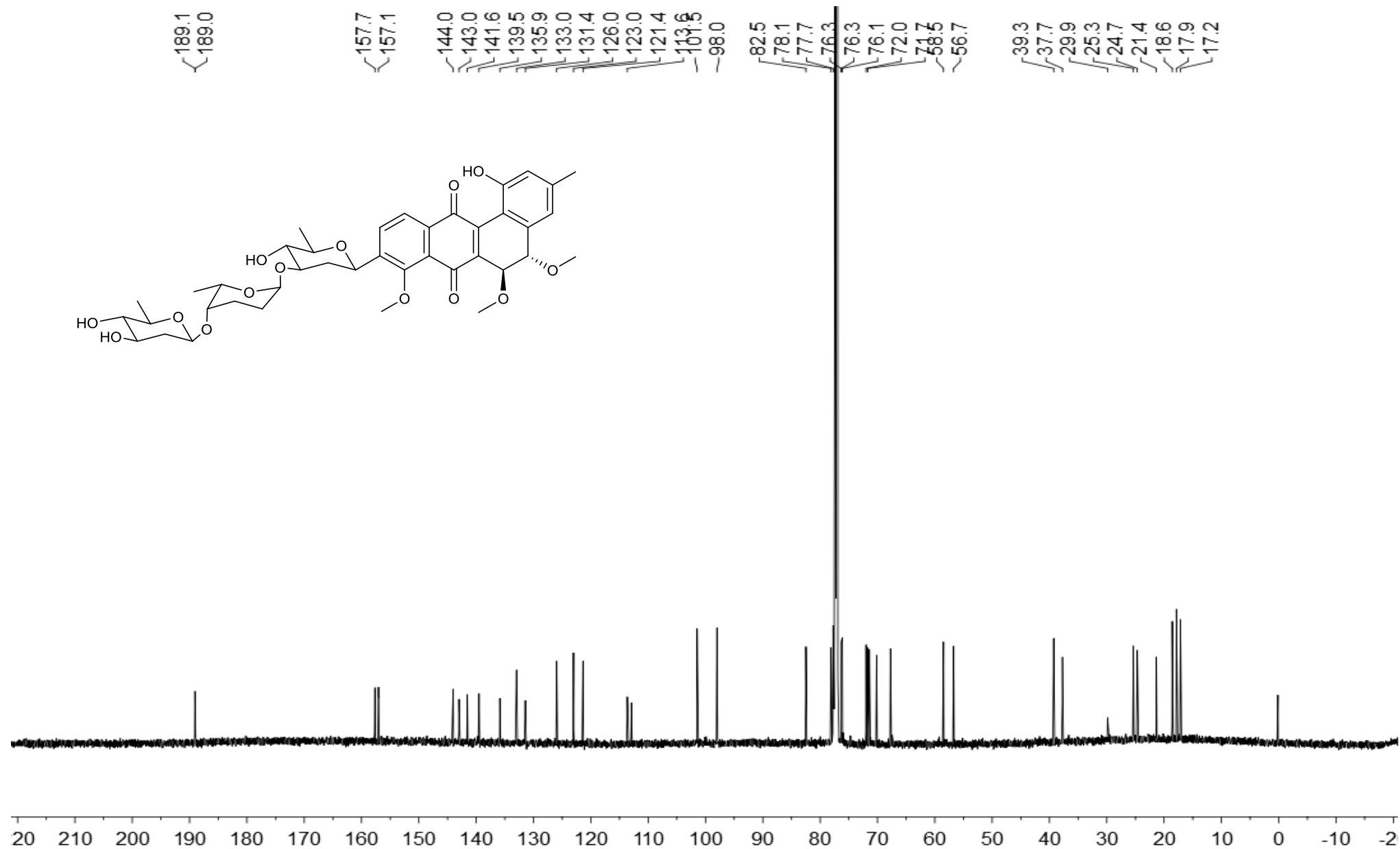


Figure S59. ^{13}C DEPT spectrum of compound **9** in CDCl_3 .

