Supporting Information

Protein Tyrosine Phosphatase 1B Inhibitory Iridoids from *Psydrax subcordata*

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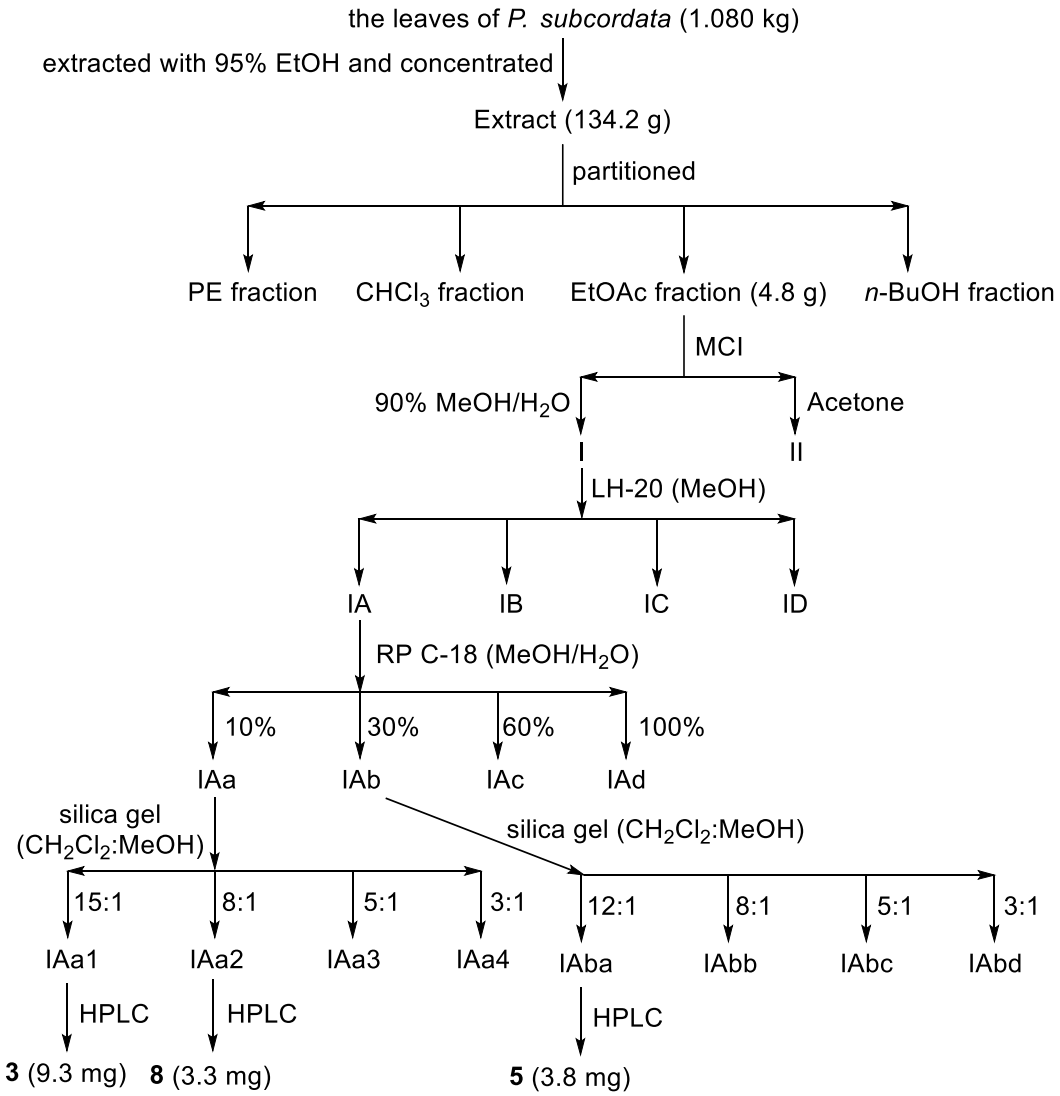
the leaves of *P. subcordata* (1.080 kg)
extracted with 95% EtOH and concentrated
Extract (134.2 g)
partitioned
PE fraction
$CHCl_3$ fraction
EtOAc fraction (4.8 g)
n-BuOH fraction
MCI
90% $MeOH/H_2O$
Acetone
I
II
LH-20 (MeOH)
IA
IB
IC
ID
RP C-18 ($MeOH/H_2O$)
10%
30%
60%
100%
IAa
IAb
IAc
IAd
silica gel (CH_2Cl_2:MeOH)
silica gel (CH_2Cl_2:MeOH)
15:1
8:1
5:1
3:1
12:1
8:1
5:1
3:1
IAa1
IAa2
IAa3
IAa4
IAba
IAbb
IAbc
IAbd
HPLC
HPLC
HPLC
3 (9.3 mg)
8 (3.3 mg)
5 (3.8 mg)

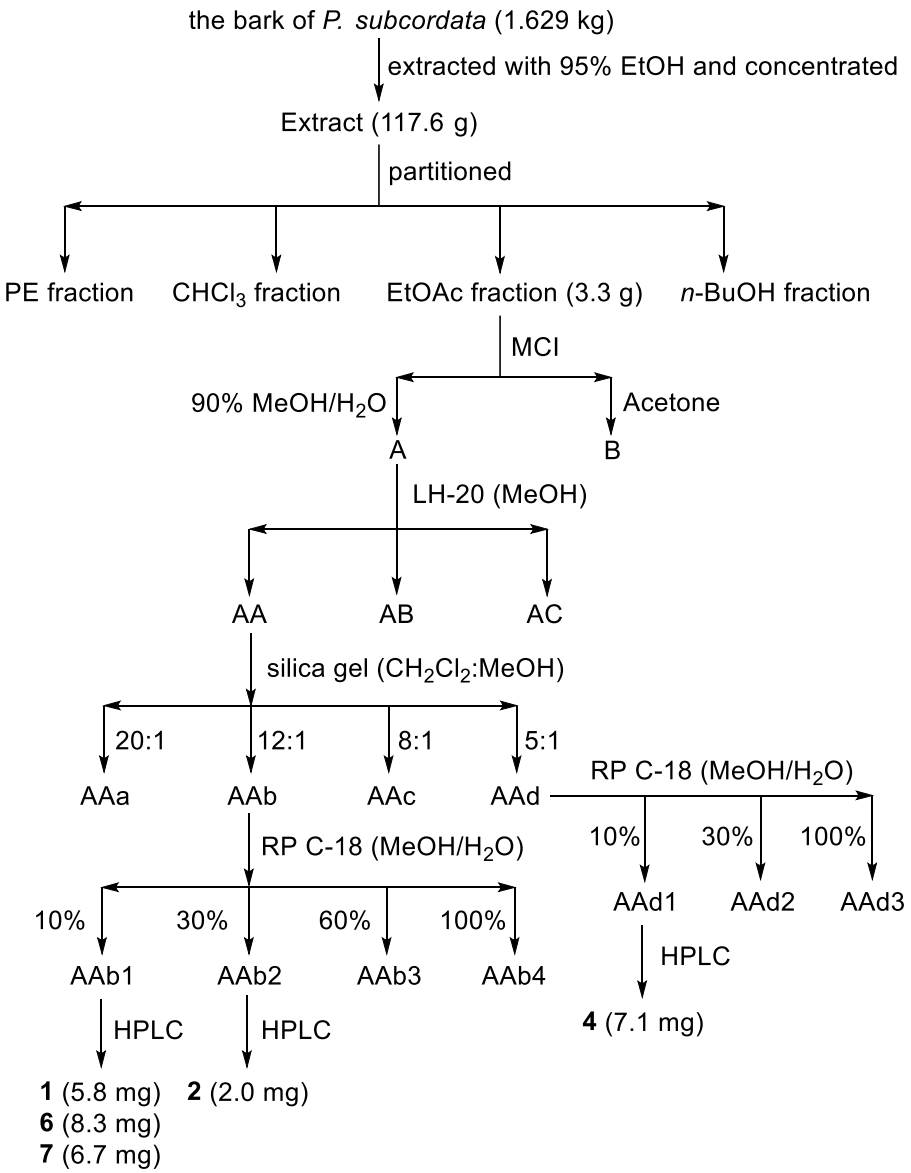

Figure S1. Flow charts of the extraction and isolation of the leaves and bark of *P. subcordata*.

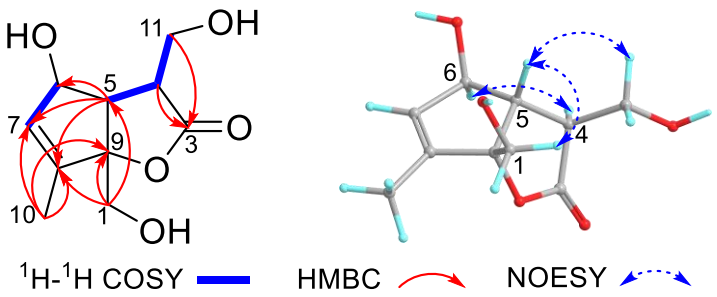

Figure S2. ^{1}H–^{1}H COSY, key HMBC, and NOESY correlations of **2**.

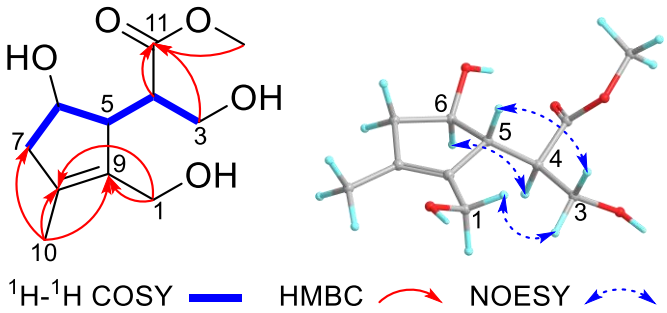

Figure S3. ^{1}H–^{1}H COSY, key HMBC, and NOESY correlations of **3**.

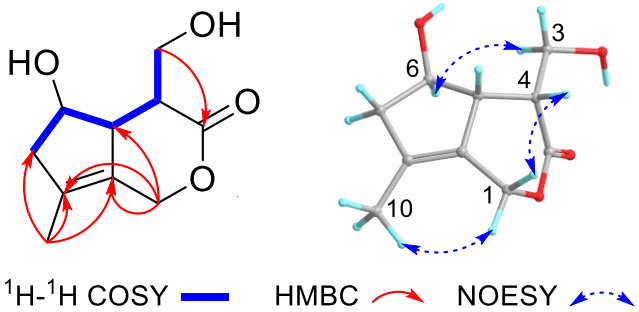

Figure S4. ^{1}H–^{1}H COSY, key HMBC, and NOESY correlations of **3a**.

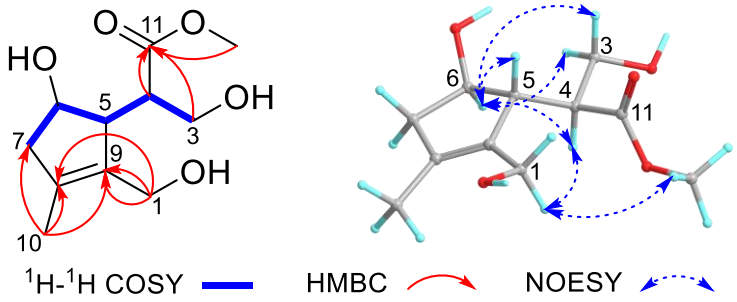

Figure S5. ^{1}H–^{1}H COSY, key HMBC, and NOESY correlations of **4**.

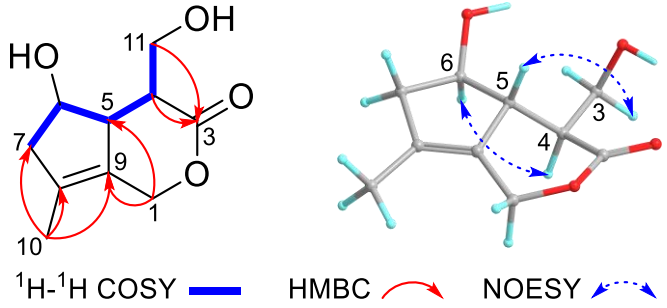

Figure S6. ^{1}H–^{1}H COSY, key HMBC, and NOESY correlations of **4a**.

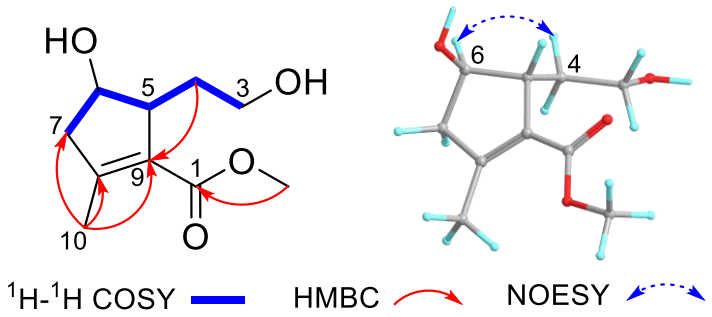

Figure S7. ^{1}H–^{1}H COSY, key HMBC, and NOESY correlations of **5**.

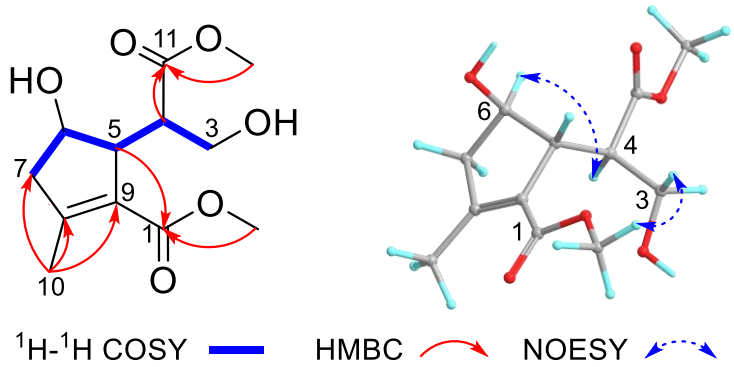

Figure S8. ^{1}H–^{1}H COSY, key HMBC, and NOESY correlations of **6**.

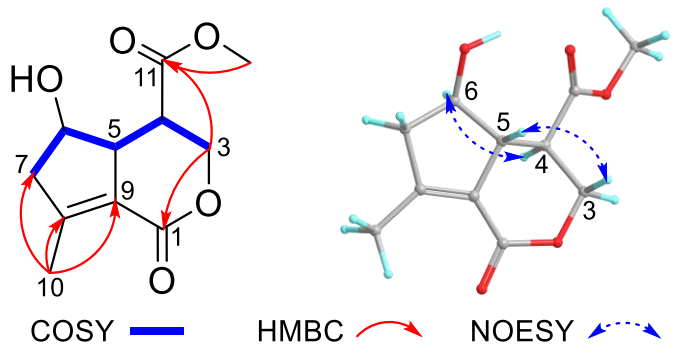

Figure S9. ^{1}H–^{1}H COSY, key HMBC, and NOESY correlations of **6a**.

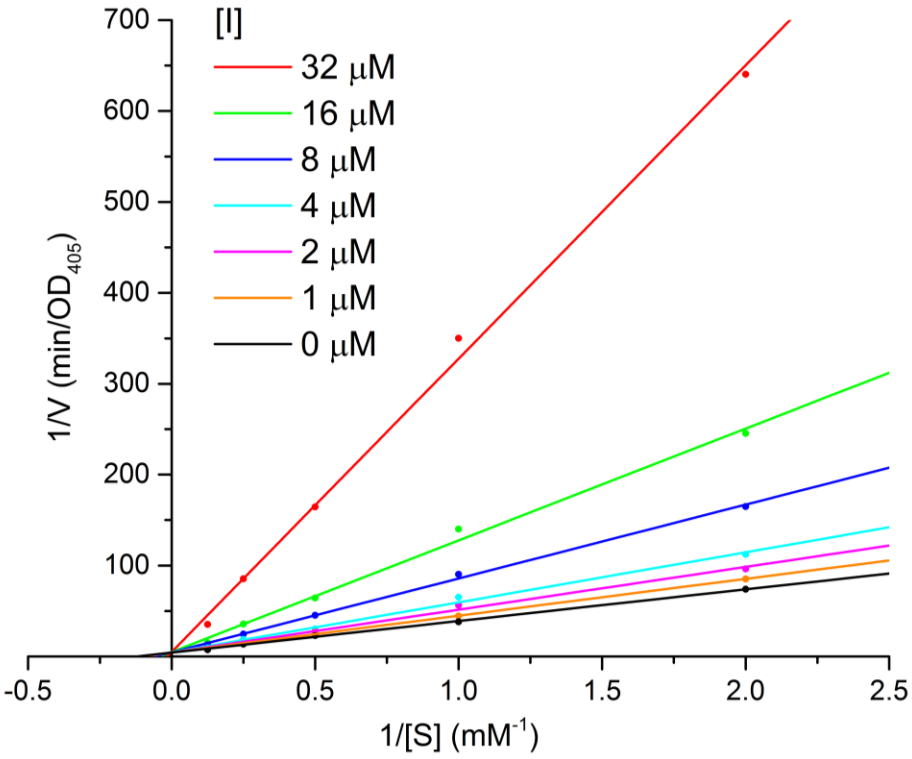

Figure S10. Lineweaver-Burk plots for the inhibition of PTP1B by **3a**.

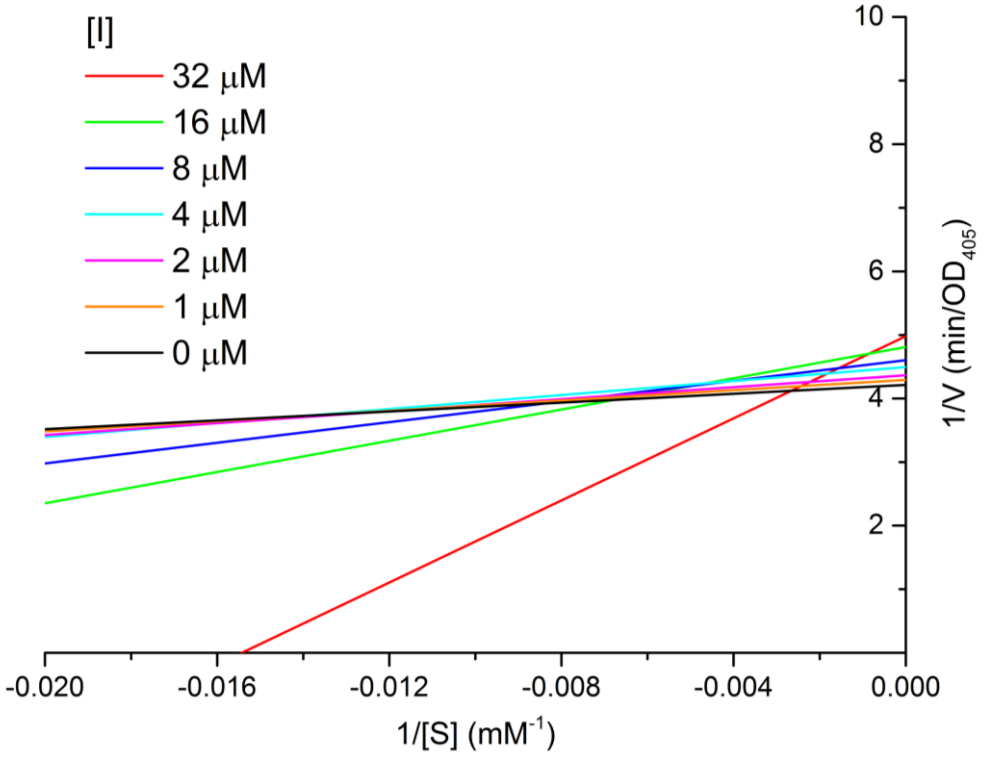

Figure S11. Lineweaver-Burk plots for the inhibition of PTP1B by **3a** (amplify).

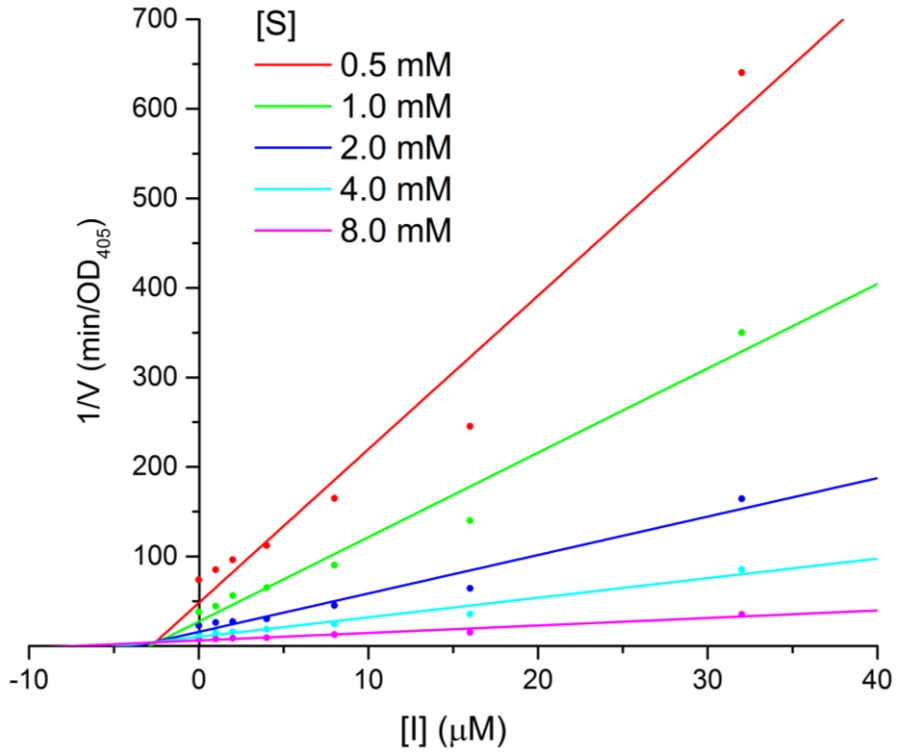

Figure S12. Dixon plots for the inhibition of PTP1B by **3a**.

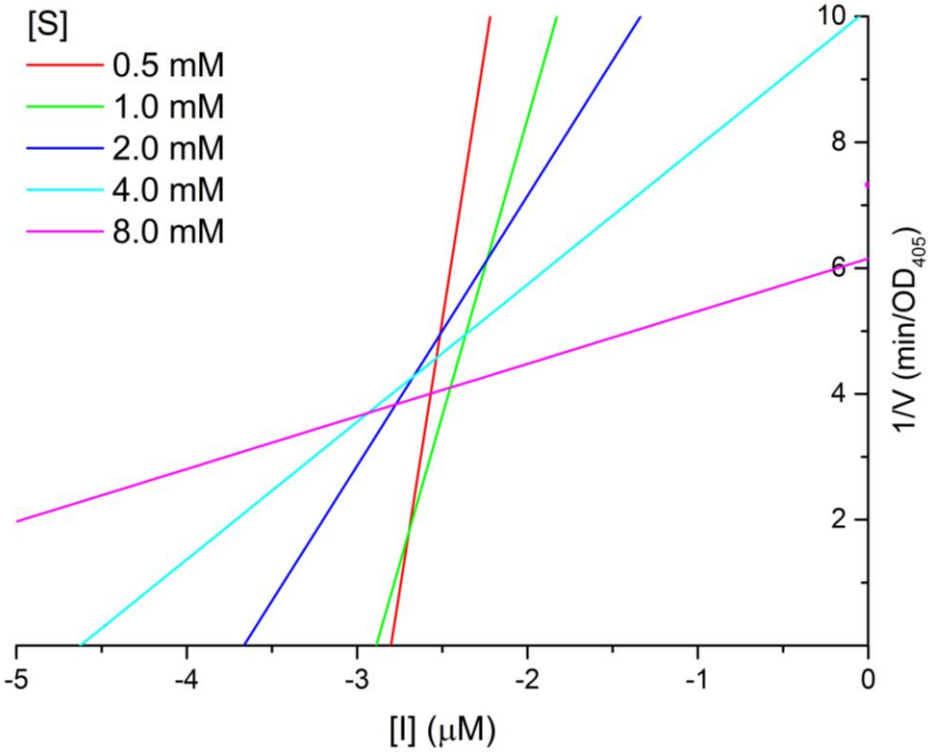

Figure S13. Dixon plots for the inhibition of PTP1B by **3a** (amplify)

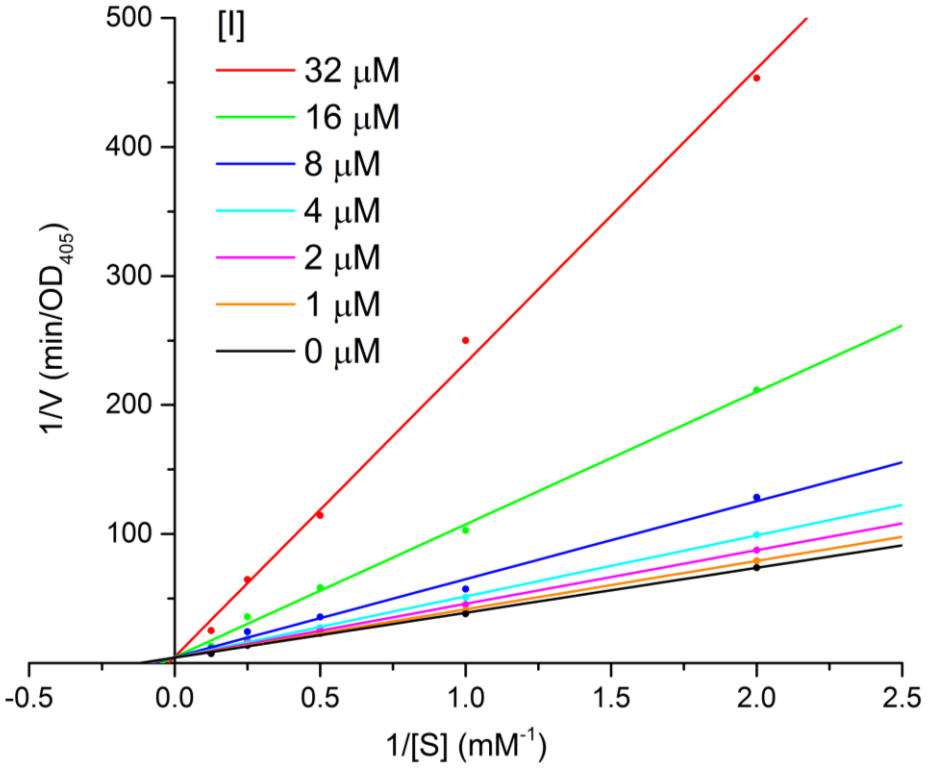

Figure S14. Lineweaver-Burk plots for the inhibition of PTP1B by **4a**.

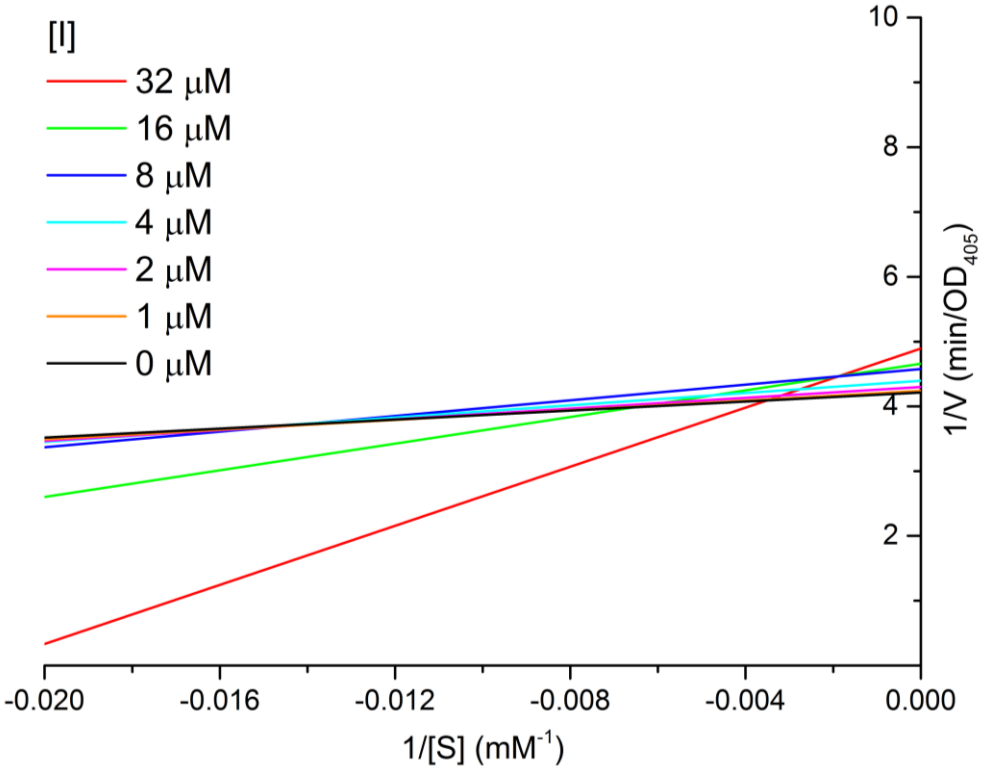

Figure S15. Lineweaver-Burk plots for the inhibition of PTP1B by **4a** (amplify).

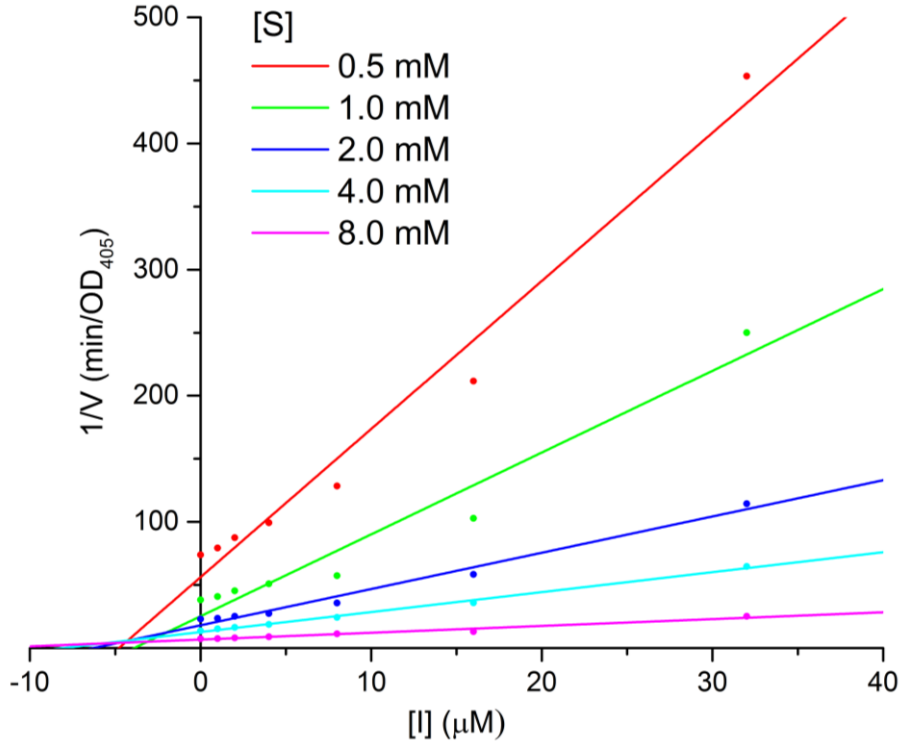

Figure S16. Dixon plots for the inhibition of PTP1B by **4a**.

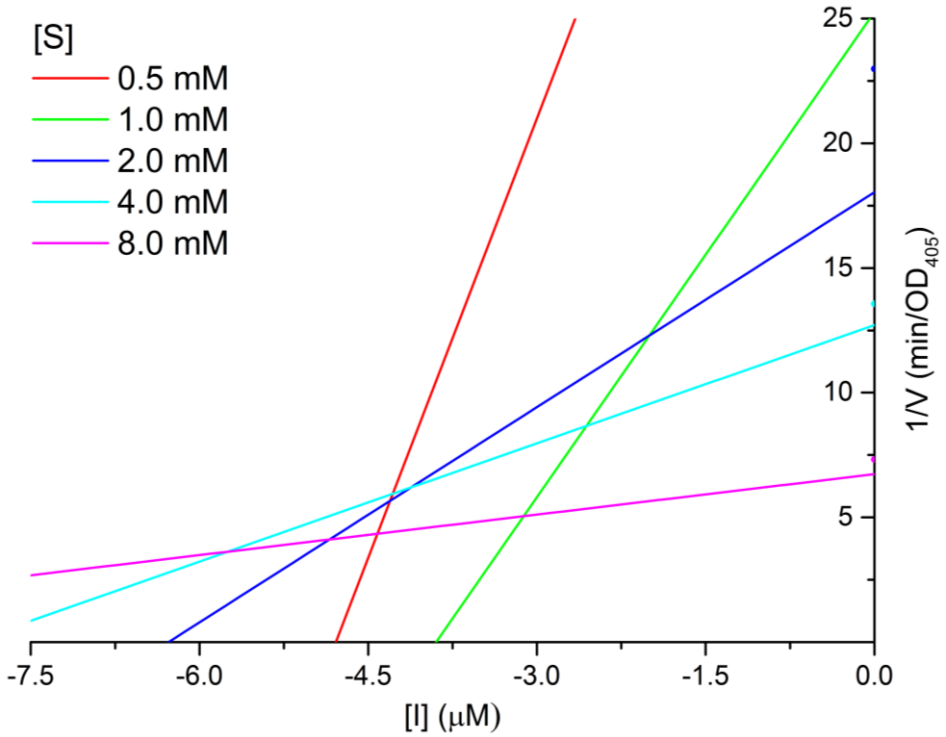

Figure S17. Dixon plots for the inhibition of PTP1B by **4a** (amplify).

Table S1. Effect of different concentrations of **3a** on V_{max}, K_m, and the K_{ik} to K_{iv} ratio using *p*NPP as a substrate.

V_{max} and K_m values were calculated according to Lineweaver-Burk from the data shown in Figures S10 and S11. K_{ik}/K_{iv} ratio was calculated according to Yang et al.[S1]

Inhibitor (**3a**)	Substrate (*p*NPP)				
[I] (μM)	V_{max}	K_m	K_{iv}	K_{ik}	K_{ik}/K_{iv}
0	0.2374	8.258			
1	0.2329	9.439	52.44	6.993	7.499
2	0.2290	10.78	27.50	3.280	8.382
4	0.2224	12.23	14.84	2.077	7.145
8	0.2171	17.63	10.74	0.8815	12.18
16	0.2078	25.55	7.042	0.4777	14.74
32	0.2008	64.79	5.489	0.1461	37.58

Table S2. Effect of different concentrations of **4a** on V_{max}, K_m, and the K_{ik} to K_{iv} ratio using *p*NPP as a substrate.

V_{max} and K_m values were calculated according to Lineweaver-Burk from the data shown in Figures S14 and S15. K_{ik}/K_{iv} ratio was calculated according to Yang et al.[S1]

Inhibitor (**4a**)	Substrate (*p*NPP)				
[I] (μM)	V_{max}	K_m	K_{iv}	K_{ik}	K_{ik}/K_{iv}
0	0.2374	8.258			
1	0.2358	8.828	149.6	14.50	10.32
2	0.2326	9.668	48.93	5.858	8.354
4	0.2275	10.75	22.99	3.316	6.934
8	0.2184	13.19	11.50	1.675	6.864
16	0.2146	22.06	9.426	0.5984	15.75
32	0.2043	46.57	6.188	0.2155	28.71

Table S3. The calculated energies (kcal/mol) of compounds **1**−**8**, **3a**, **4a**, **6a**, and oleanolic acid to PTP1B by Autidock 4.2.6.[S2]

Inhibitors	Binding Energy	Intermolecular	Internal Energy	Torsional Energy	Unbound Extended Energy
1	−6.26	−7.75	−0.94	1.49	−0.94
2	−5.35	−6.84	−0.84	1.49	−0.84
3	−6.85	−9.23	−1.38	2.39	−1.38
3a	−7.16	−8.05	−0.41	0.89	−0.41
4	−6.45	−8.84	−1.61	2.39	−1.61
4a	−6.84	−7.74	−0.3	0.89	−0.3
5	−6.42	−8.21	−1.62	1.79	−1.62
6	−6.9	−9.28	−1.84	2.39	−1.84
6a	−7.62	−8.52	−0.56	0.89	−0.56
7	−5.69	−7.48	−1.22	1.79	−1.22
8	−6.03	−6.33	0.03	0.3	0.03
oleanolic acid	−9.19	−10.08	0.13	0.89	0.13

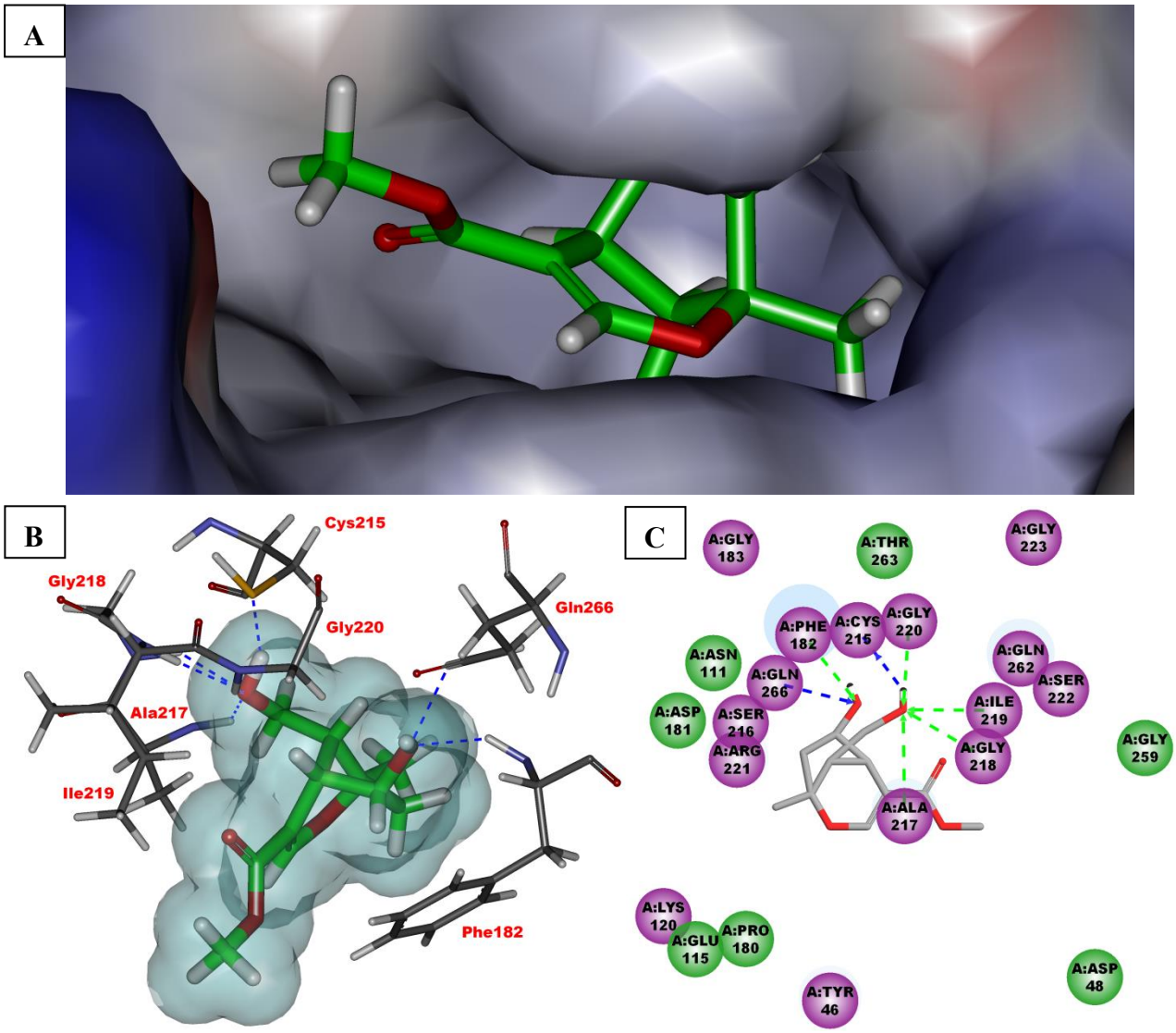

Figure S18. Molecular docking models for PTP1B inhibition of subcordatanol I (**1**).

A: 3D docking surfaces of the PTP1B protein active site and subcordatanol I (**1**). **B** and **C**: Ligand interaction models of subcordatanol I (**1**).

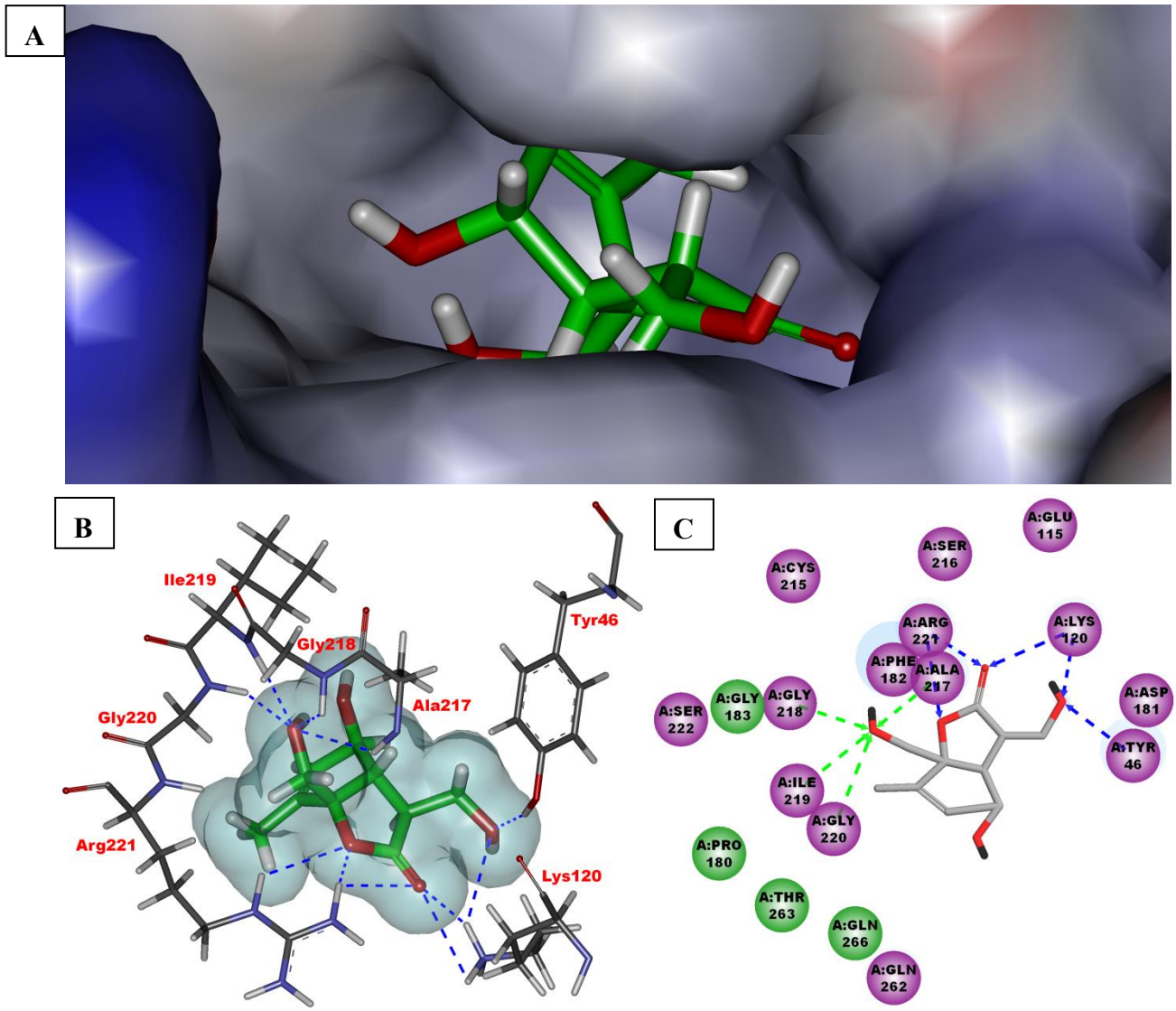

Figure S19. Molecular docking models for PTP1B inhibition of subcordatanol II (**2**).

A: 3D docking surfaces of the PTP1B protein active site and subcordatanol II (**2**). **B** and **C**: Ligand interaction models of subcordatanol II (**2**).

