Myrmenaphthol A, Isolated From a Hawaiian Sponge of Genus *Myrmekioderma*

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Figure S1. [1]H NMR Spectrum (500 MHz) of Myrmenaphthol A **(1)** in MeOH-d_4

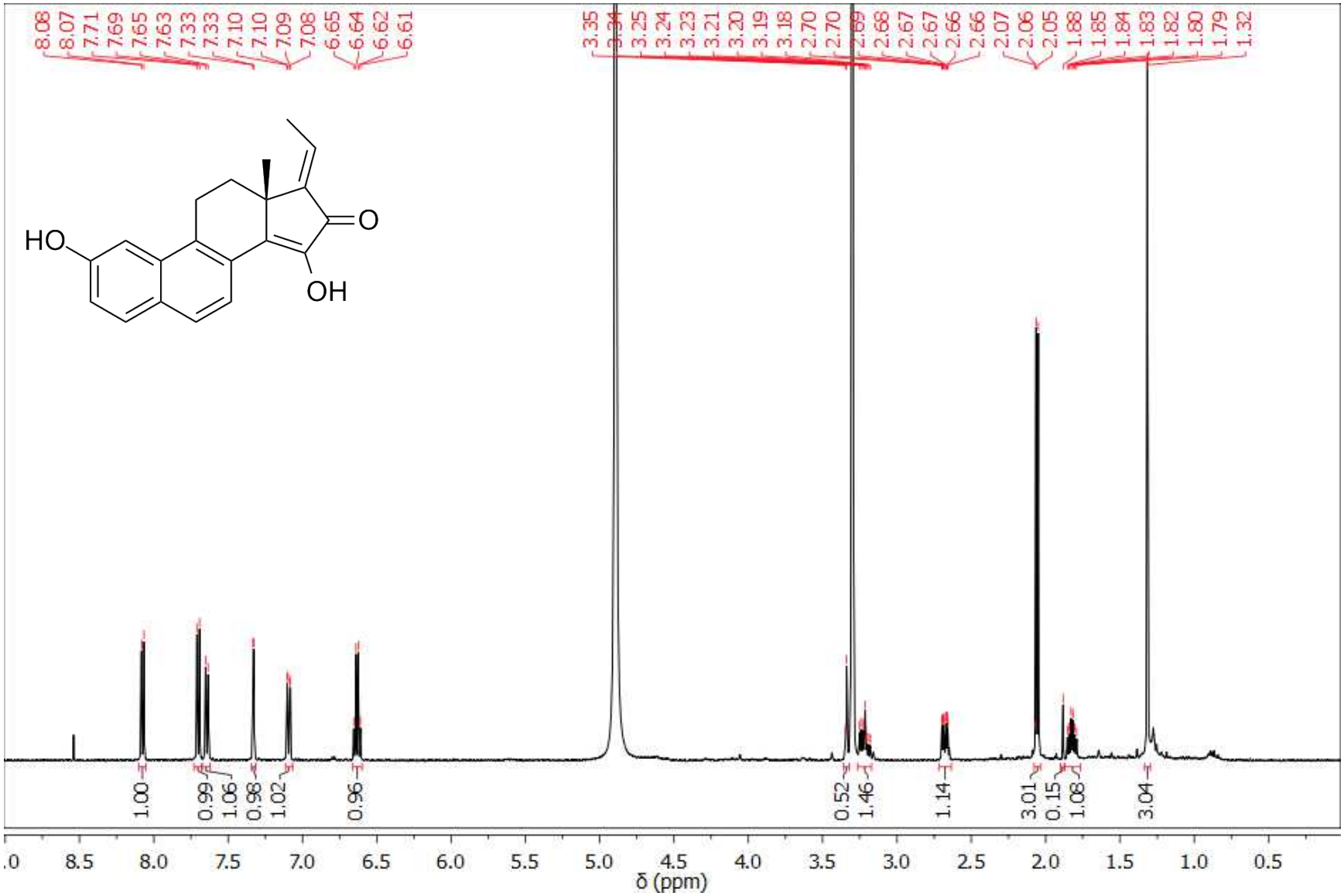


Figure S2. ^{13}C NMR Spectrum (125 MHz) of Myrmenaphthol A **(1)** in MeOH-d_4