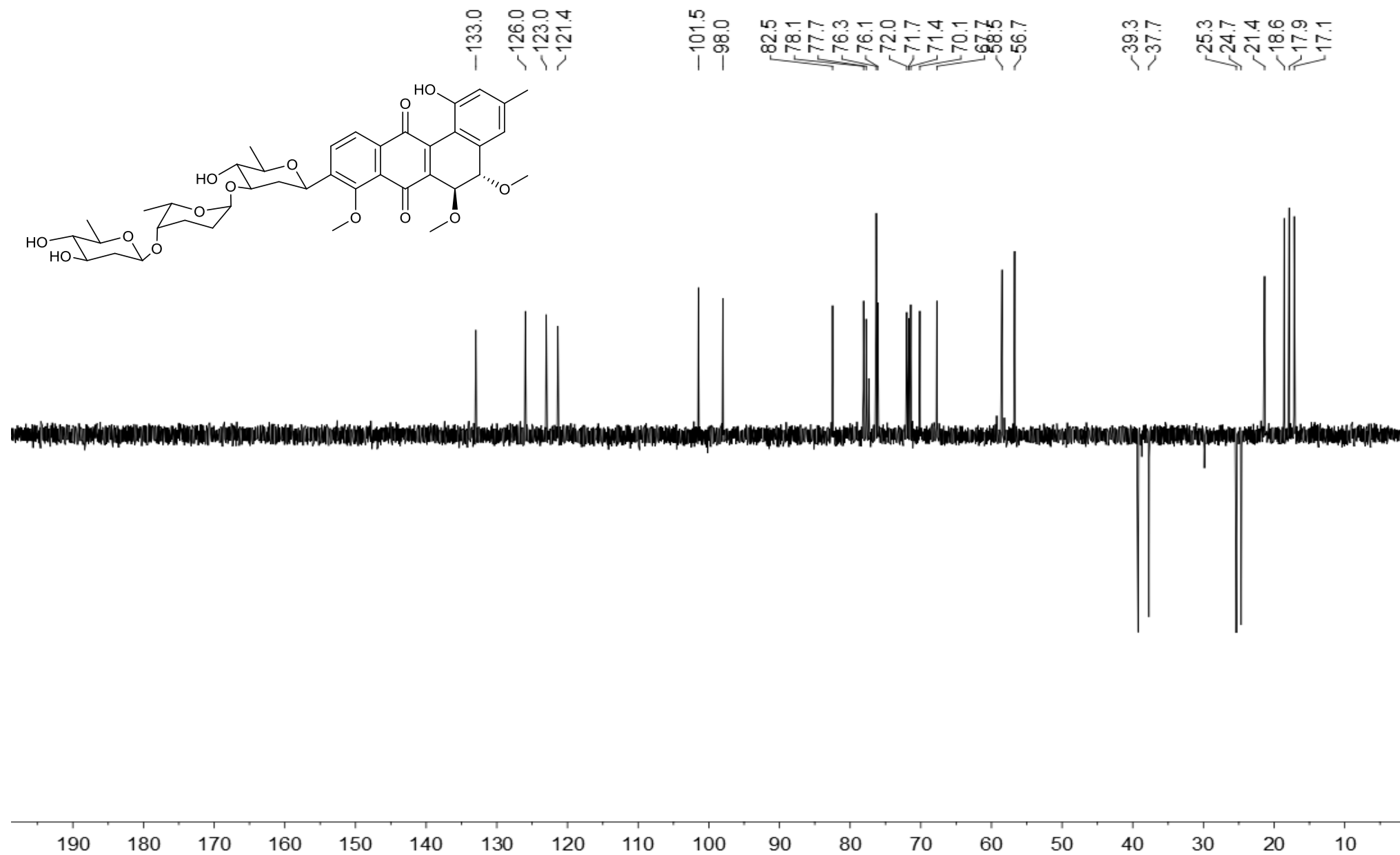


Figure S60. ^1H - ^1H COSY spectrum of compound **9** in CDCl_3 .