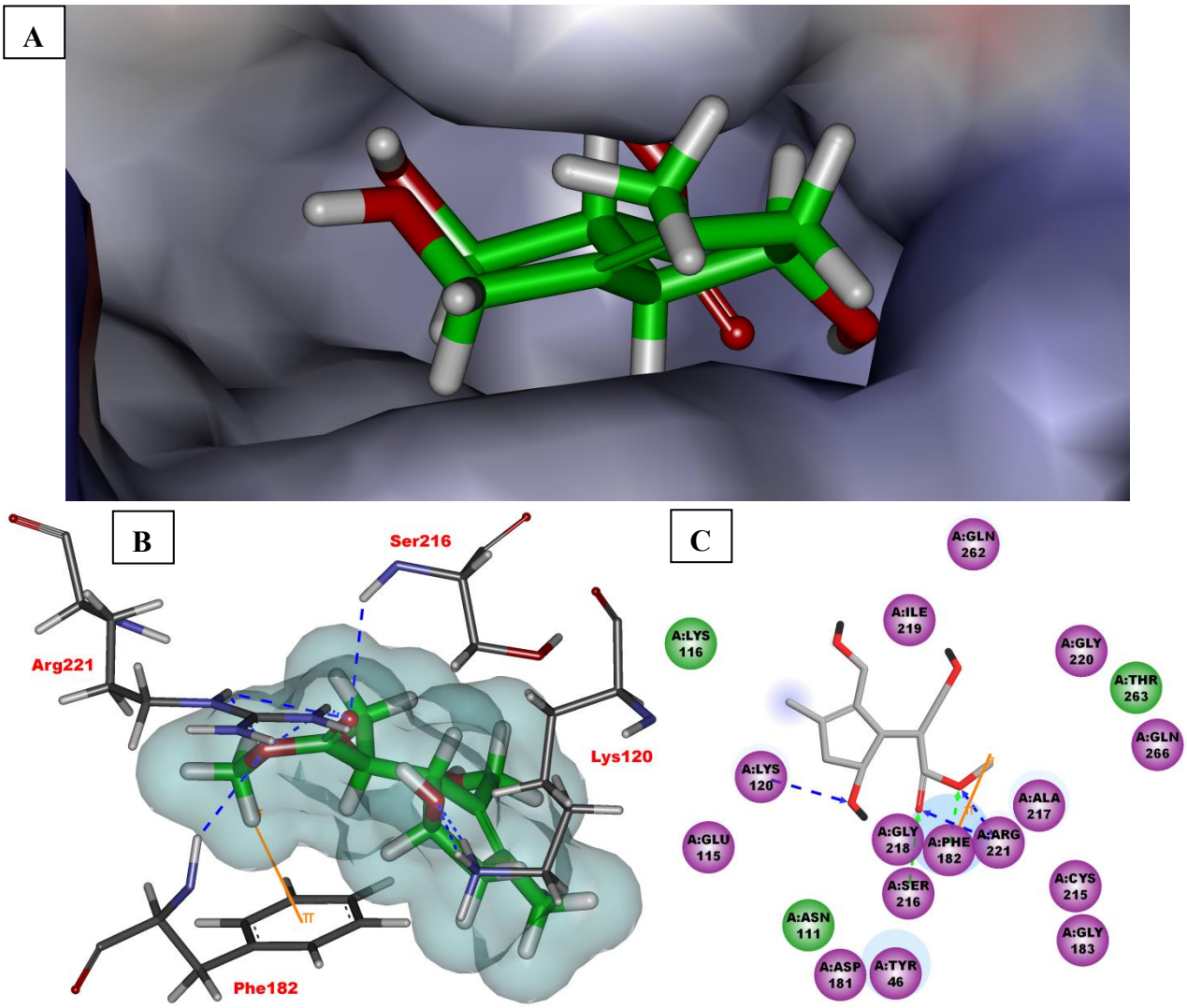

Figure S20. Molecular docking models for PTP1B inhibition of subcordatanol III (**3**).

A: 3D docking surfaces of the PTP1B protein active site and subcordatanol III (**3**). **B** and **C**: Ligand interaction models of subcordatanol III (**3**).

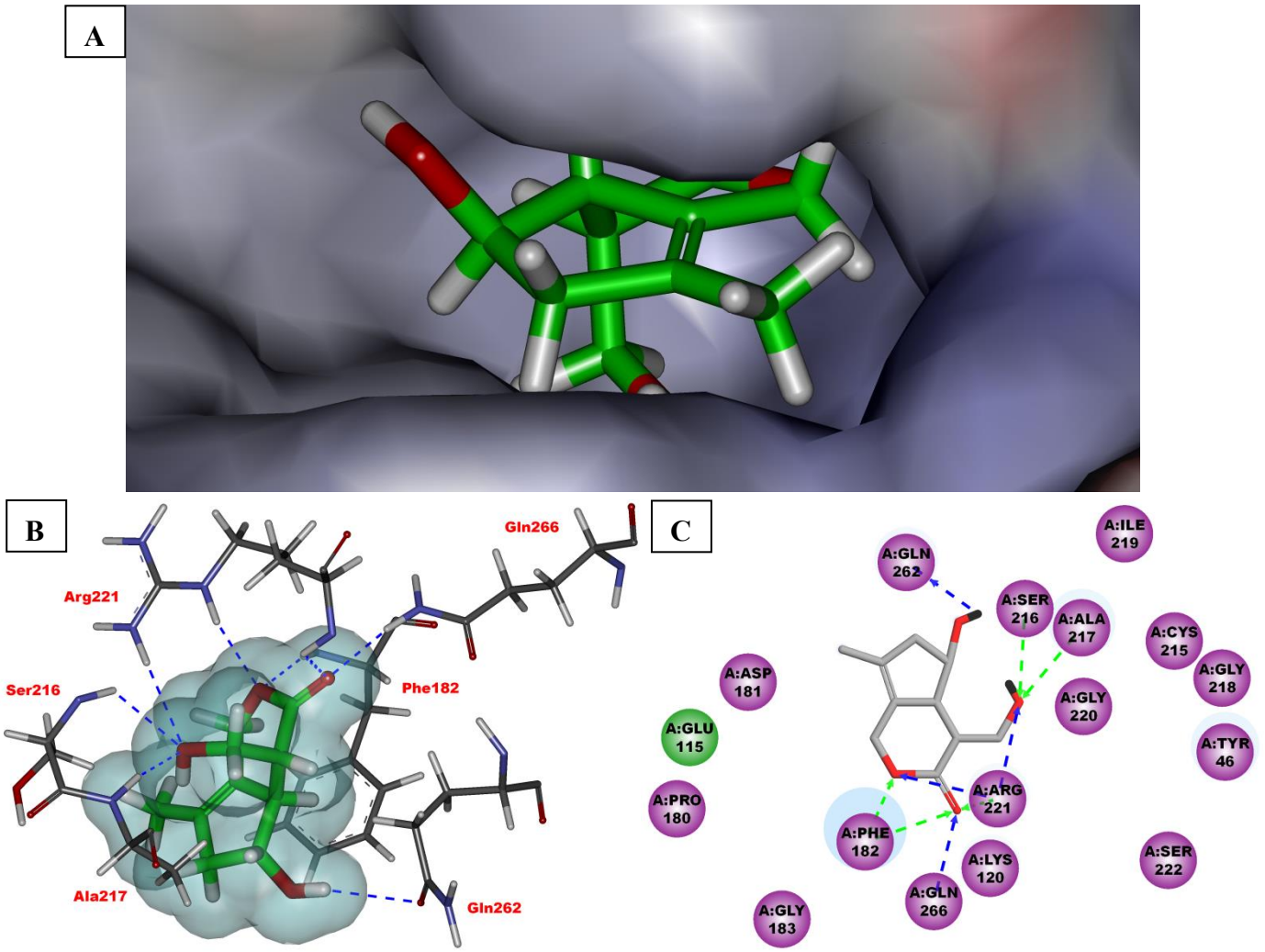

Figure S21. Molecular docking models for PTP1B inhibition of subcordatalactone A (**3a**).

A: 3D docking surfaces of the PTP1B protein active site and subcordatalactone A (**3a**). **B** and **C**: Ligand interaction models of subcordatalactone A (**3a**).

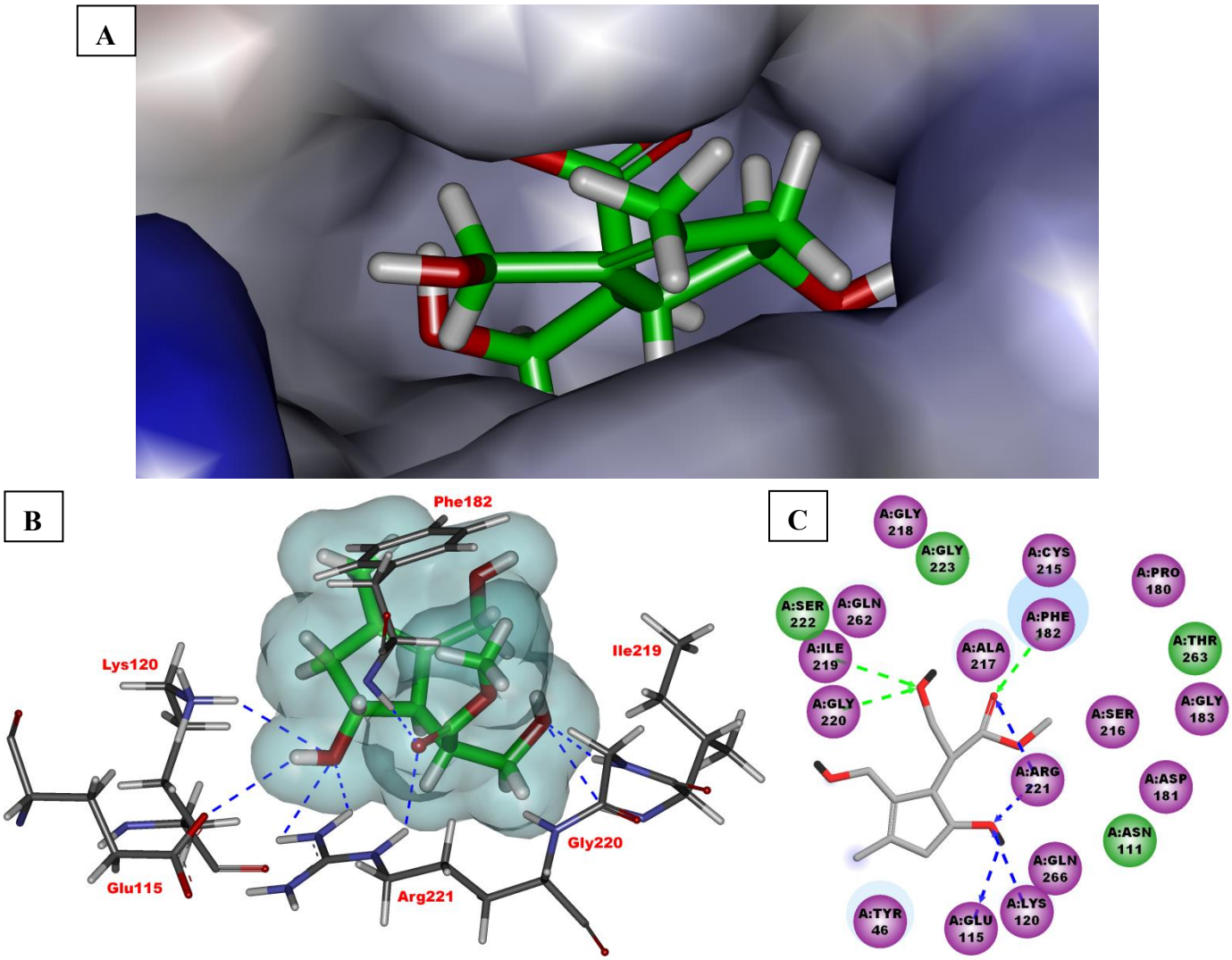

Figure S22. Molecular docking models for PTP1B inhibition of subcordatanol IV (**4**).

A: 3D docking surfaces of the PTP1B protein active site and subcordatanol IV (**4**). **B** and **C**: Ligand interaction models of subcordatanol IV (**4**).

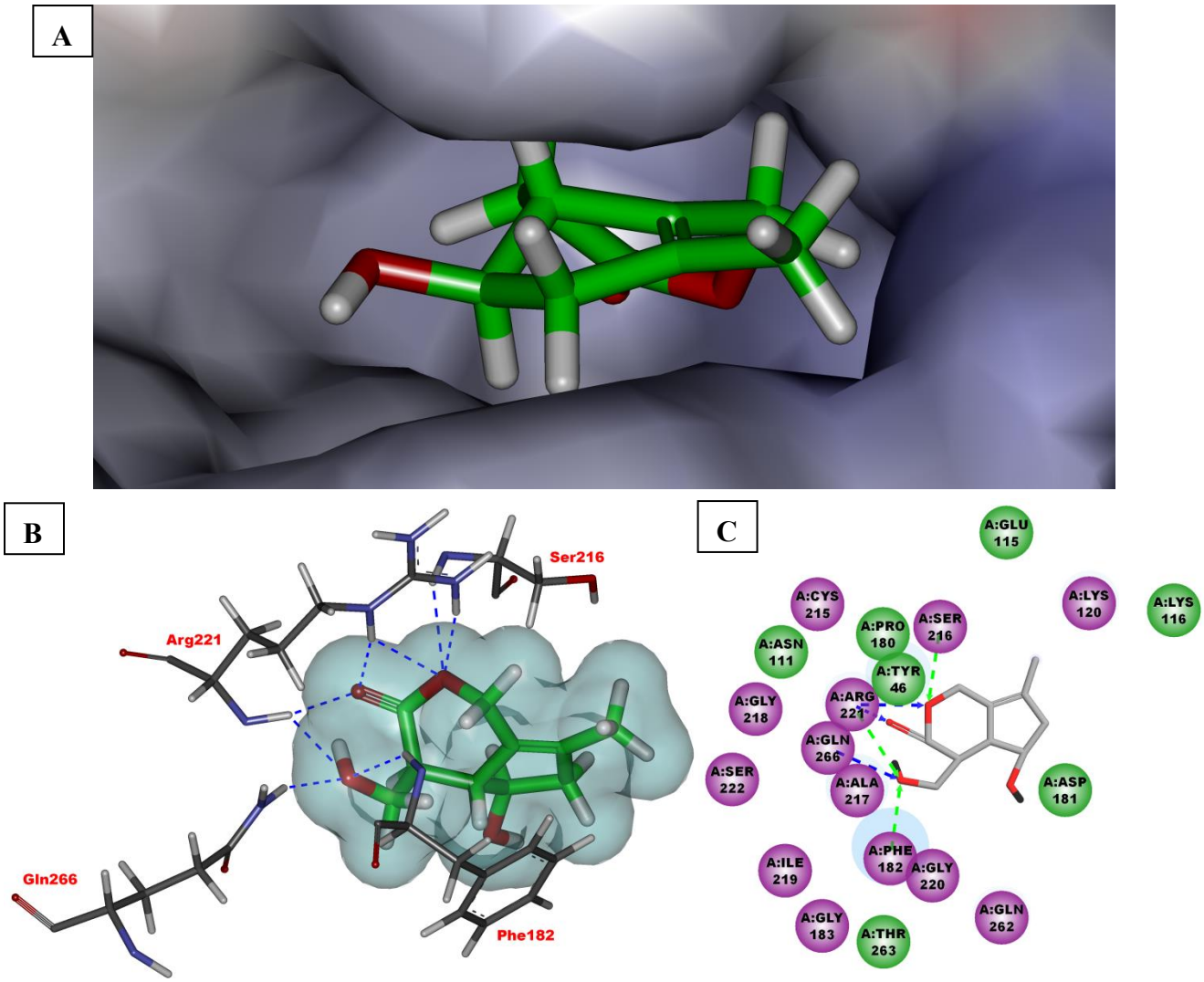

Figure S23. Molecular docking models for PTP1B inhibition of subcordatalactone B (**4a**).

A: 3D docking surfaces of the PTP1B protein active site and subcordatalactone B (**4a**). **B** and **C**: Ligand interaction models of subcordatalactone B (**4a**).

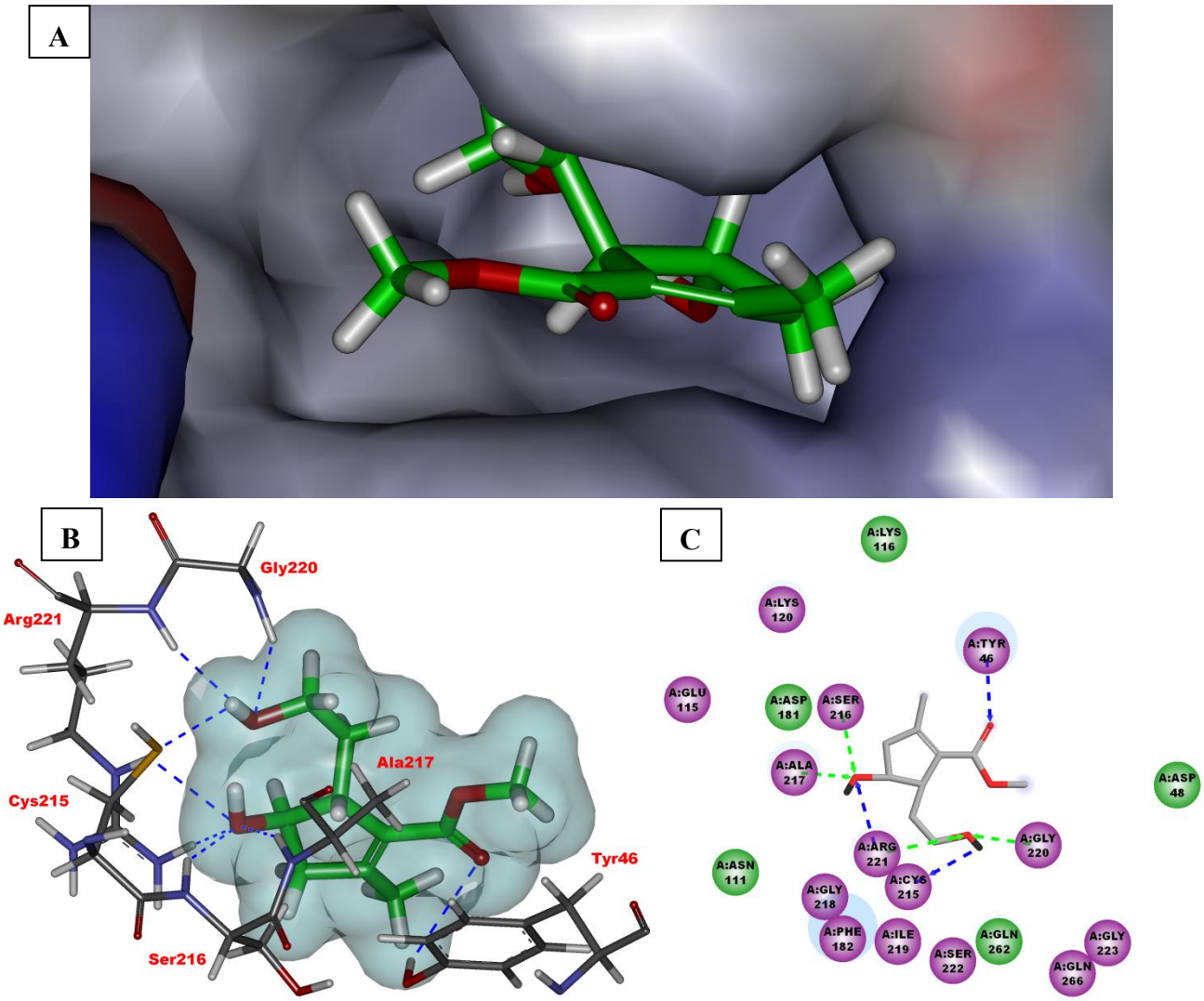

Figure S24. Molecular docking models for PTP1B inhibition of 1-*O*-methylcrescentin I (**5**).

A: 3D docking surfaces of the PTP1B protein active site and 1-*O*-methylcrescentin I (**5**). **B** and **C**: Ligand interaction models of 1-*O*-methylcrescentin I (**5**).

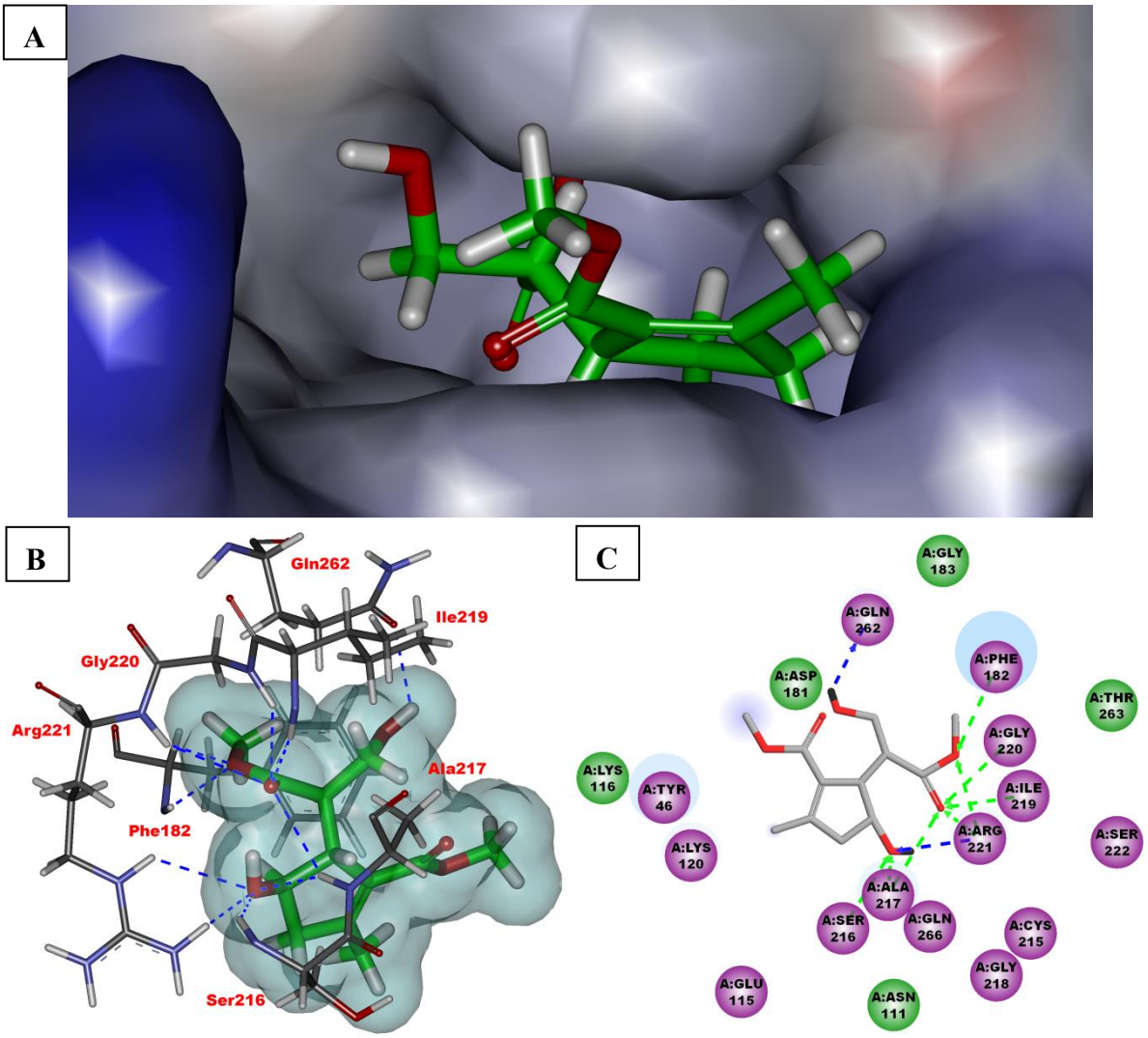

Figure S25. Molecular docking models for PTP1B inhibition of subcordatanol V (**6**).

A: 3D docking surfaces of the PTP1B protein active site and subcordatanol V (**6**). **B** and **C**: Ligand interaction models of subcordatanol V (**6**).

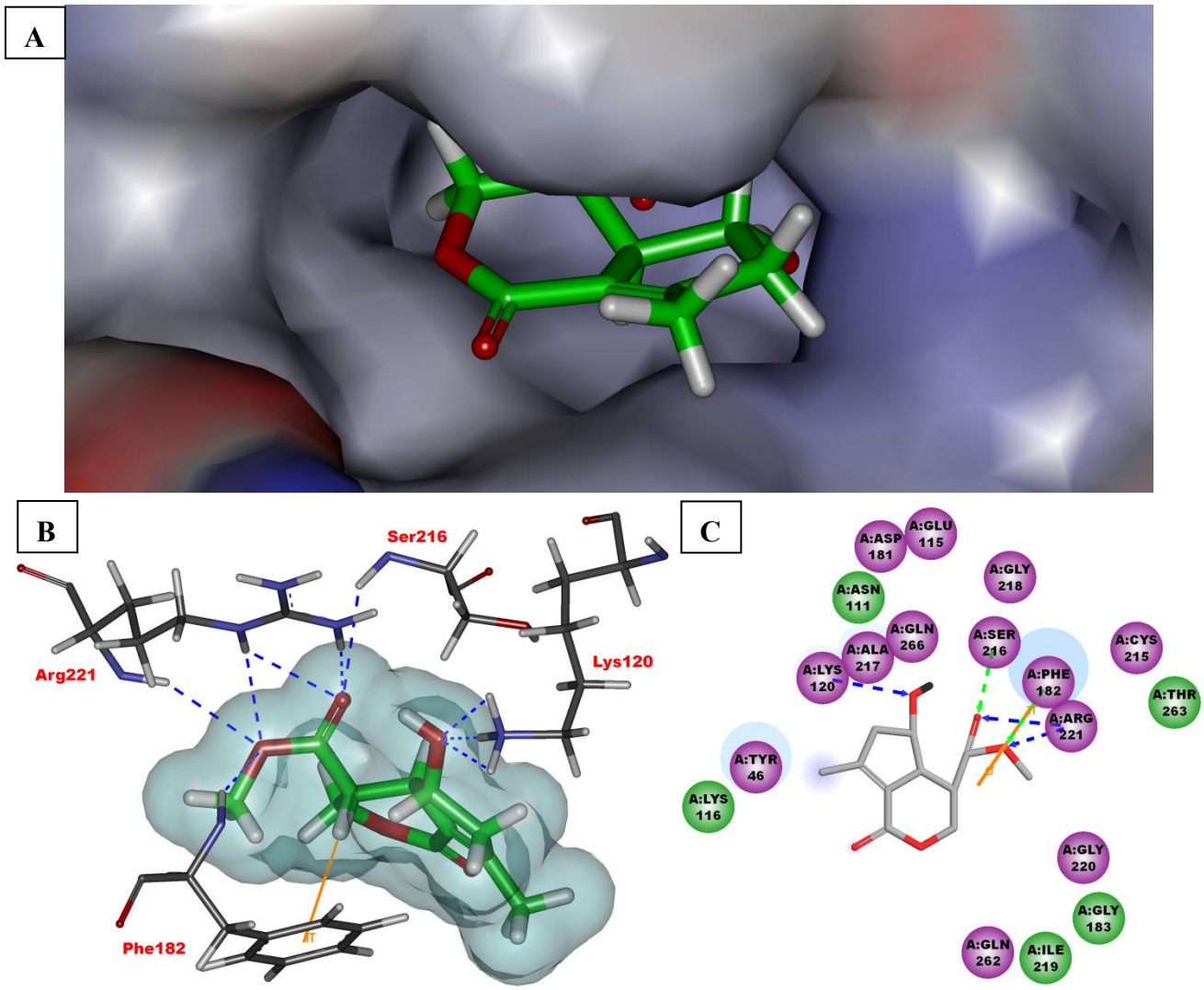

Figure S26. Molecular docking models for PTP1B inhibition of subcordatalactone C (**6a**).

A: 3D docking surfaces of the PTP1B protein active site and subcordatalactone C (**6a**). **B** and **C**: Ligand interaction models of subcordatalactone C (**6a**).

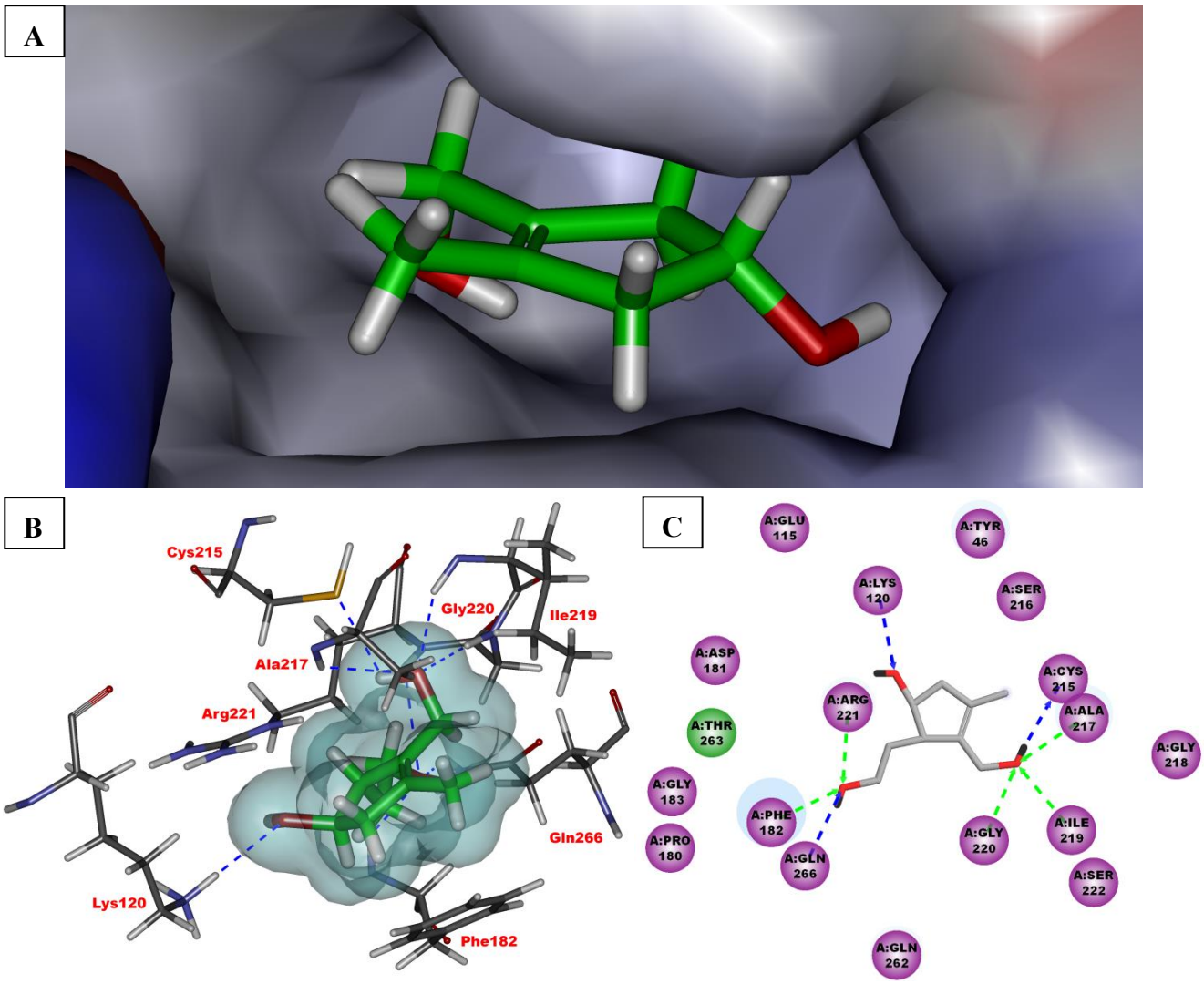

Figure S27. Molecular docking models for PTP1B inhibition of 10-deoxyeucommiol (**7**).

A: 3D docking surfaces of the PTP1B protein active site and 10-deoxyeucommiol (**7**). **B** and **C**: Ligand interaction models of 10-deoxyeucommiol (**7**).

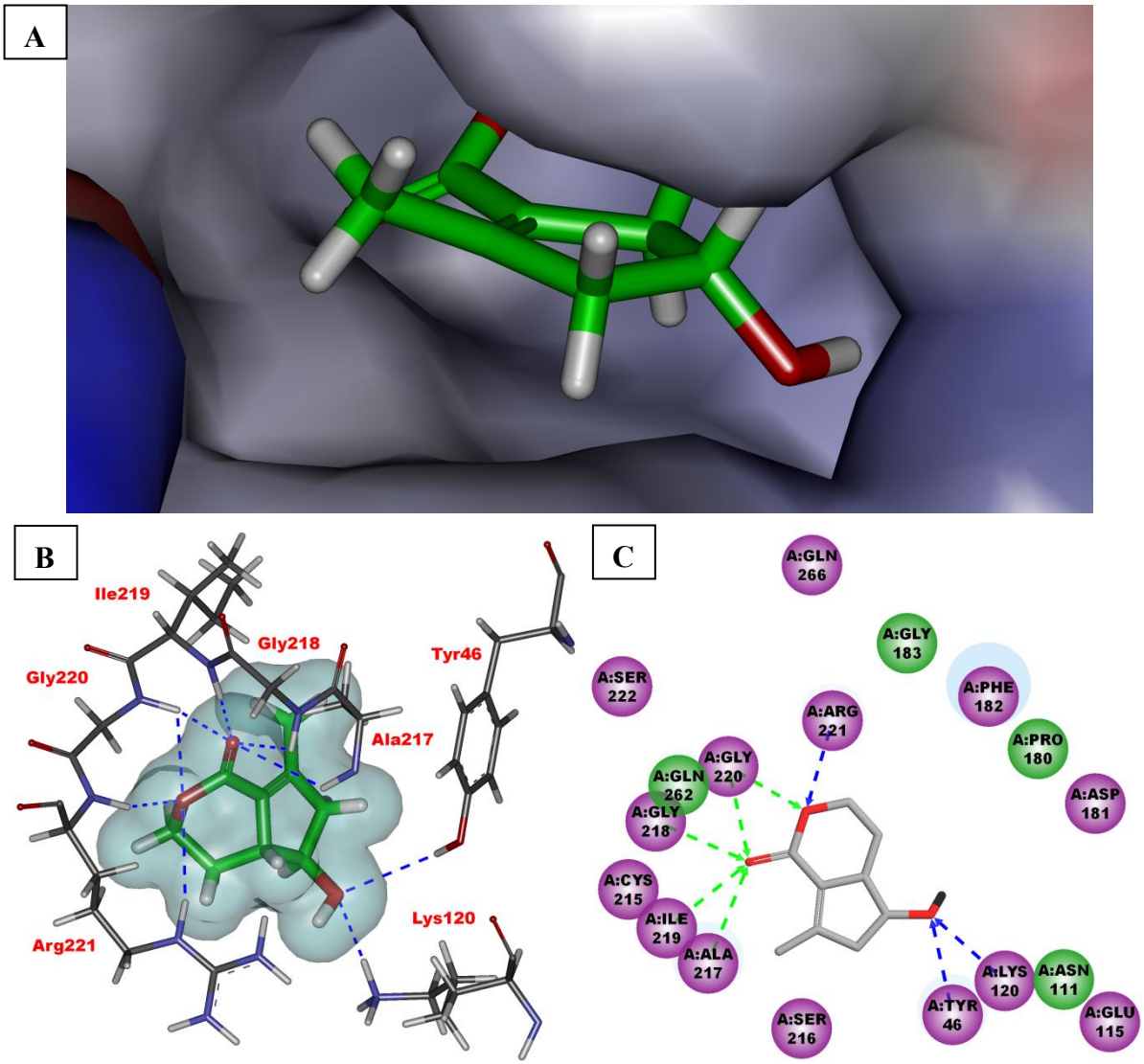

Figure S28. Molecular docking models for PTP1B inhibition of 6*β*-hydroxy-2-oxabicyclo[4.3.0]Δ^{8-9}-nonen-1-one (**8**).

A: 3D docking surfaces of the PTP1B protein active site and 6*β*-hydroxy-2-oxabicyclo[4.3.0]Δ^{8-9}-nonen-1-one (**8**). **B** and **C**: Ligand interaction models of 6*β*-hydroxy-2-oxabicyclo[4.3.0]Δ^{8-9}-nonen- 1-one (**8**).

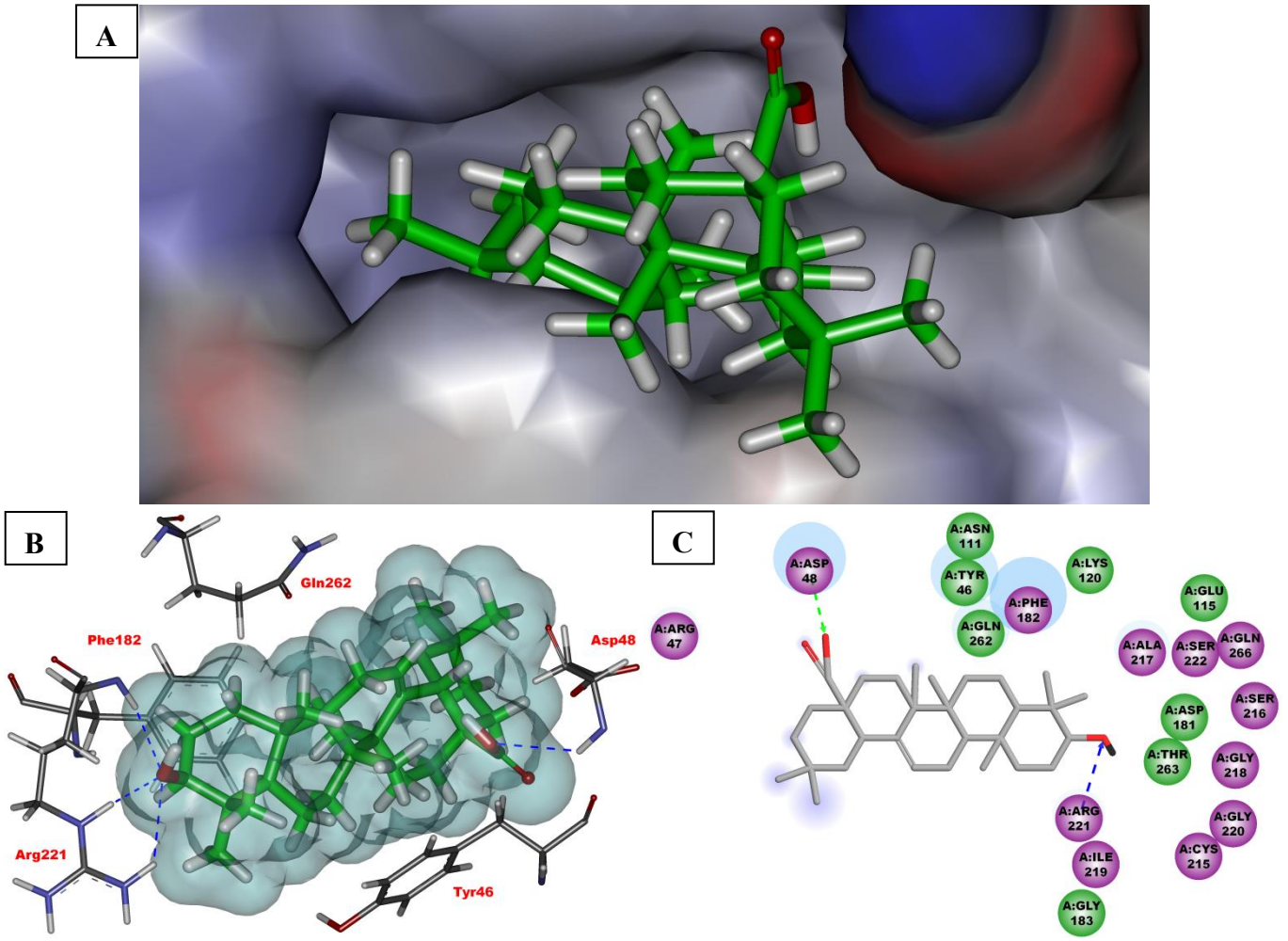

Figure S29. Molecular docking models for PTP1B inhibition of oleanolic acid.

A: 3D docking surfaces of the PTP1B protein active site and oleanolic acid. **B** and **C**: Ligand interaction models of oleanolic acid.

Table S4. Cartesian coordinate of **1** [E(RB3LYP) = −804.928766230 a.u.]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	−0.47023	1.948143	−0.04145
2	6	0	−0.07385	0.65359	0.713852
3	6	0	−1.45721	1.439143	−1.12528
4	6	0	−1.73093	−0.050862	−0.8063
5	8	0	−0.7624	−0.880315	−1.55804
6	6	0	0.955492	−0.096619	−0.10898
7	6	0	0.526795	−0.804307	−1.17969
8	6	0	−1.39866	−0.144279	0.702226
9	6	0	−3.09238	−0.54218	−1.27021
10	8	0	−1.18417	2.875668	0.783266
11	6	0	−1.35012	−1.533105	1.348441
12	8	0	−2.64289	−2.023645	1.721281
13	6	0	2.375538	0.007414	0.248383
14	8	0	2.798351	0.684169	1.174369
15	8	0	3.193657	−0.723984	−0.55461
16	6	0	4.596714	−0.653292	−0.24973
17	1	0	−2.15322	0.439259	1.243521
18	1	0	0.40831	2.44058	−0.47683
19	1	0	0.312302	0.859036	1.715868
20	1	0	−1.07024	1.55085	−2.14298
21	1	0	−2.38388	2.018138	−1.05412
22	1	0	1.177658	−1.386154	−1.82324
23	1	0	−3.18404	−1.628666	−1.16018
24	1	0	−3.88558	−0.057675	−0.69192
25	1	0	−3.24247	−0.309587	−2.33056
26	1	0	−0.57005	3.246817	1.437006
27	1	0	−0.79353	−1.467852	2.288632
28	1	0	−0.83377	−2.261793	0.710942
29	1	0	−3.11726	−2.304499	0.92506
30	1	0	4.956787	0.37567	−0.33565
31	1	0	4.787948	−1.017758	0.763288
32	1	0	5.083622	−1.29339	−0.98657

Table S5. Cartesian coordinate of **2** [E(RB3LYP) = − 765.618118831 a.u.]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.082829	−0.783286	−0.24805
2	1	0	0.165467	−1.278002	−1.22292
3	6	0	−0.68518	0.562607	−0.33678
4	6	0	−1.49458	0.603195	0.952506
5	6	0	−1.51884	−0.613883	1.517465
6	1	0	−2.06917	−0.872126	2.419109
7	6	0	−0.7477	−1.653187	0.726655
8	1	0	−0.11445	−2.282528	1.360747
9	8	0	−1.6083	−2.5713	0.051841
10	1	0	−2.0959	−2.063361	−0.6255
11	6	0	−2.16089	1.860322	1.428163
12	1	0	−2.69579	1.693428	2.36819
13	1	0	−1.42227	2.656072	1.5856
14	1	0	−2.88103	2.246439	0.693005
15	8	0	0.319042	1.617424	−0.38154
16	6	0	1.549808	1.129137	−0.07519
17	6	0	1.470546	−0.355403	0.257104
18	1	0	1.528417	−0.434742	1.352367
19	6	0	2.665782	−1.126511	−0.33132
20	1	0	2.549646	−2.194388	−0.12126
21	1	0	2.681539	−1.000389	−1.42636
22	8	0	3.895893	−0.733899	0.247909
23	1	0	3.976107	0.231602	0.138754
24	8	0	2.539872	1.826045	−0.09288
25	6	0	−1.5412	0.735192	−1.60321
26	1	0	−1.99479	1.733379	−1.6283
27	1	0	−0.90607	0.629439	−2.48692
28	8	0	−2.53929	−0.285872	−1.69725
29	1	0	−3.30299	−0.033104	−1.15522

Table S6. Cartesian coordinate of **3** [E(RB3LYP) = −806.135135427 a.u.]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.24026	−0.65744	0.521675
2	1	0	0.419161	−1.33486	1.371541
3	6	0	1.492782	0.190402	0.310466
4	6	0	1.812347	1.354237	1.203728
5	1	0	2.770215	1.81333	0.928022
6	1	0	1.045848	2.130811	1.13142
7	8	0	1.818085	0.987437	2.597129
8	1	0	2.483225	0.29221	2.72537
9	6	0	2.27226	−0.33086	−0.66013
10	6	0	1.645549	−1.57162	−1.25866
11	1	0	2.13784	−2.47943	−0.87693
12	1	0	1.718768	−1.61038	−2.3533
13	6	0	0.190974	−1.53294	−0.76406
14	1	0	−0.42036	−1.01589	−1.5216
15	8	0	−0.29972	−2.84654	−0.56856
16	1	0	−1.21742	−2.7587	−0.23616
17	6	0	3.621446	0.12482	−1.13442
18	1	0	4.354969	−0.6893	−1.04878
19	1	0	3.585387	0.397589	−2.19855
20	1	0	4.006683	0.986892	−0.582
21	6	0	−1.06784	0.107585	0.902692
22	1	0	−0.80494	0.797187	1.715276
23	6	0	−2.16497	−0.82525	1.454976
24	1	0	−1.7543	−1.41307	2.280783
25	1	0	−2.99679	−0.22442	1.848293
26	8	0	−2.66291	−1.7687	0.503788
27	1	0	−3.04044	−1.24076	−0.22567
28	6	0	−1.63415	0.939481	−0.23714
29	8	0	−2.59575	0.617542	−0.9217
30	8	0	−0.96616	2.08893	−0.43019
31	6	0	−1.42108	2.922273	−1.5179
32	1	0	−0.75635	3.786023	−1.5133
33	1	0	−1.34854	2.380964	−2.46432
34	1	0	−2.45676	3.228292	−1.35127

Table S7. Cartesian coordinate of **3a** [E(RB3LYP) = −690.388071075 a.u.]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.05701	−0.44558	0.611143
2	1	0	−0.14019	−0.92671	1.598175
3	6	0	1.222804	0.356226	0.524555
4	6	0	1.126593	1.793563	0.896246
5	1	0	2.048967	2.35551	0.744695
6	1	0	0.793993	1.941345	1.933285
7	8	0	0.153817	2.441472	0.017013
8	6	0	−0.98054	1.780805	−0.32341
9	6	0	−1.29944	0.484072	0.431271
10	1	0	−1.58267	0.824316	1.4419
11	6	0	−2.53126	−0.18488	−0.20072
12	1	0	−3.39279	0.488916	−0.16567
13	1	0	−2.34546	−0.41849	−1.25089
14	8	0	−2.84955	−1.44308	0.415843
15	1	0	−3.18798	−1.29629	1.312806
16	8	0	−1.71535	2.260093	−1.15977
17	6	0	2.225961	−0.34176	−0.03695
18	6	0	1.737965	−1.73018	−0.40495
19	1	0	2.137817	−2.0826	−1.36376
20	1	0	2.021327	−2.47525	0.354035
21	6	0	0.202156	−1.57838	−0.41966
22	1	0	−0.10172	−1.2272	−1.42054
23	8	0	−0.41902	−2.81468	−0.1224
24	1	0	−1.36647	−2.63966	0.039675
25	6	0	3.636825	0.089327	−0.29675
26	1	0	3.885596	−0.02136	−1.36084
27	1	0	3.820998	1.129749	−0.01076
28	1	0	4.345093	−0.54202	0.257786