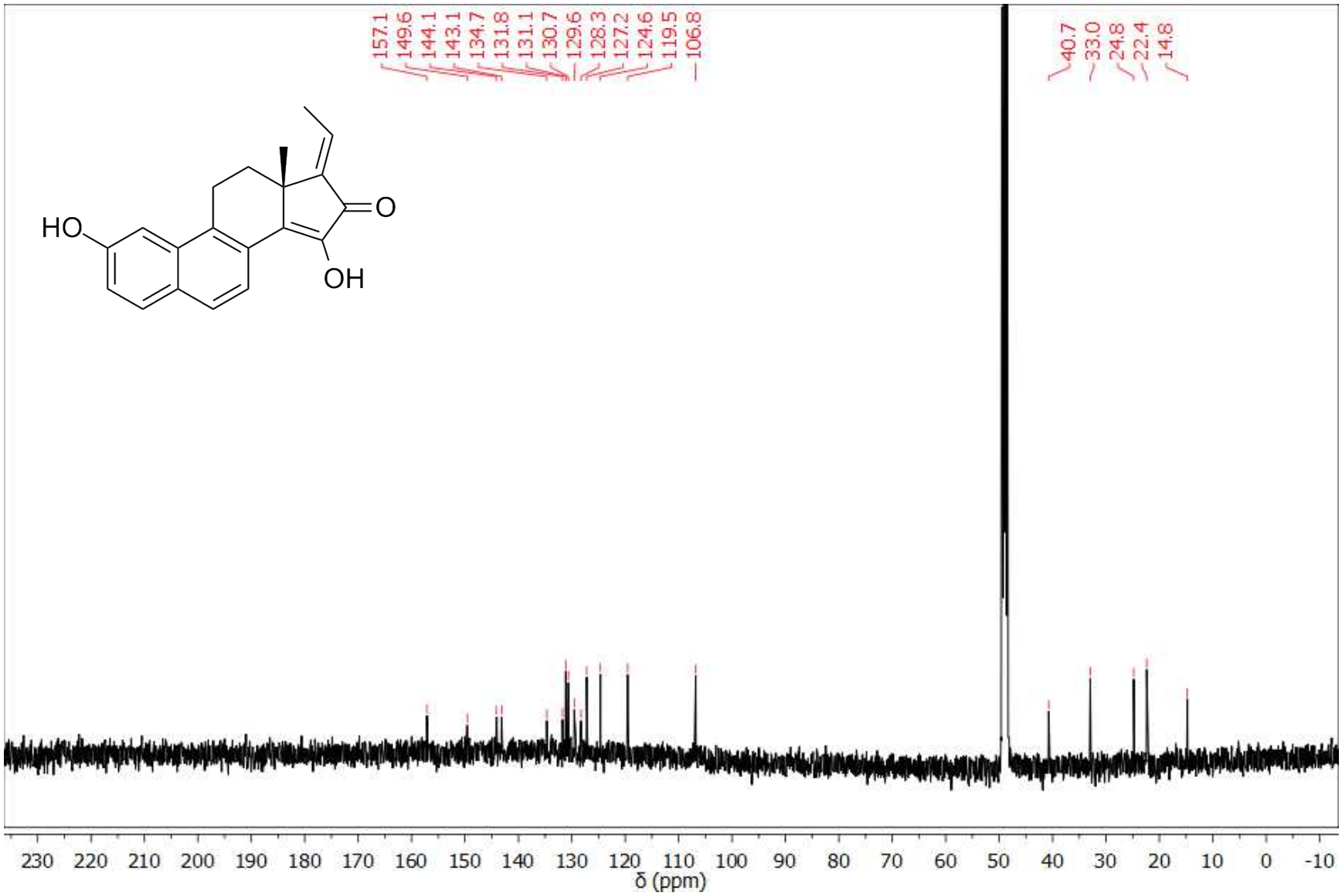


Figure S3. gHSQC NMR Spectrum (500 MHz) of Myrmenaphthol A **(1)** in MeOH-d_4

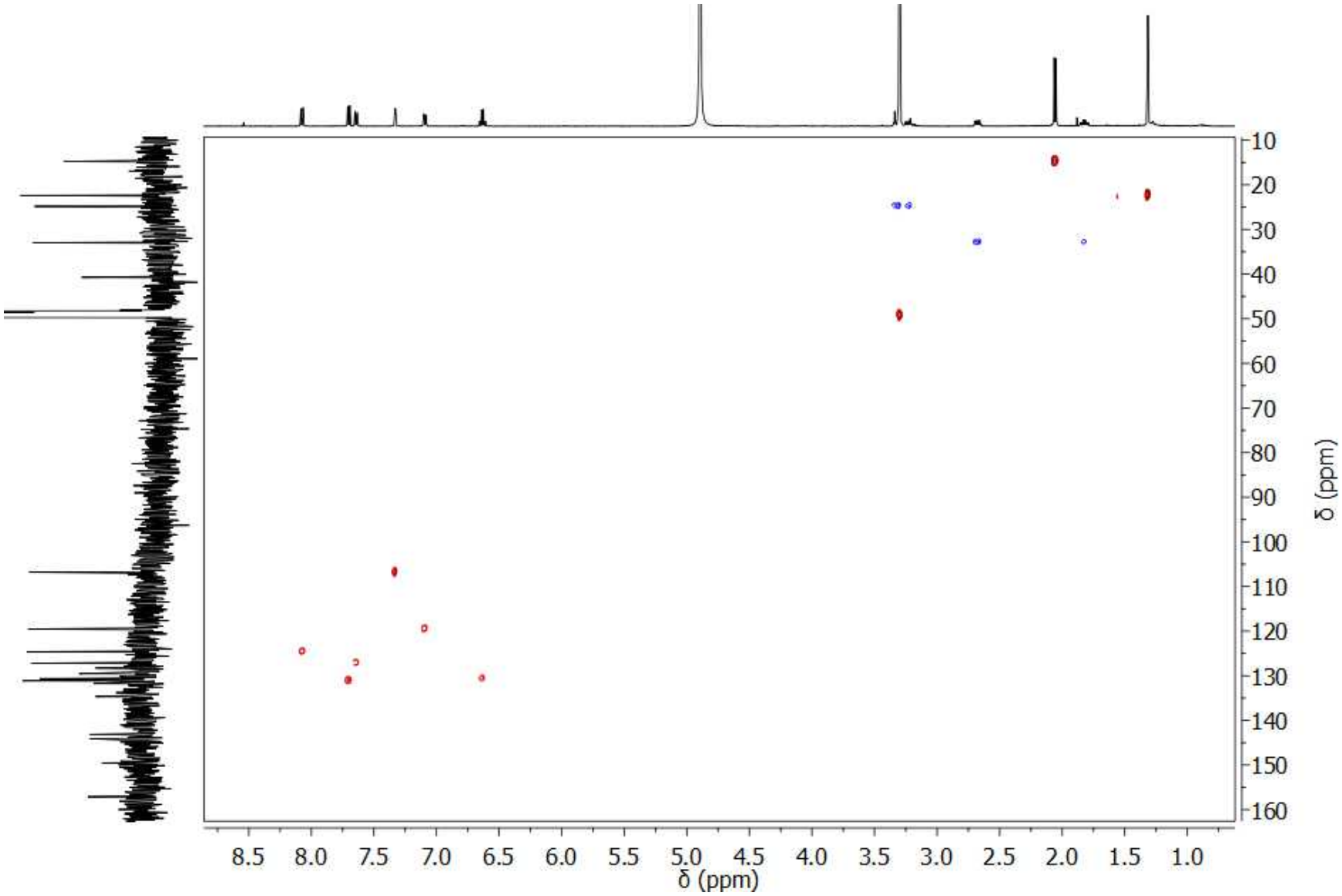


Figure S4. gCOSY NMR Spectrum (500 MHz) of Myrmenaphthol A **(1)** in MeOH-d_4

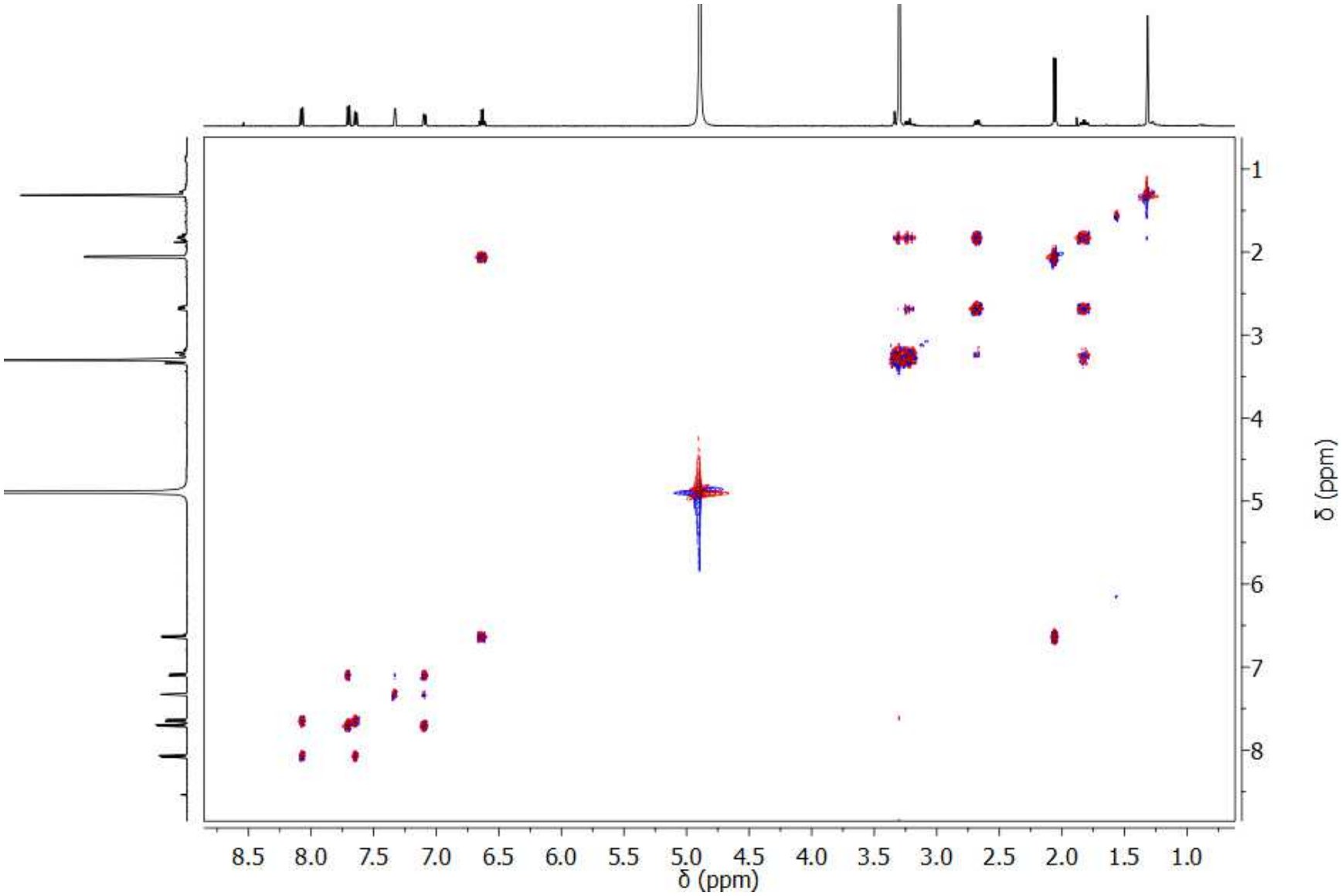