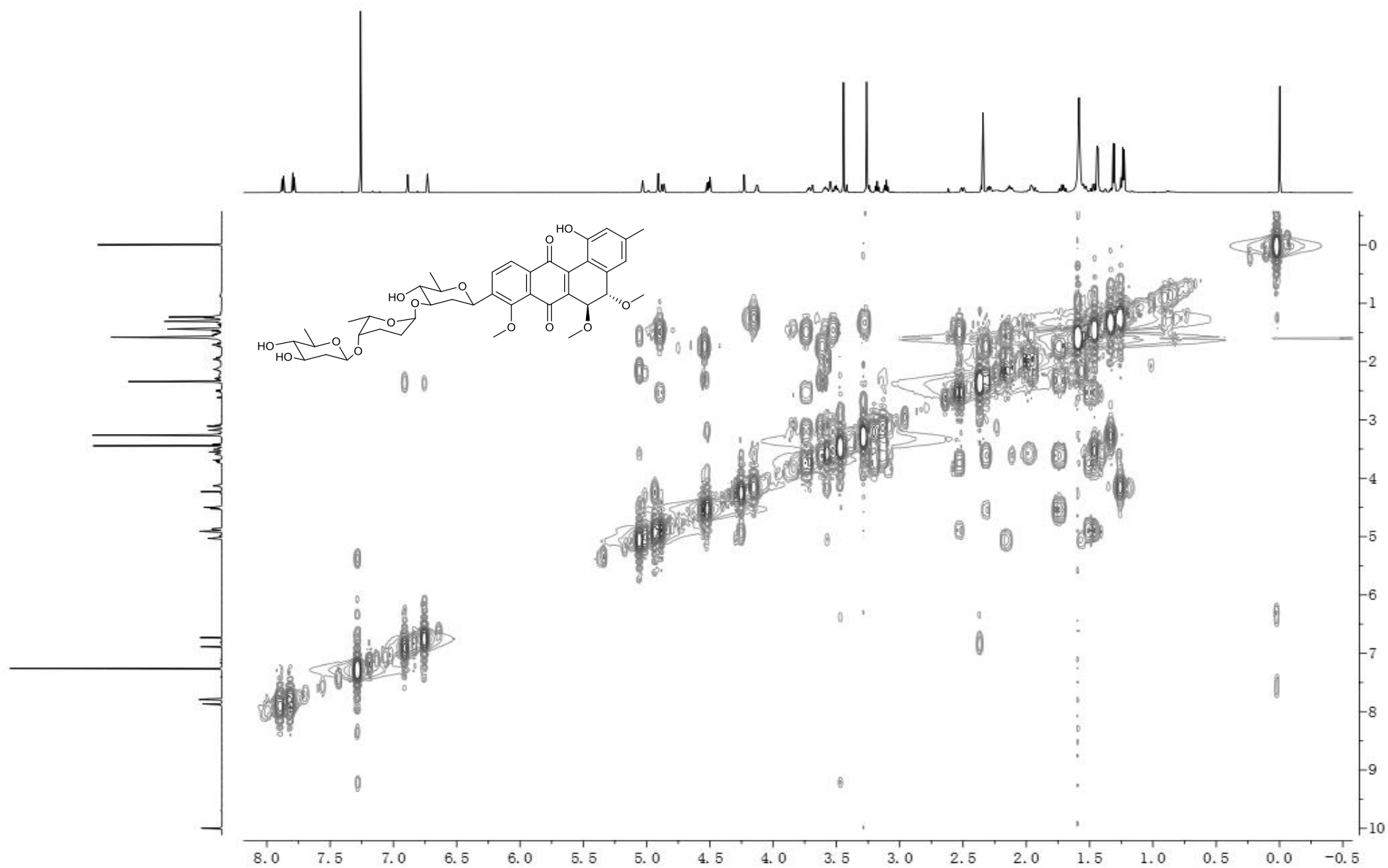


Figure S61. HSQC spectrum of compound **9** in CDCl₃.