Table S8. Cartesian coordinate of **4** [E(RB3LYP) = −806.131628606 a.u.]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.51517	0.412487	0.124827
2	1	0	−0.30698	0.439428	1.204402
3	6	0	−1.35378	−0.83259	−0.19075
4	6	0	−0.76132	−2.21549	−0.28197
5	1	0	−1.48217	−2.90899	−0.72078
6	1	0	0.120918	−2.21947	−0.94258
7	8	0	−0.42315	−2.76711	0.991717
8	1	0	0.326082	−2.25069	1.34288
9	6	0	−2.66748	−0.53337	−0.24613
10	6	0	−2.90281	0.939713	0.014267
11	1	0	−3.23777	1.10042	1.051229
12	1	0	−3.66388	1.38153	−0.64425
13	6	0	−1.50757	1.552447	−0.18704
14	1	0	−1.39847	1.855308	−1.23957
15	8	0	−1.22247	2.680968	0.657861
16	1	0	−1.81302	3.415864	0.430304
17	6	0	−3.83814	−1.45012	−0.44293
18	1	0	−4.43983	−1.13763	−1.30816
19	1	0	−3.54519	−2.49278	−0.59046
20	1	0	−4.50359	−1.41366	0.431354
21	6	0	0.843989	0.531282	−0.61048
22	1	0	0.727809	0.21965	−1.65912
23	6	0	1.409461	1.980144	−0.66151
24	1	0	2.380915	1.962467	−1.16148
25	1	0	0.735481	2.601835	−1.26697
26	8	0	1.616429	2.551808	0.615492
27	1	0	0.736787	2.789389	0.96475
28	6	0	1.896157	−0.37888	0.011884
29	8	0	1.794217	−0.97025	1.073295
30	8	0	3.001113	−0.4505	−0.7533
31	6	0	4.0895	−1.24167	−0.2328
32	1	0	4.879673	−1.16741	−0.98007
33	1	0	4.422419	−0.83813	0.726499
34	1	0	3.774639	−2.28021	−0.10275

Table S9. Cartesian coordinate of **4a** [E(RB3LYP) = −690.390689796 a.u.]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	−0.047118	0.36334	0.374092
2	1	0	0.139504	0.550352	1.445974
3	6	0	−1.114586	−0.68809	0.208576
4	6	0	−0.741499	−2.09857	0.504936
5	1	0	−1.403345	−2.82745	0.031716
6	1	0	−0.744573	−2.29054	1.587532
7	8	0	0.594079	−2.45722	0.051085
8	6	0	1.595445	−1.56933	−0.14569
9	6	0	1.275571	−0.0731	−0.286
10	1	0	1.168272	0.064589	−1.37548
11	6	0	2.488823	0.753652	0.17792
12	1	0	2.593959	0.687071	1.26531
13	1	0	3.407533	0.373419	−0.27451
14	8	0	2.326073	2.155106	−0.10628
15	1	0	2.611783	2.331748	−1.01561
16	8	0	2.721872	−1.99537	−0.29289
17	6	0	−2.313651	−0.16651	−0.1062
18	6	0	−2.228758	1.346357	−0.16582
19	1	0	−2.778298	1.775294	−1.01336
20	1	0	−2.646478	1.799939	0.745846
21	6	0	−0.716738	1.629453	−0.23802
22	1	0	−0.423426	1.685255	−1.3002
23	8	0	−0.39963	2.844582	0.41288
24	1	0	0.570652	2.943725	0.354011
25	6	0	−3.616673	−0.88045	−0.30588
26	1	0	−4.075902	−0.59081	−1.26059
27	1	0	−3.508702	−1.96995	−0.29764
28	1	0	−4.335026	−0.61	0.481087

Table S10. Cartesian coordinate of **5** [E(RB3LYP) = −691.607660318 a.u.]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.801854	−0.12164	0.301795
2	1	0	0.982016	−0.24231	1.382523
3	6	0	−0.66333	0.268102	0.089996
4	6	0	−1.72668	−0.74938	0.226817
5	8	0	−2.90283	−0.41186	−0.36144
6	6	0	−3.96909	−1.36774	−0.21753
7	1	0	−4.20089	−1.52859	0.838859
8	1	0	−4.82119	−0.92805	−0.73743
9	1	0	−3.69055	−2.32188	−0.67302
10	8	0	−1.576	−1.81313	0.808767
11	6	0	−0.81294	1.609104	−0.04622
12	6	0	0.530534	2.296074	0.038071
13	1	0	0.667815	2.737867	1.037646
14	1	0	0.641918	3.11343	−0.68568
15	6	0	1.542548	1.164381	−0.16709
16	1	0	1.736627	1.063721	−1.24935
17	8	0	2.749875	1.451073	0.513691
18	1	0	3.362072	0.712414	0.32161
19	6	0	−2.05005	2.4436	−0.1766
20	1	0	−2.03566	3.249538	0.570066
21	1	0	−2.06629	2.934843	−1.16027
22	1	0	−2.96896	1.868262	−0.06867
23	6	0	1.254256	−1.41608	−0.40048
24	1	0	0.548373	−2.21837	−0.15689
25	1	0	1.214671	−1.2808	−1.49354
26	6	0	2.641513	−1.91508	0.005136
27	1	0	2.713114	−2.00313	1.093682
28	1	0	2.825628	−2.90975	−0.42278
29	8	0	3.725588	−1.03512	−0.36039
30	1	0	3.826492	−1.04301	−1.32517

Table S11. Cartesian coordinate of **6** [E(RB3LYP) = −919.493282263 a.u.]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.503975	0.721237	0.654811
2	1	0	0.574538	1.215635	1.63599
3	6	0	−0.961	0.719246	0.217804
4	6	0	−1.91664	−0.20742	0.858552
5	8	0	−3.06794	−0.39446	0.1684
6	6	0	−4.02841	−1.27158	0.785287
7	1	0	−4.87599	−1.29724	0.099253
8	1	0	−3.60422	−2.27106	0.912883
9	1	0	−4.33229	−0.8829	1.761006
10	8	0	−1.699	−0.76786	1.922823
11	6	0	−1.23069	1.749113	−0.62096
12	6	0	0.018649	2.559326	−0.87782
13	1	0	0.123299	2.866725	−1.92601
14	1	0	−0.00021	3.482837	−0.27831
15	6	0	1.164651	1.661715	−0.39572
16	1	0	1.510765	1.05236	−1.24641
17	8	0	2.232399	2.446233	0.097629
18	1	0	2.938557	1.821133	0.366376
19	6	0	−2.52818	2.204883	−1.21449
20	1	0	−2.48883	2.113266	−2.30955
21	1	0	−3.38651	1.638447	−0.8549
22	1	0	−2.68154	3.271594	−1.00039
23	6	0	1.184271	−0.67009	0.853134
24	1	0	0.520804	−1.24325	1.511267
25	6	0	2.548668	−0.57593	1.562301
26	1	0	2.435303	−0.00692	2.48941
27	1	0	2.894927	−1.58475	1.825524
28	8	0	3.561976	0.094246	0.806343
29	1	0	3.67089	−0.42382	−0.01404
30	6	0	1.326598	−1.45418	−0.44028
31	8	0	2.377104	−1.6186	−1.04653
32	8	0	0.159107	−1.96114	−0.86851
33	6	0	0.190864	−2.69146	−2.11265
34	1	0	0.551474	−2.04925	−2.91998
35	1	0	0.843533	−3.56332	−2.02191
36	1	0	−0.84023	−2.99596	−2.29131

Table S12. Cartesian coordinate of **6a** [E(RB3LYP) = −803.751549217 a.u.]

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.217636	0.429079	−0.34564
2	6	0	1.559558	−0.25154	−0.12692
3	6	0	1.69252	−1.72238	−0.11946
4	8	0	0.525103	−2.444	−0.11775
5	6	0	−0.76434	−1.85061	−0.34389
6	6	0	−0.89223	−0.44107	0.257126
7	6	0	0.457117	1.848175	0.238907
8	6	0	1.977757	2.048875	0.107437
9	6	0	2.544889	0.646232	0.115252
10	6	0	4.001687	0.411833	0.353701
11	1	0	0.01785	0.542069	−1.42396
12	8	0	−0.22776	2.893969	−0.42048
13	6	0	−2.29305	0.124224	0.06668
14	8	0	2.735003	−2.34265	−0.06109
15	8	0	−2.5526	1.266886	−0.27121
16	8	0	−3.24349	−0.78143	0.348782
17	6	0	−4.61365	−0.33161	0.250622
18	1	0	−0.94368	−1.81676	−1.4271
19	1	0	−1.47557	−2.54533	0.10281
20	1	0	−0.74191	−0.5239	1.345355
21	1	0	0.189414	1.831403	1.310228
22	1	0	2.397697	2.679337	0.900441
23	1	0	2.197296	2.551305	−0.84728
24	1	0	4.252017	−0.64885	0.365078
25	1	0	4.590343	0.907342	−0.43209
26	1	0	4.306657	0.873581	1.303079
27	1	0	−1.17202	2.649681	−0.43899
28	1	0	−5.2173	−1.19986	0.513489
29	1	0	−4.78927	0.49096	0.947982
30	1	0	−4.82899	−0.00045	−0.76792

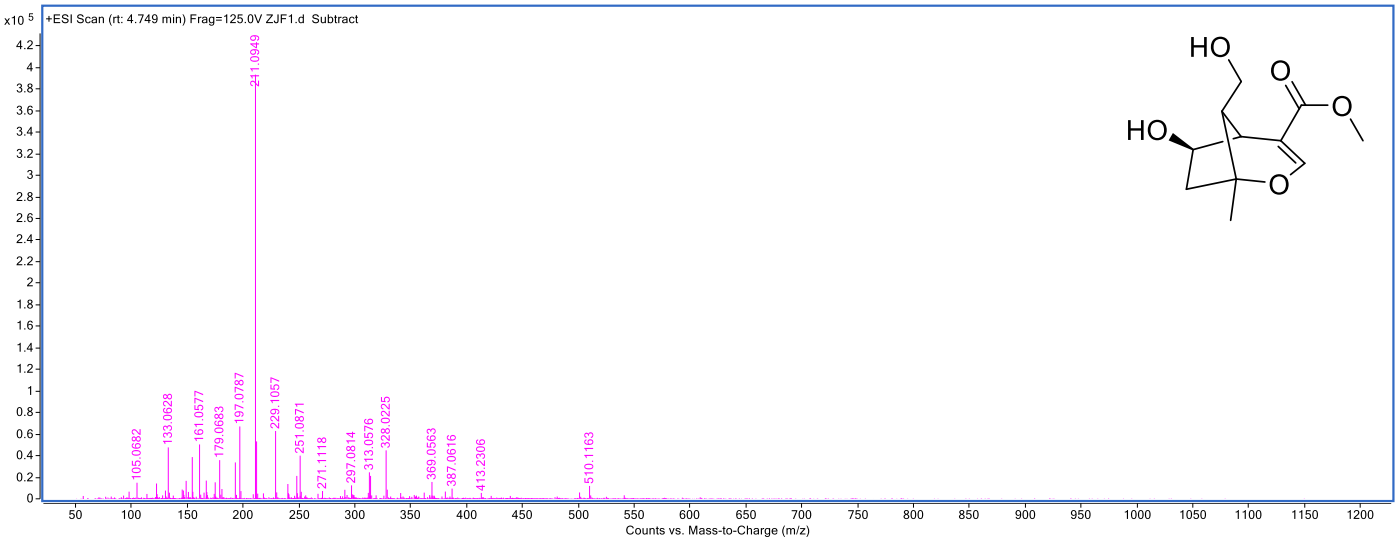

Figure S30. (+)-HR-ESI-MS spectrum of **1**

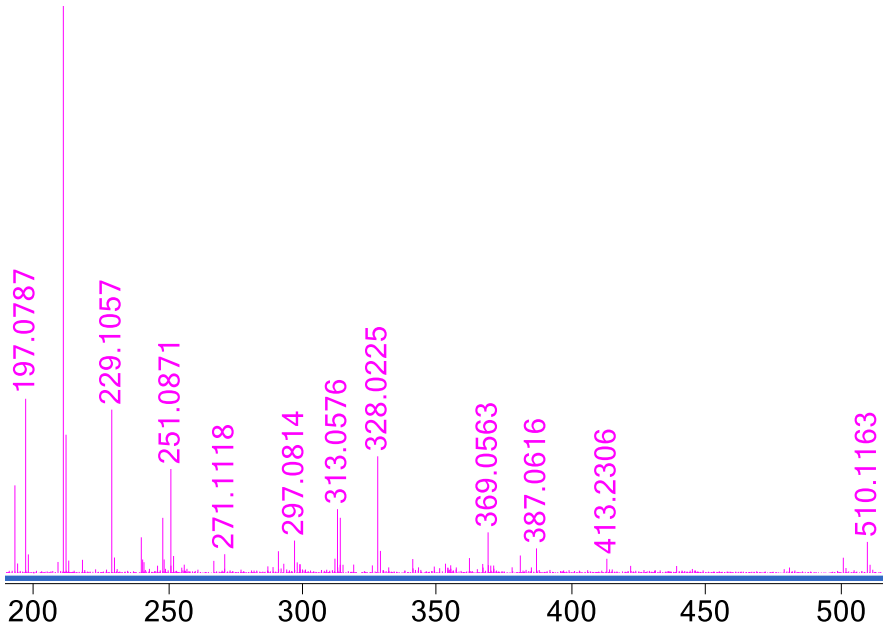

Figure S31. (+)-HR-ESI-MS spectrum of **1** (amplified)

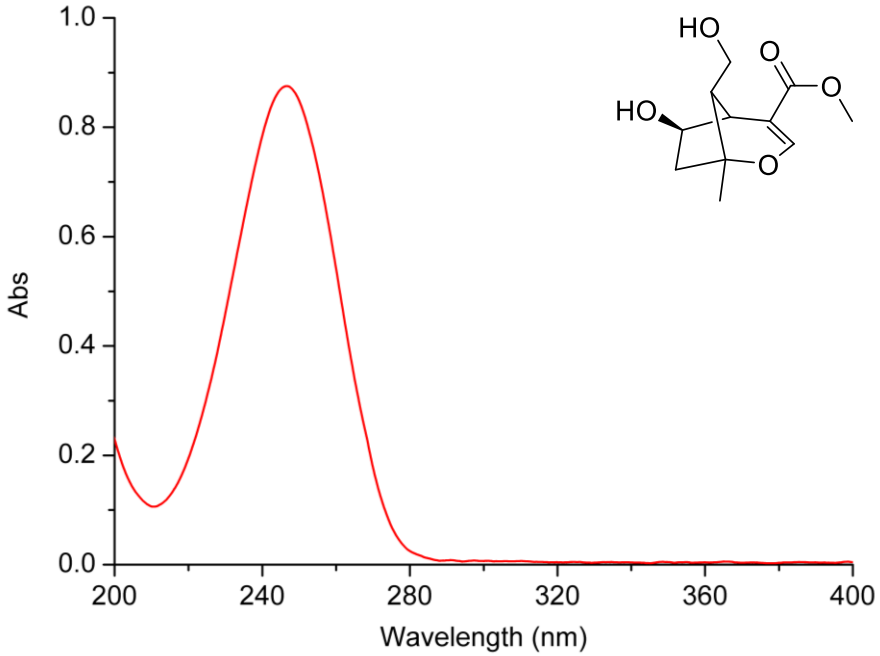

Figure S32. UV spectrum of compound **1**

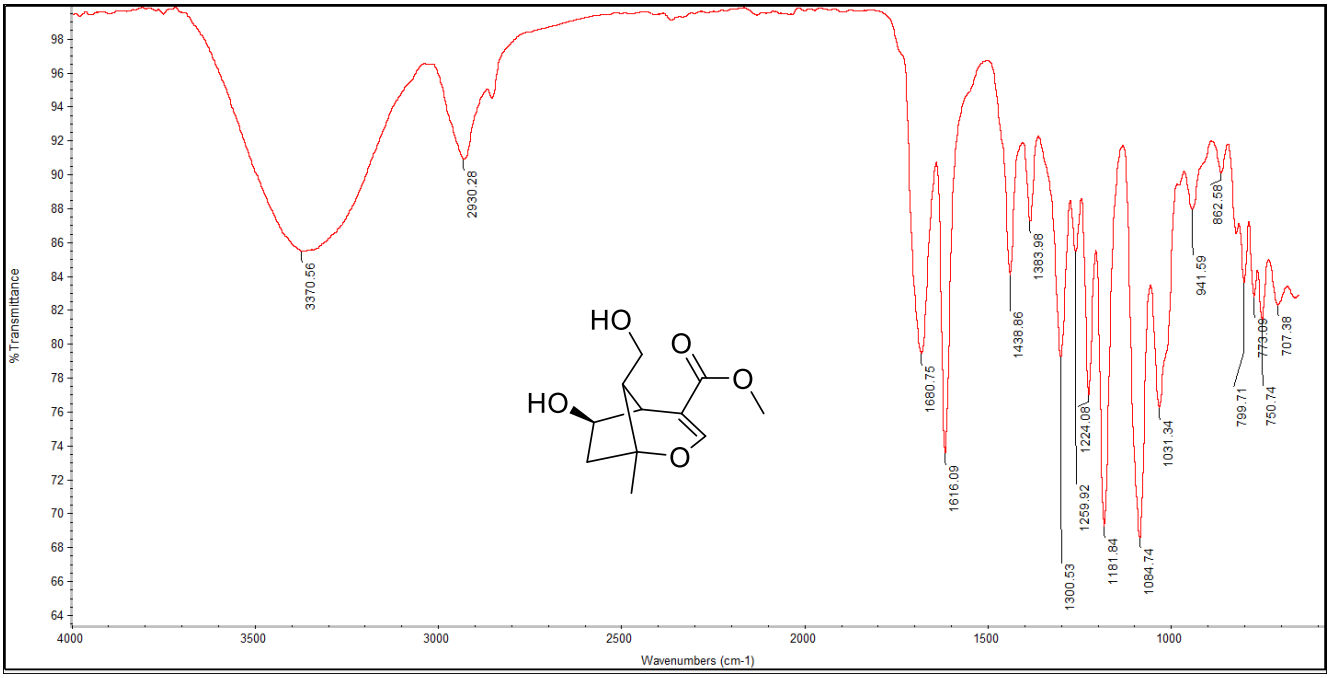

Figure S33. IR spectrum of compound **1**

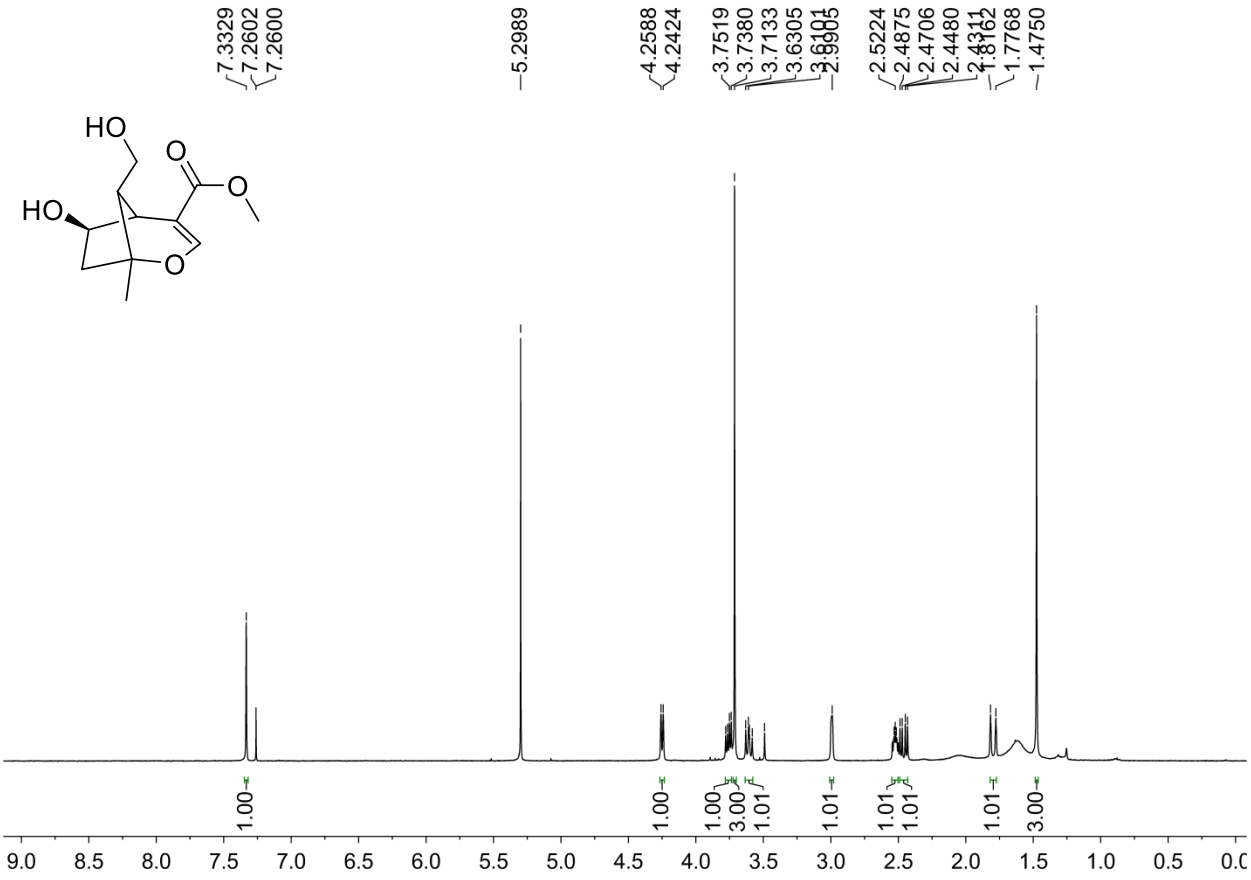

Figure S34. [1]H NMR (400 MHz, chloroform-*d*) spectrum of compound **1**

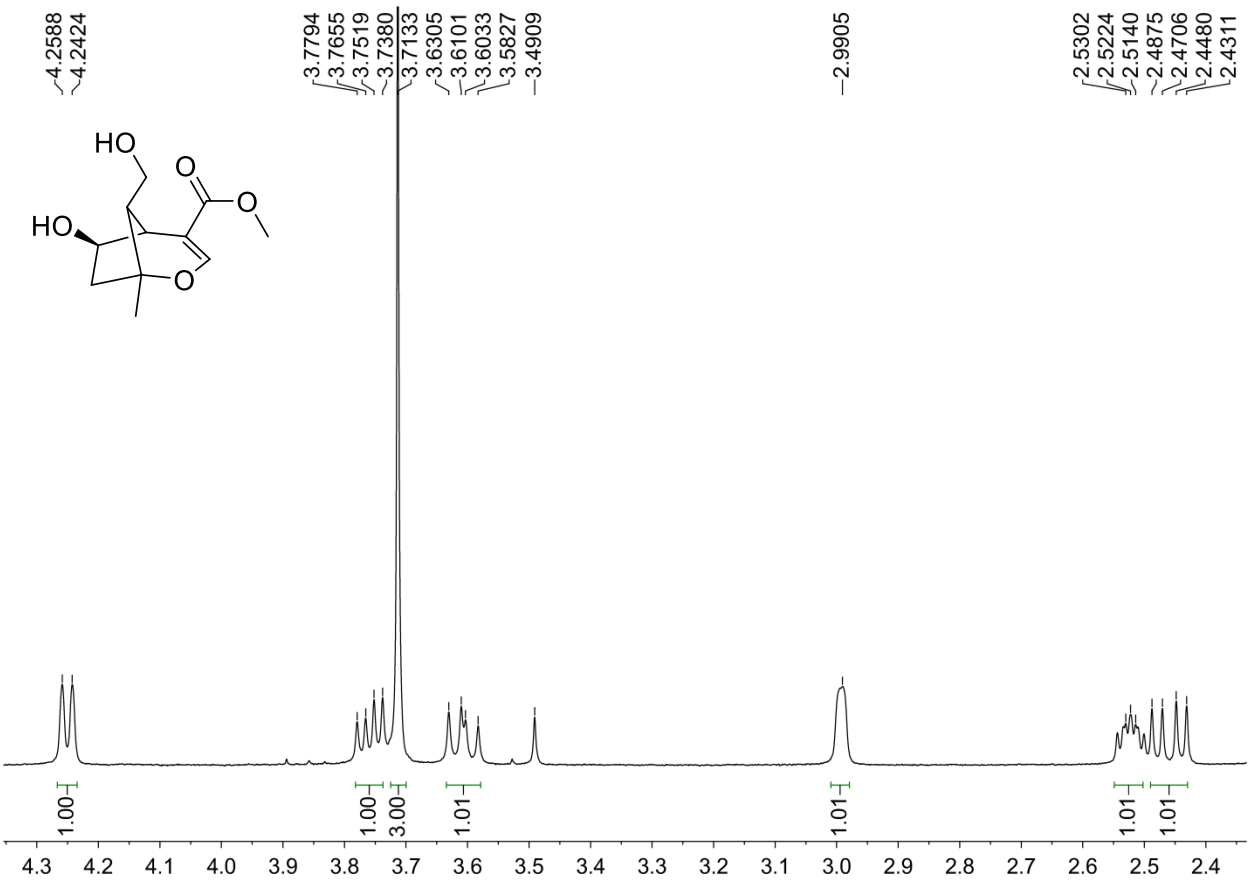

Figure S35. [1]H NMR (400 MHz, chloroform-*d*) spectrum of compound **1** (amplified)

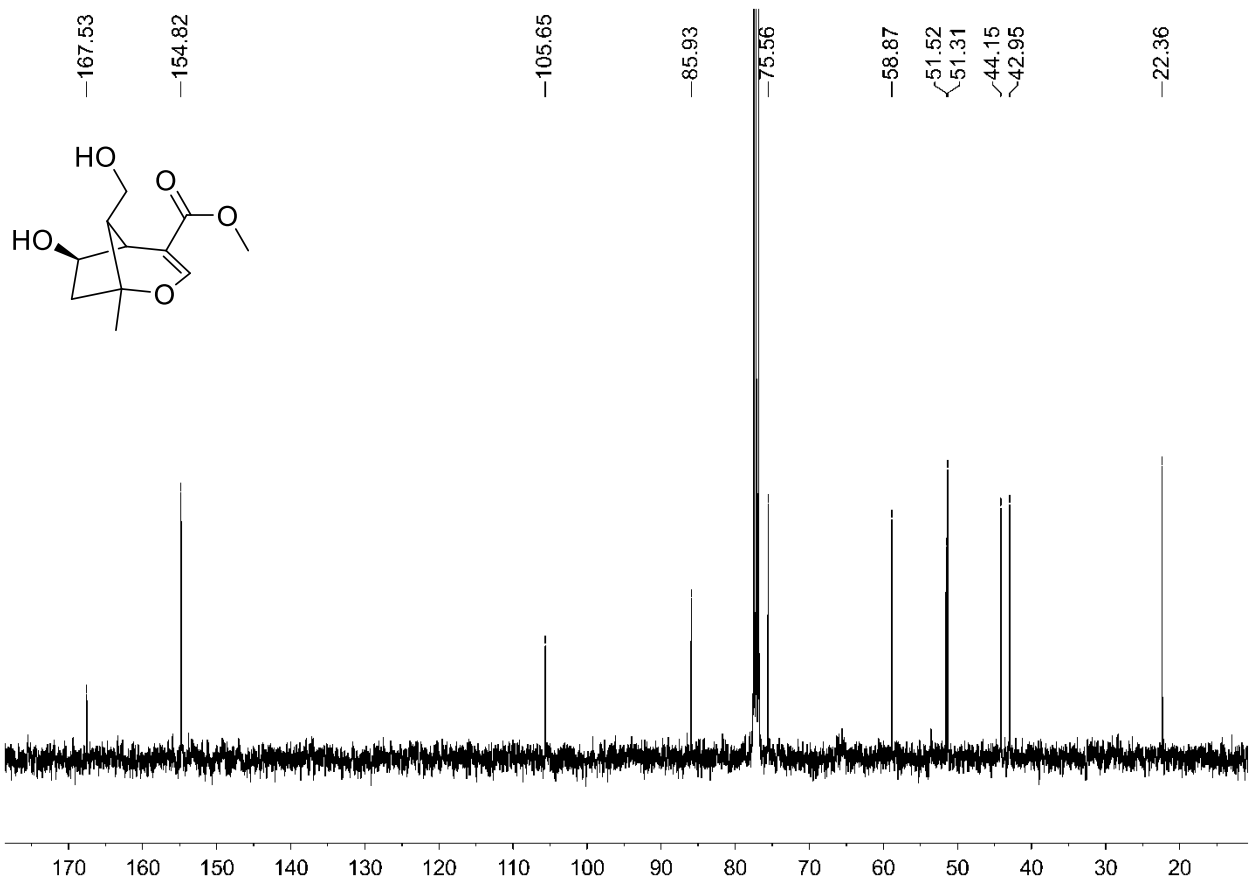

Figure S36. ^{13}C NMR (100 MHz, chloroform-*d*) spectrum of compound **1**

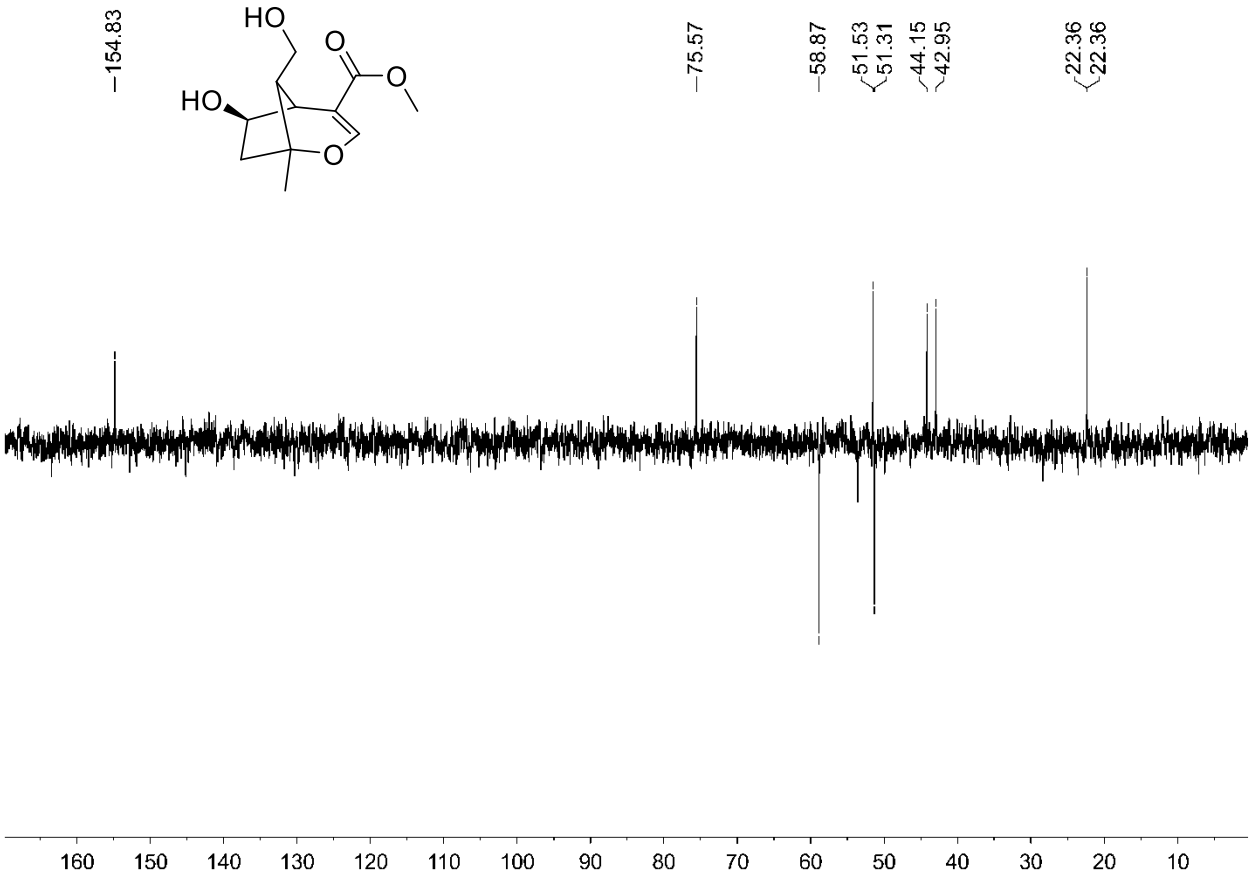

Figure S37. DEPT135 (100 MHz, chloroform-*d*) spectrum of compound **1**

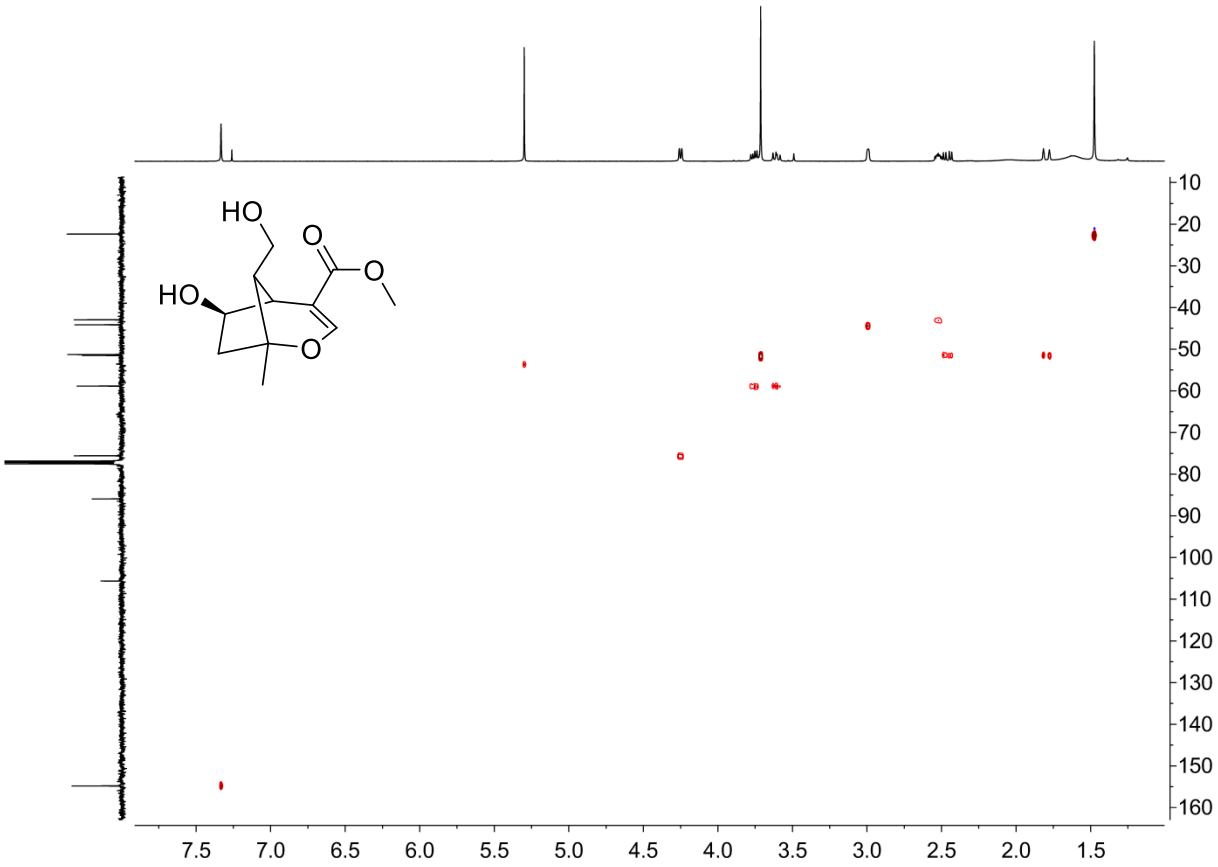

Figure S38. HSQC spectrum (chloroform-*d*) of compound **1** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

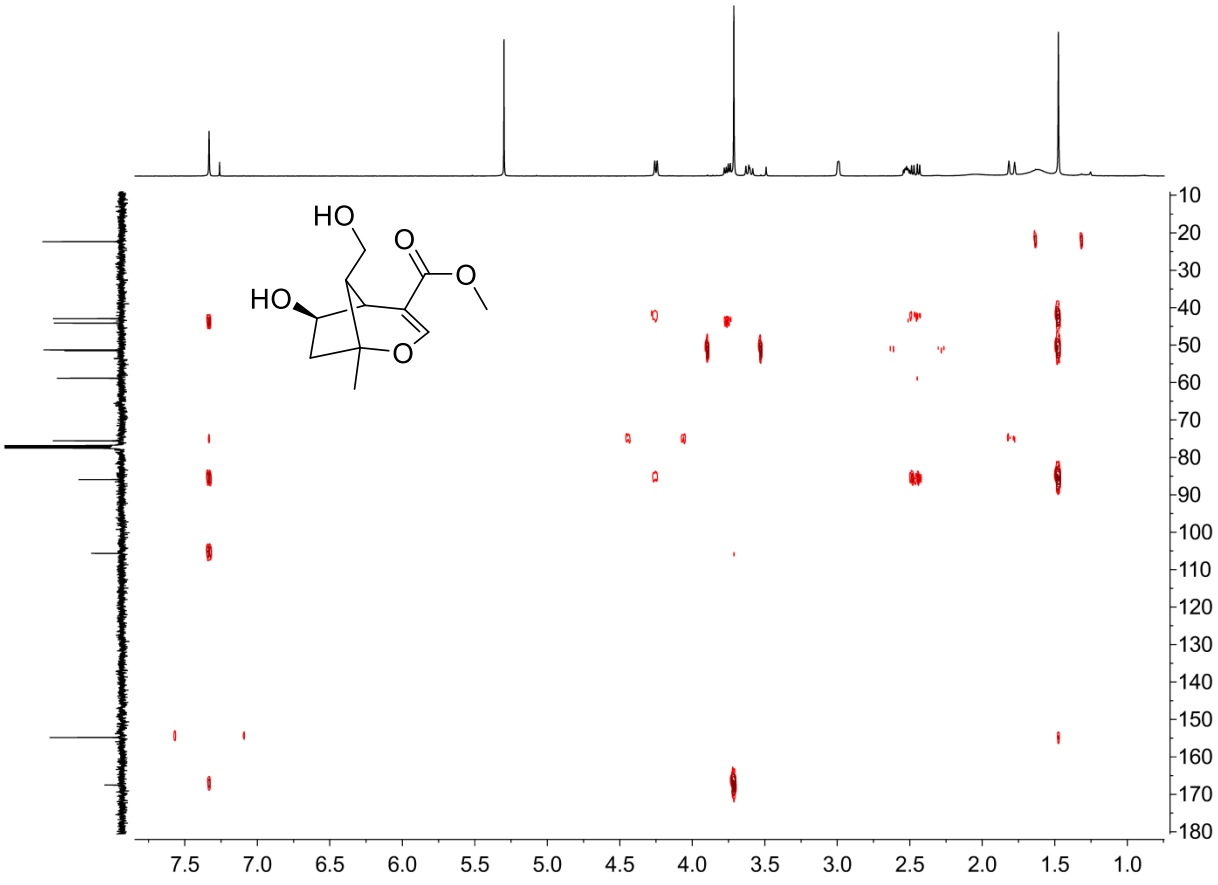

Figure S39. HMBC spectrum (chloroform-*d*) of compound **1** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

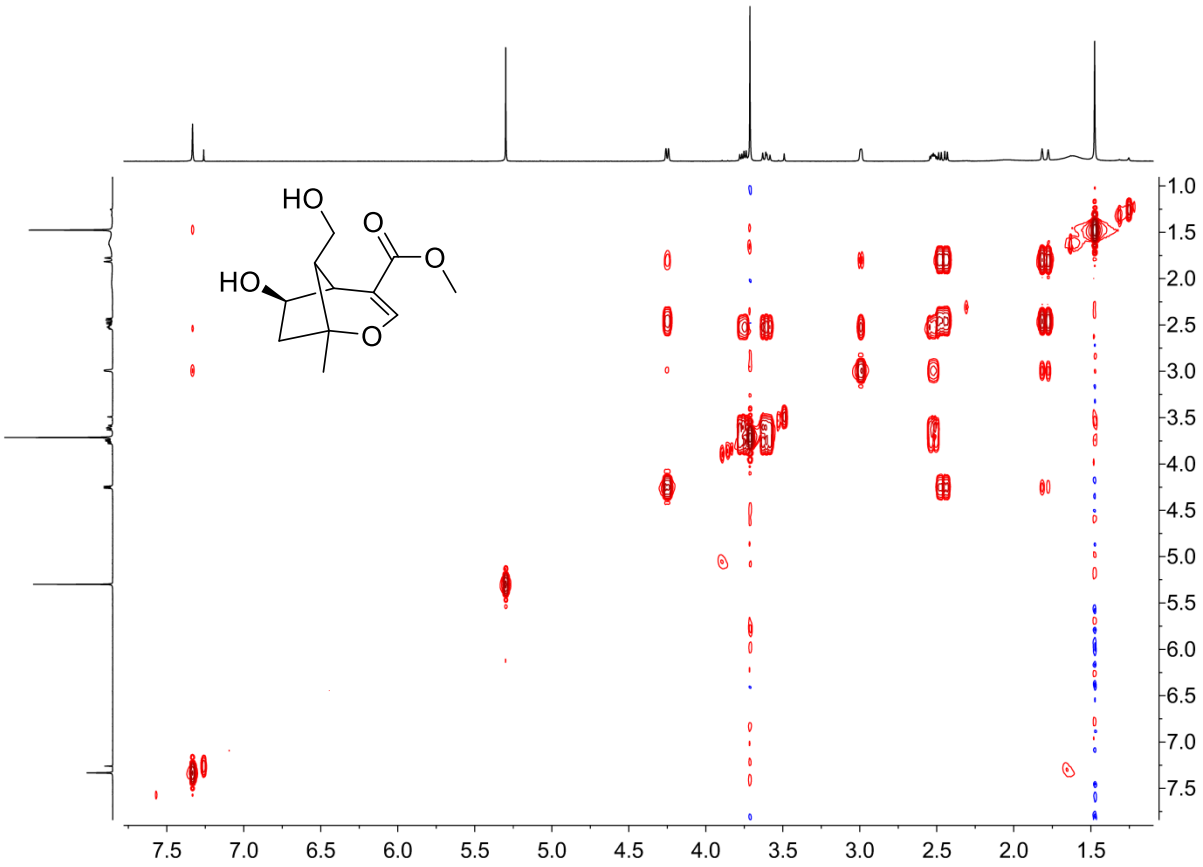

Figure S40. $^{1}H–^{1}H$ COSY spectrum (400 MHz, chloroform-*d*) of compound **1**