Figure S5. gHMBC NMR Spectrum (500 MHz) of Myrmenaphthol A **(1)** in MeOH-d_4

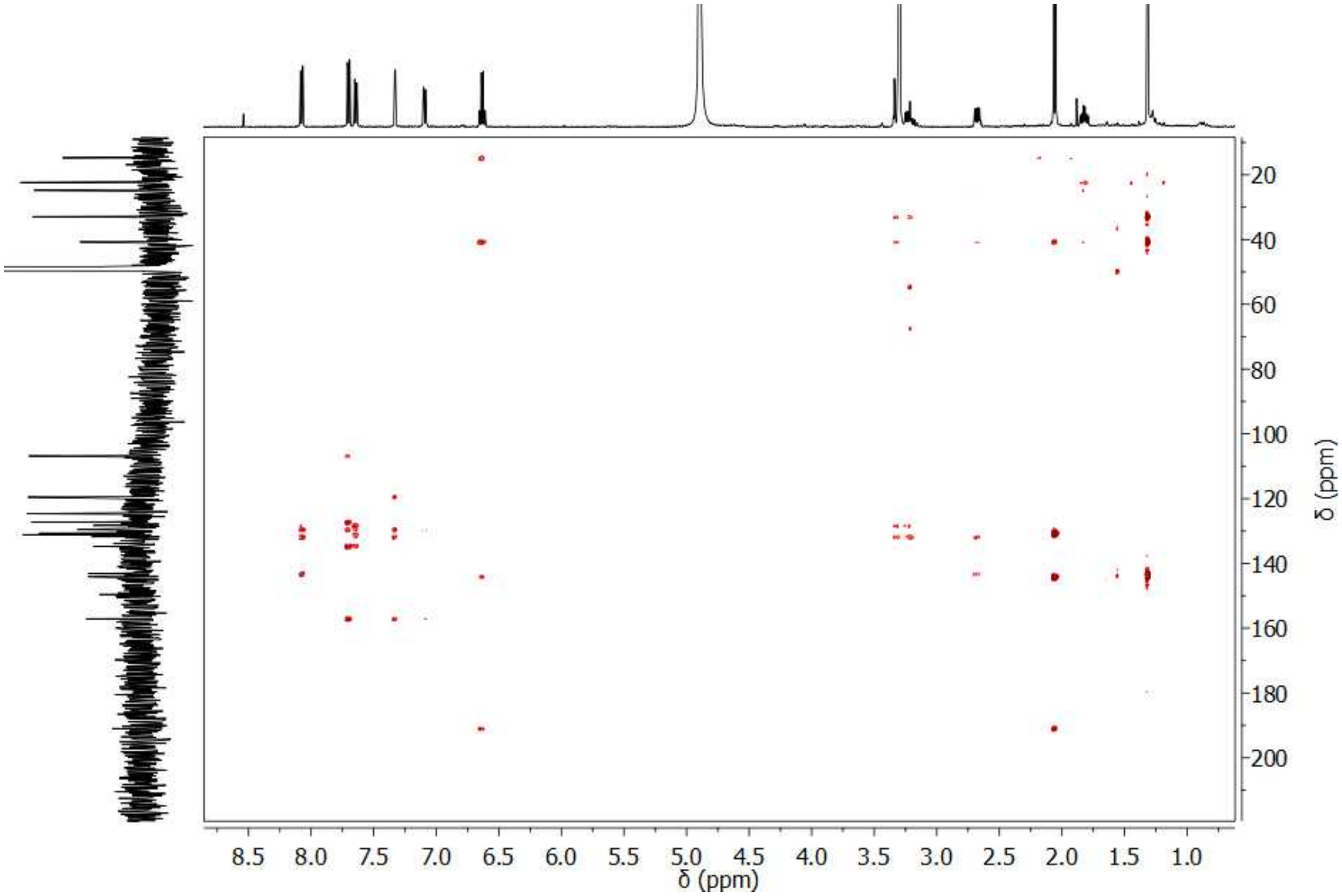


Figure S6. gROESY Spectrum (500 MHz) of Myrmenaphthol A **(1)** in MeOH-d_4

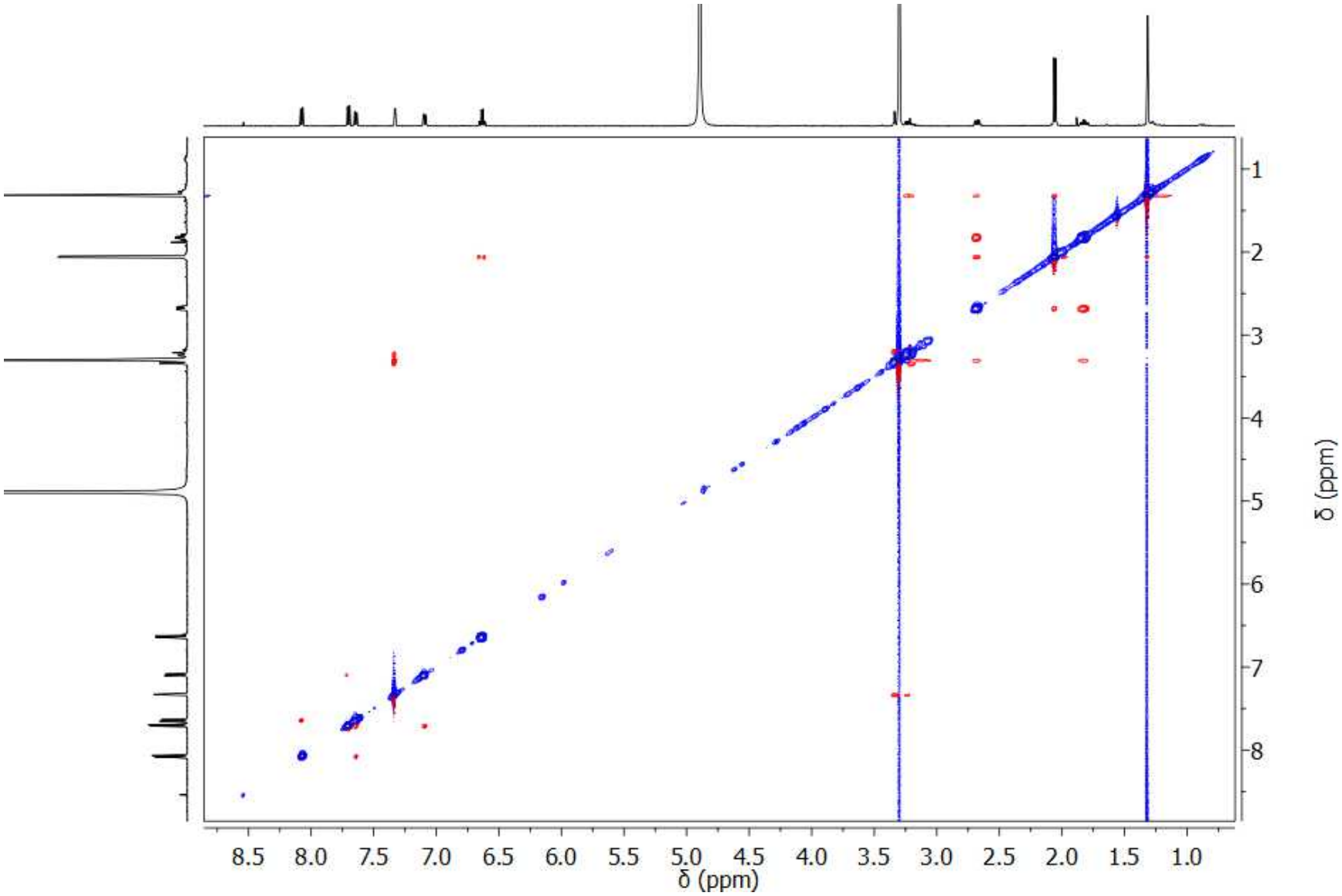


Figure S7. ^{1}H NMR Spectrum (500 MHz) of Cinanthrenol A **(2)** in MeOH-d_4