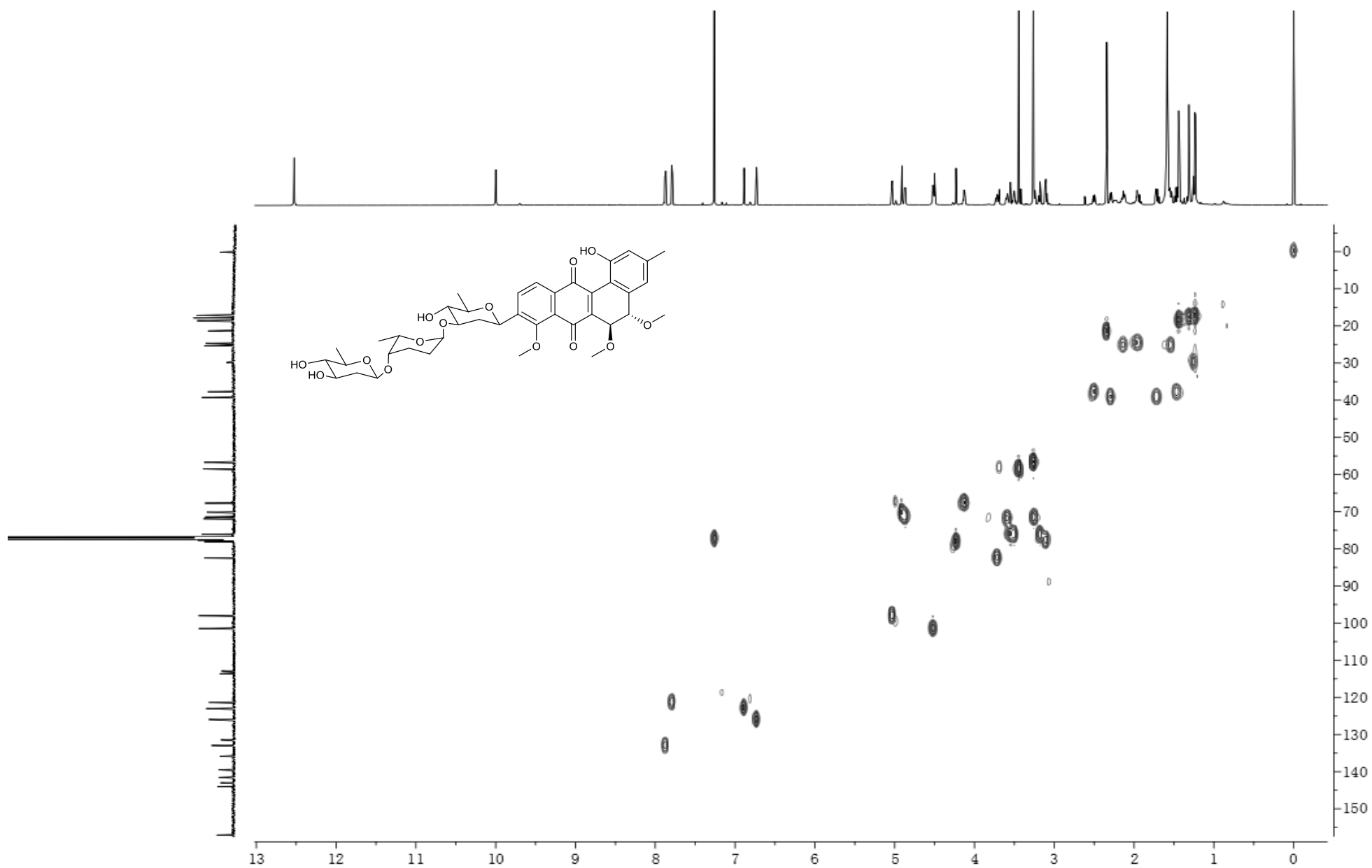


Figure S62. HMBC spectrum of compound **9** in CDCl₃.