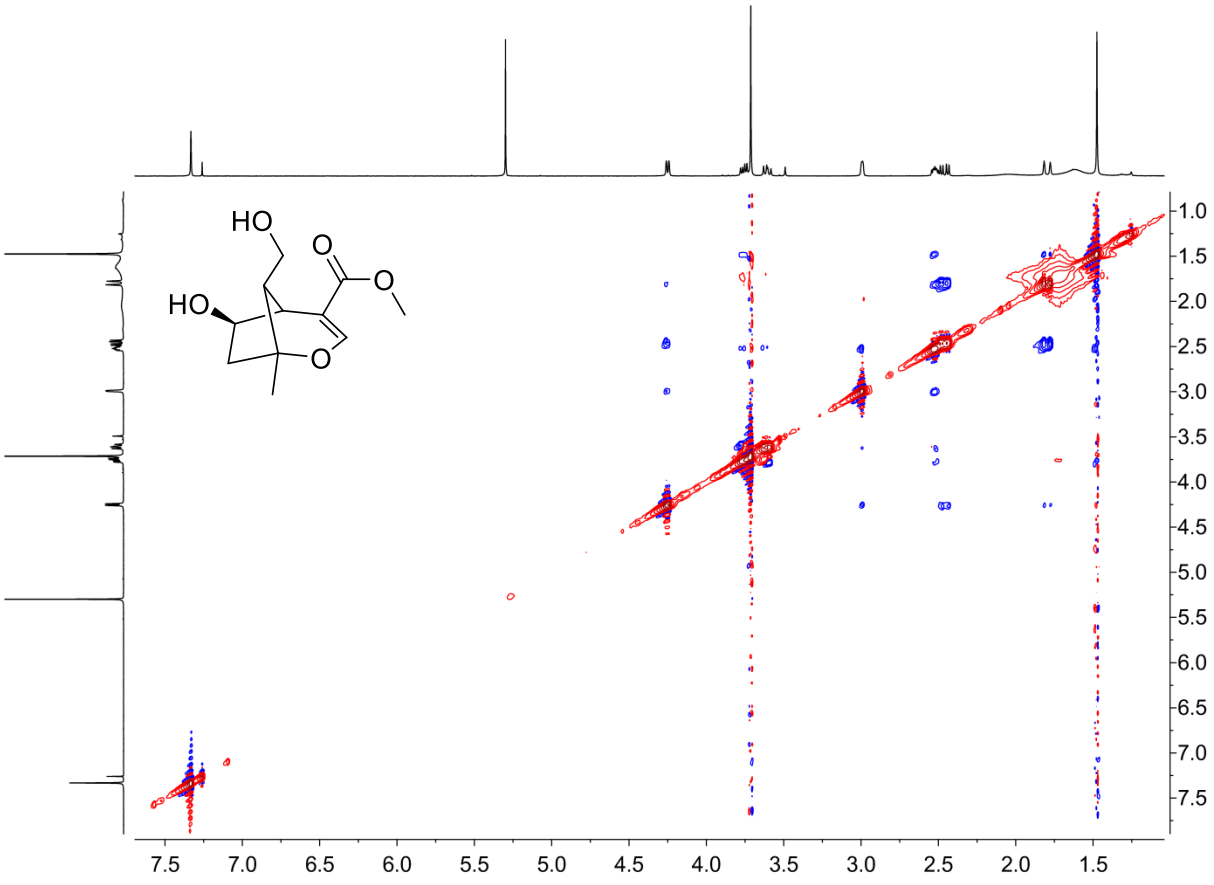

Figure S41. NOESY spectrum (400 MHz, chloroform-*d*) of compound **1**

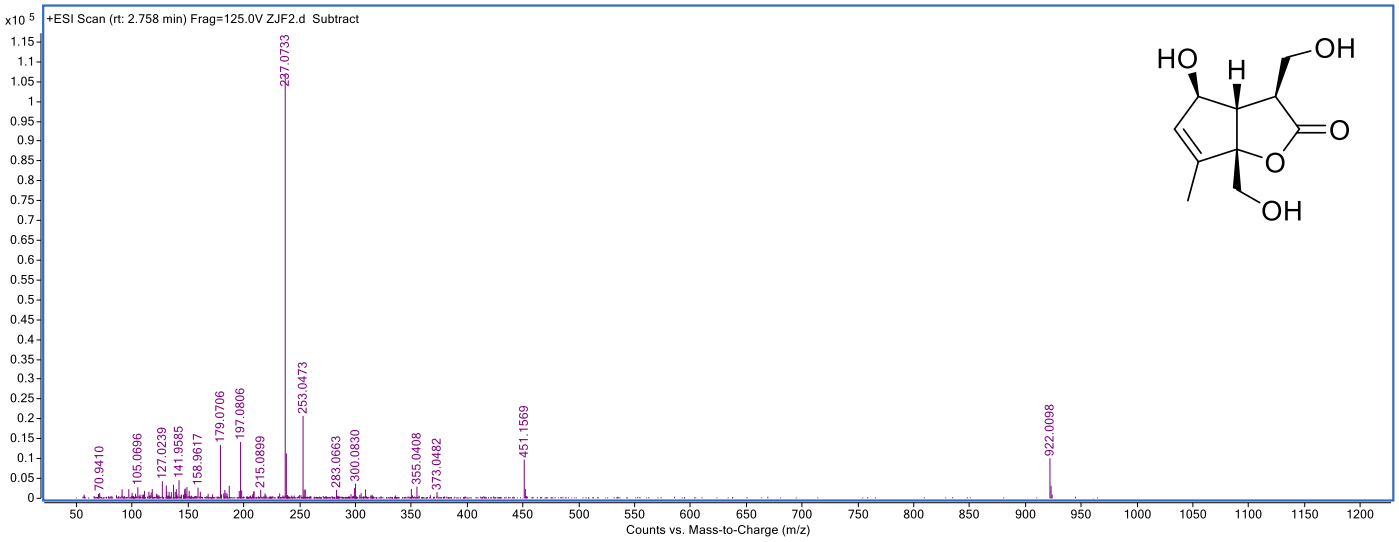

Figure S42. (+)-HR-ESI-MS spectrum of **2**

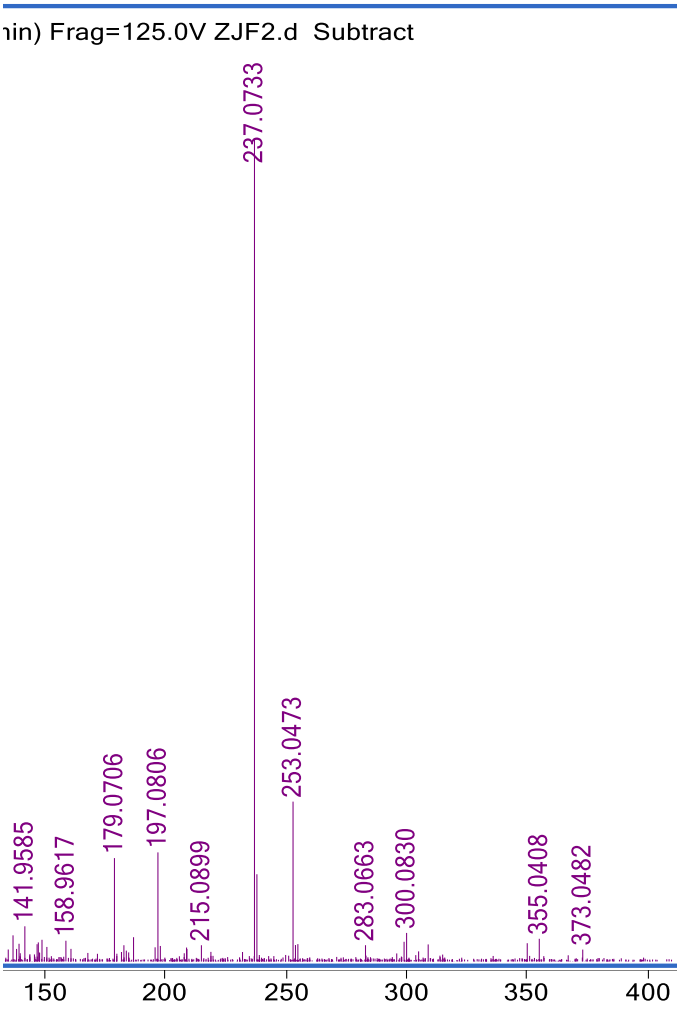

Figure S43. (+)-HR-ESI-MS spectrum of **2** (amplified)

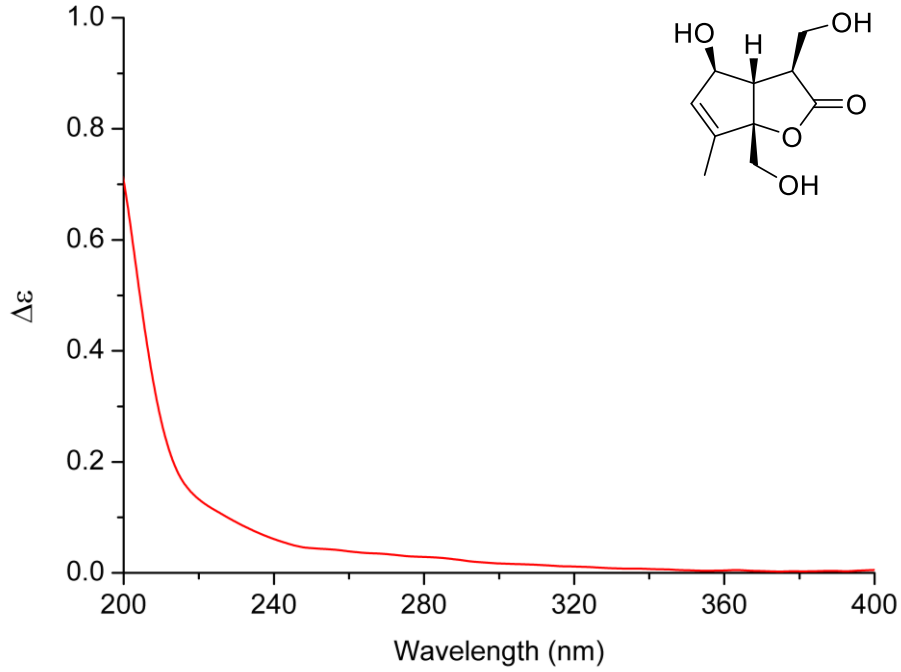

Figure S44. UV spectrum of compound **2**

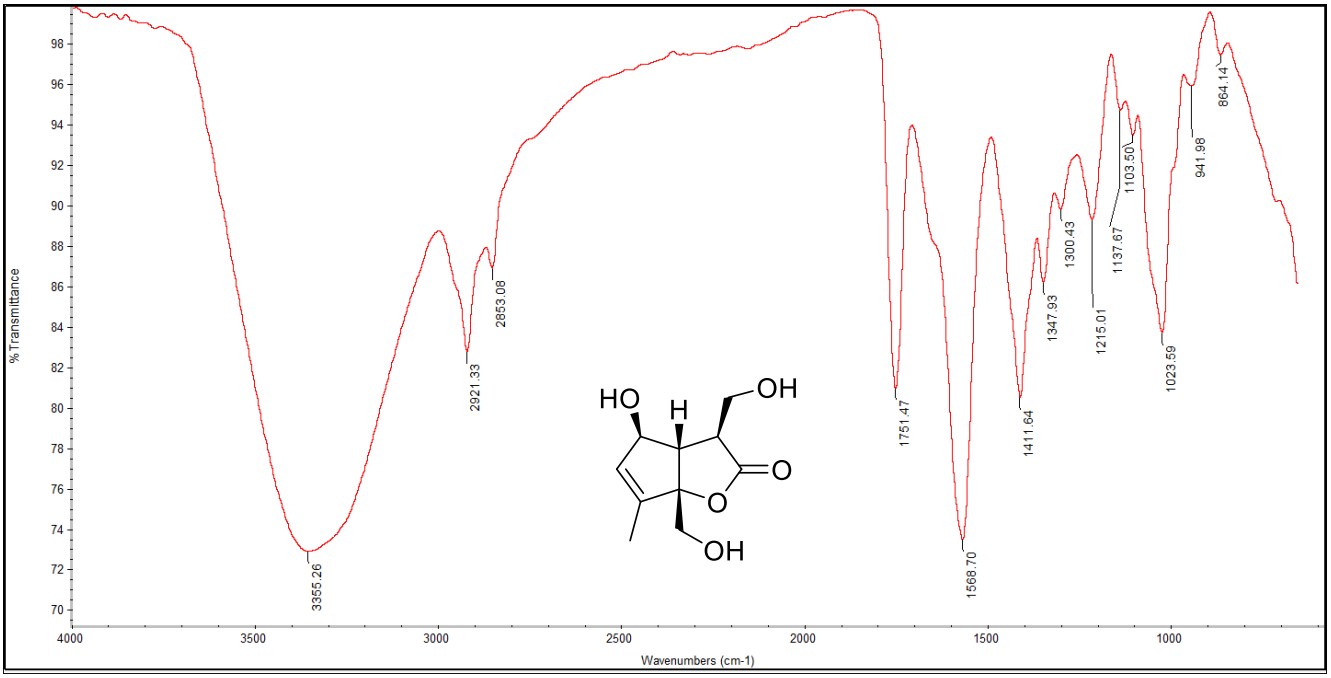

Figure S45. IR spectrum of compound **2**

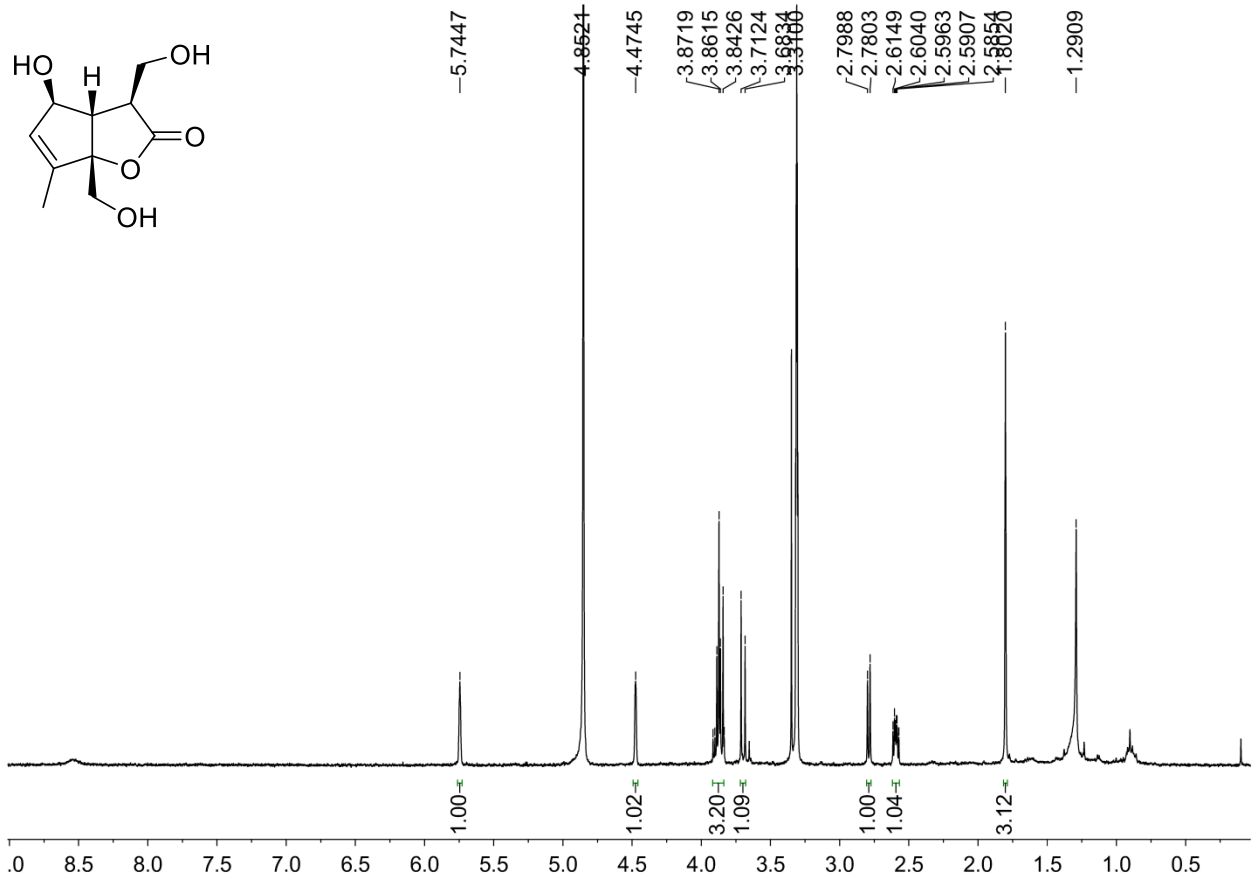

Figure S46. ^{1}H NMR (400 MHz, methanol-d_4) spectrum of compound **2**

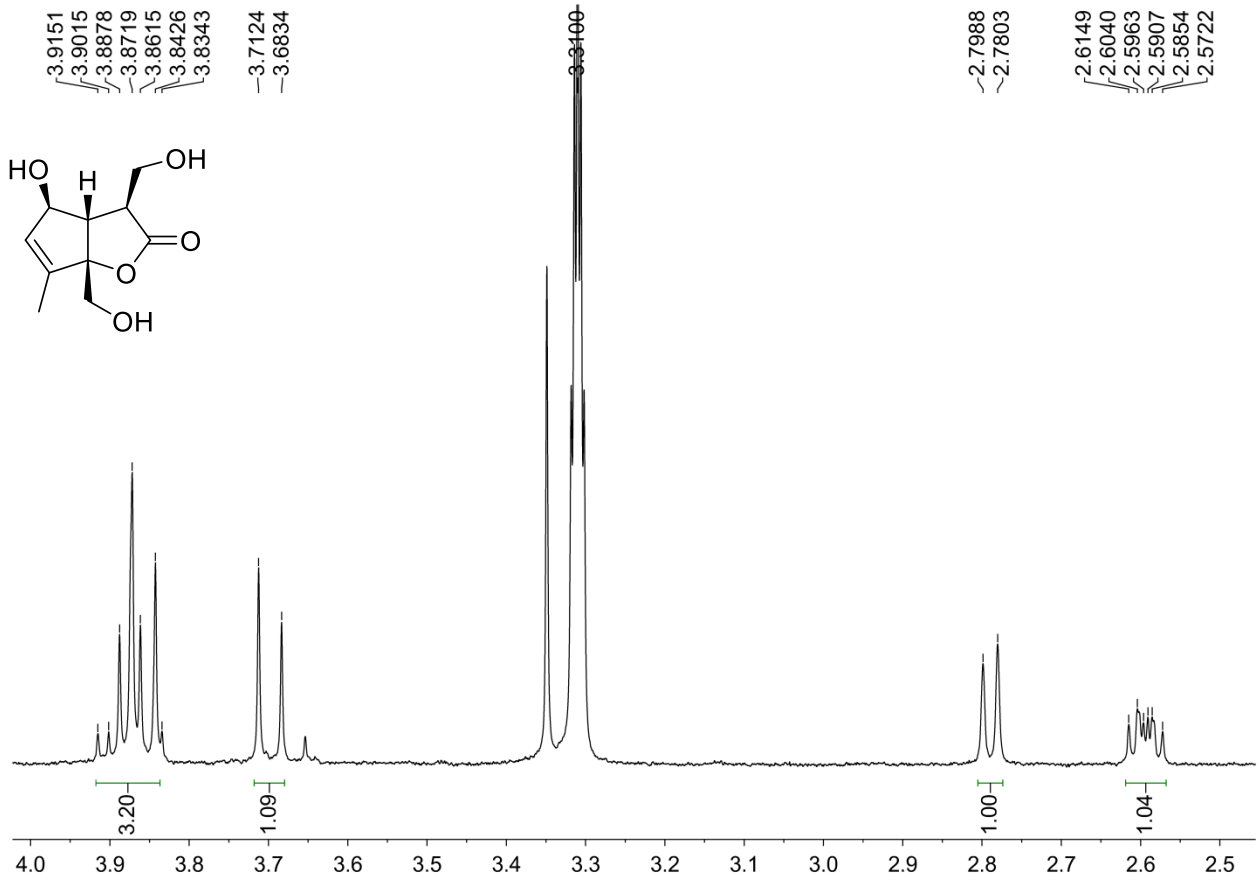

Figure S47. ^{1}H NMR (400 MHz, methanol-d_4) spectrum of compound **2** (amplified)

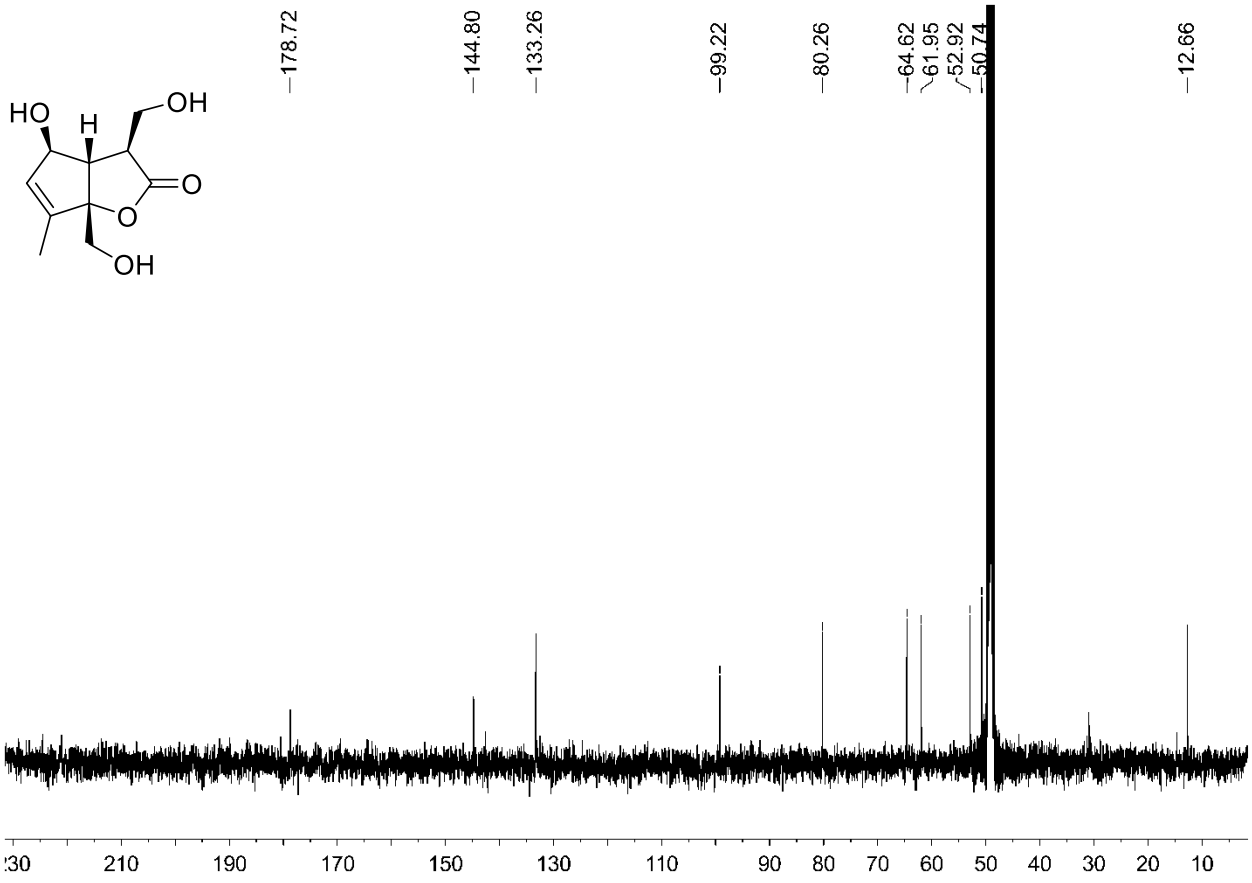

Figure S48. ^{13}C NMR (100 MHz, methanol-d_4) spectrum of compound **2**

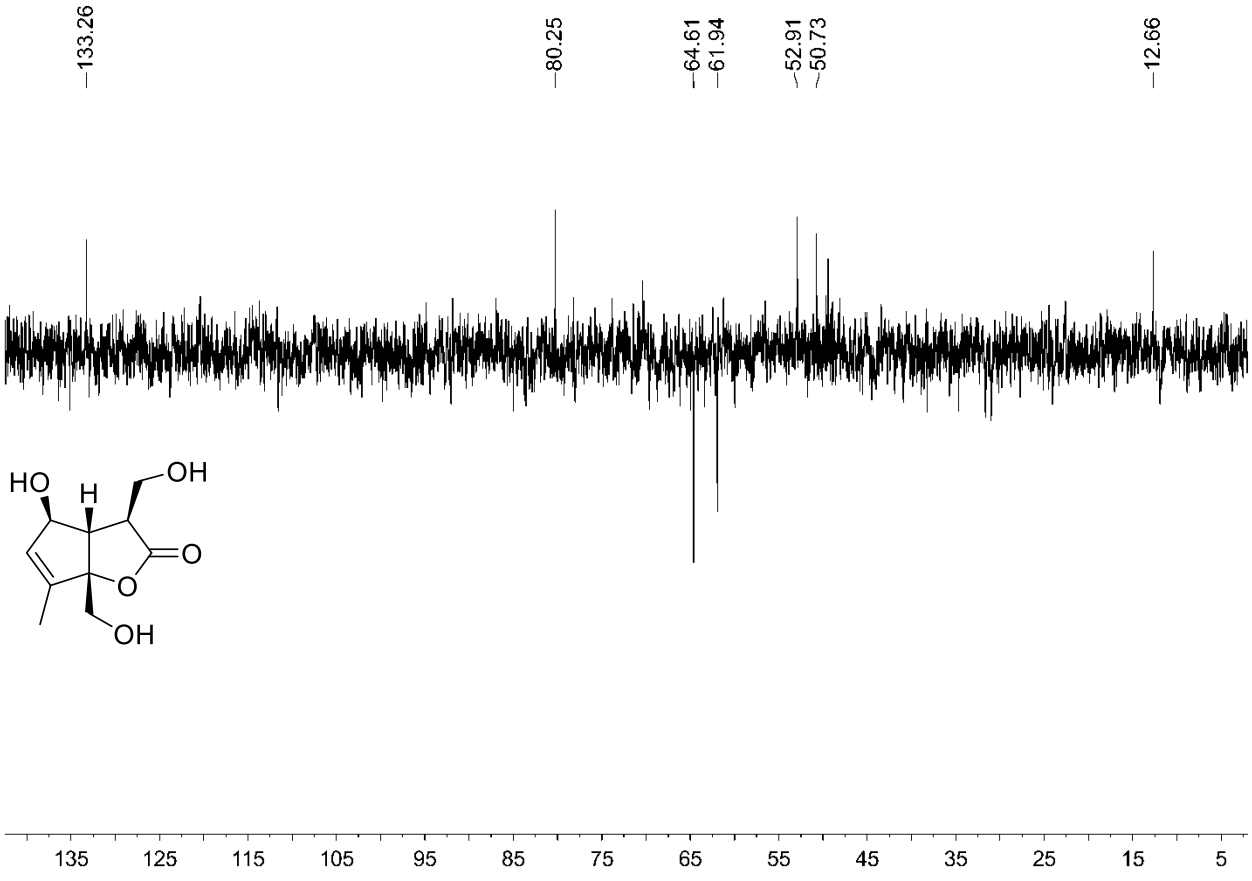

Figure S49. DEPT135 (100 MHz, methanol-d_4) spectrum of compound **2**

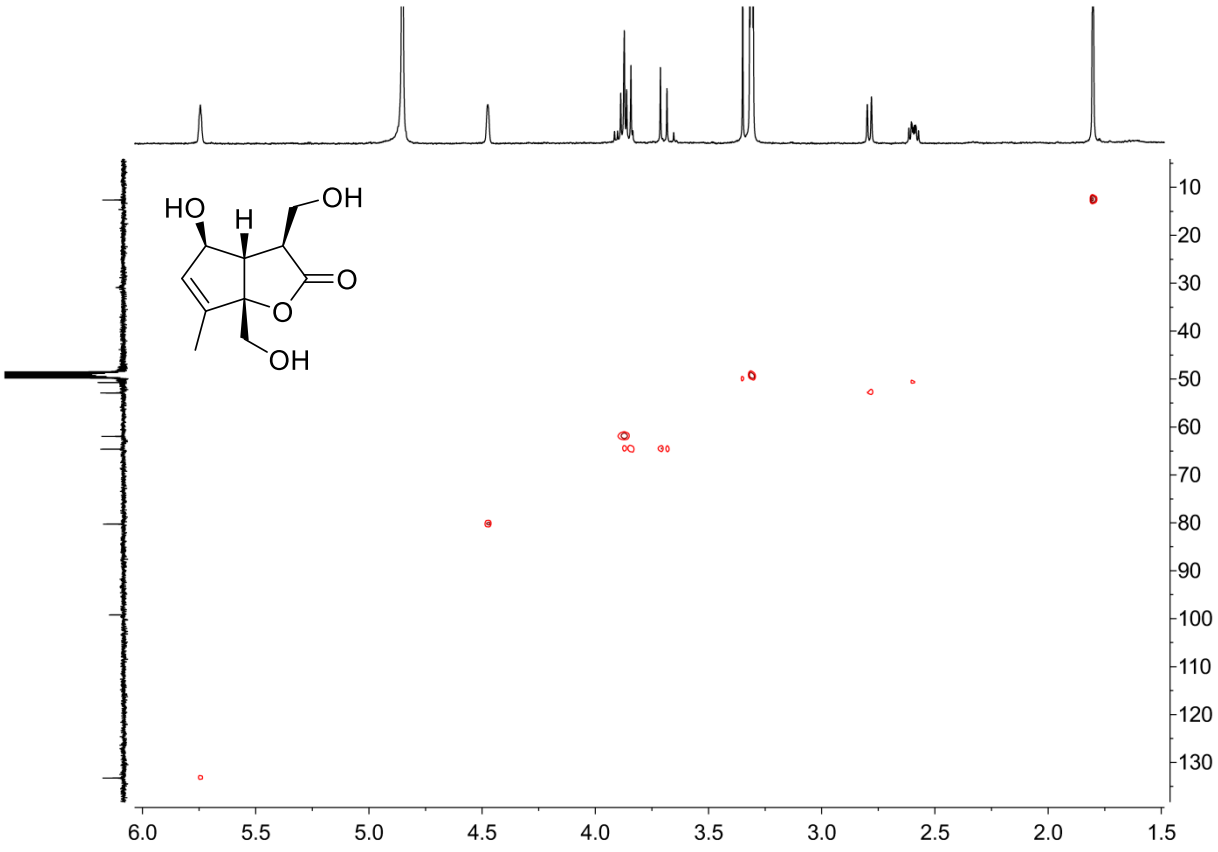

Figure S50. HSQC spectrum (methanol-d_4) of compound **2** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

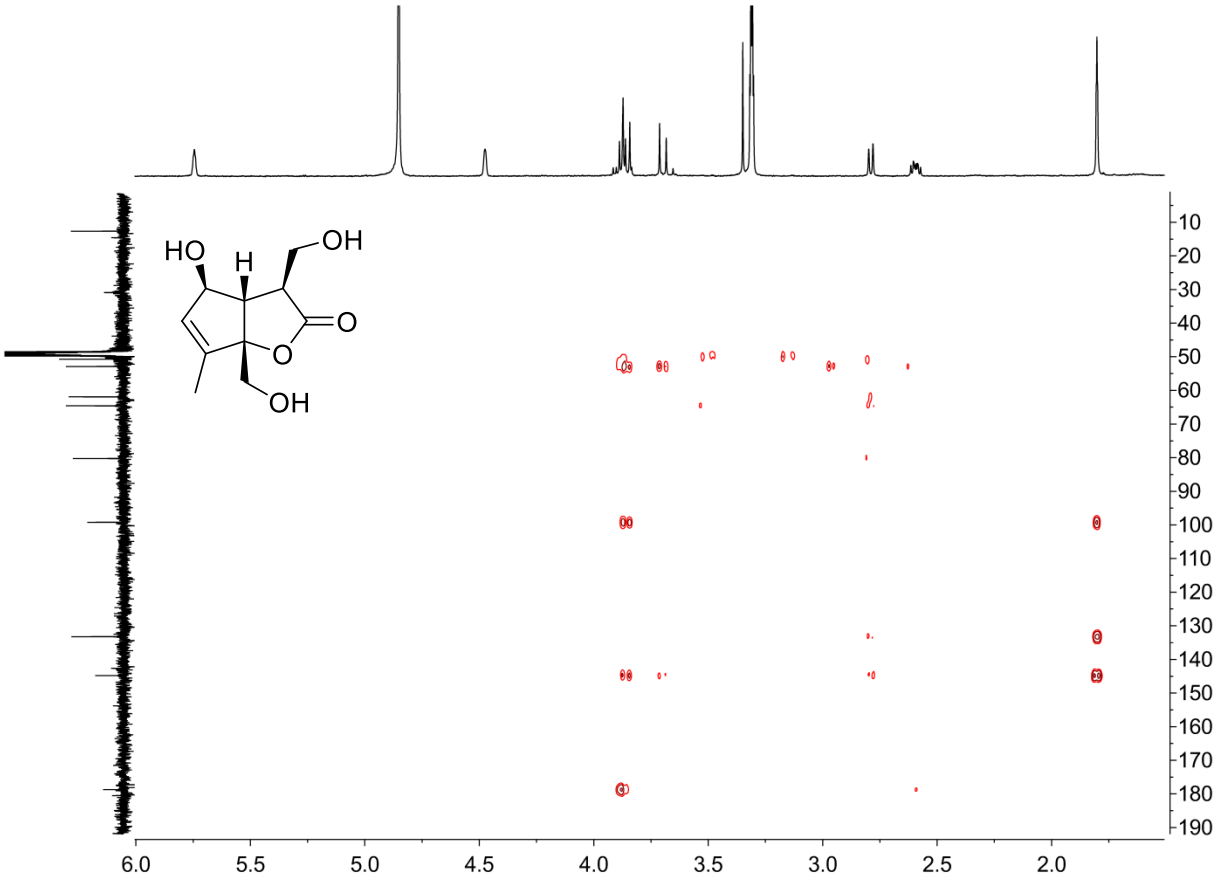

Figure S51. HMBC spectrum (methanol-d_4) of compound **2** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

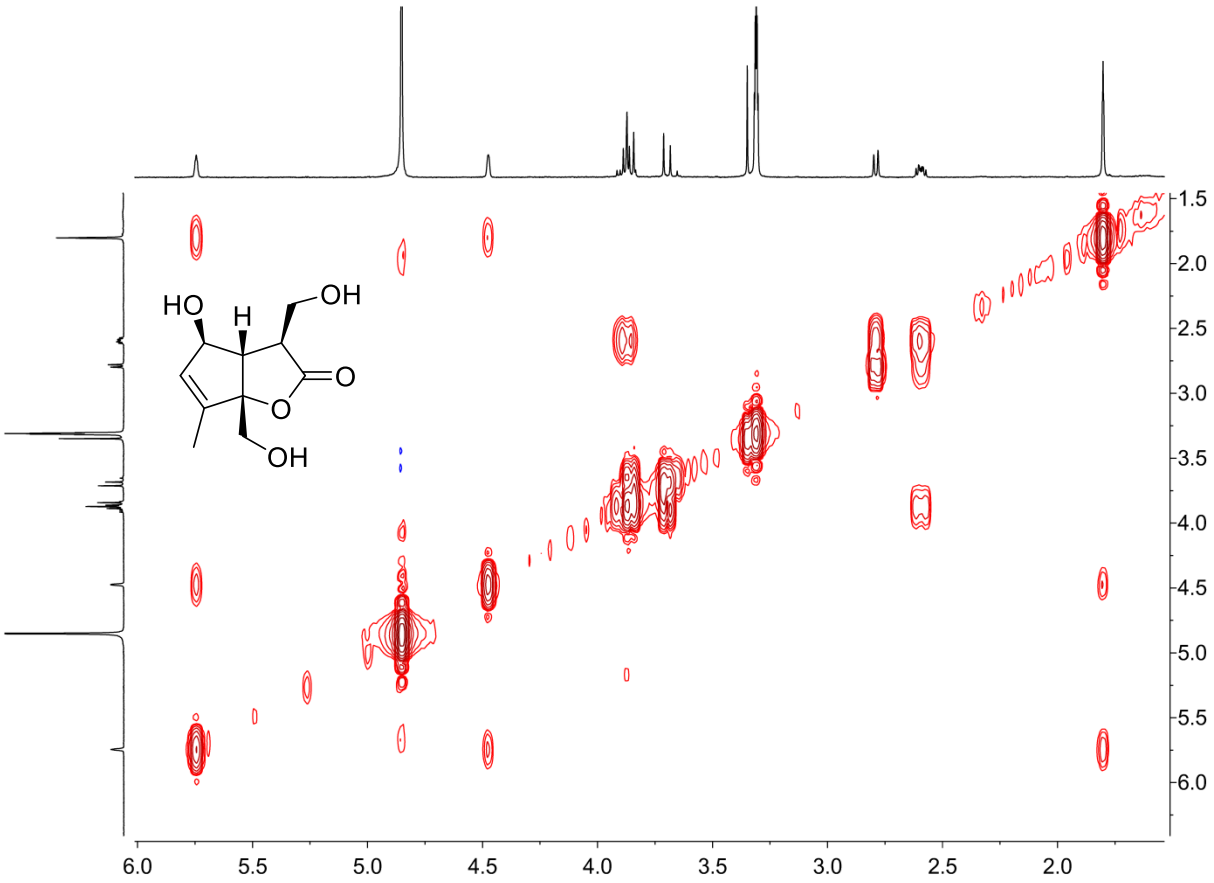

Figure S52. $^{1}H–^{1}H$ COSY spectrum (400 MHz, methanol-d_4) of compound **2**

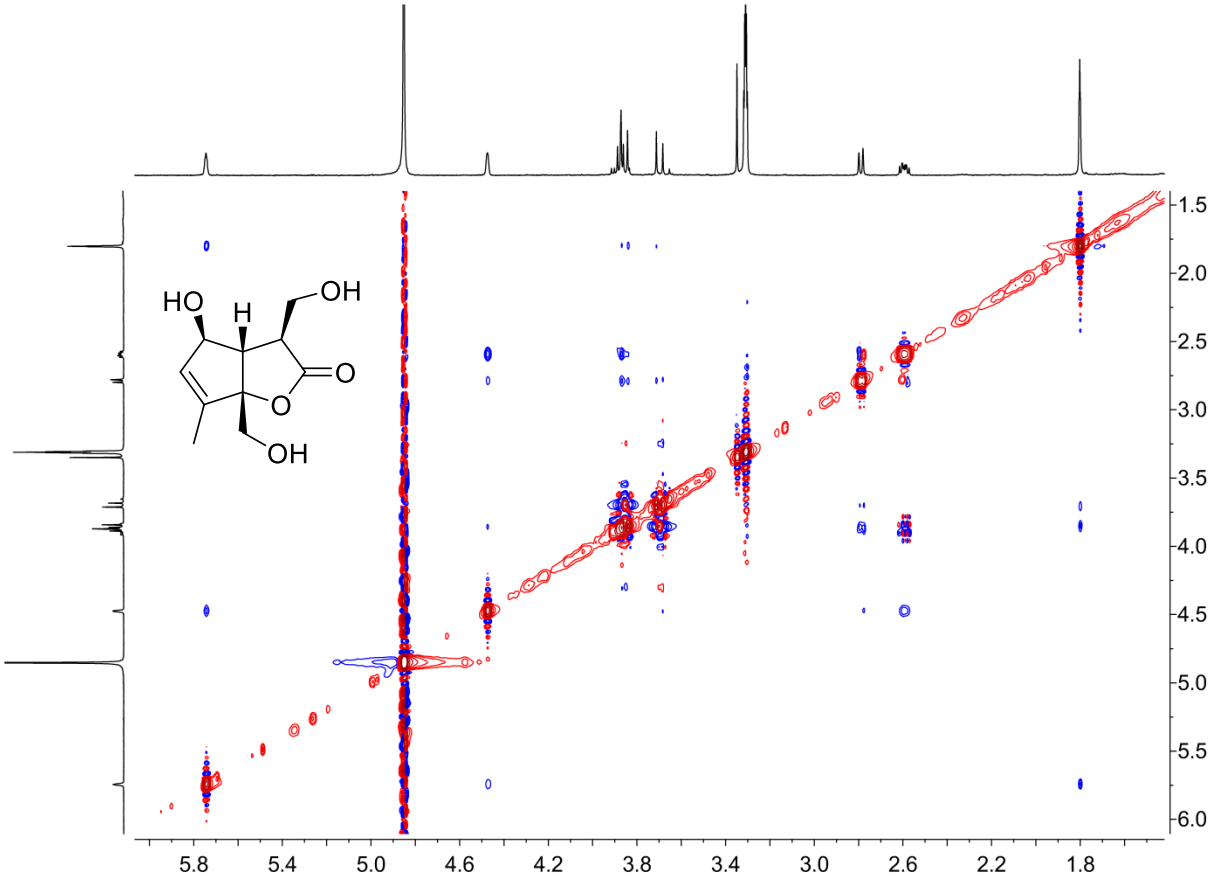

Figure S53. NOESY spectrum (400 MHz, methanol-d_4) of compound **2**

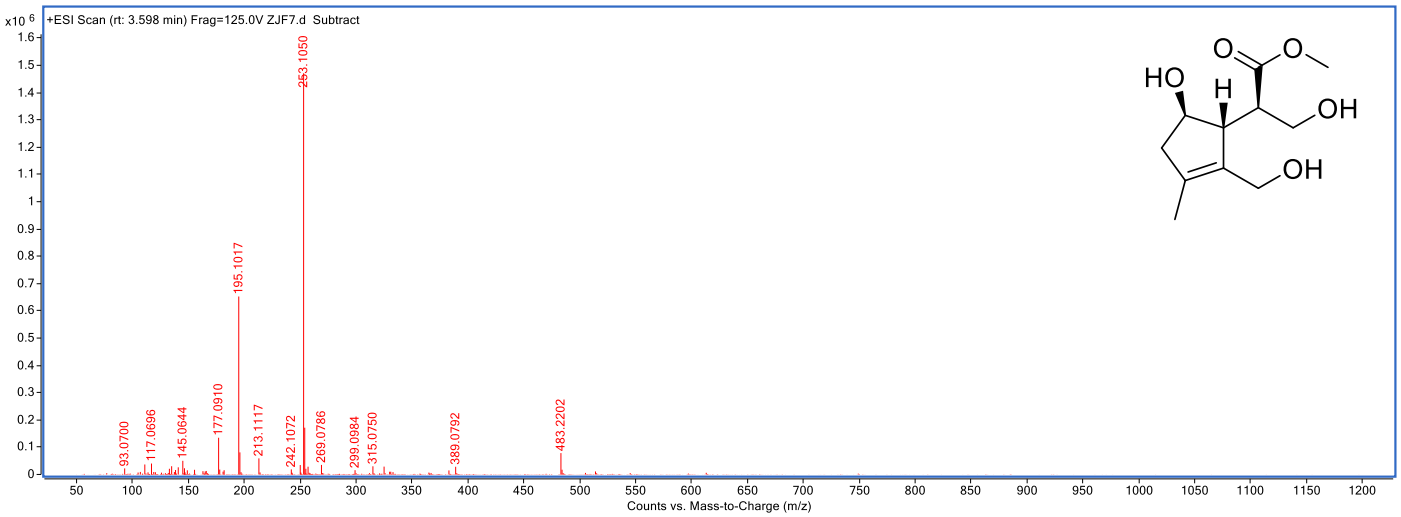

Figure S54. (+)-HR-ESI-MS spectrum of **3**

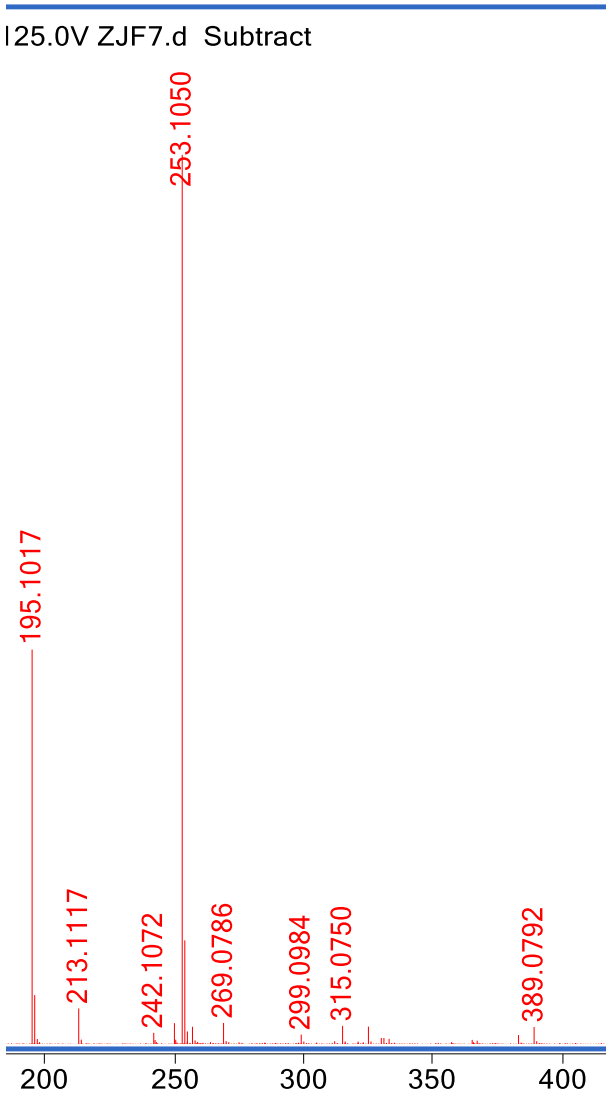

Figure S55. (+)-HR-ESI-MS spectrum of **3** (amplified)