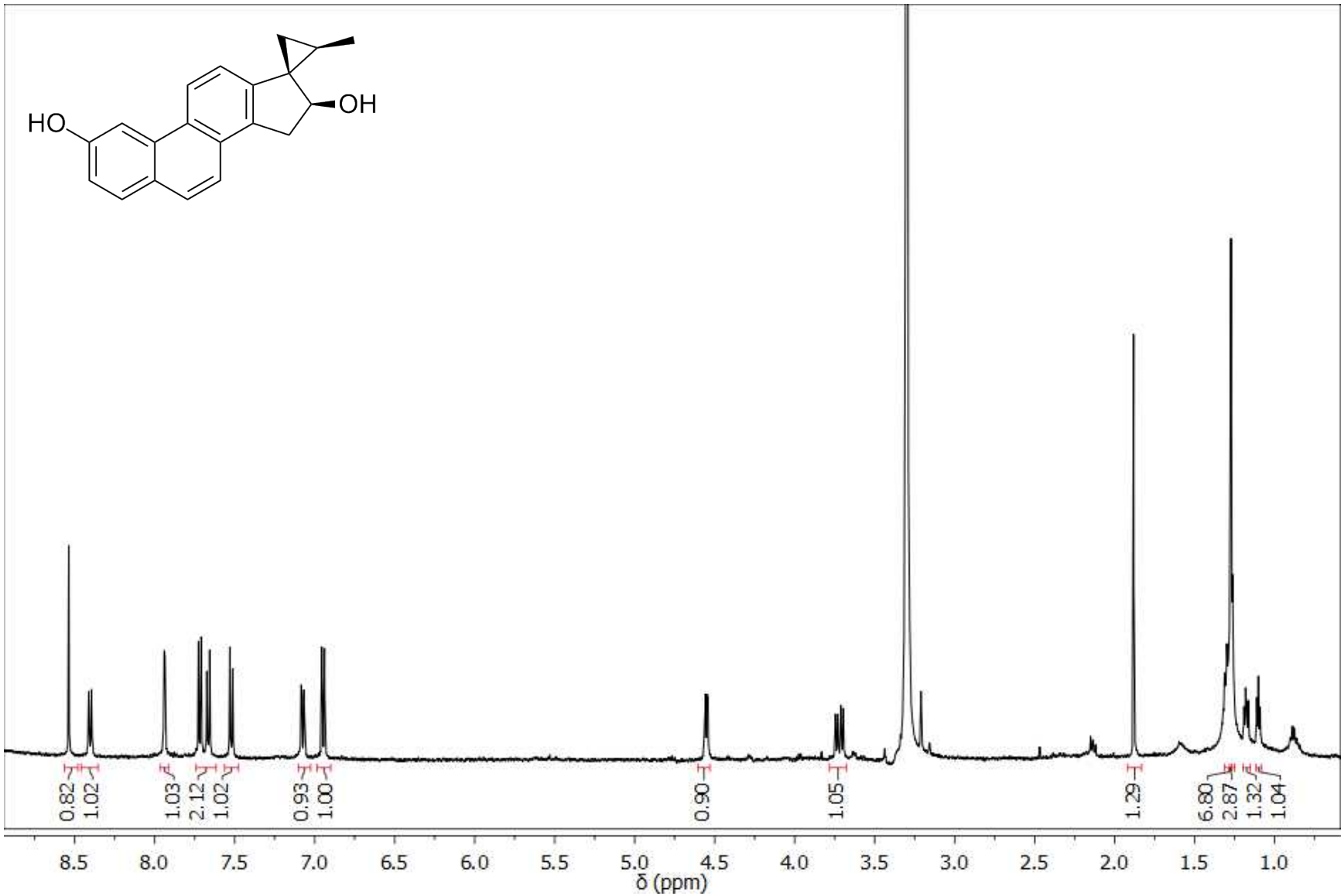


Figure S9. gHSQC NMR Spectrum (500 MHz) of Cinanthrenol A **(2)** in MeOH-d_4

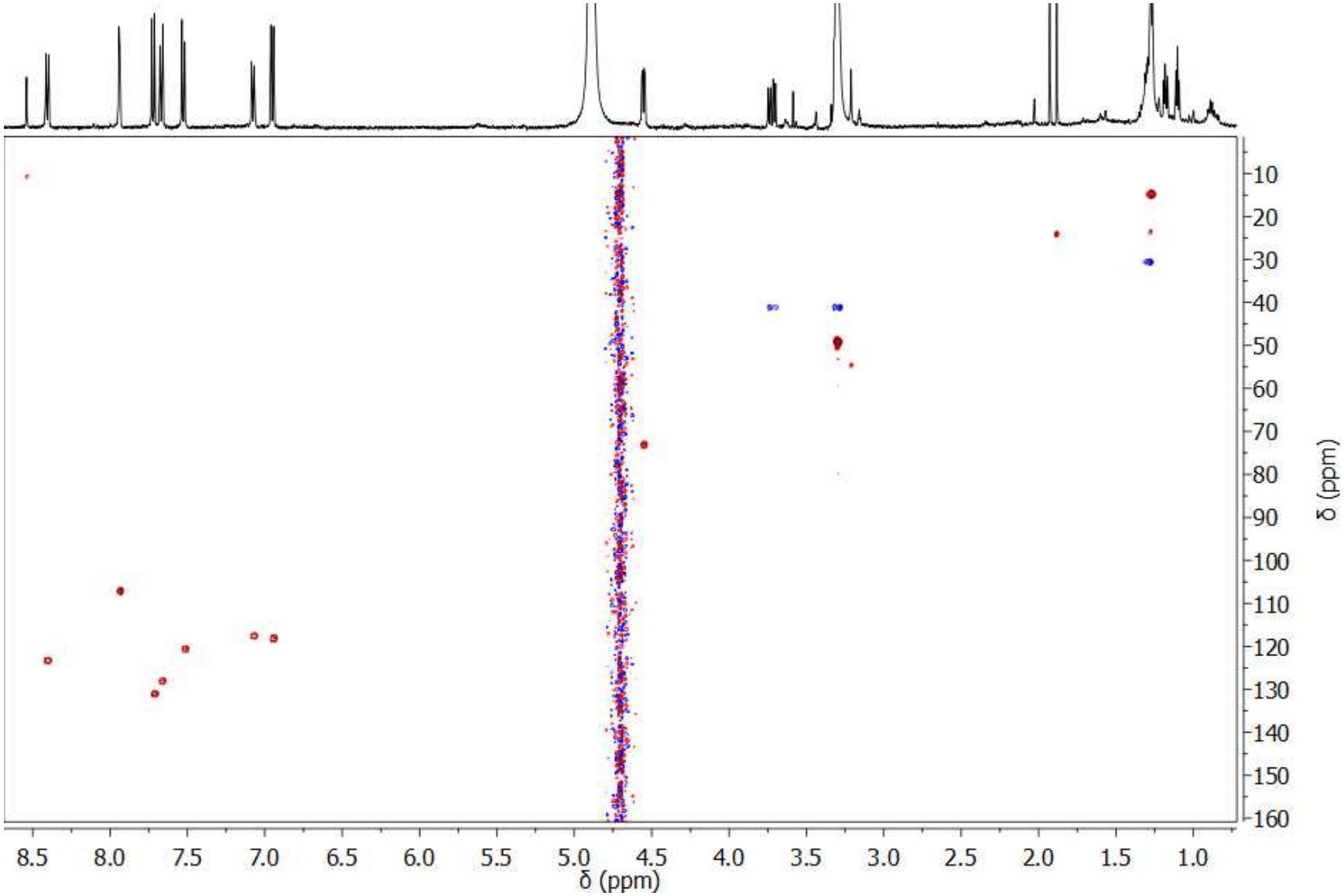


Figure 10: ^{1}H NMR Spectrum of 3,4-dihydroxypregna-5,17-diene-10,2-carbolactone (3) (CD_3OD, 500 MHz)