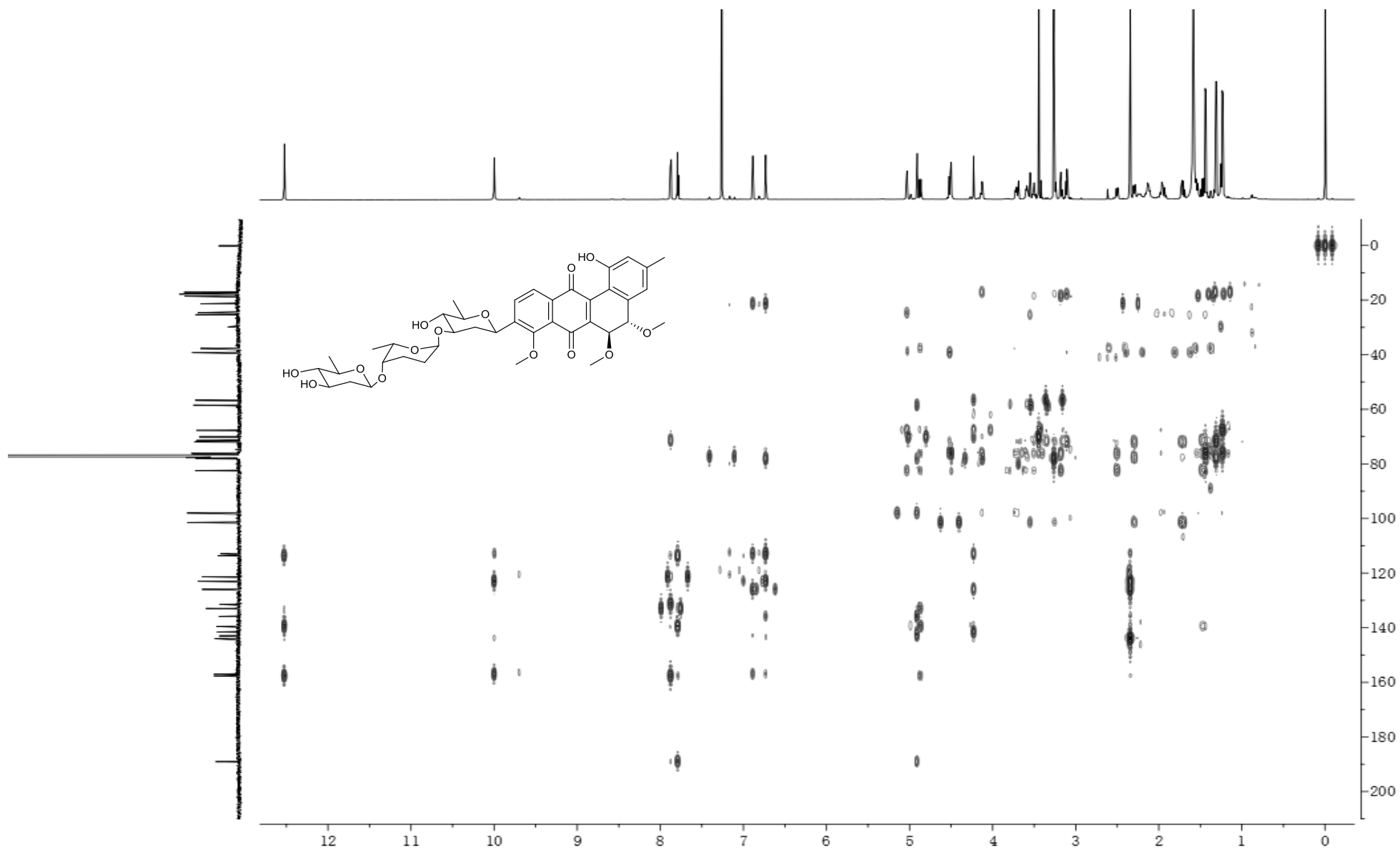


Figure S63. NOESY spectrum of compound **9** in CDCl₃.