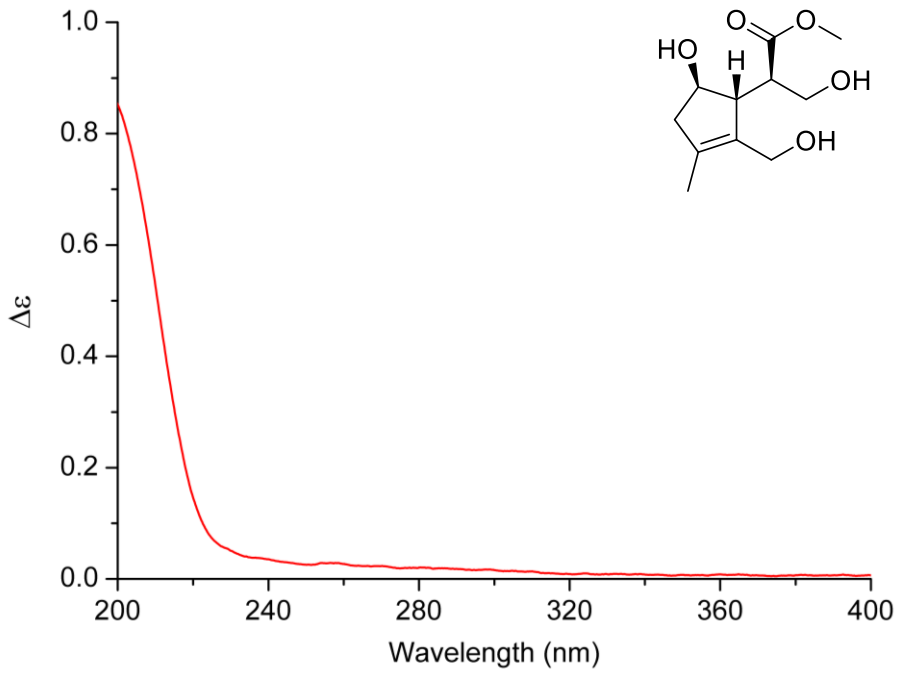

Figure S56. UV spectrum of compound **3**

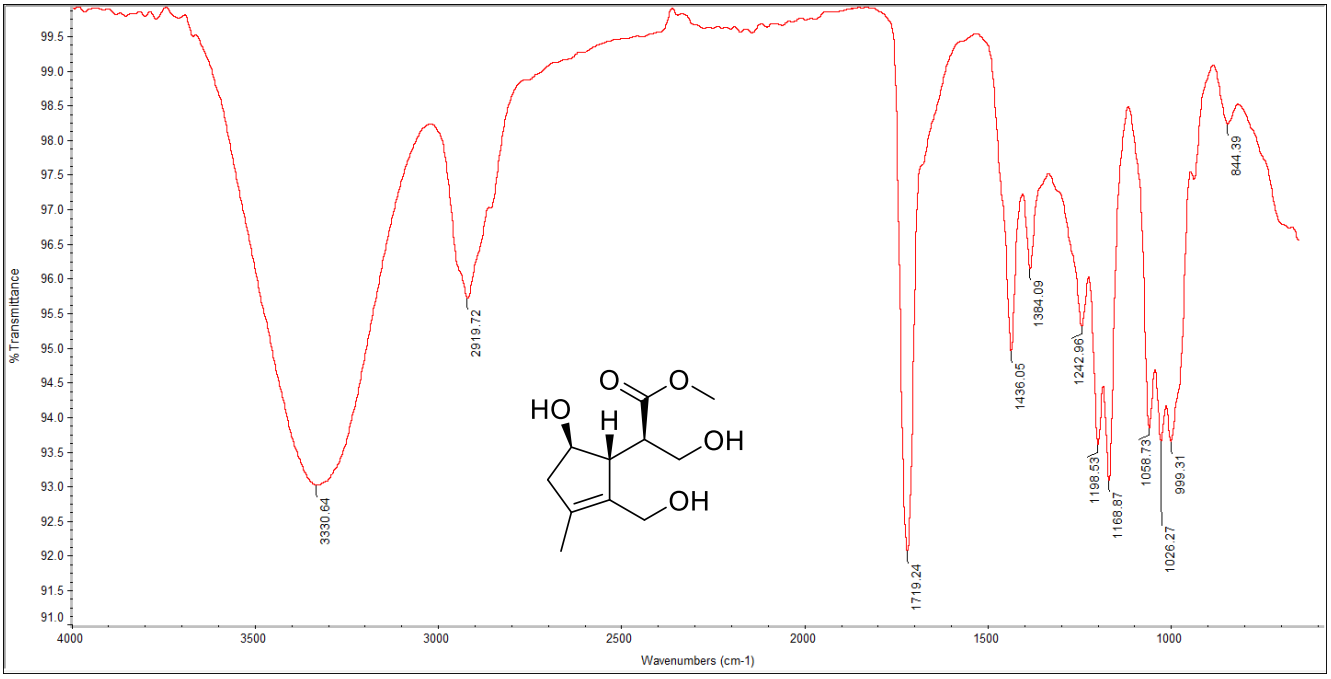

Figure S57. IR spectrum of compound **3**

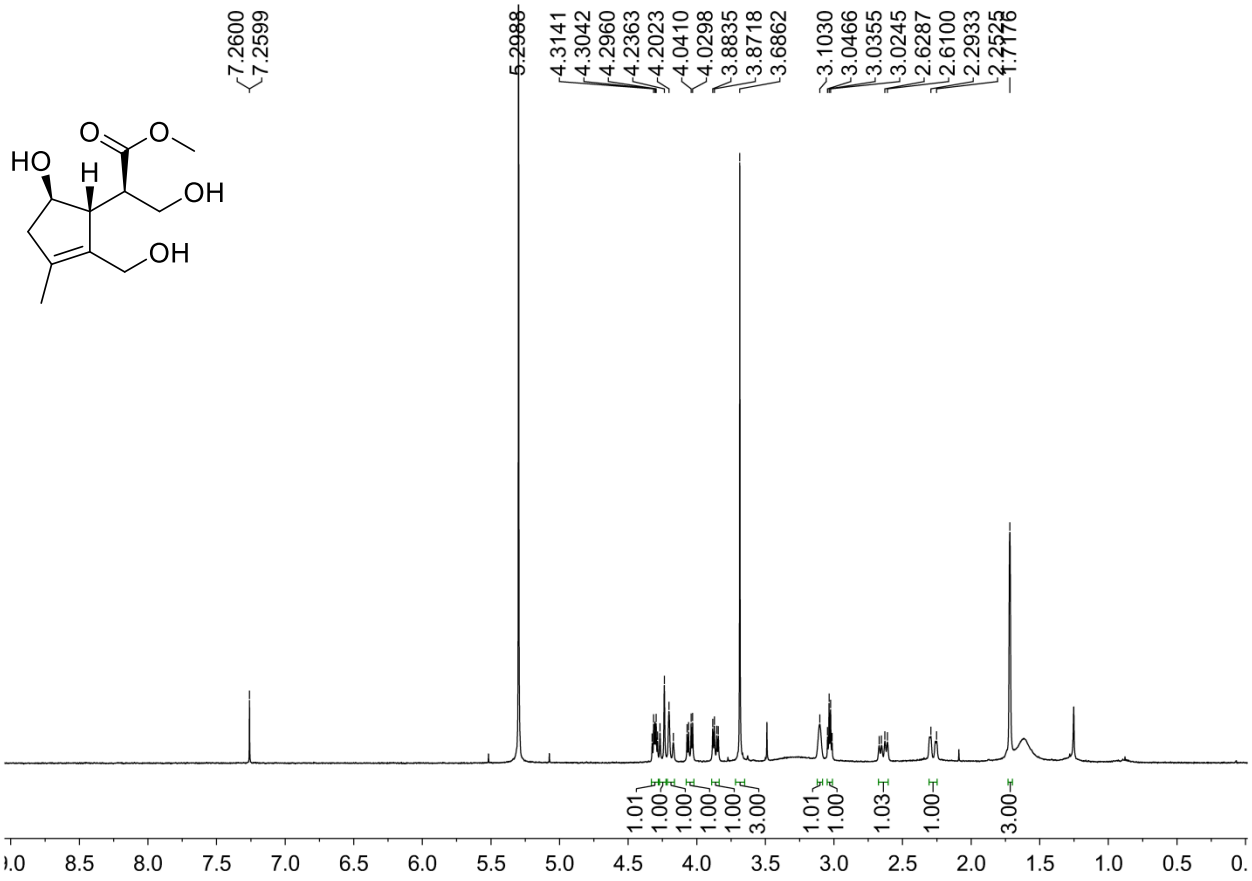

Figure S58. ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of compound **3**

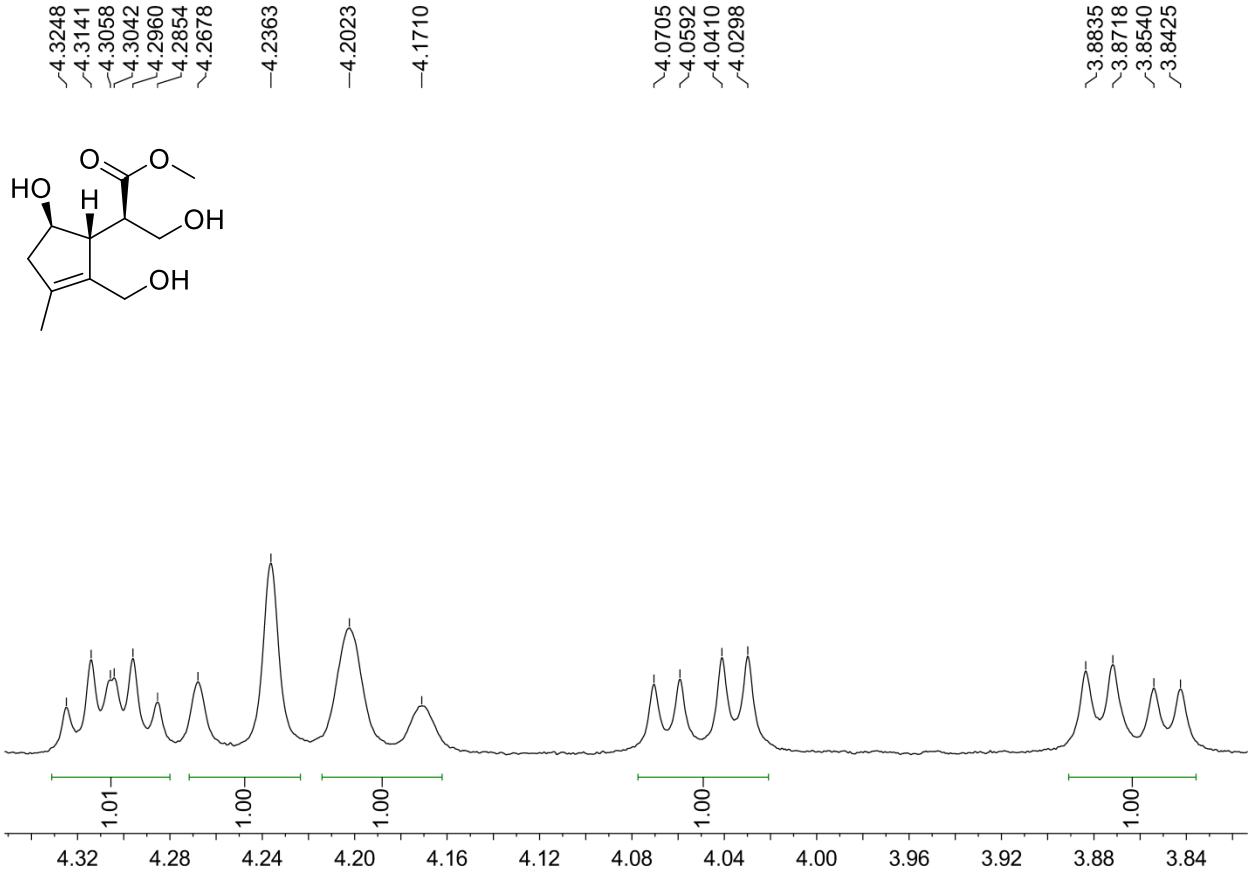

Figure S59. ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of compound **3** (amplified)

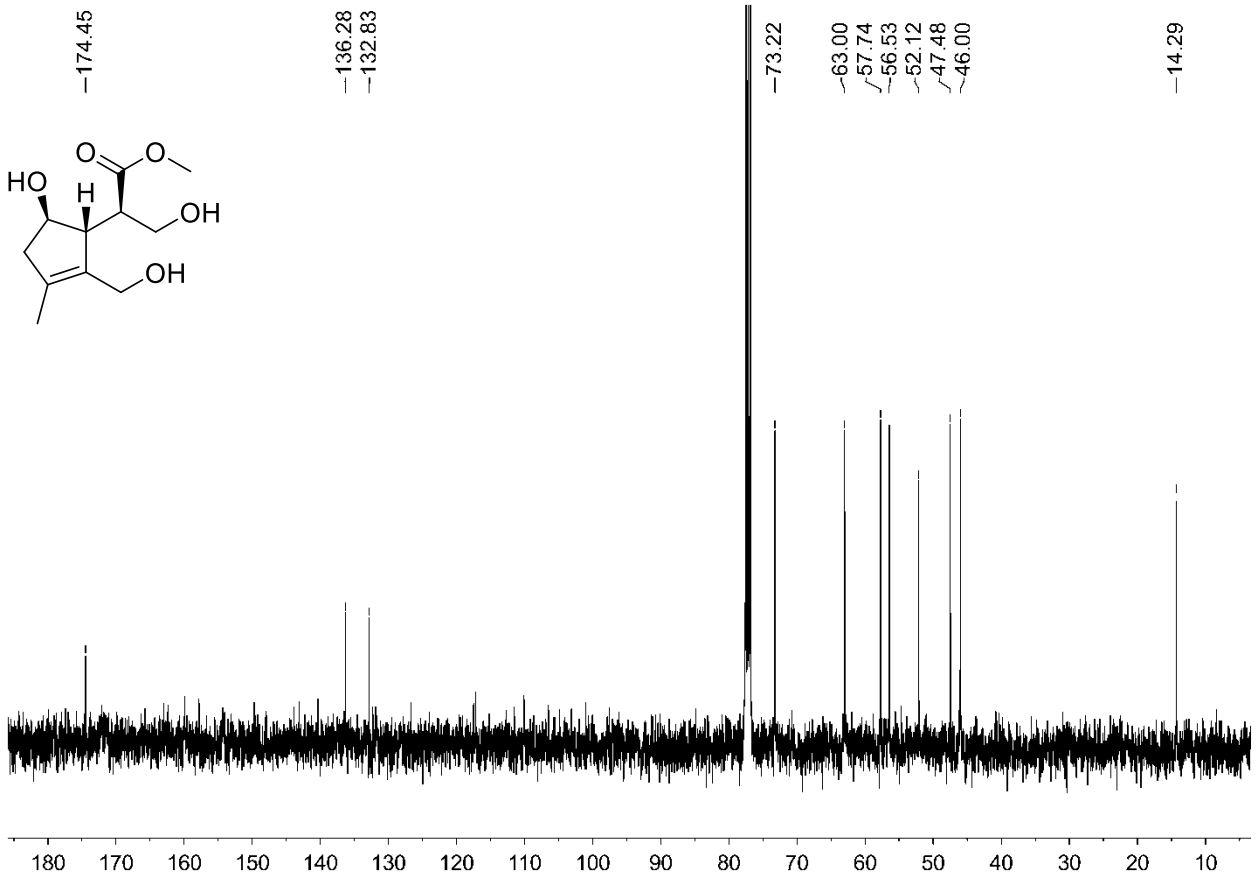

Figure S60. ^{13}C NMR (100 MHz, chloroform-*d*) spectrum of compound **3**

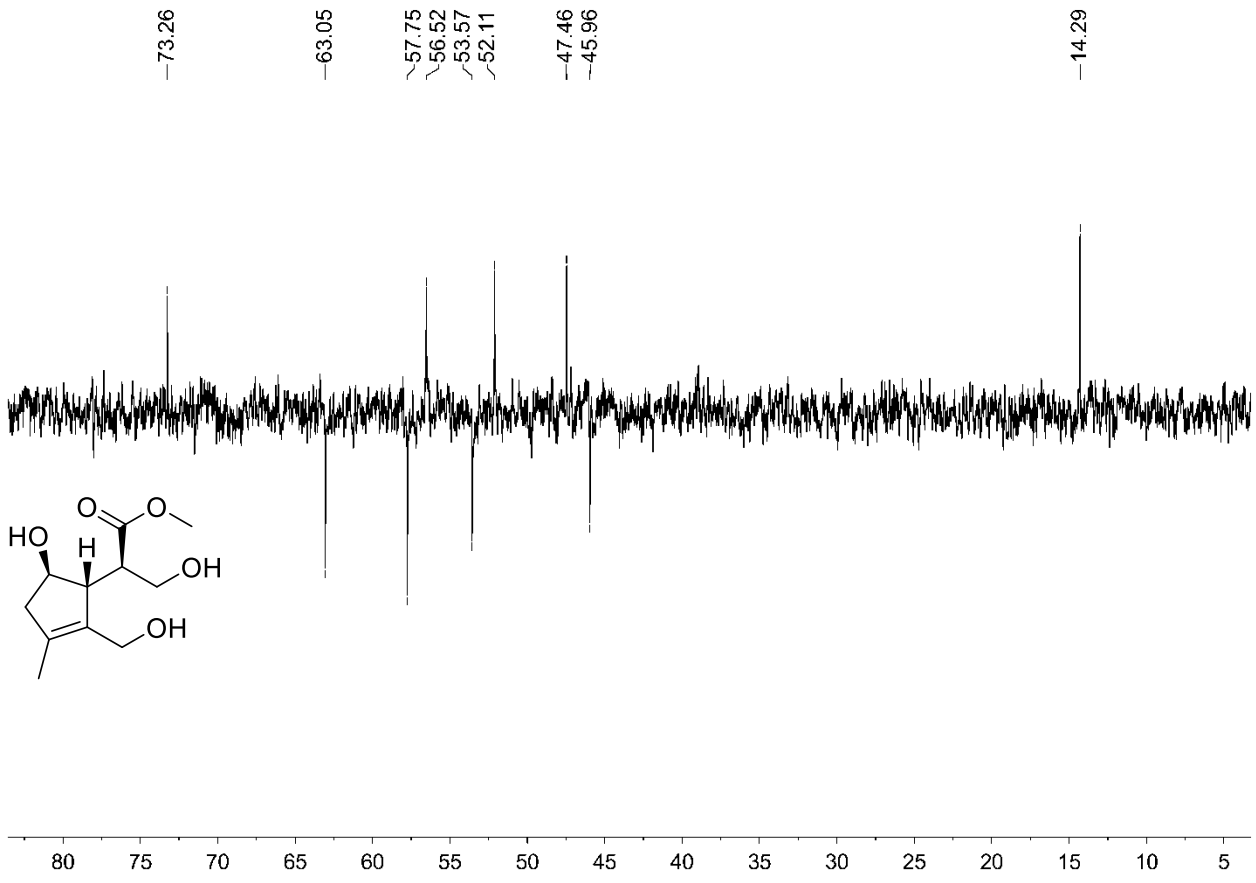

Figure S61. DEPT135 (100 MHz, chloroform-*d*) spectrum of compound **3**

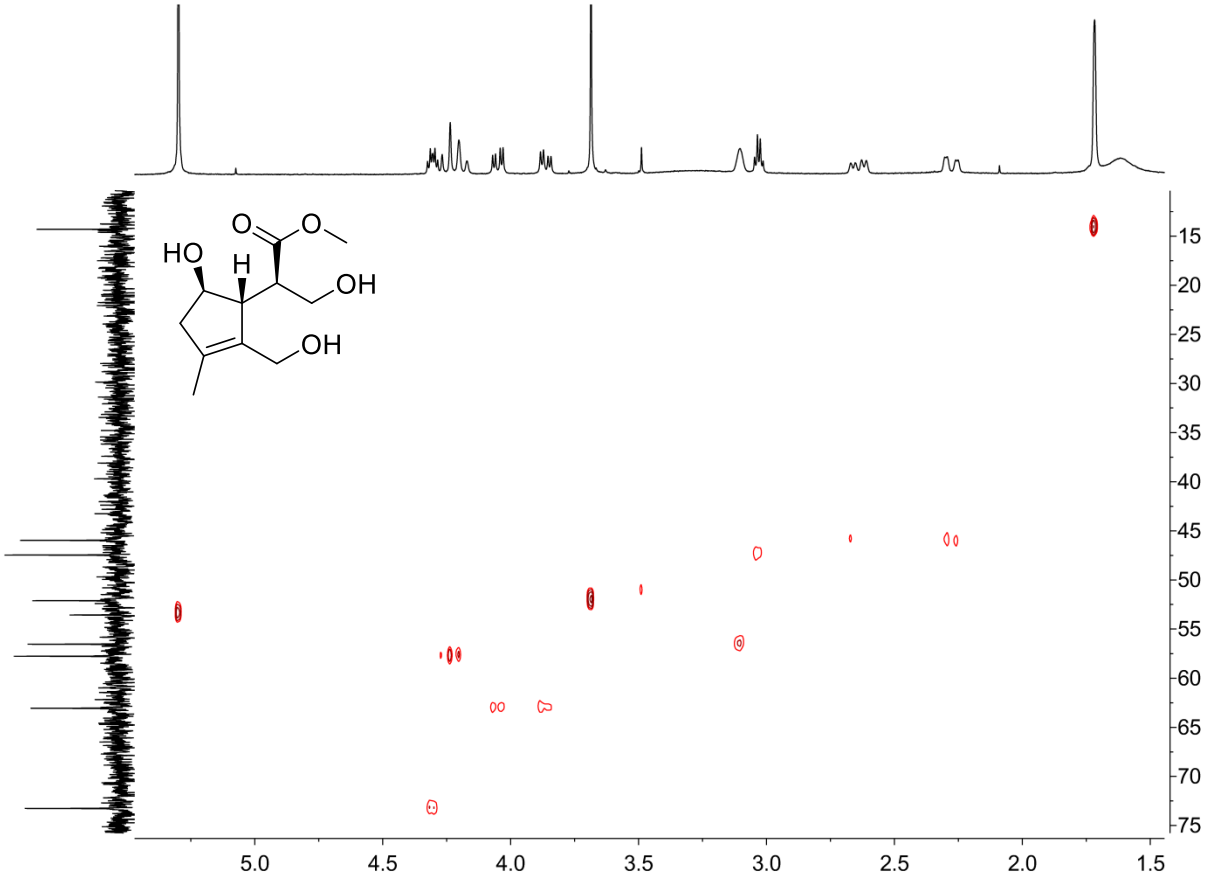

Figure S62. HSQC spectrum (chloroform-*d*) of compound **3** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

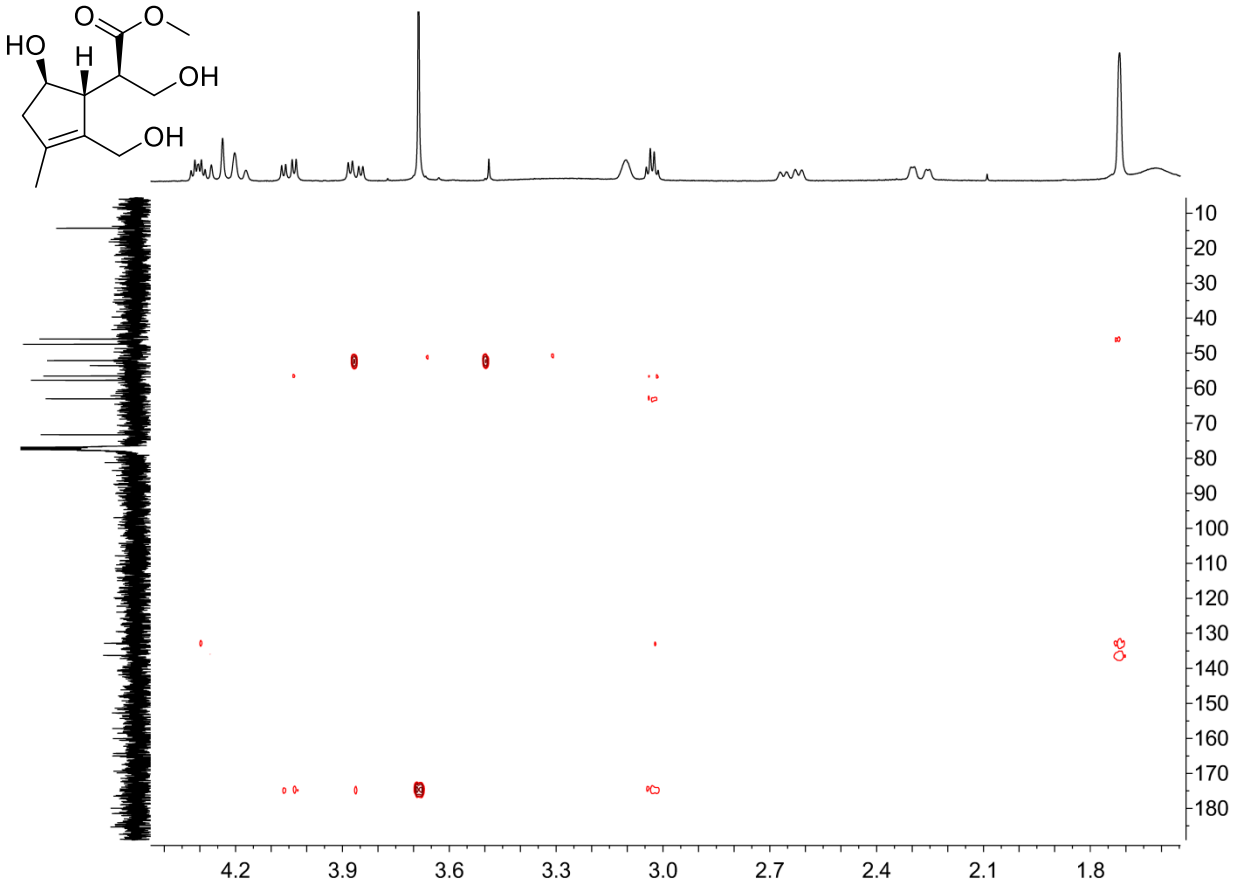

Figure S63. HMBC spectrum (chloroform-*d*) of compound **3** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

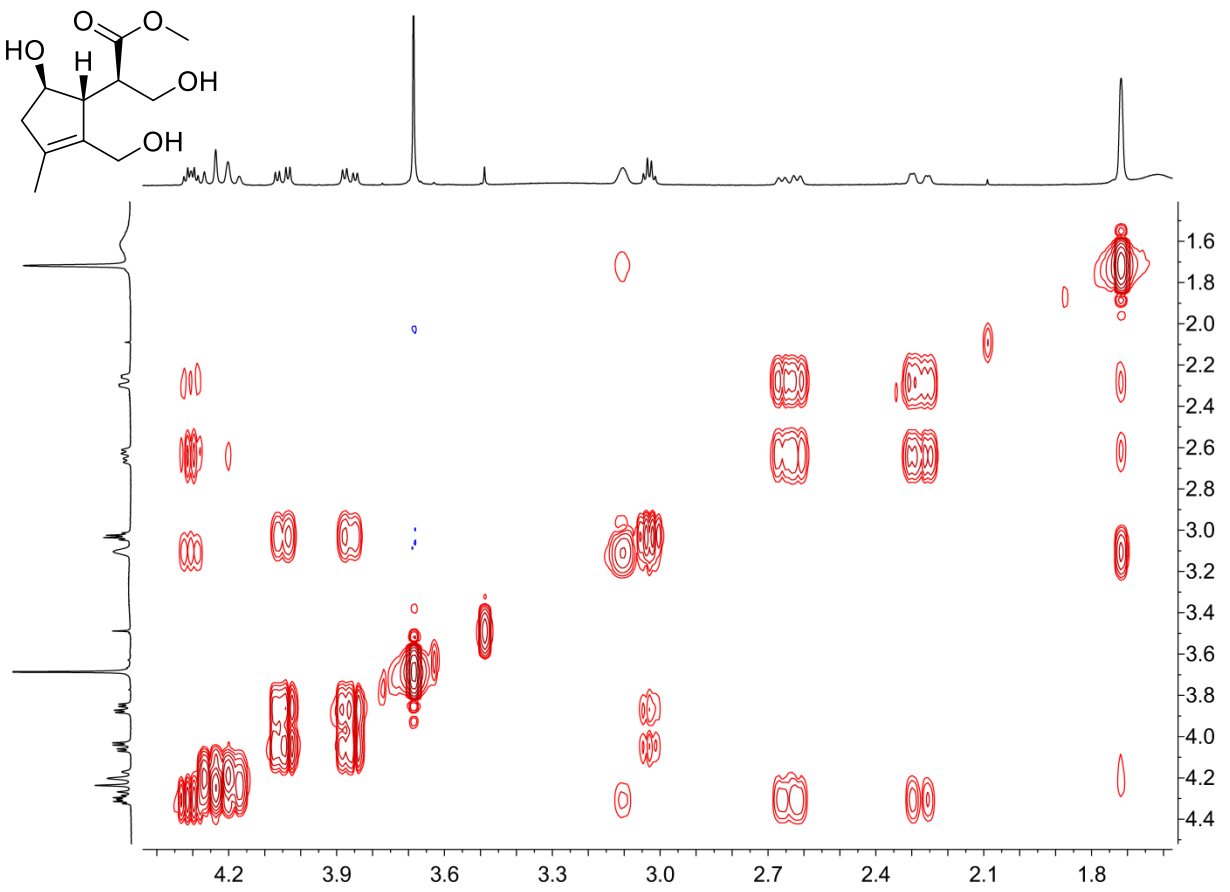

Figure S64. ^{1}H–^{1}H COSY spectrum (400 MHz, chloroform-*d*) of compound **3**

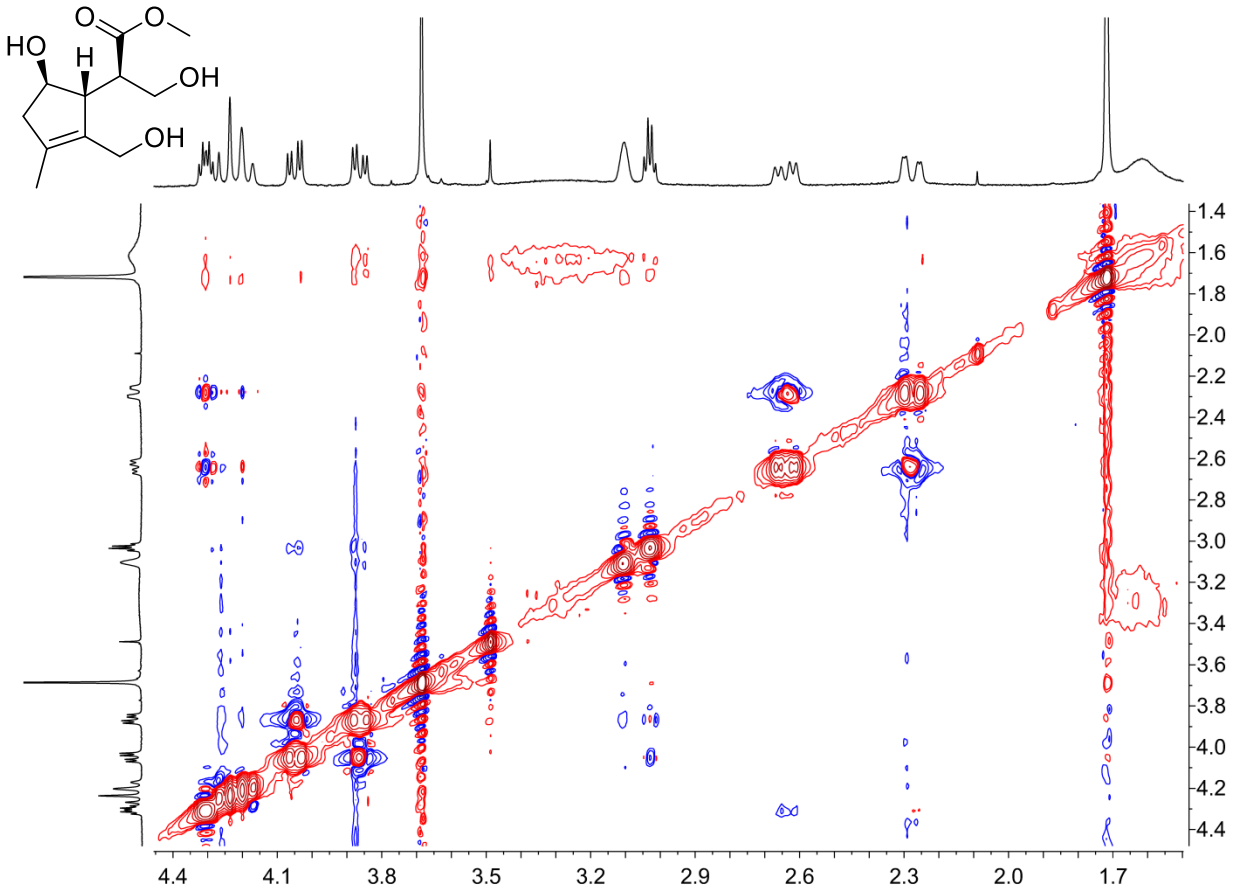

Figure S65. NOESY spectrum (400 MHz, chloroform-*d*) of compound **3**

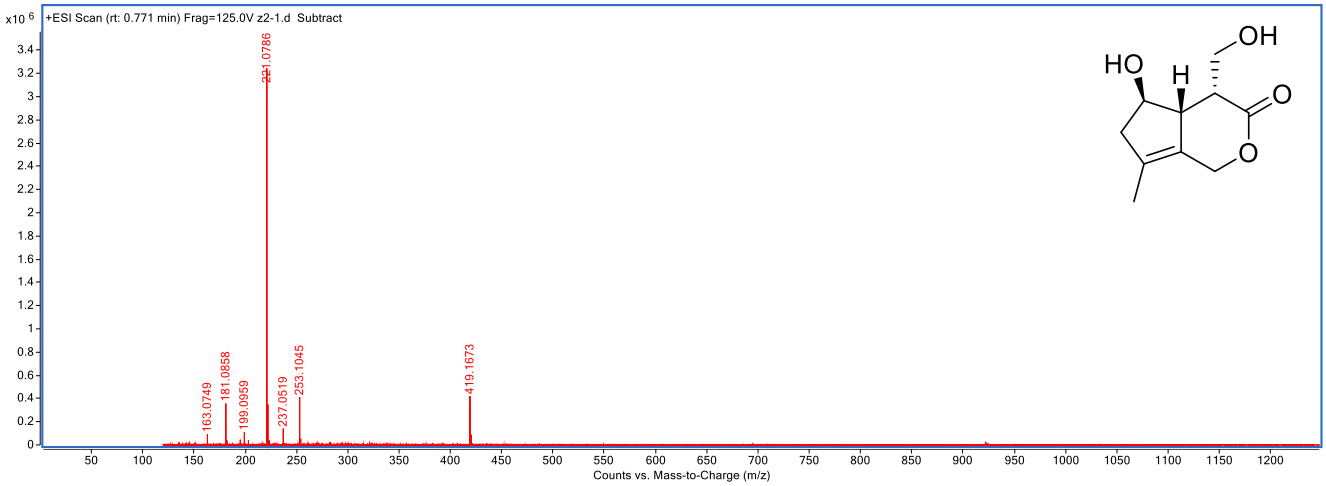

Figure S66. (+)-HR-ESI-MS spectrum of **3a**

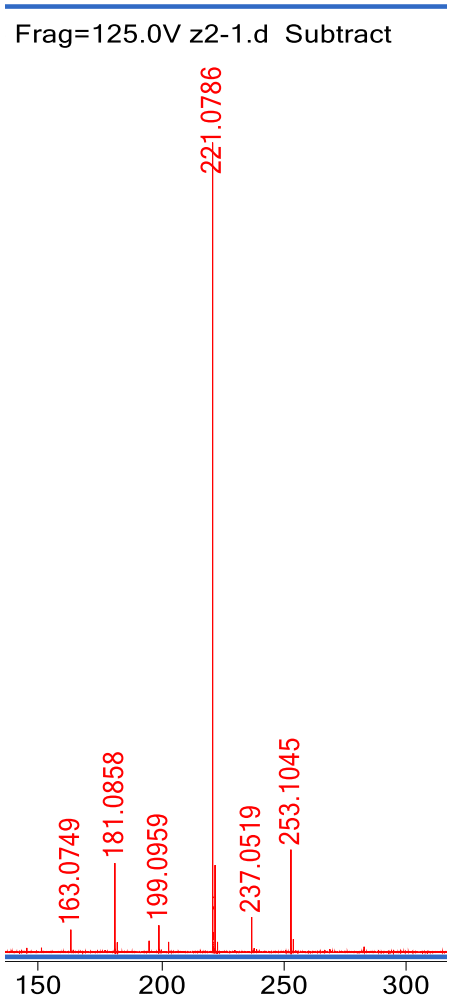

Figure S67. (+)-HR-ESI-MS spectrum of **3a** (amplified)

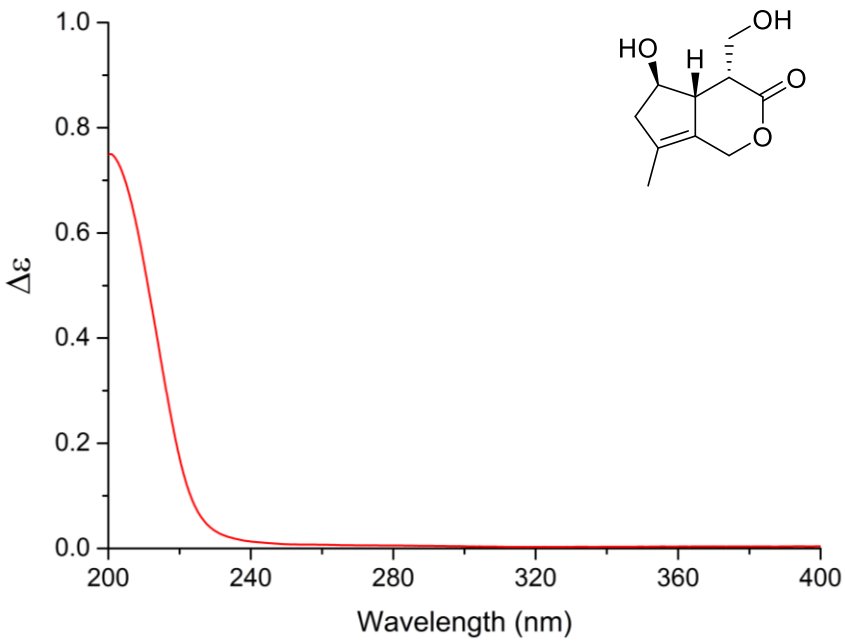

Figure S68. UV spectrum of compound **3a**

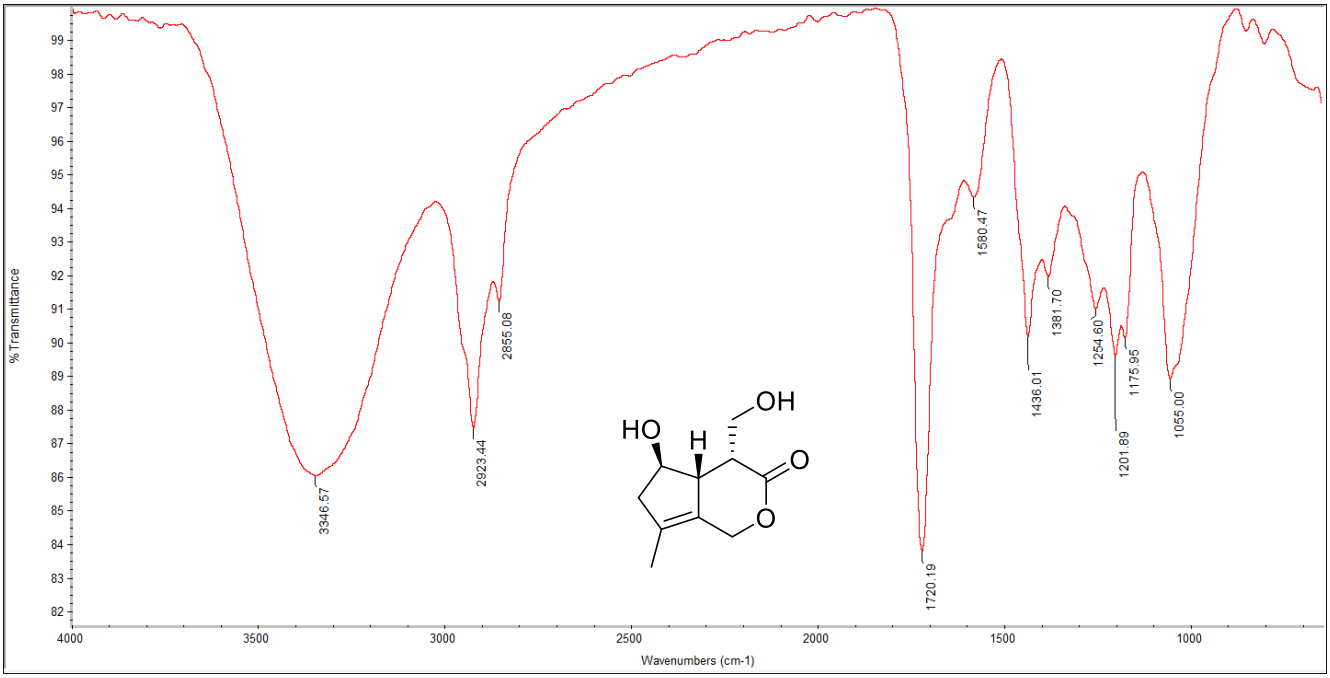

Figure S69. IR spectrum of compound **3a**

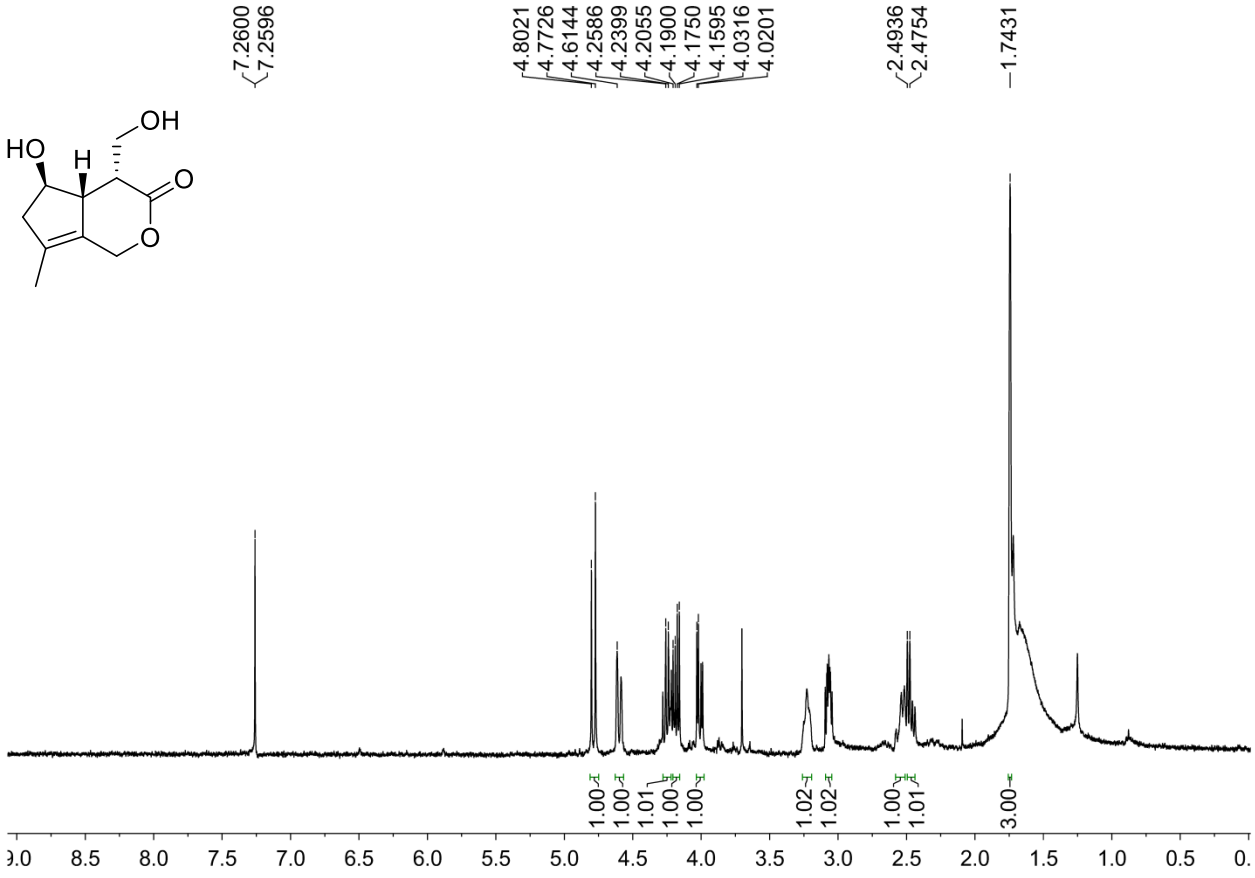

Figure S70. ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of compound **3a**

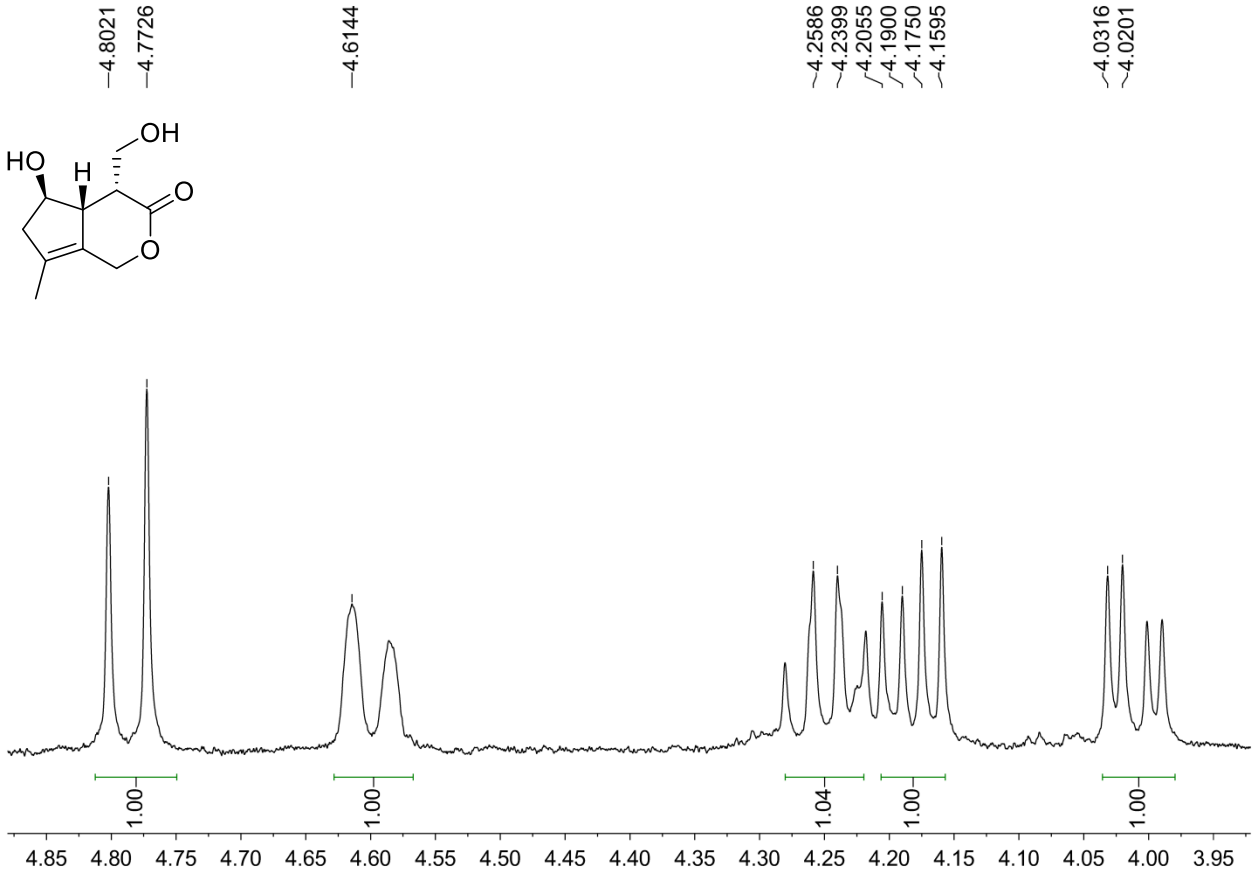

Figure S71. ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of compound **3a** (amplified)