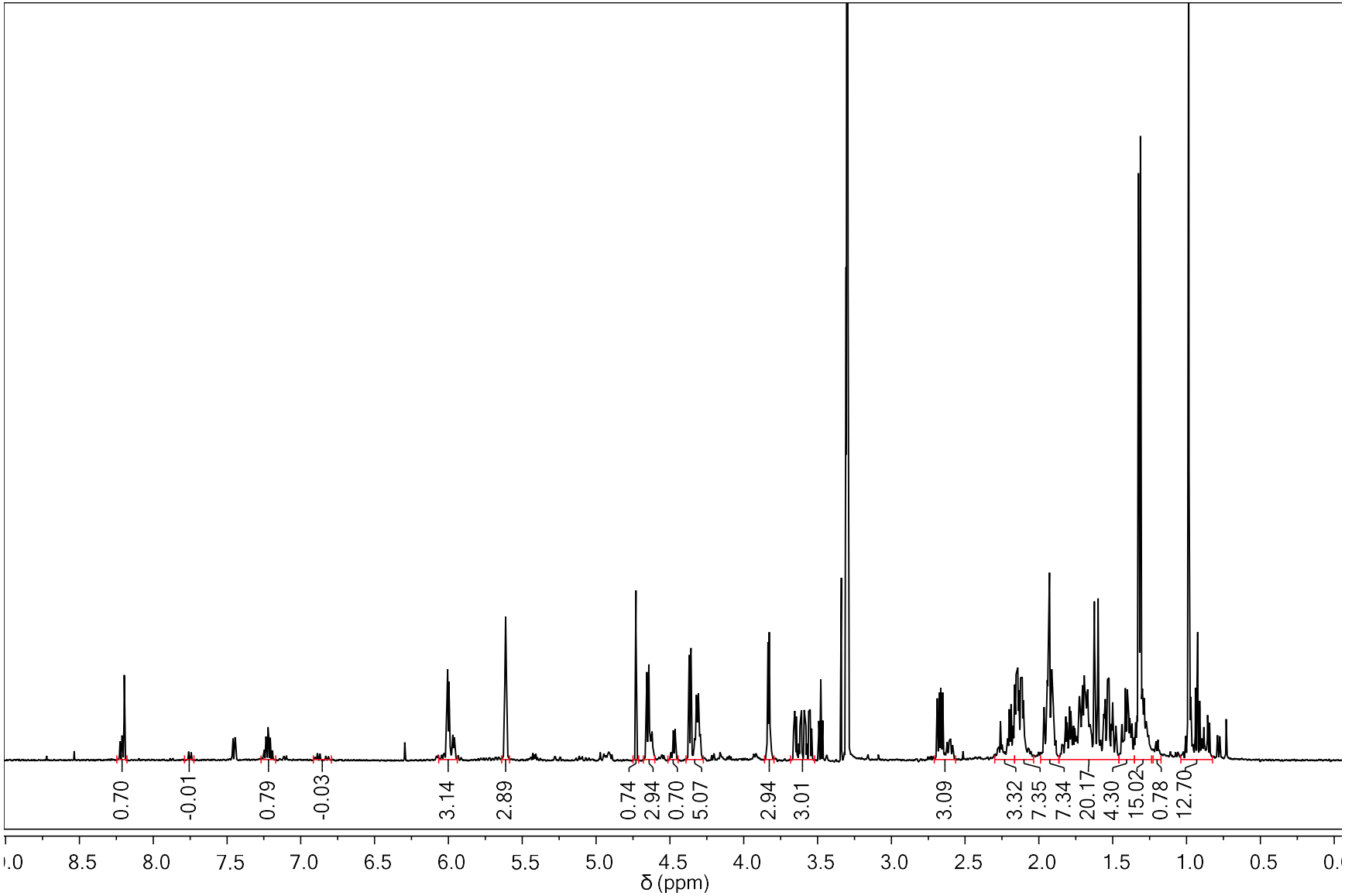


Figure 11: ^{1}H NMR Spectrum of 3,4-dihydroxypregna-5,20-diene-10,2-carbolactone (4) (CD3OD, 500 MHz)

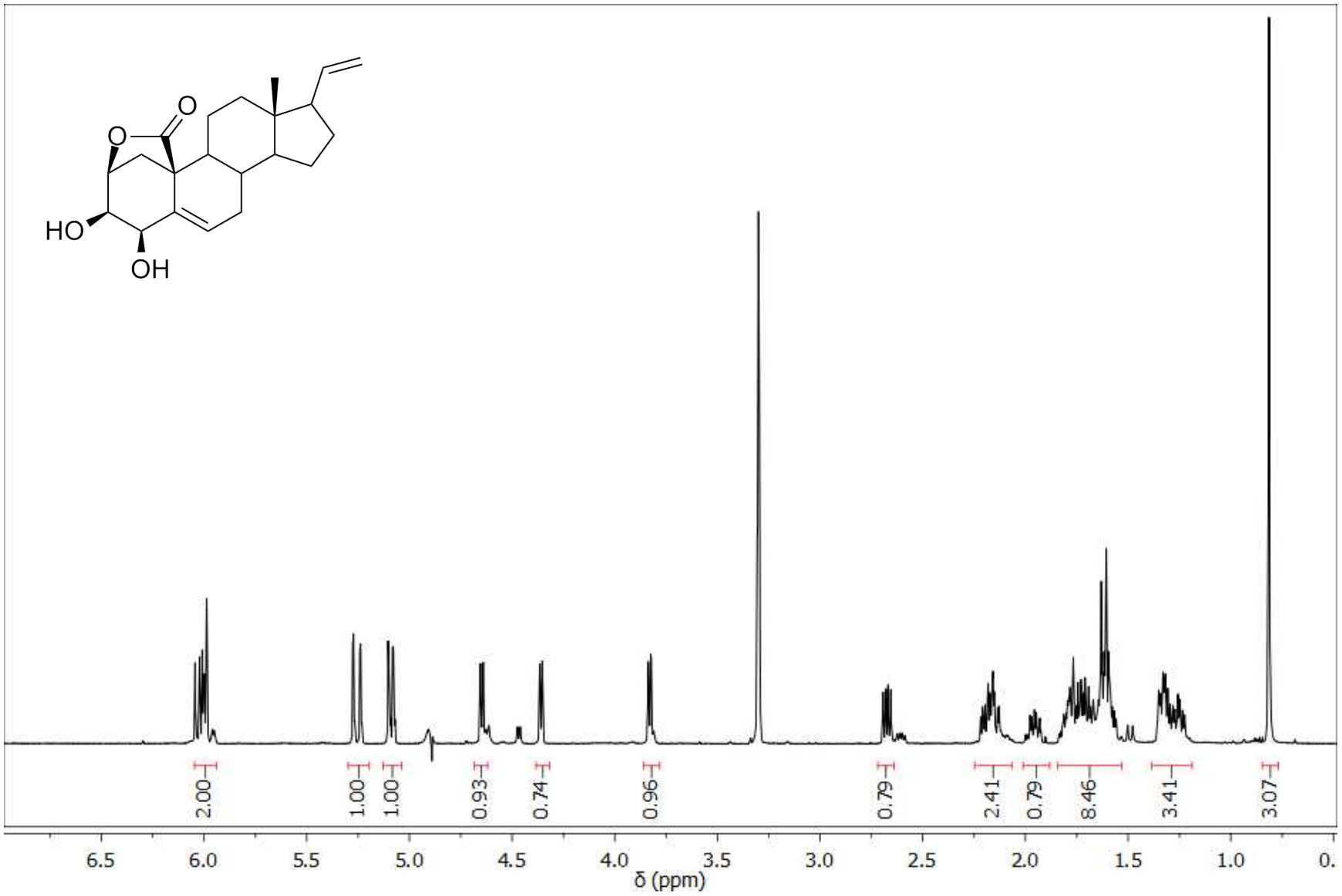


Figure S12. Image of *Myrmekioderma* sp.

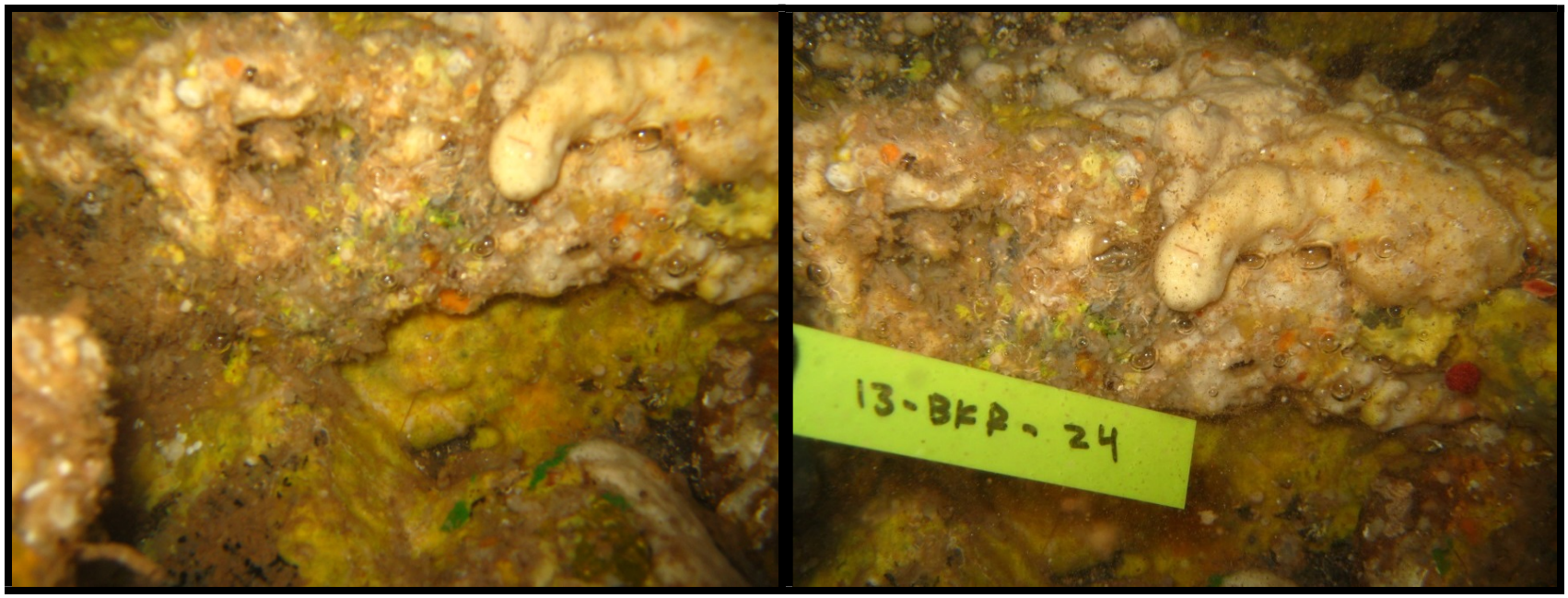
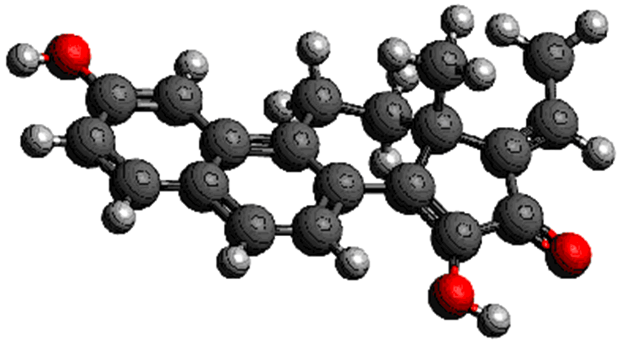


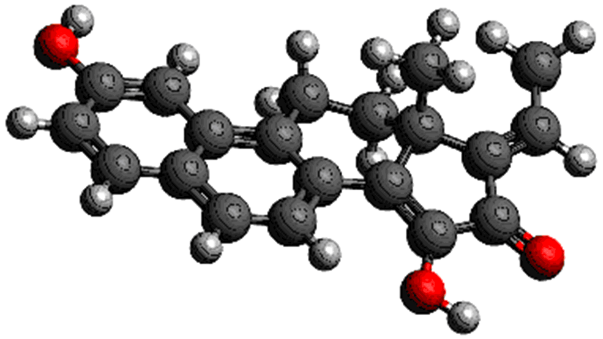
Table S1. Optimized Conformers Energy and Abundance.

Filename	Energy (kcal/mol)	Relative Energy (kcal/mol)	Boltzmann Factor	Equilibrium Mole Fraction	Number of Imaginary Frequencies
SP1-opt_freq-conf-1.out	-626268.4843	0.312499677	0.58976892	0.369809964	0
SP1-opt_freq-conf-3.out	-626265.1258	3.670929937	0.00202396	0.001269111	0
SP1-opt_freq-conf-4.out	-626265.358	3.438751463	0.00299626	0.001878782	0
SP1-opt_freq-conf-2.out	-626268.7968	0	1	0.627042143	0

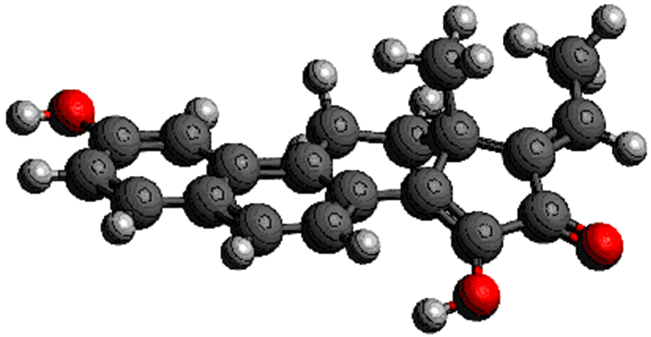
Conformer 1



Conformer 2



Conformer 3



Conformer 4

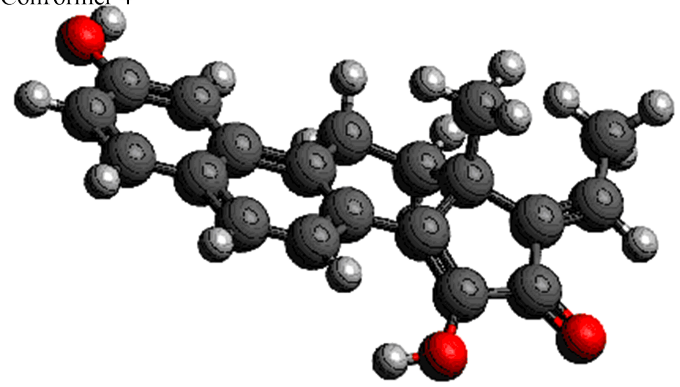


Table S2. Cartesian Coordinates For The Re-Optimized Conformer 1 Of Compound (1)