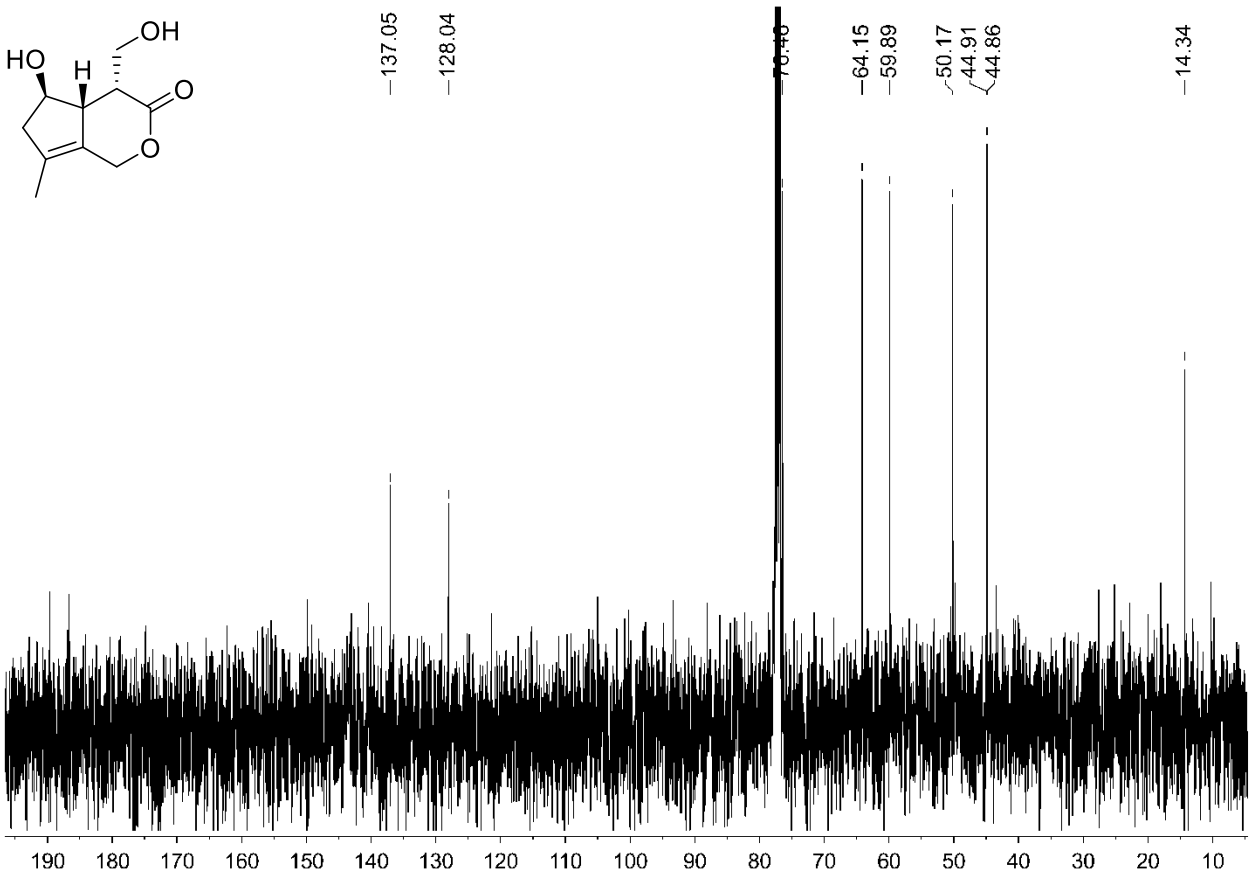

Figure S72. ^{13}C NMR (100 MHz, chloroform-*d*) spectrum of compound **3a**

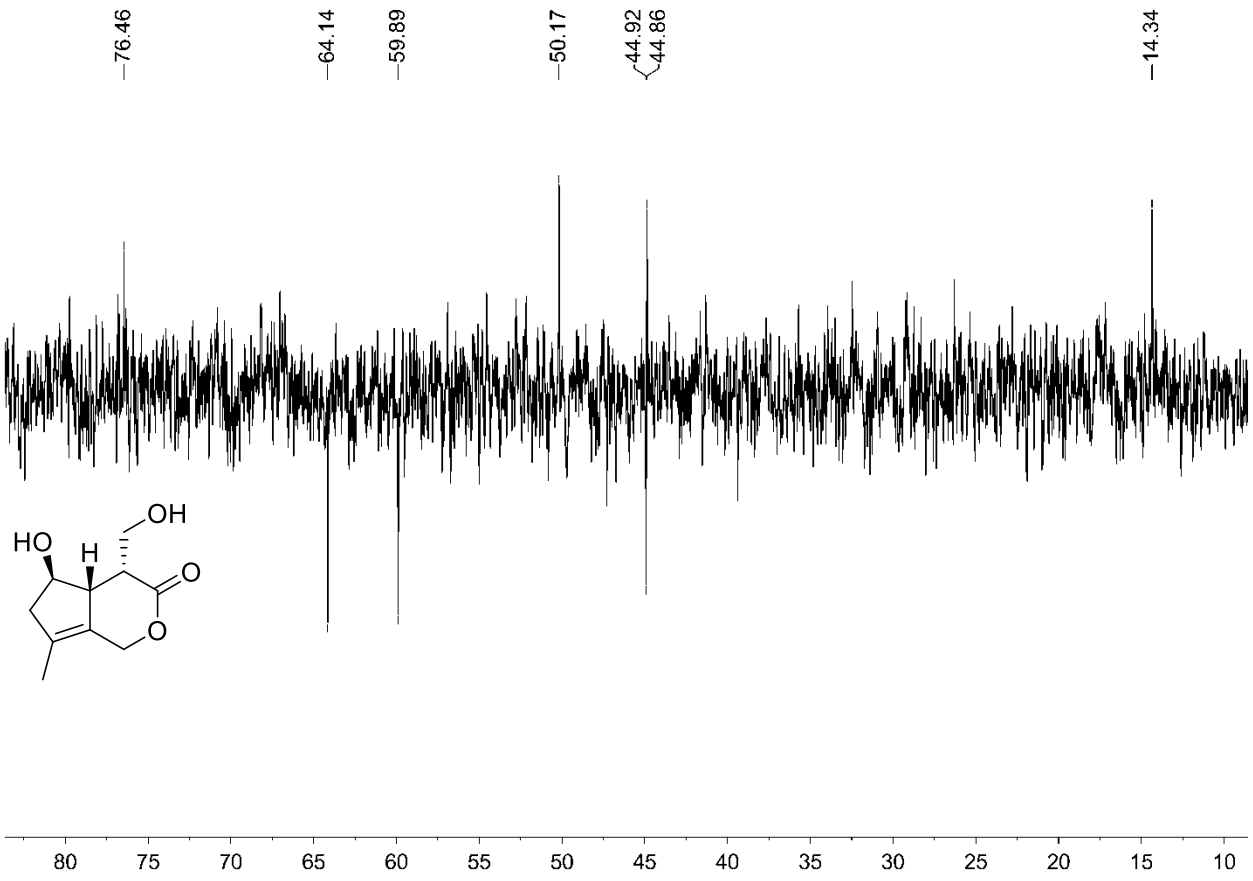

Figure S73. DEPT135 (100 MHz, chloroform-*d*) spectrum of compound **3a**

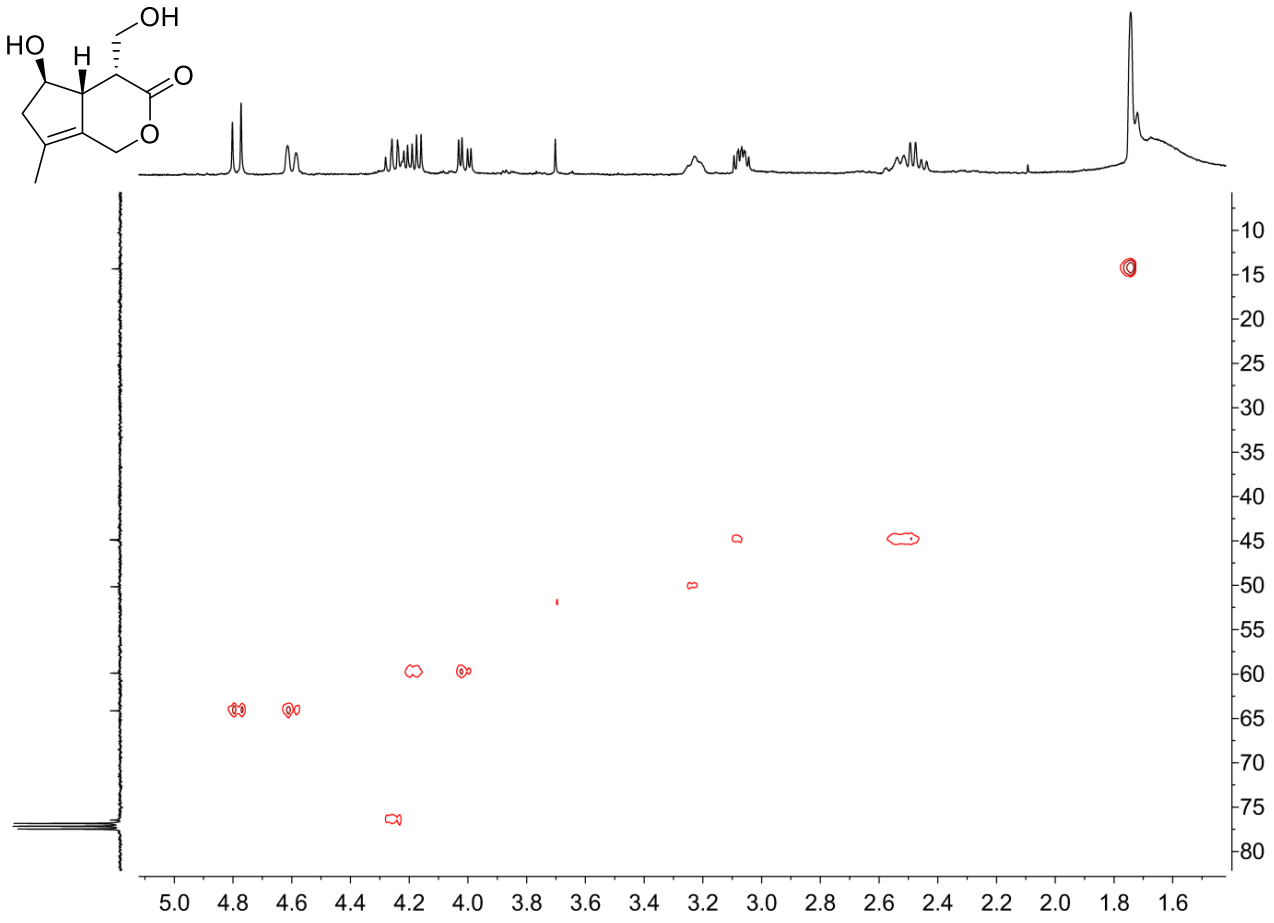

Figure S74. HSQC spectrum (chloroform-*d*) of compound **3a** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

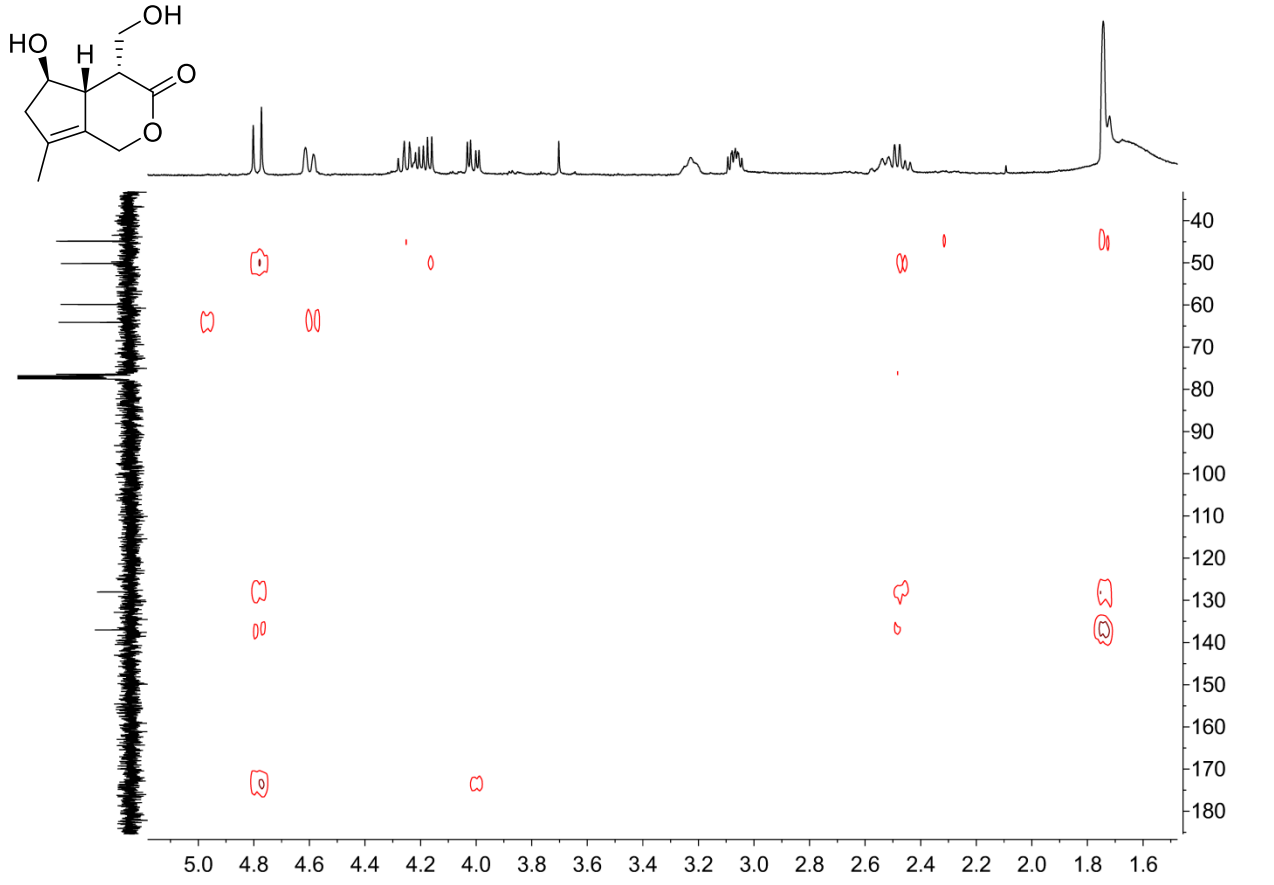

Figure S75. HMBC spectrum (chloroform-*d*) of compound **3a** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

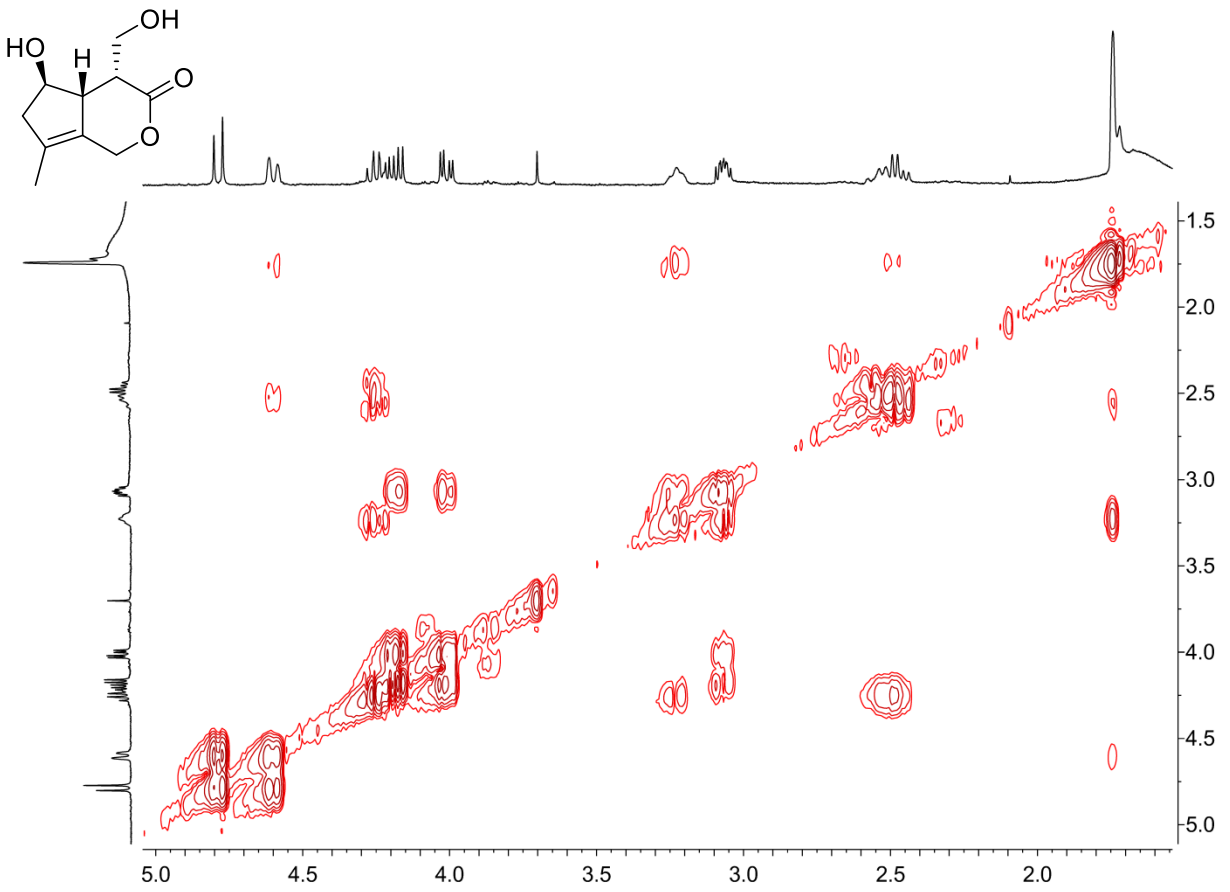

Figure S76. $^{1}H–^{1}H$ COSY spectrum (400 MHz, chloroform-*d*) of compound **3a**

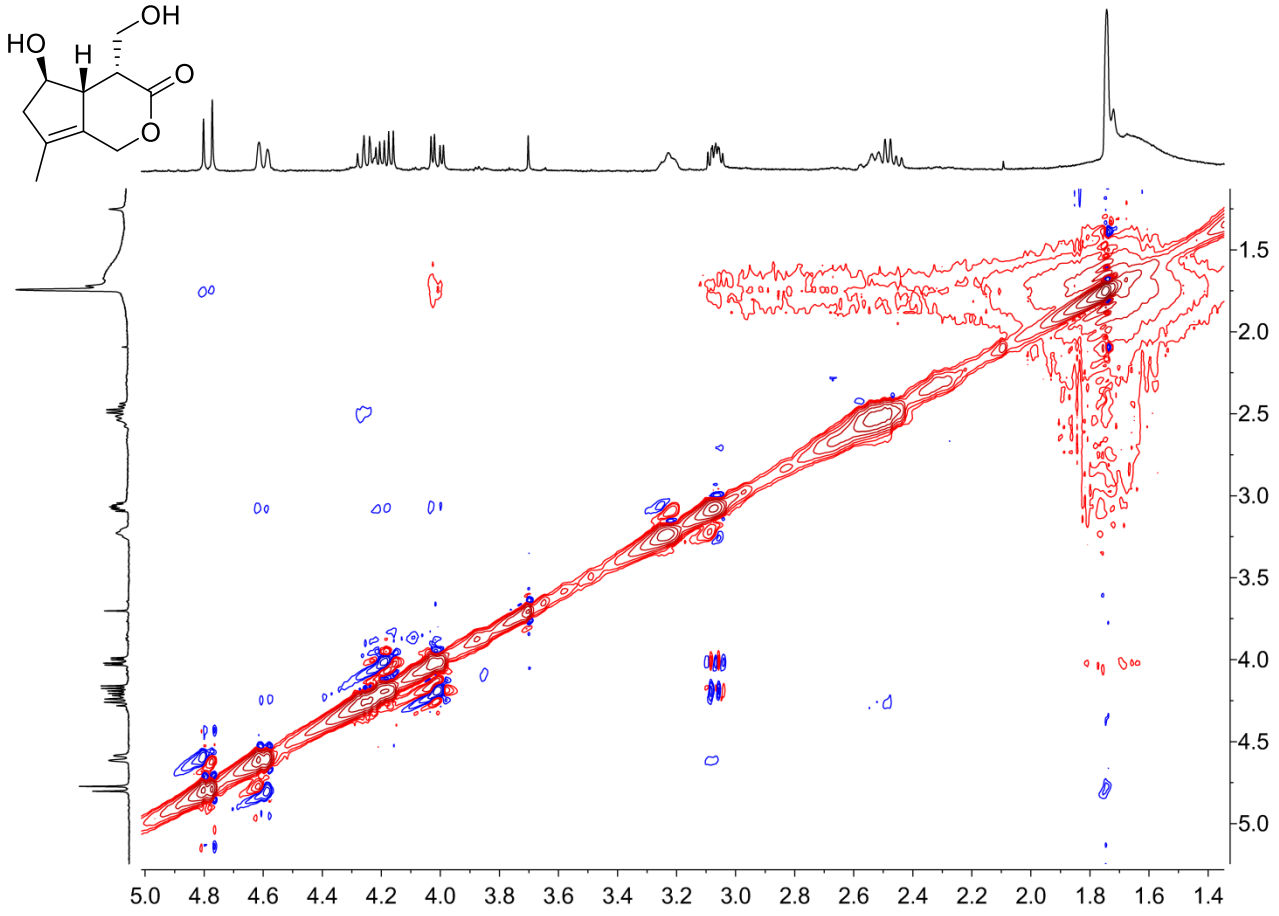

Figure S77. NOESY spectrum (400 MHz, chloroform-*d*) of compound **3a**

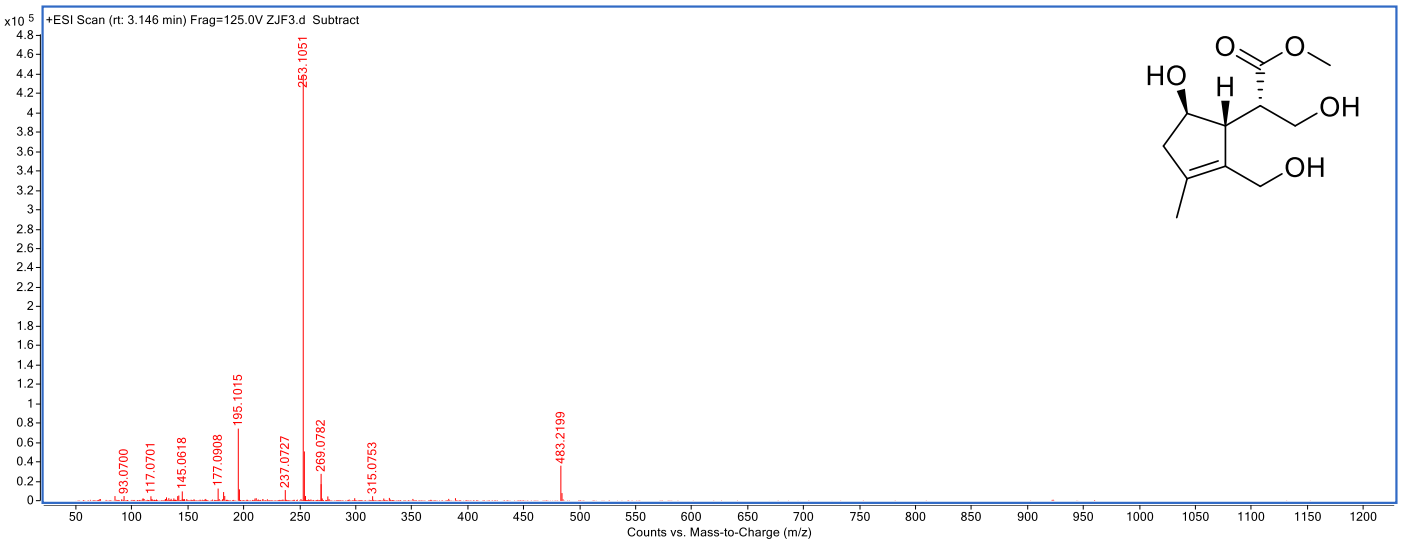

Figure S78. (+)-HR-ESI-MS spectrum of **4**

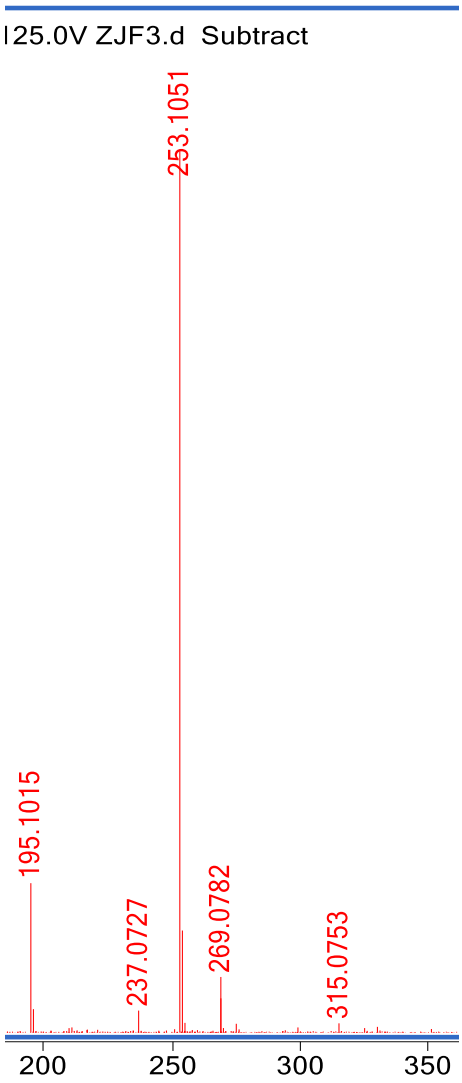

Figure S79. (+)-HR-ESI-MS spectrum of **4** (amplified)

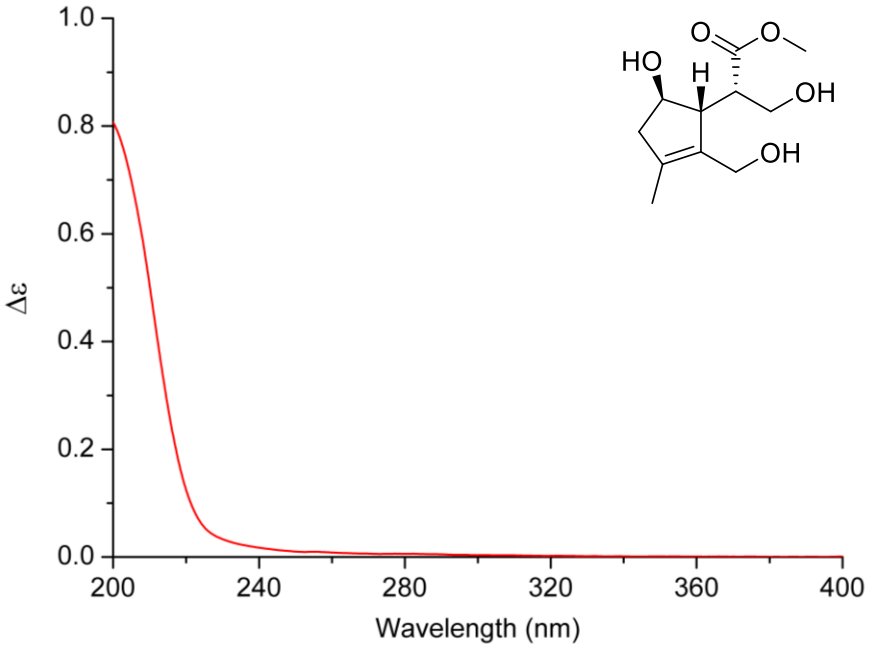

Figure S80. UV spectrum of compound **4**

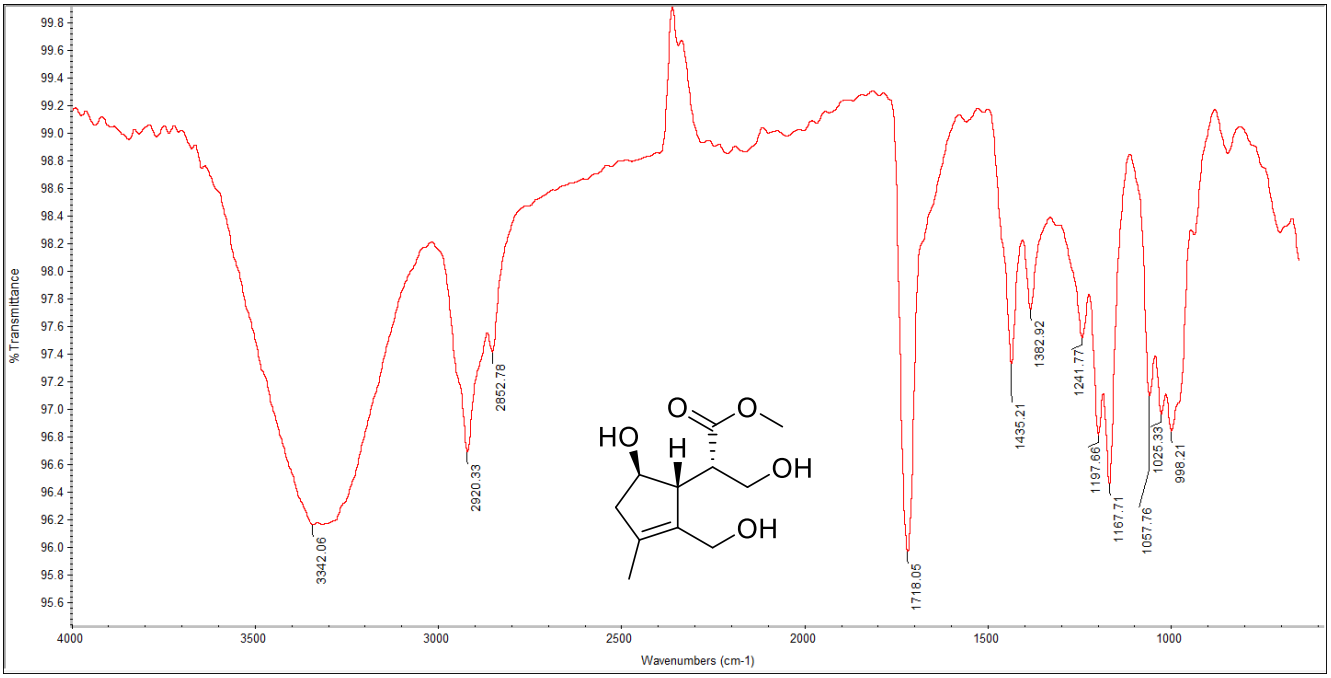

Figure S81. IR spectrum of compound **4**

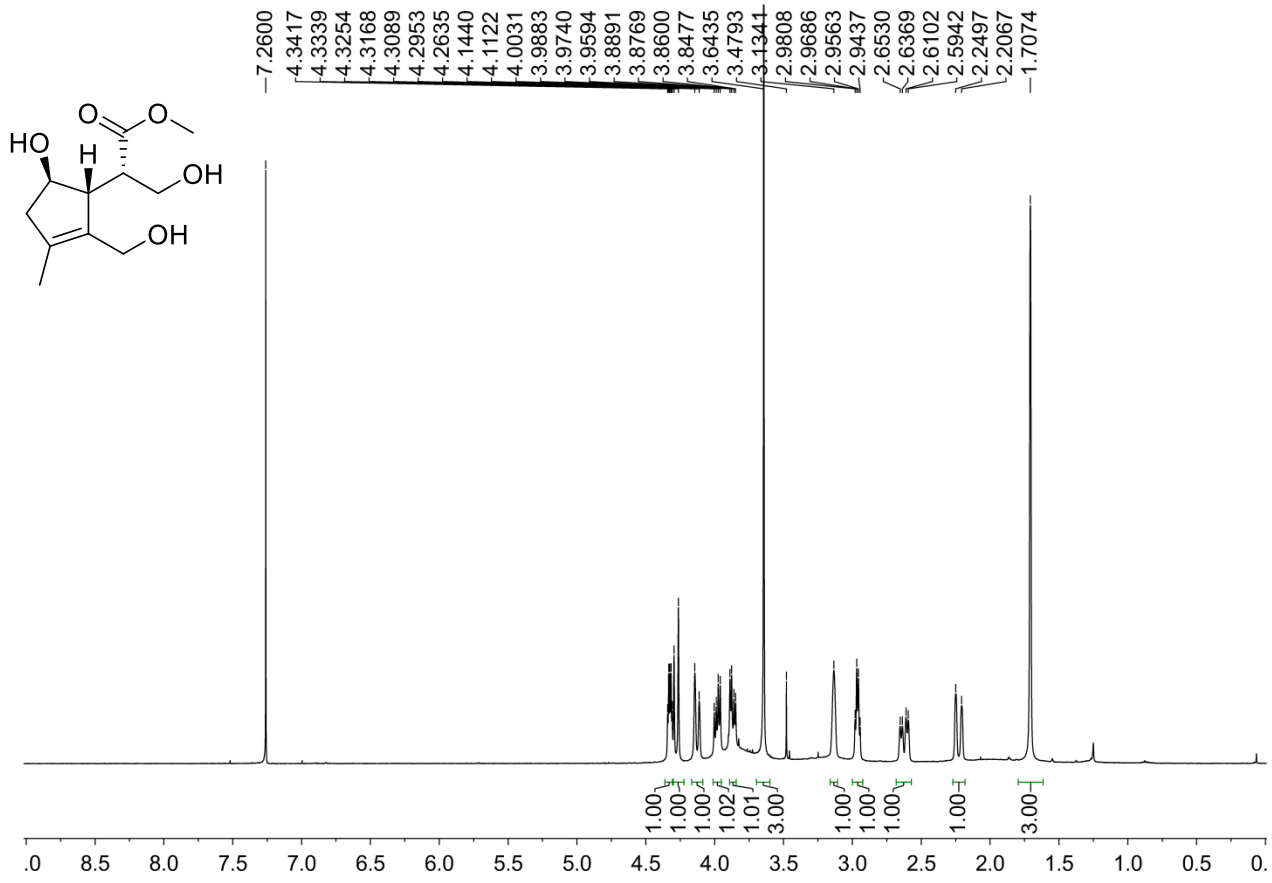

Figure S82. ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of compound **4**

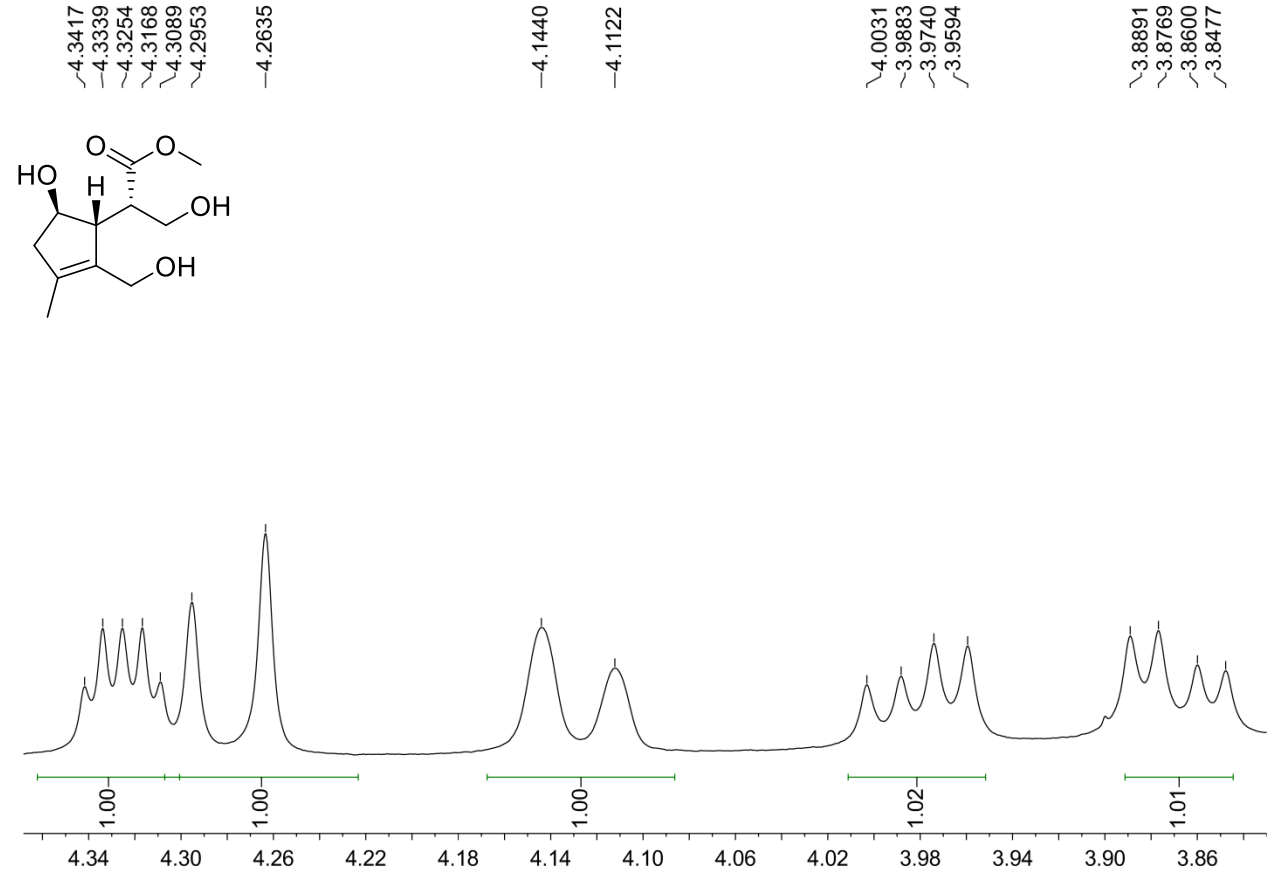

Figure S83. ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of compound **4** (amplified)

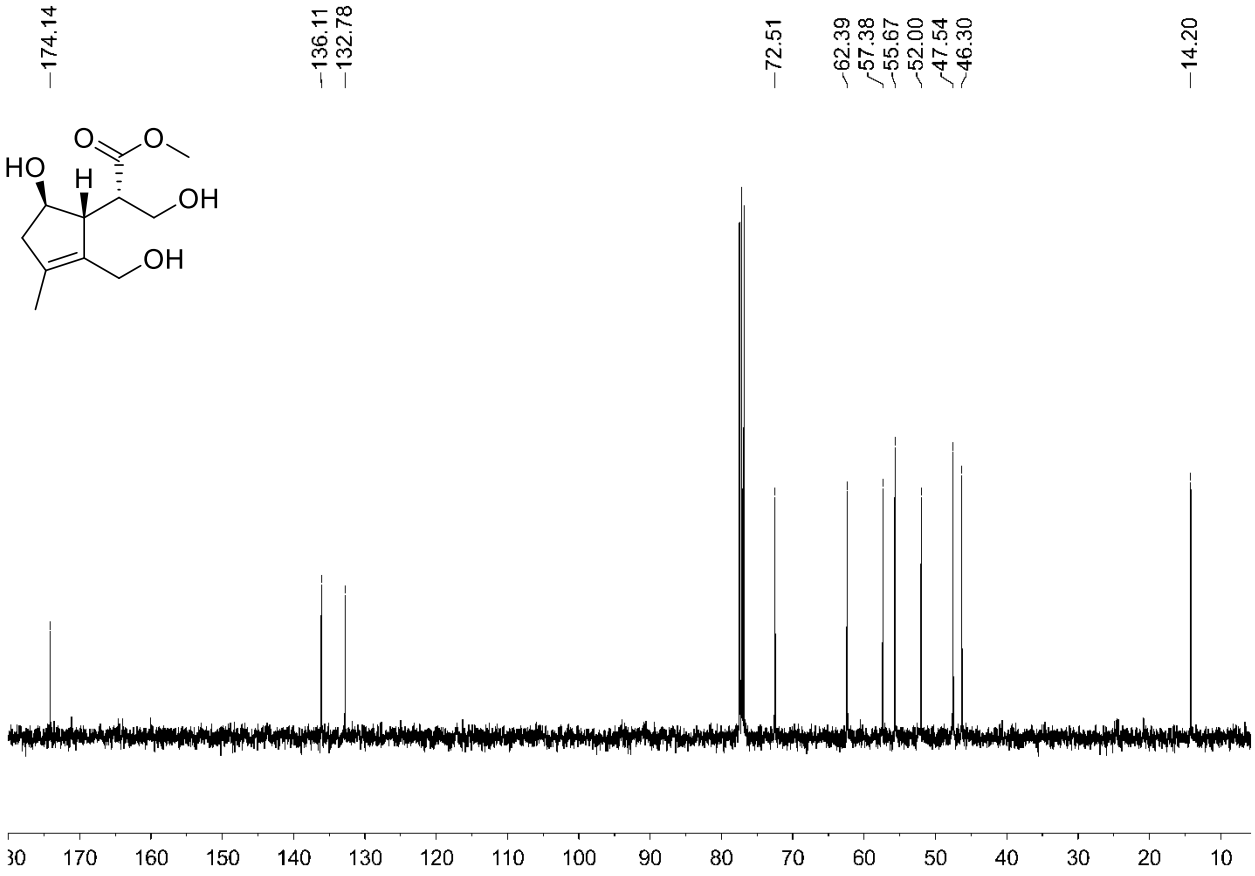

Figure S84. ^{13}C NMR (100 MHz, chloroform-*d*) spectrum of compound **4**

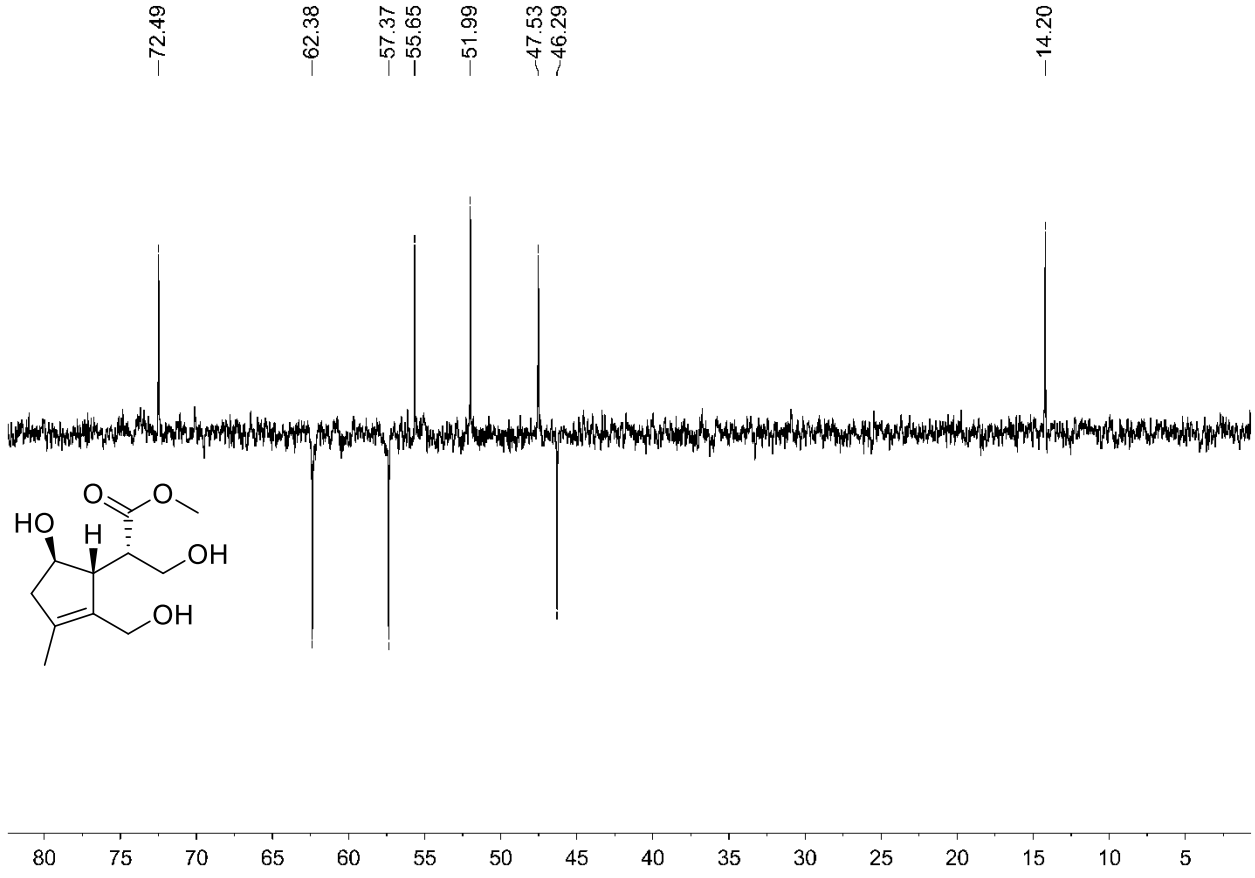

Figure S85. DEPT135 (100 MHz, chloroform-*d*) spectrum of compound **4**

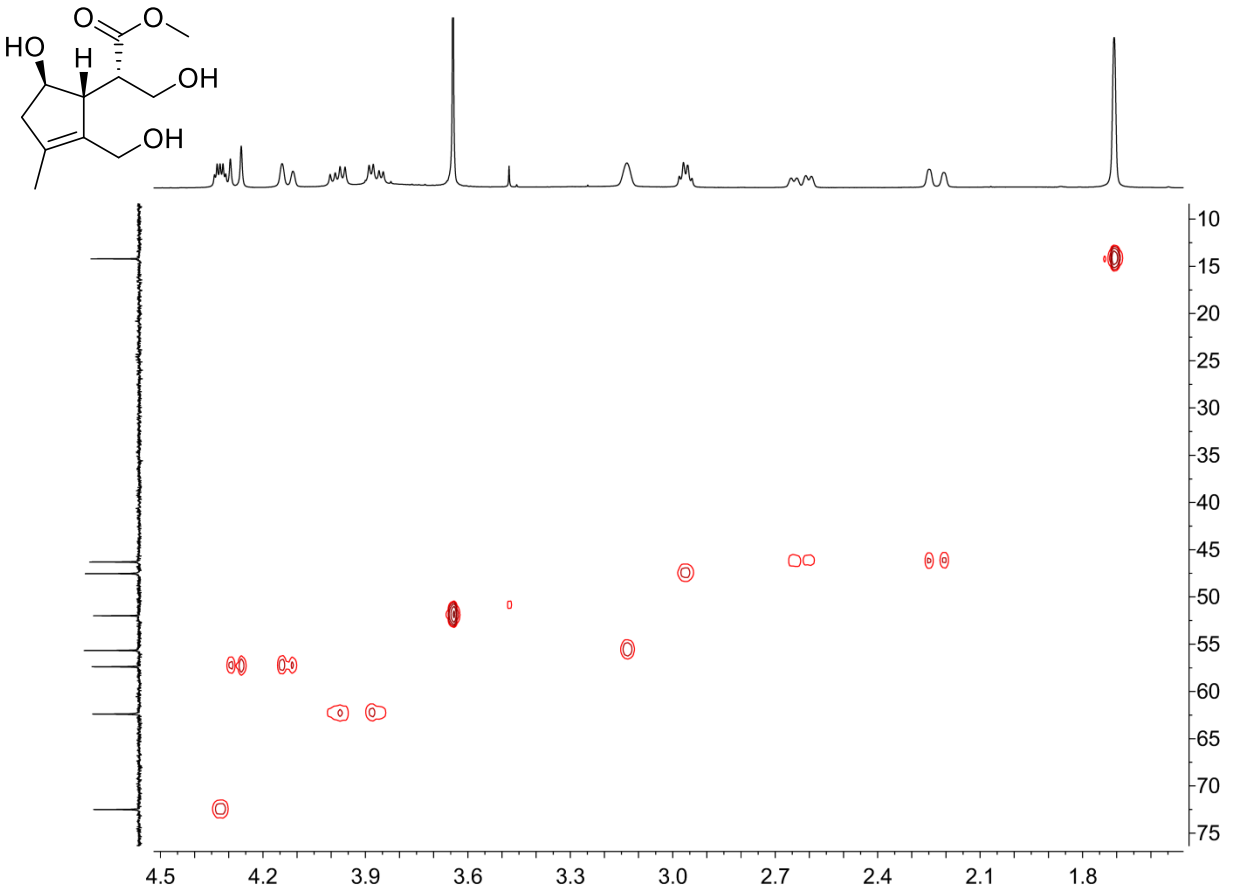

Figure S86. HSQC spectrum (chloroform-*d*) of compound **4** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