Number	Atomic	Coordinates (Angstrom)		
		X	Y	Z
1	C	4.330634	1.35584	0.206493
2	C	2.920039	1.209219	0.161322
3	C	2.364438	-0.08278	-0.07172
4	C	3.245318	-1.18449	-0.23973
5	C	4.609504	-1.00656	-0.18244
6	C	5.164254	0.279162	0.038967
7	C	2.056564	2.32343	0.347766
8	C	0.699874	2.16344	0.314812
9	C	0.129199	0.873948	0.088255
10	C	0.939931	-0.23685	-0.12088
11	C	-1.32159	0.703284	0.076284
12	C	-1.90278	-0.68947	0.284019
13	C	-1.14992	-1.61185	-0.68749
14	C	0.355094	-1.60631	-0.39744
15	C	-3.37549	-0.49427	-0.03553
16	C	-3.60263	0.953716	-0.26089
17	C	-2.29183	1.613533	-0.16686
18	O	5.403156	-2.10009	-0.34393
19	O	-2.17028	2.935868	-0.39241
20	O	-4.64811	1.541486	-0.51792
21	C	-4.38414	-1.37112	-0.11222
22	C	-4.33348	-2.84978	0.100741
23	C	-1.71235	-1.13002	1.748585
24	H	4.748197	2.345111	0.38043
25	H	2.867973	-2.18775	-0.40687
26	H	6.245257	0.397598	0.076321
27	H	2.495476	3.302709	0.525554
28	H	0.038769	3.009417	0.469277
29	H	-1.3341	-1.25861	-1.70937
30	H	-1.523	-2.63898	-0.6276
31	H	0.875785	-2.05263	-1.25175
32	H	0.572636	-2.26184	0.457755
33	H	6.343921	-1.85673	-0.2859
34	H	-3.0586	3.295447	-0.5893
35	H	-5.36149	-0.95324	-0.36204
36	H	-5.05793	-3.13979	0.869319

37	H	-4.6253	-3.37132	-0.81774
38	H	-3.34833	-3.20536	0.402129
39	H	-2.29165	-0.48405	2.414367
40	H	-2.04824	-2.1617	1.891158
41	H	-0.66145	-1.06886	2.046008

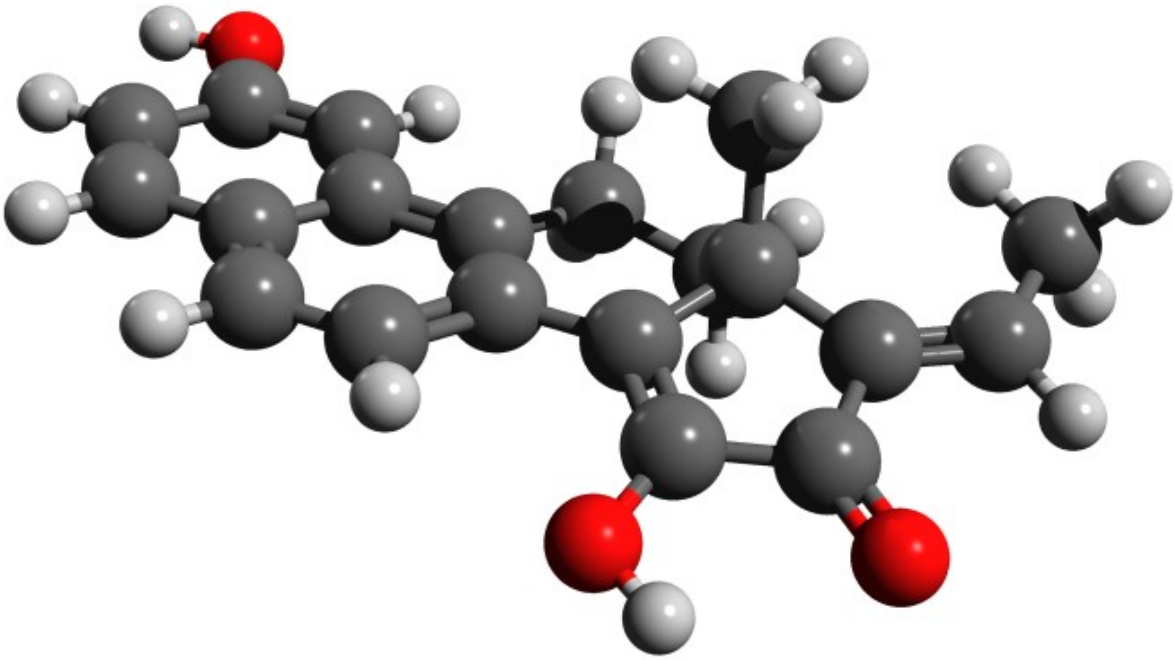


Table S3. Cartesian Coordinates For The Re-Optimized Conformer 2 Of Compound (1)

Center Number	Atomic Number	Coordinates (Angstrom)		
		X	Y	Z
1	C	4.334731	1.360531	0.207675
2	C	2.921933	1.212171	0.163804
3	C	2.366905	-0.0793	-0.06781
4	C	3.250959	-1.18179	-0.23717
5	C	4.614208	-0.99964	-0.18302
6	C	5.168335	0.286647	0.038684
7	C	2.058616	2.32531	0.349629
8	C	0.701209	2.165151	0.316369
9	C	0.131627	0.876325	0.090813
10	C	0.943854	-0.2348	-0.11656
11	C	-1.31901	0.704825	0.076975
12	C	-1.90008	-0.68772	0.286223
13	C	-1.14574	-1.61139	-0.6828
14	C	0.359097	-1.60485	-0.3915
15	C	-3.37239	-0.49359	-0.03611
16	C	-3.59945	0.953822	-0.26518
17	C	-2.28907	1.614233	-0.16993
18	O	5.507	-2.01395	-0.33453
19	O	-2.16736	2.936048	-0.39814
20	O	-4.64452	1.540701	-0.52589
21	C	-4.38066	-1.37087	-0.11242
22	C	-4.32993	-2.84899	0.10428
23	C	-1.71152	-1.12562	1.751803
24	H	4.74947	2.351039	0.381411
25	H	2.862808	-2.1828	-0.40344
26	H	6.24896	0.391884	0.071884
27	H	2.497061	3.304915	0.526727
28	H	0.040127	3.01131	0.470031
29	H	-1.32902	-1.2601	-1.70552
30	H	-1.51834	-2.63862	-0.62151
31	H	0.879696	-2.05252	-1.24524
32	H	0.575649	-2.25919	0.464924
33	H	5.04494	-2.85917	-0.47991
34	H	-3.05534	3.294941	-0.59782
35	H	-5.35775	-0.9539	-0.36479
36	H	-5.05566	-3.13733	0.87228

37	H	-4.6199	-3.37288	-0.81345
38	H	-3.34522	-3.20347	0.408375
39	H	-2.29208	-0.47871	2.415576
40	H	-2.04702	-2.15722	1.895877
41	H	-0.66106	-1.06323	2.050612

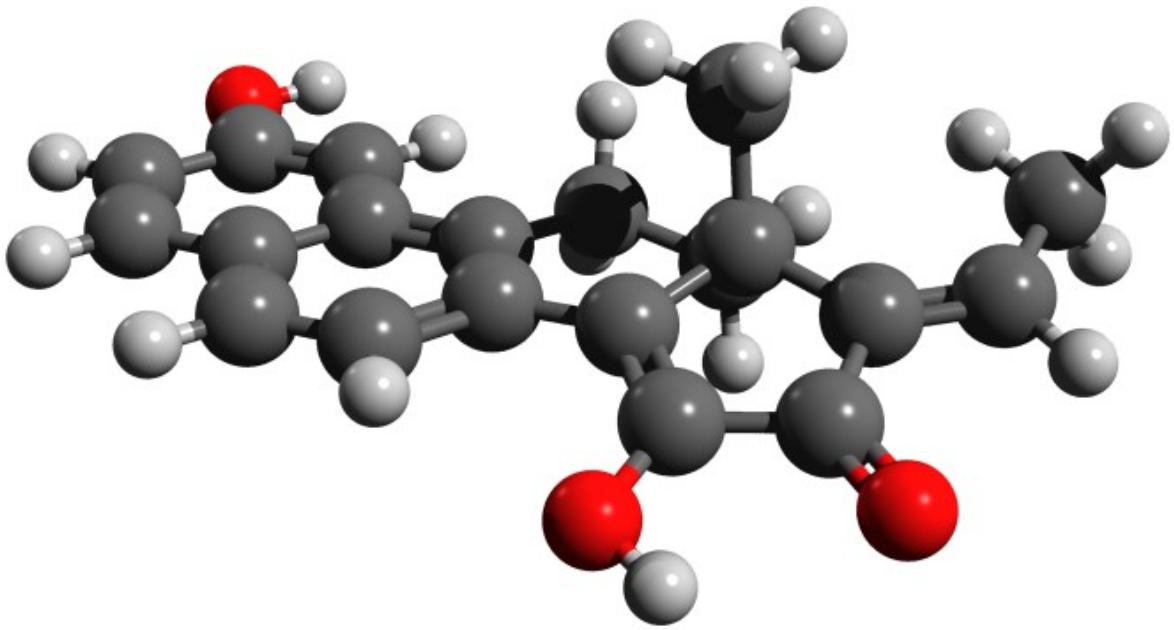


Table S4. Cartesian Coordinates For The Re-Optimized Conformer 3 Of Compound (1)

Center Number	Atomic Number	Coordinates (Angstrom)		
		X	Y	Z
1	C	4.328564	1.315938	0.317626
2	C	2.917104	1.18307	0.251108
3	C	2.353511	-0.08502	-0.07677
4	C	3.227601	-1.17854	-0.31546
5	C	4.592686	-1.01444	-0.23794
6	C	5.155254	0.248055	0.078658
7	C	2.061265	2.283121	0.525994
8	C	0.703582	2.135086	0.464518
9	C	0.124293	0.878847	0.113535
10	C	0.928324	-0.22446	-0.14782
11	C	-1.32992	0.718657	0.058769
12	C	-1.9092	-0.66952	0.291554
13	C	-1.18068	-1.58894	-0.70458
14	C	0.335299	-1.58039	-0.47149
15	C	-3.38417	-0.47224	-0.0043
16	C	-3.61094	0.966777	-0.30803
17	C	-2.28473	1.616973	-0.27347
18	O	5.37952	-2.09795	-0.4742
19	O	-2.21911	2.920436	-0.61848
20	O	-4.67042	1.518156	-0.57057
21	C	-4.39861	-1.34497	-0.02143
22	C	-4.35172	-2.81487	0.247429
23	C	-1.68236	-1.11	1.749195
24	H	4.751354	2.286809	0.566265
25	H	2.844913	-2.16405	-0.55837
26	H	6.236761	0.355091	0.131779
27	H	2.503145	3.237507	0.803206
28	H	0.056962	2.967624	0.731655
29	H	-1.4048	-1.23723	-1.71876
30	H	-1.54796	-2.6176	-0.63124
31	H	0.827728	-1.9893	-1.36073
32	H	0.588291	-2.26704	0.348863
33	H	6.321852	-1.86712	-0.39279
34	H	-1.31592	3.181819	-0.86857
35	H	-5.37934	-0.93024	-0.26301
36	H	-5.00721	-3.06079	1.090264

37	H	-4.73452	-3.36642	-0.61819
38	H	-3.34905	-3.17784	0.472745
39	H	-2.23171	-0.45423	2.430727
40	H	-2.0293	-2.13573	1.904732
41	H	-0.62206	-1.06528	2.014803

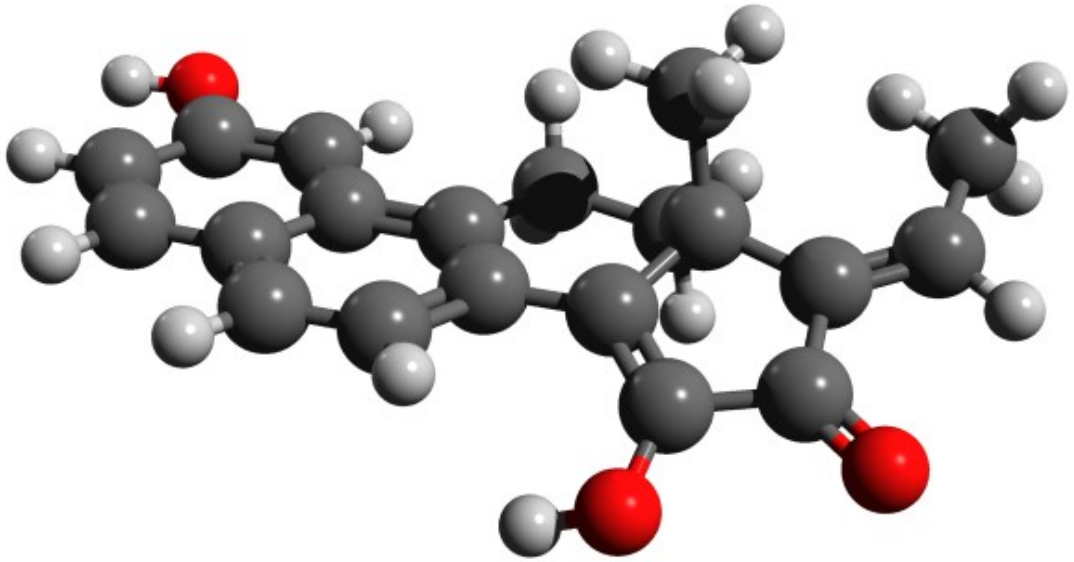


Table S5. Cartesian Coordinates For The Re-Optimized Conformer 4 Of Compound (1)

Center Number	Atomic Number	Coordinates (Angstrom)		
		X	Y	Z
1	C	4.332664	1.320747	0.317601
2	C	2.919007	1.185667	0.252734
3	C	2.356049	-0.0823	-0.07266
4	C	3.233355	-1.17687	-0.31145
5	C	4.597547	-1.00801	-0.23702
6	C	5.159381	0.255611	0.078333
7	C	2.063425	2.284892	0.526314
8	C	0.705013	2.136606	0.465089
9	C	0.126817	0.880715	0.116032
10	C	0.932291	-0.2232	-0.14328
11	C	-1.32723	0.719961	0.059355
12	C	-1.90669	-0.66776	0.293762
13	C	-1.1767	-1.58877	-0.69981
14	C	0.339105	-1.57974	-0.46515
15	C	-3.38131	-0.47114	-0.00487
16	C	-3.60748	0.967093	-0.31261
17	C	-2.28144	1.61756	-0.27656
18	O	5.484528	-2.01393	-0.4553
19	O	-2.21502	2.920333	-0.62384
20	O	-4.66639	1.517718	-0.57901
21	C	-4.39597	-1.34362	-0.02127
22	C	-4.35001	-2.81288	0.251492
23	C	-1.68163	-1.10523	1.752535
24	H	4.752532	2.293196	0.565044
25	H	2.839828	-2.16038	-0.55225
26	H	6.240452	0.349766	0.126044
27	H	2.504953	3.239918	0.80183
28	H	0.058476	2.969596	0.730992
29	H	-1.39959	-1.23885	-1.71487
30	H	-1.54384	-2.61738	-0.62521
31	H	0.831548	-1.99034	-1.35368
32	H	0.590724	-2.26516	0.356716
33	H	5.018922	-2.84411	-0.66337
34	H	-1.31149	3.181	-0.87349
35	H	-5.37619	-0.92928	-0.26554
36	H	-5.00588	-3.05612	1.094815

37	H	-4.73284	-3.36652	-0.61276
38	H	-3.34765	-3.17582	0.478146
39	H	-2.23266	-0.44871	2.431972
40	H	-2.02764	-2.13103	1.909665
41	H	-0.62177	-1.05876	2.019698