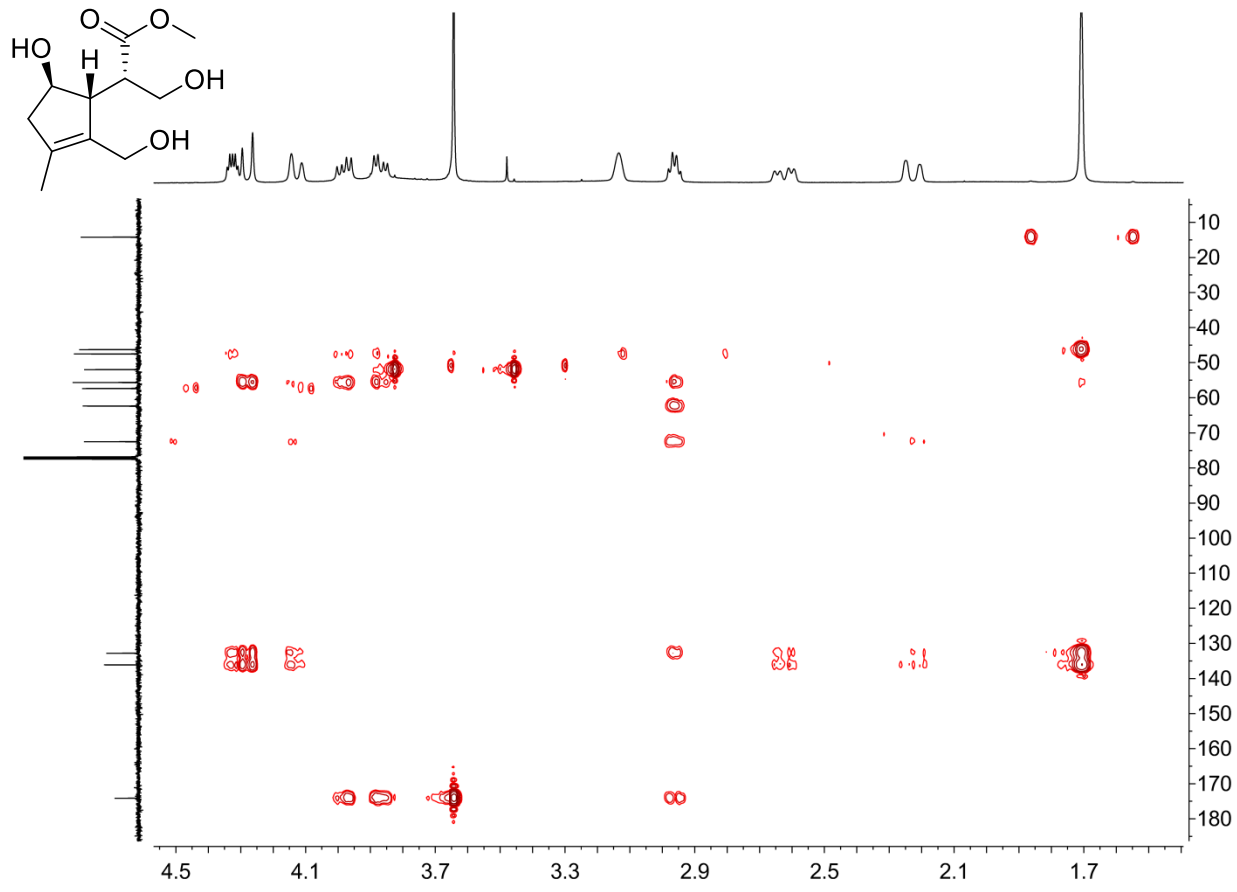

Figure S87. HMBC spectrum (chloroform-*d*) of compound **4** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

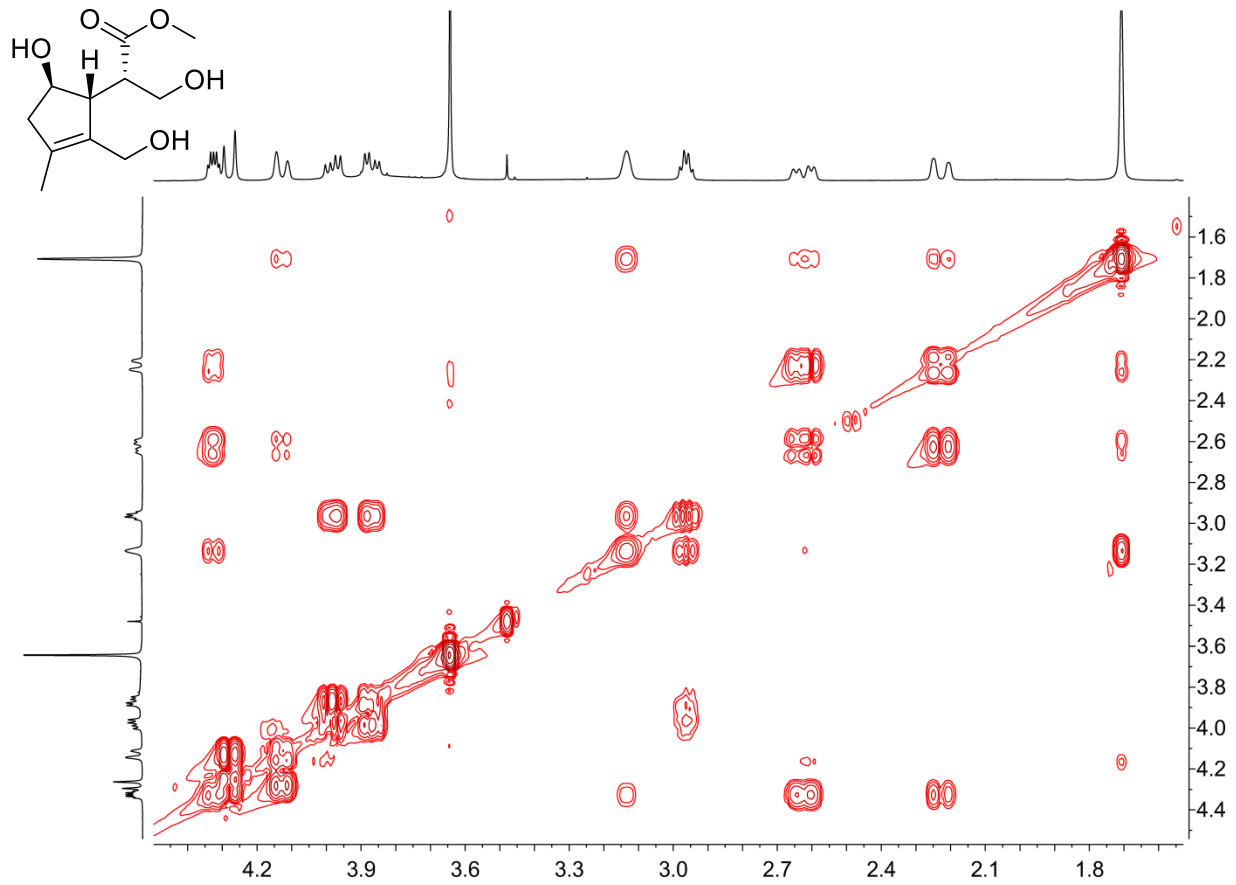

Figure S88. ^{1}H–^{1}H COSY spectrum (400 MHz, chloroform-*d*) of compound **4**

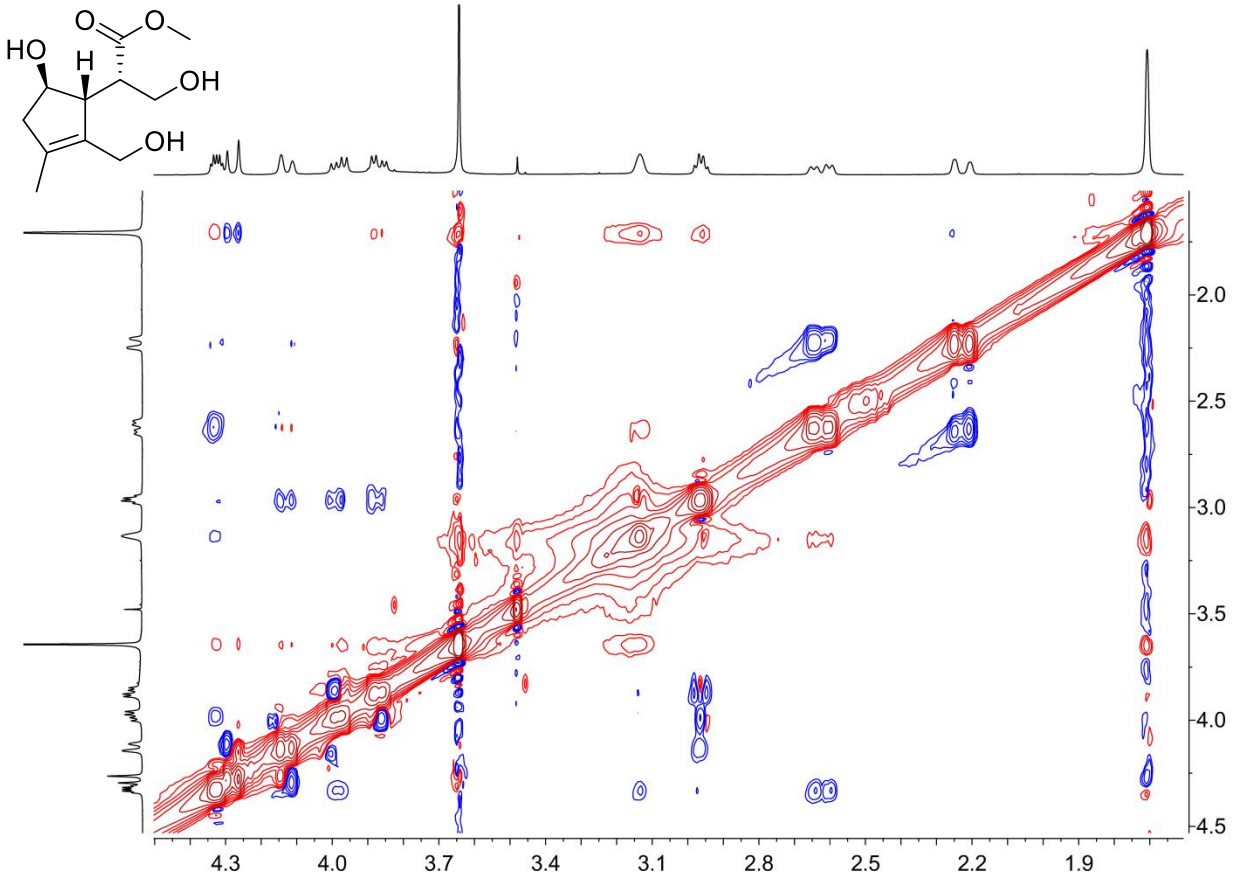

Figure S89. NOESY spectrum (400 MHz, chloroform-*d*) of compound **4**

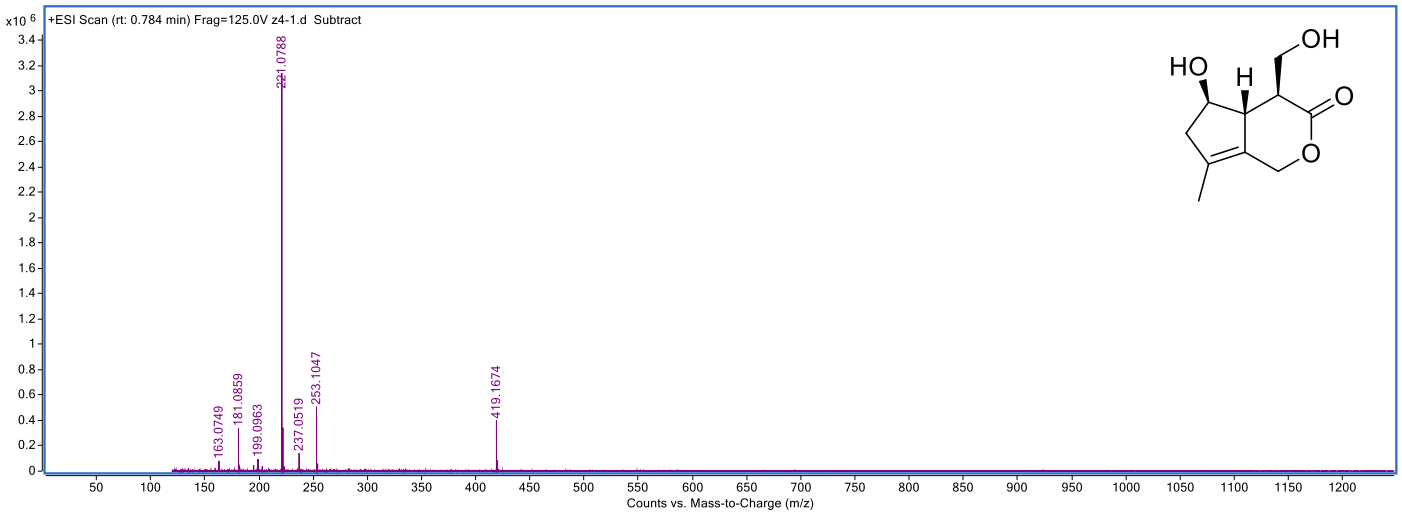

Figure S90. (+)-HR-ESI-MS spectrum of **4a**

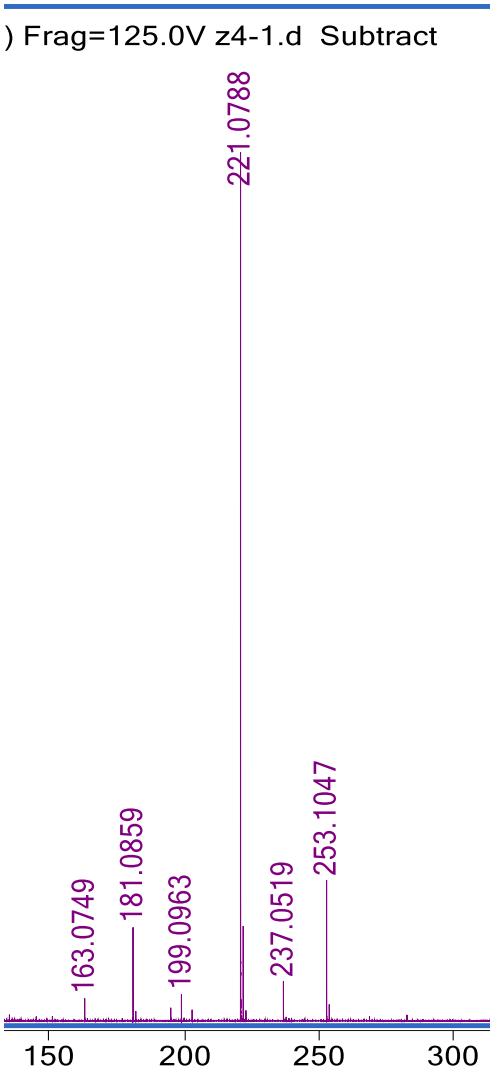

Figure S91. (+)-HR-ESI-MS spectrum of **4a** (amplified)

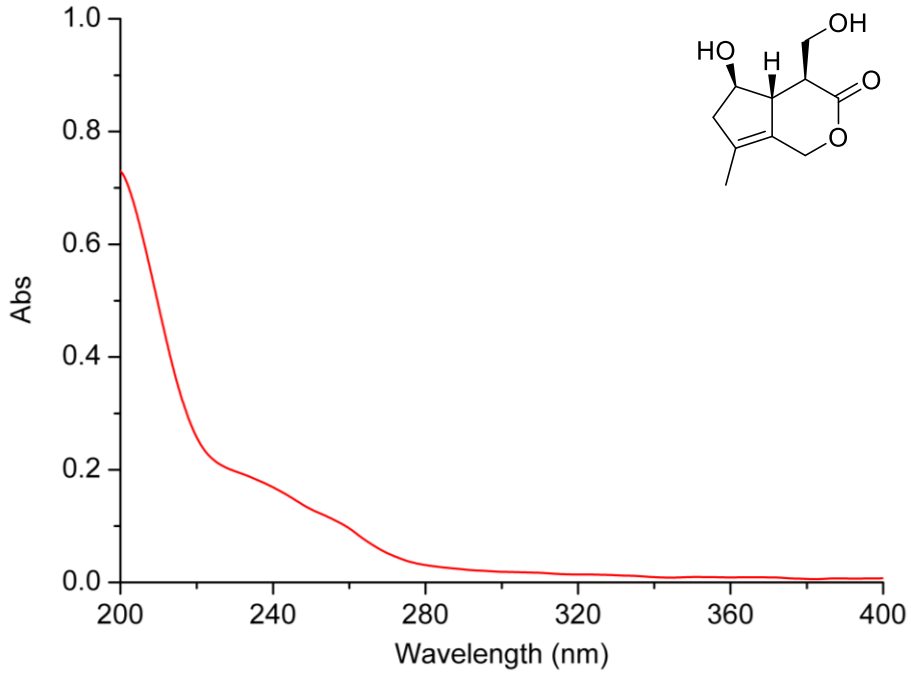

Figure S92. UV spectrum of compound **4a**

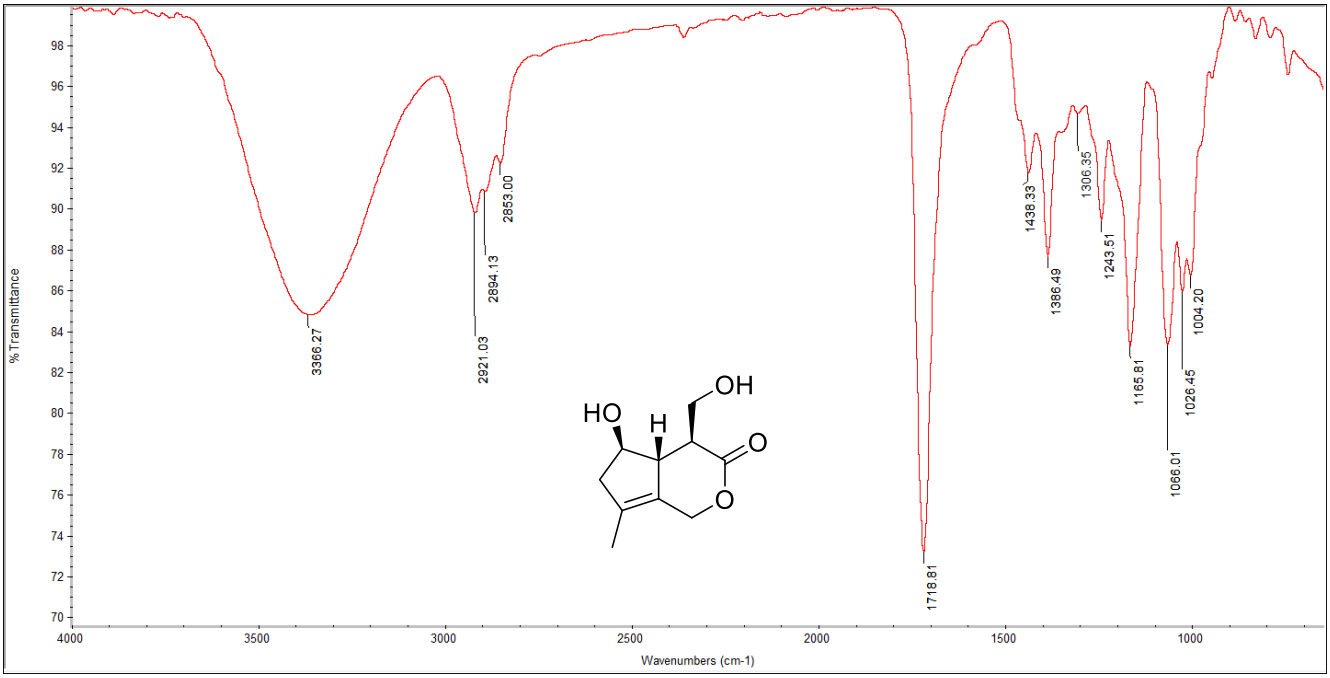

Figure S93. IR spectrum of compound **4a**

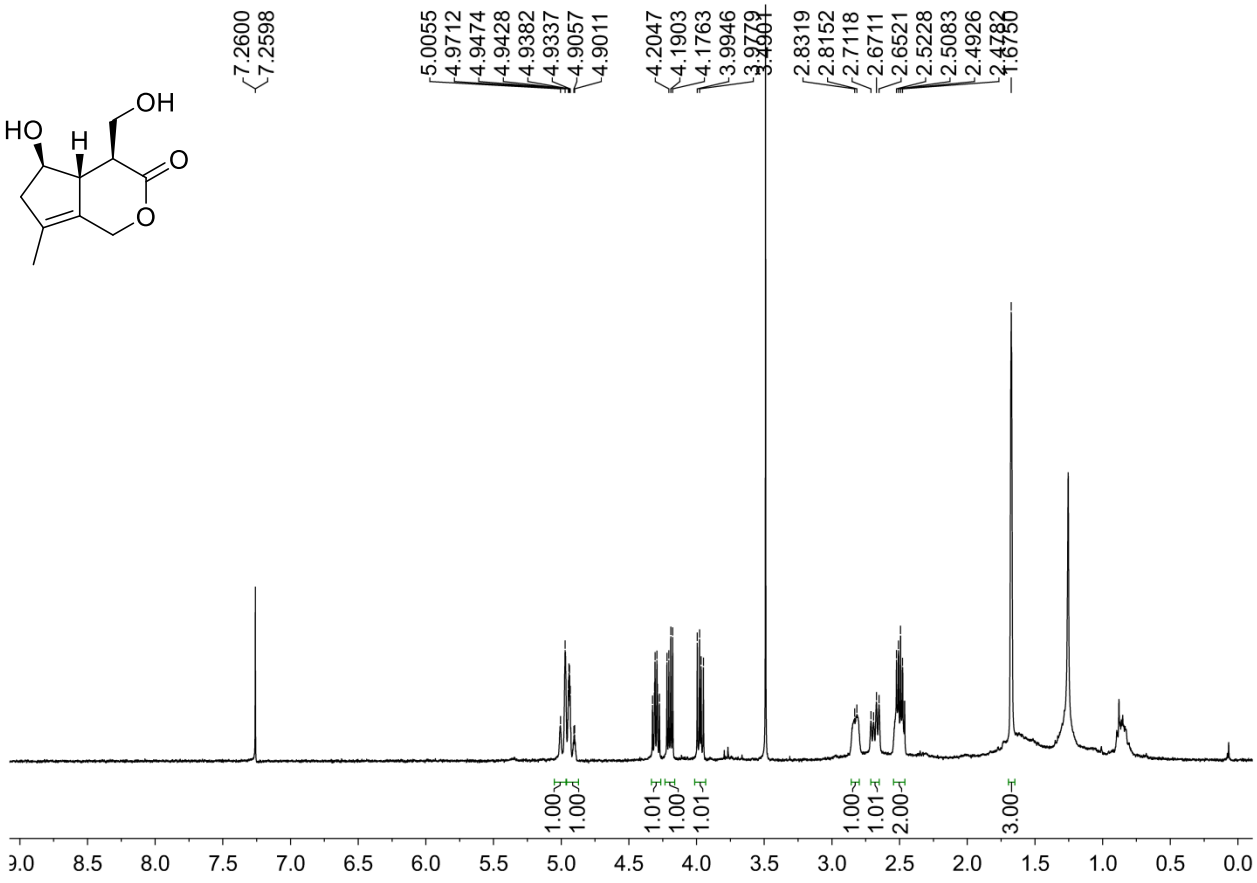

Figure S94. [1]H NMR (400 MHz, chloroform-*d*) spectrum of compound **4a**

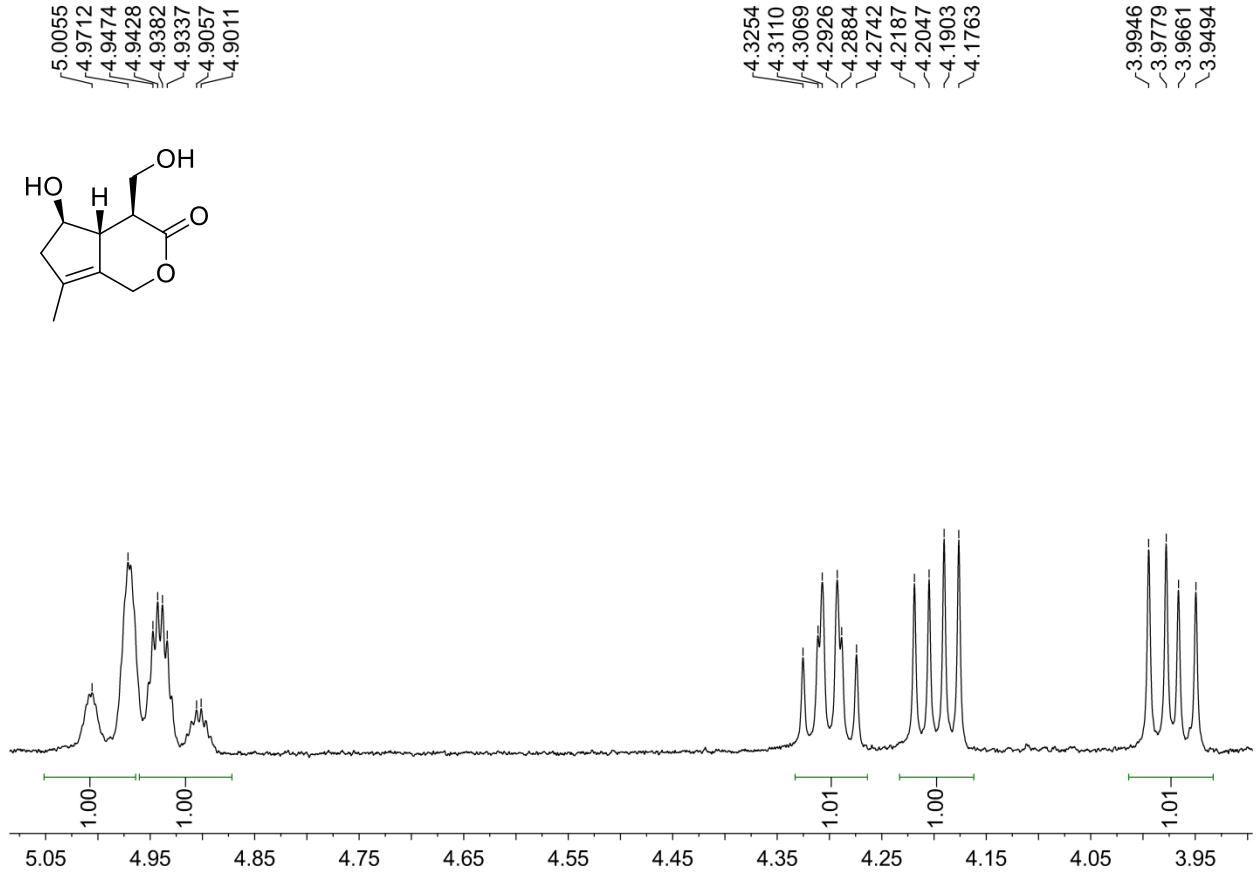

Figure S95. [1]H NMR (400 MHz, chloroform-*d*) spectrum of compound **4a** (amplified)

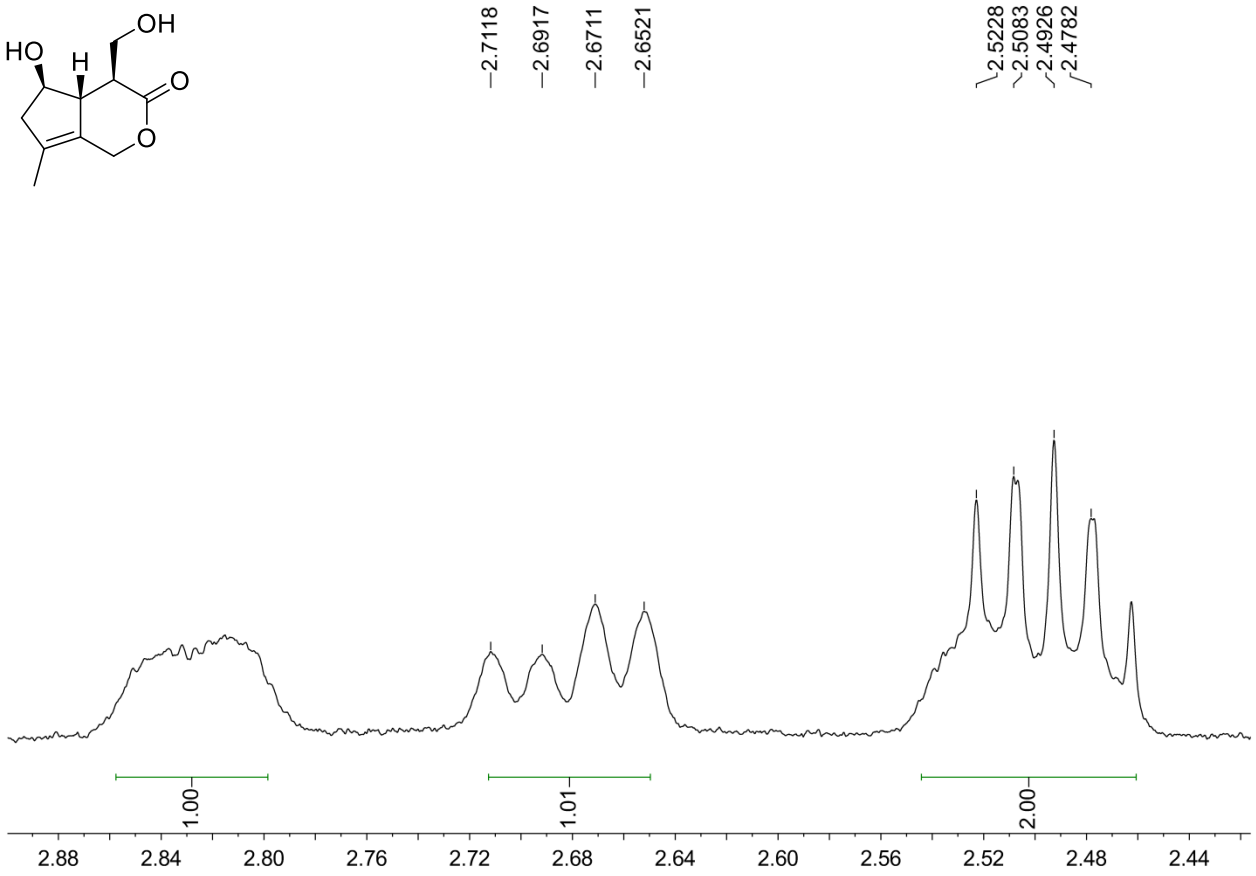

Figure S96. ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of compound **4a** (amplified)

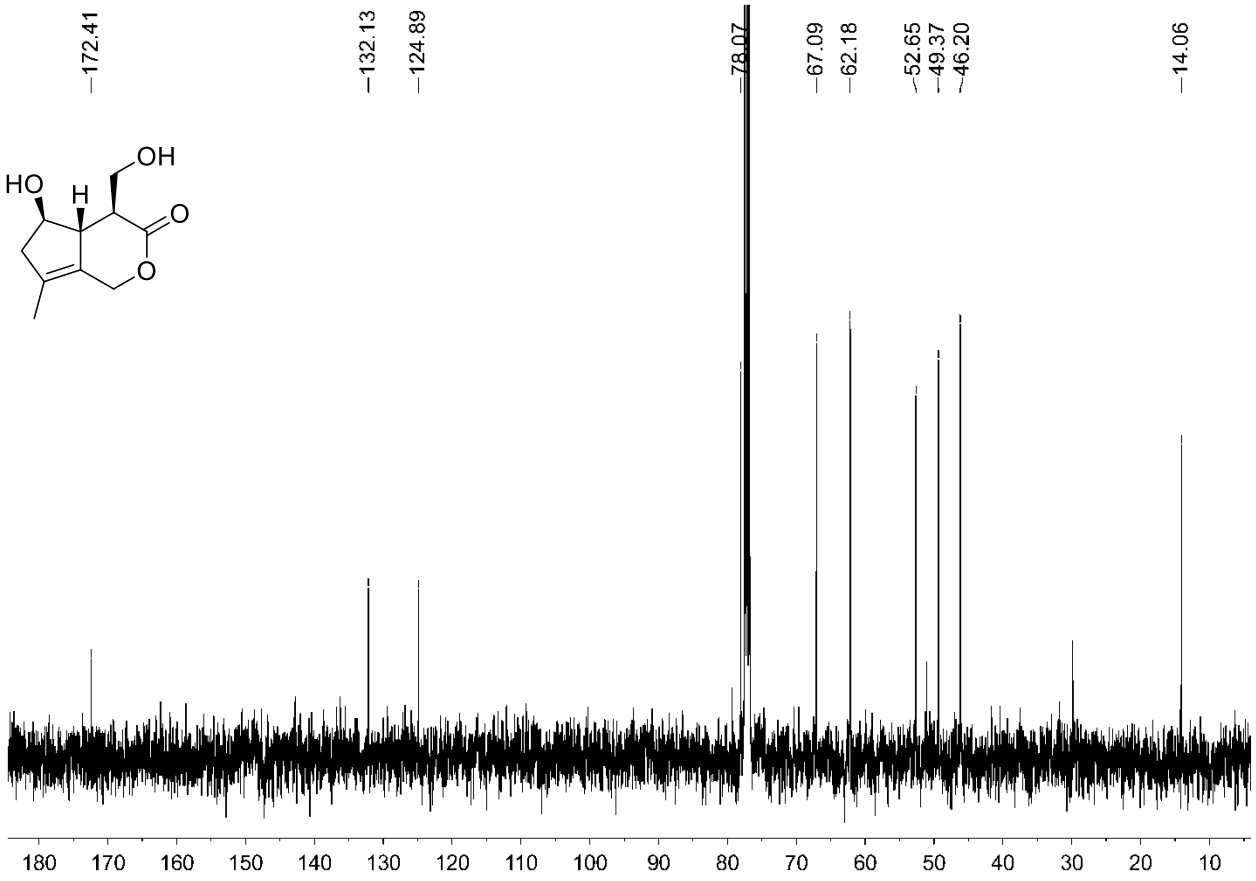

Figure S97. ^{13}C NMR (100 MHz, chloroform-*d*) spectrum of compound **4a**

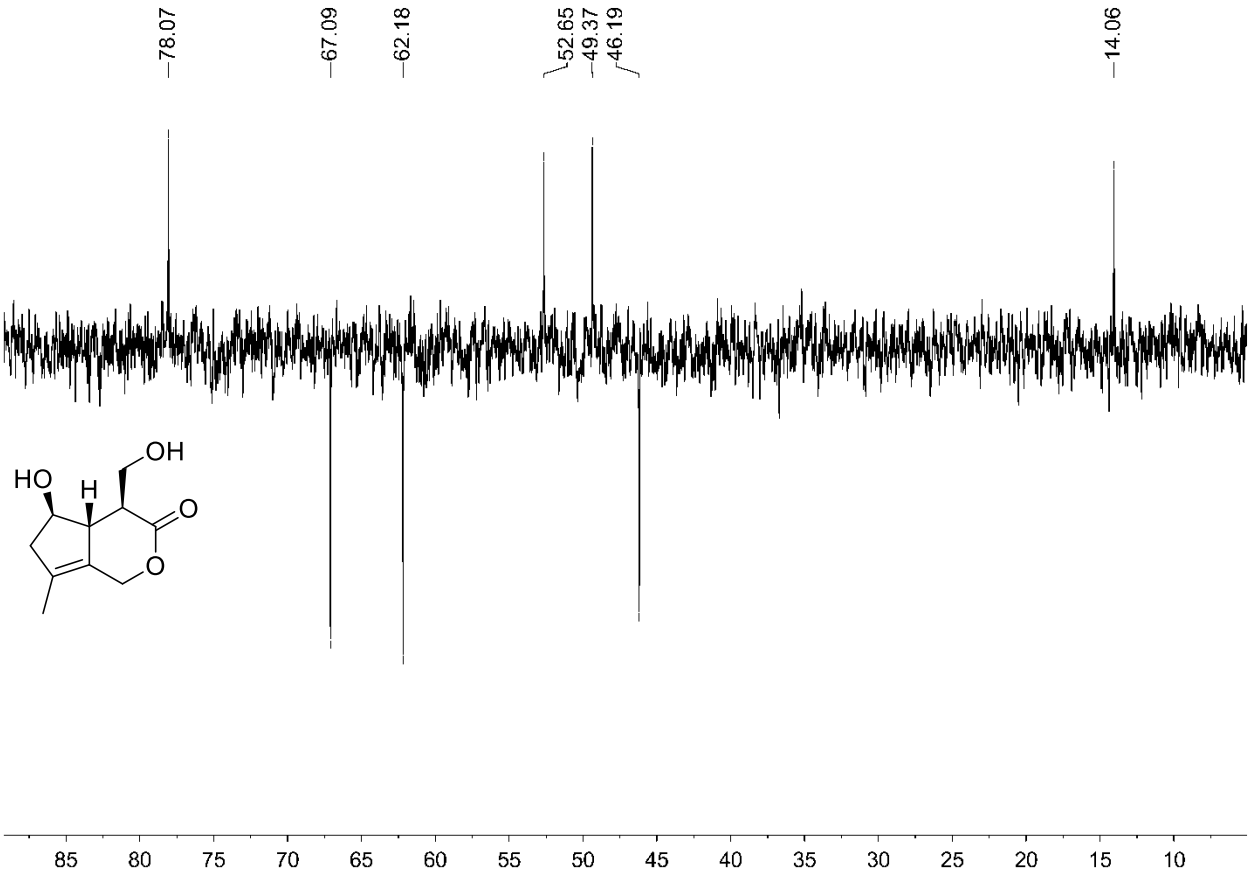

Figure S98. DEPT135 (100 MHz, chloroform-*d*) spectrum of compound **4a**

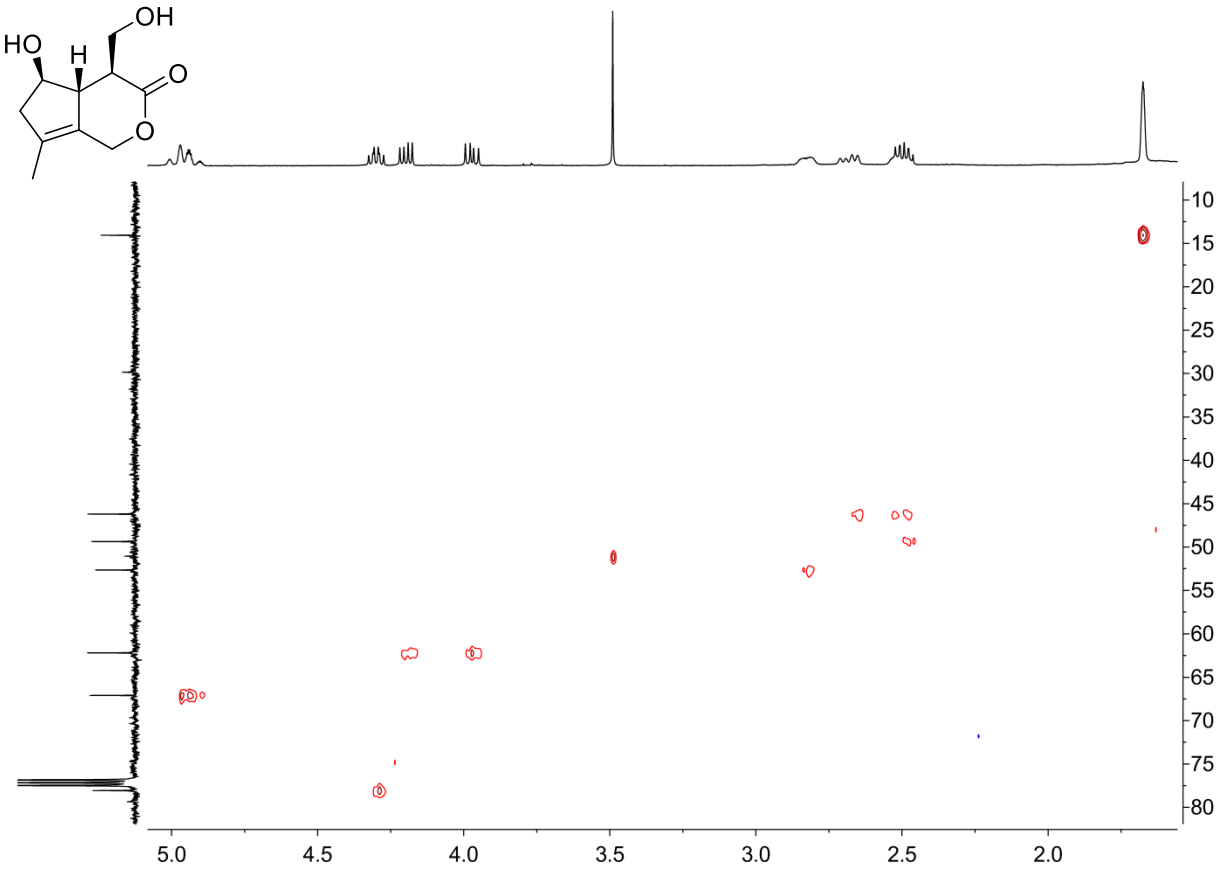

Figure S99. HSQC spectrum (chloroform-*d*) of compound **4a** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

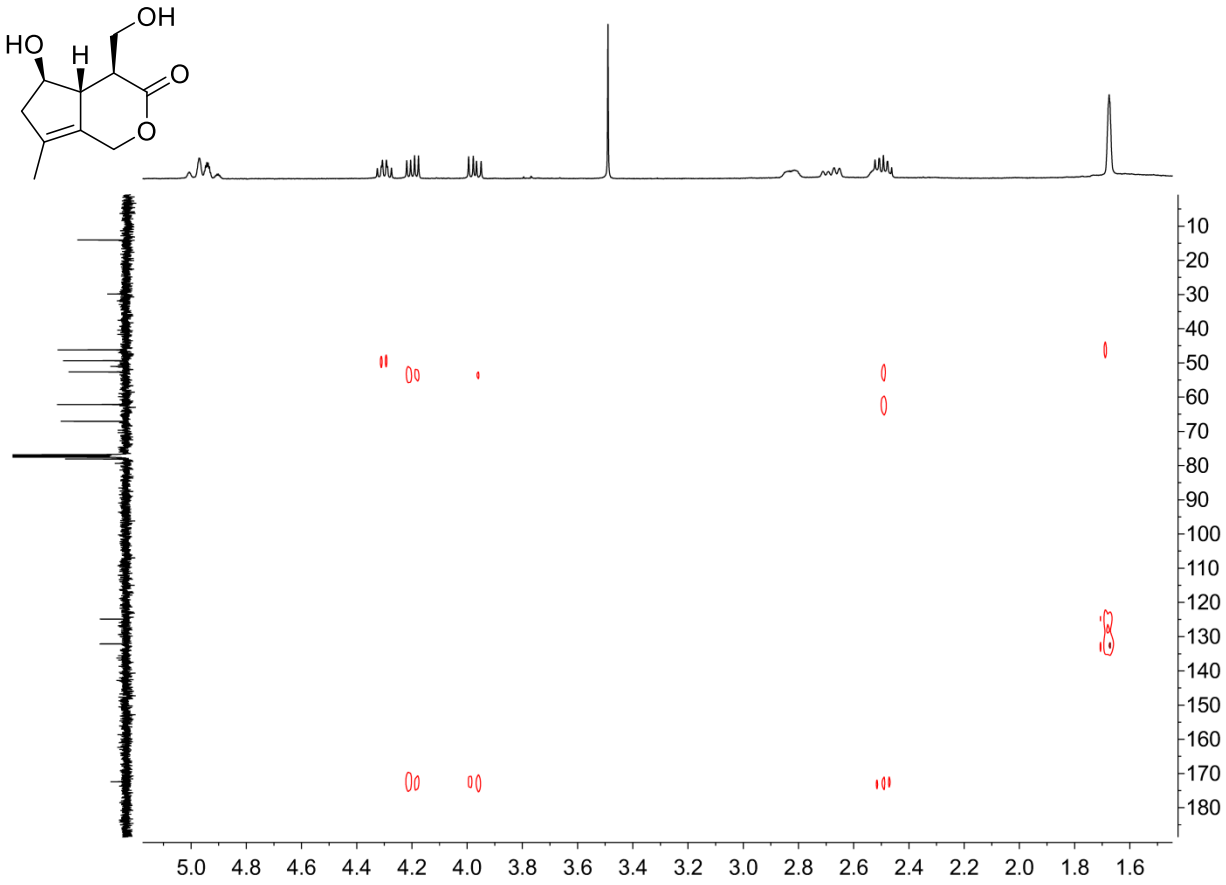

Figure S100. HMBC spectrum (chloroform-*d*) of compound **4a** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

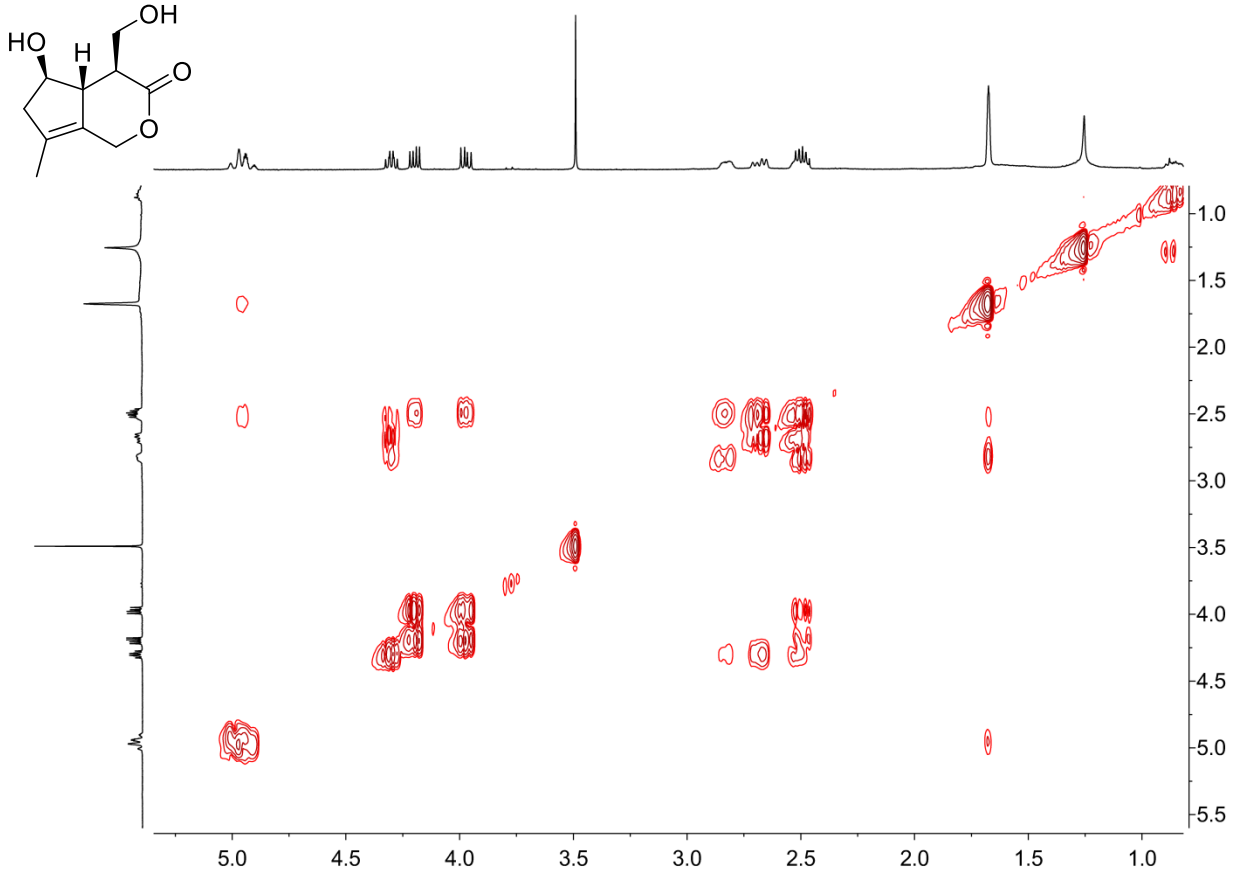

Figure S101. ^{1}H–^{1}H COSY spectrum (400 MHz, chloroform-*d*) of compound **4a**

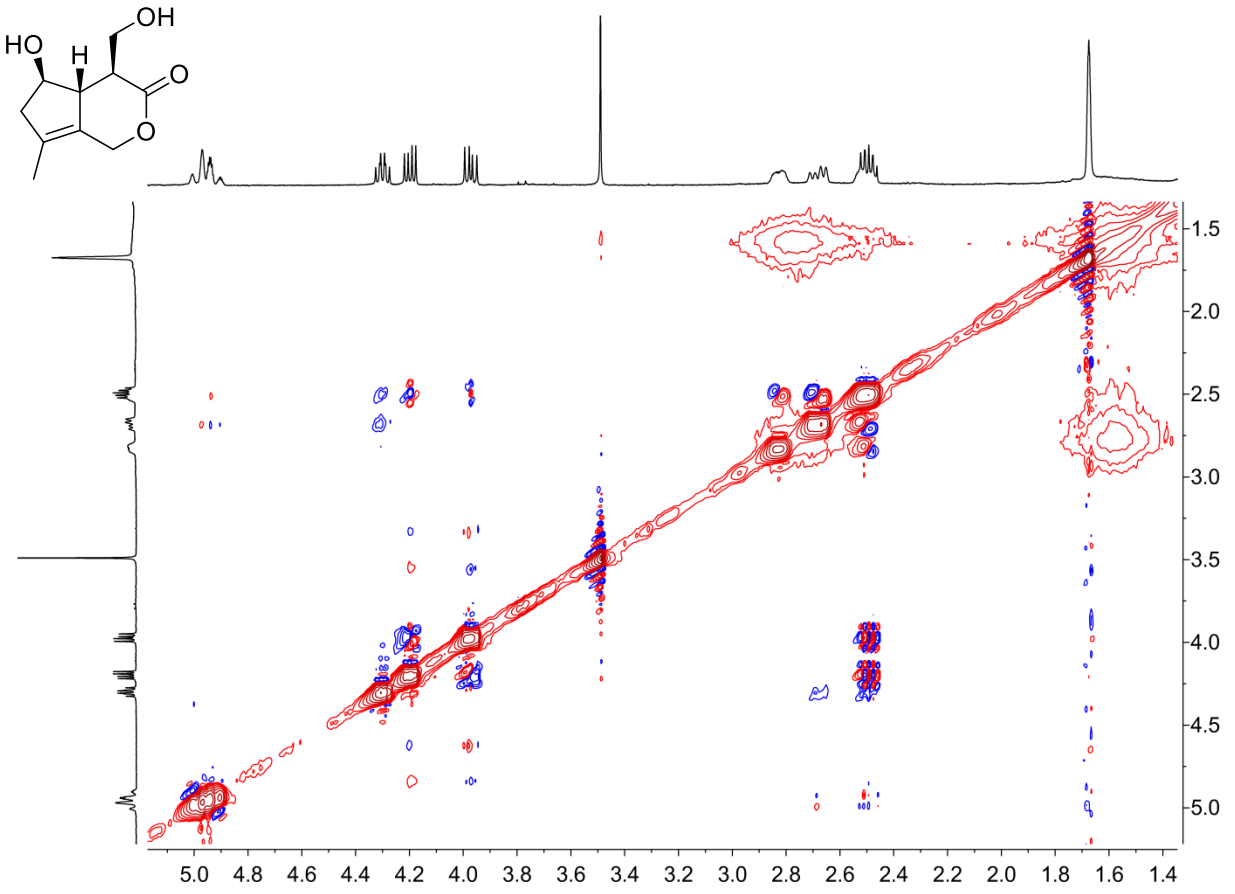

Figure S102. NOESY spectrum (400 MHz, chloroform-*d*) of compound **4a**

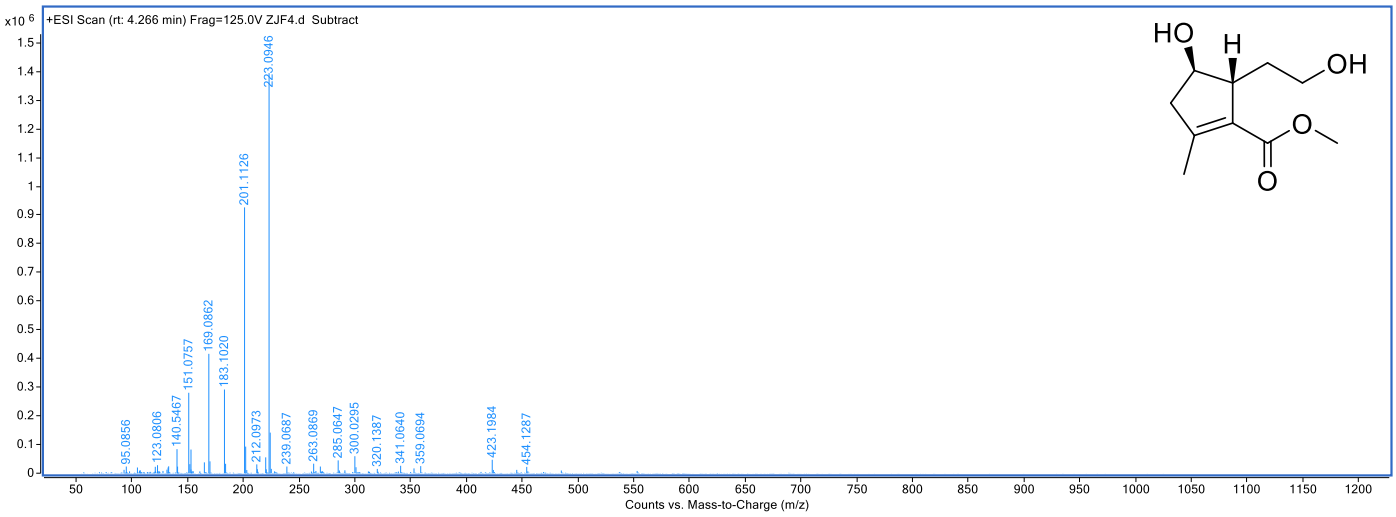

Figure S103. (+)-HR-ESI-MS spectrum of **5**

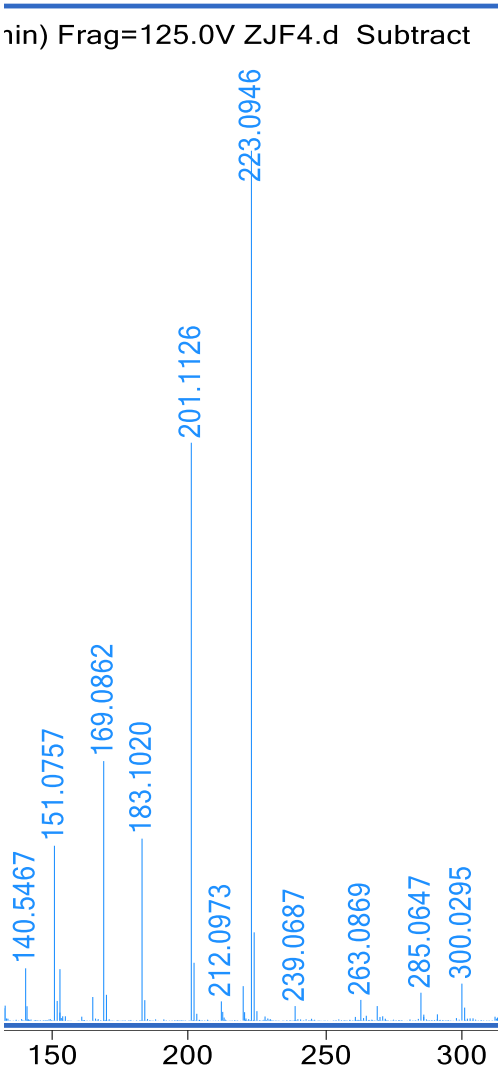

Figure S104. (+)-HR-ESI-MS spectrum of **5** (amplified)

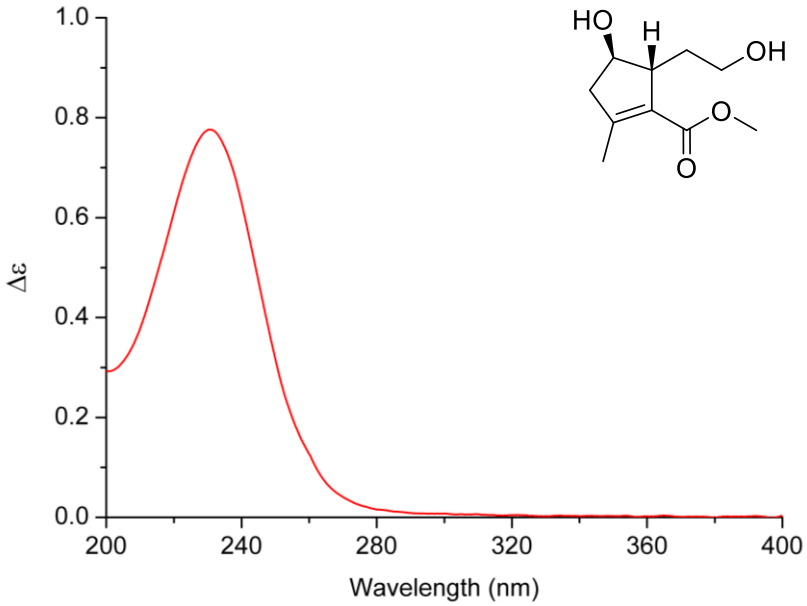

Figure S105. UV spectrum of compound **5**

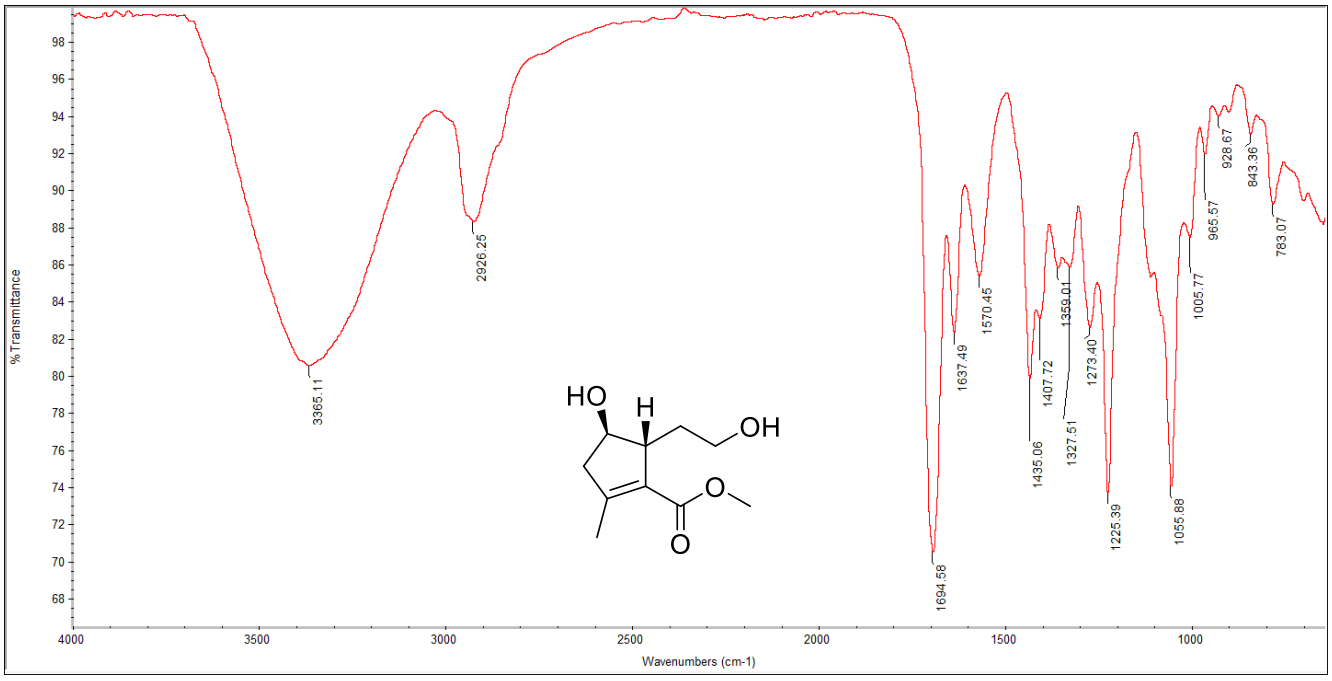

Figure S106. IR spectrum of compound **5**

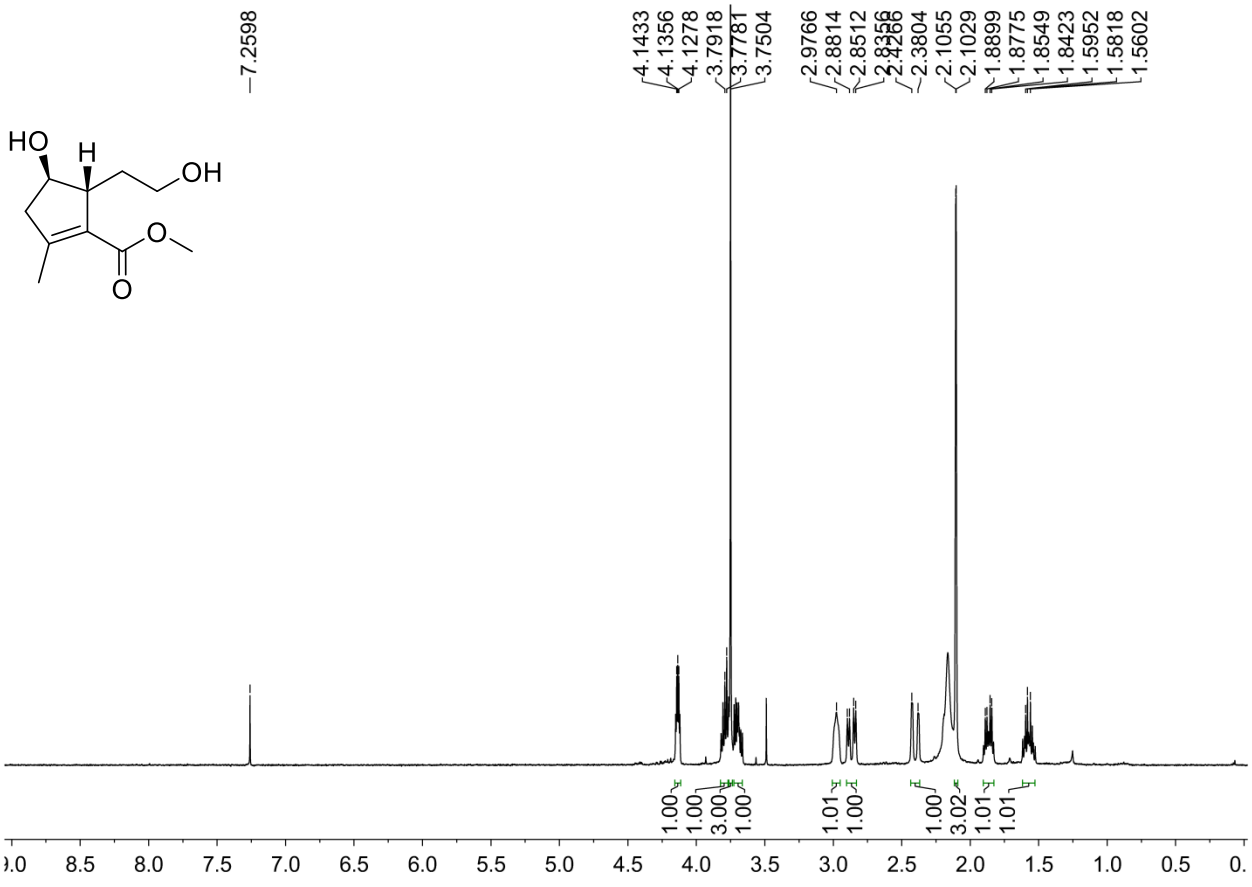

Figure S107. ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of compound **5**

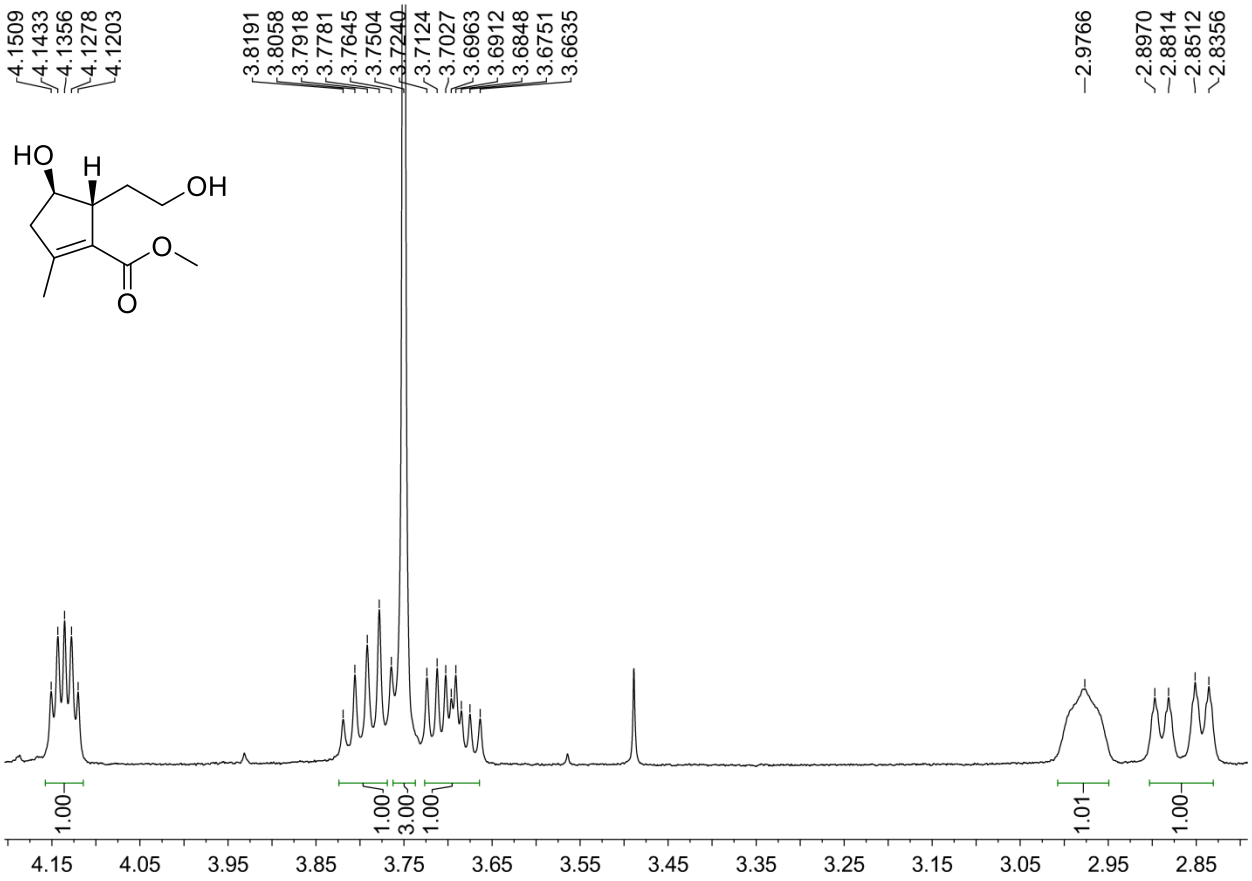

Figure S108. [1]H NMR (400 MHz, chloroform-*d*) spectrum of compound **5** (amplified)

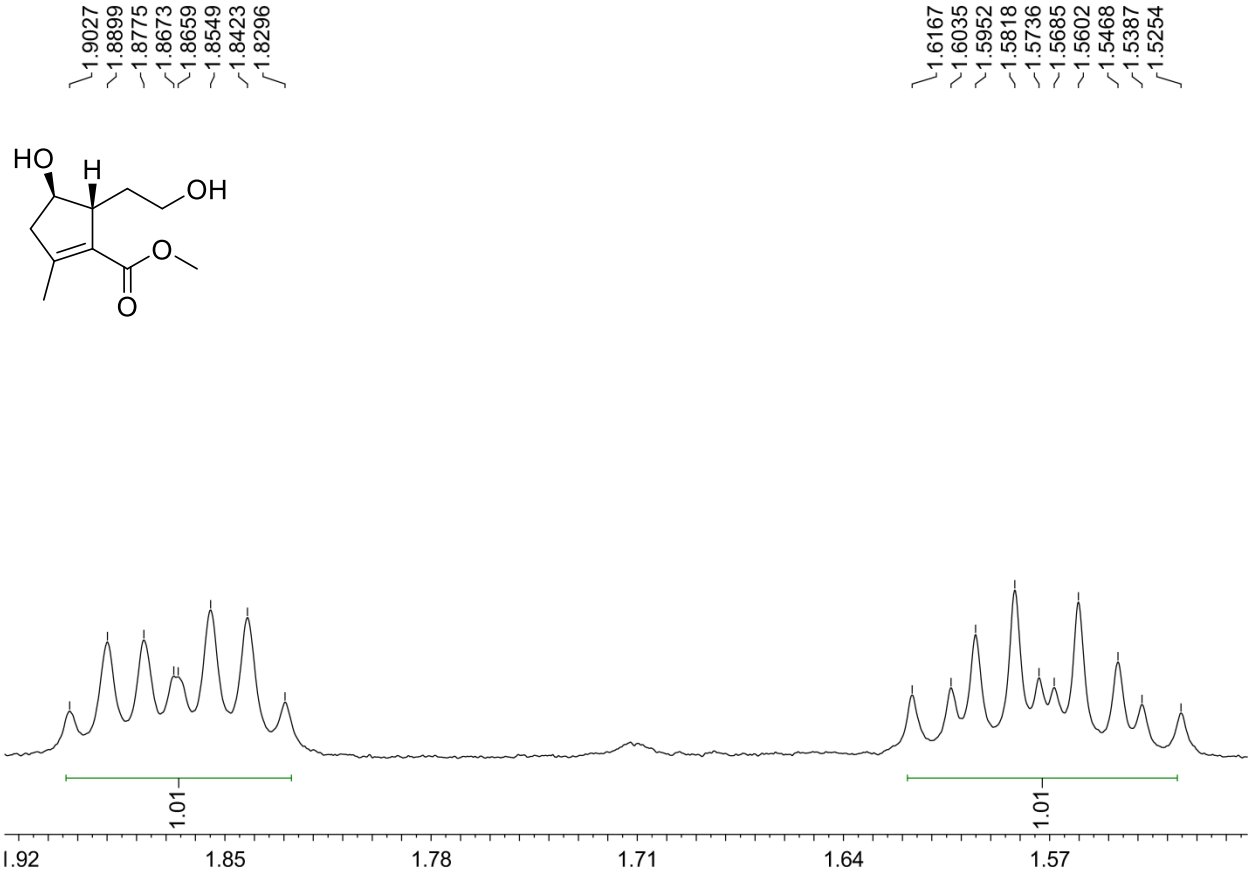

Figure S109. [1]H NMR (400 MHz, chloroform-*d*) spectrum of compound **5** (amplified)

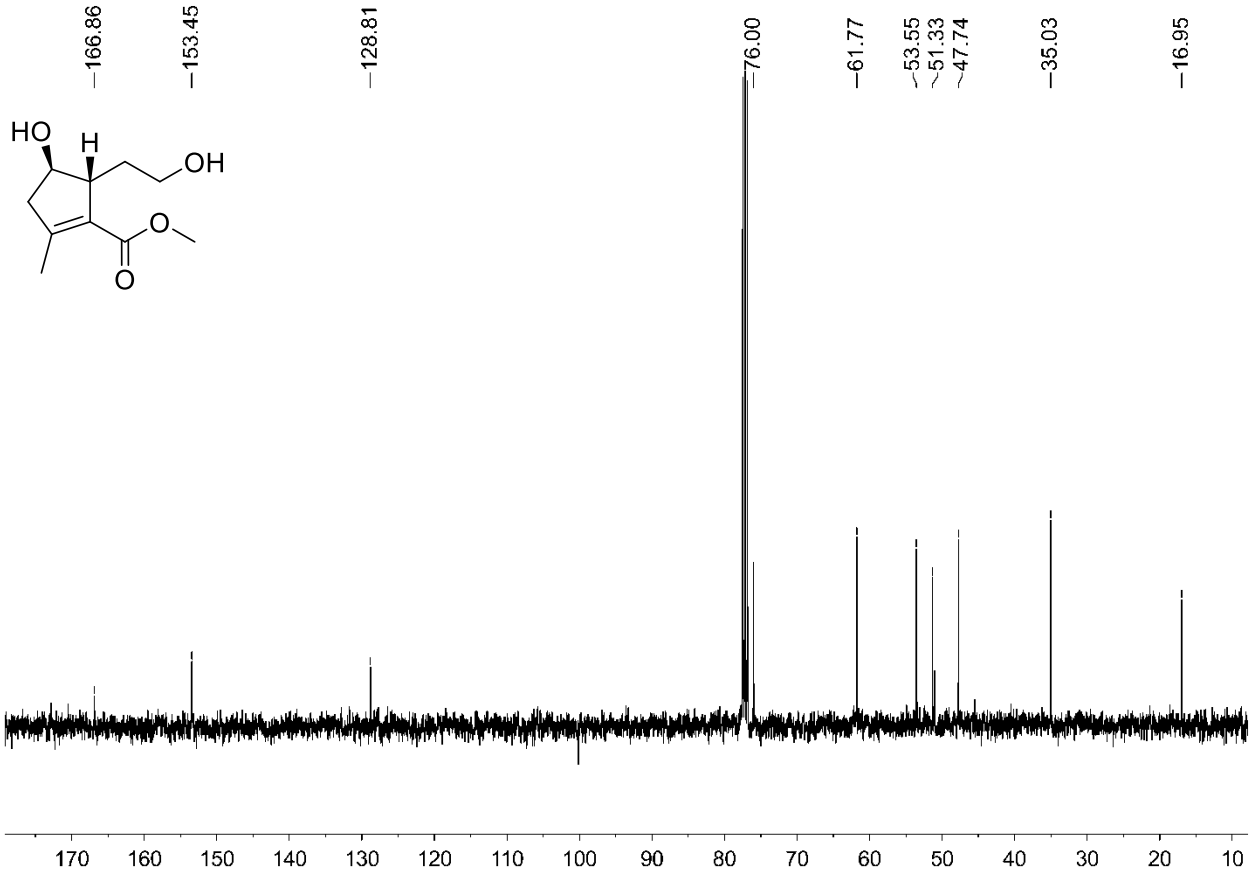

Figure S110. ^{13}C NMR (100 MHz, chloroform-*d*) spectrum of compound **5**

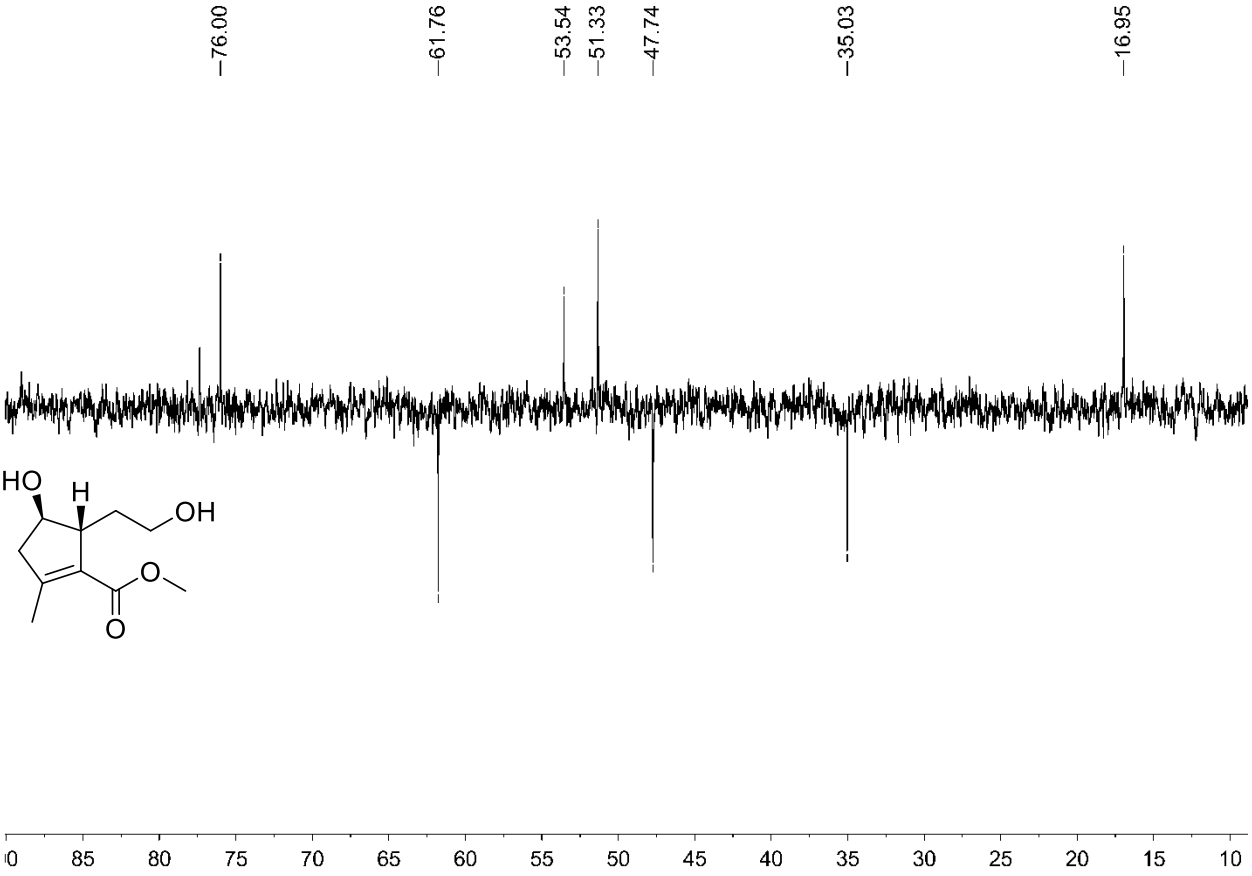

Figure S111. DEPT135 (100 MHz, chloroform-*d*) spectrum of compound **5**

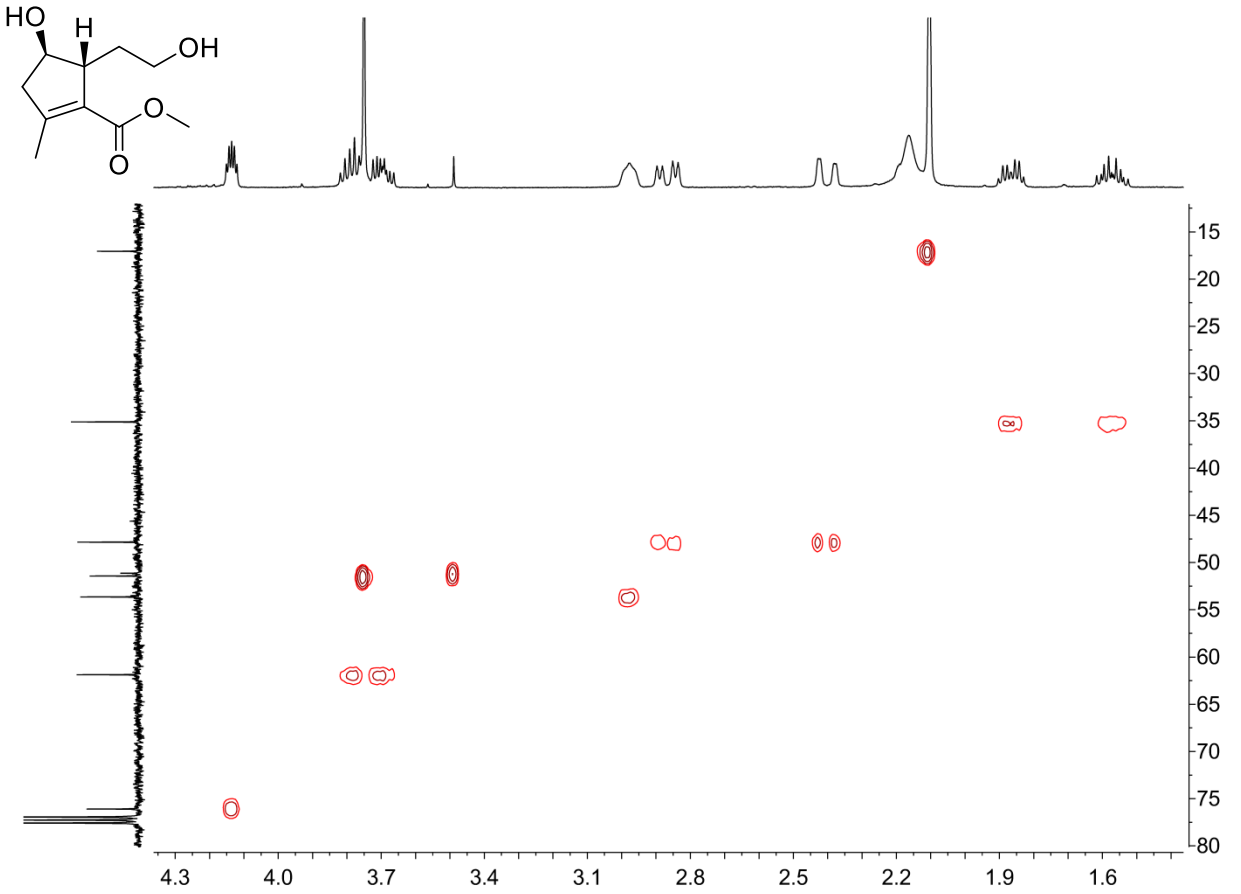

Figure S112. HSQC spectrum (chloroform-*d*) of compound **5** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

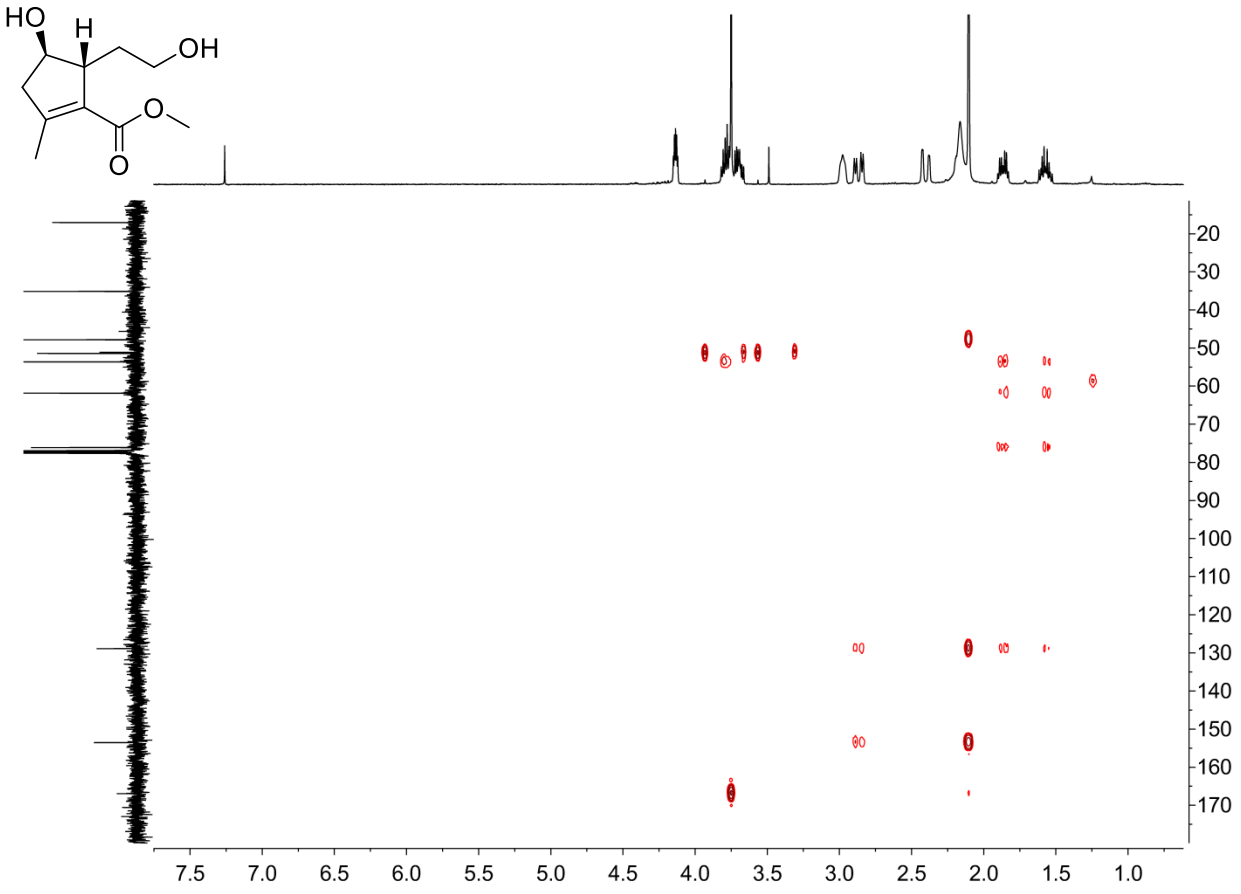

Figure S113. HMBC spectrum (chloroform-*d*) of compound **5** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

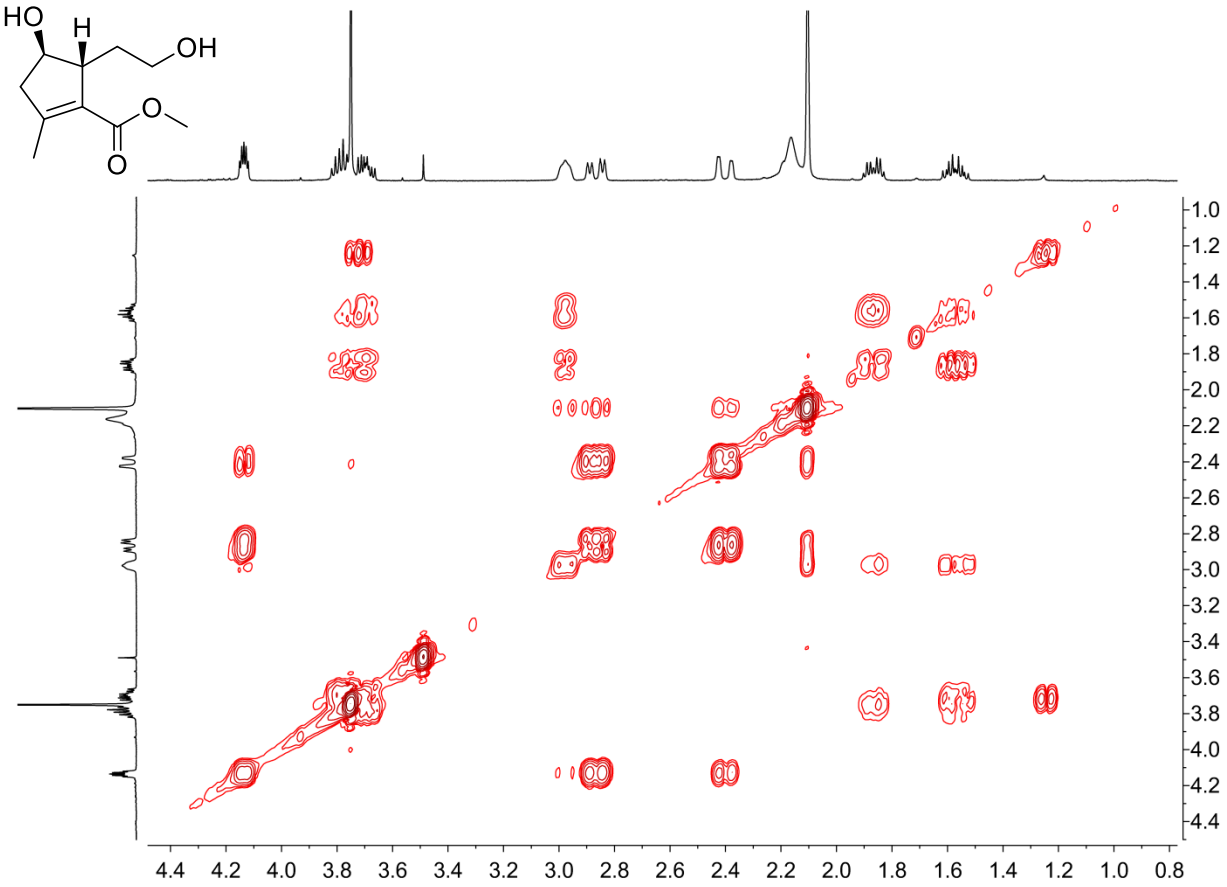

Figure S114. $^{1}H–^{1}H$ COSY spectrum (400 MHz, chloroform-*d*) of compound **5**

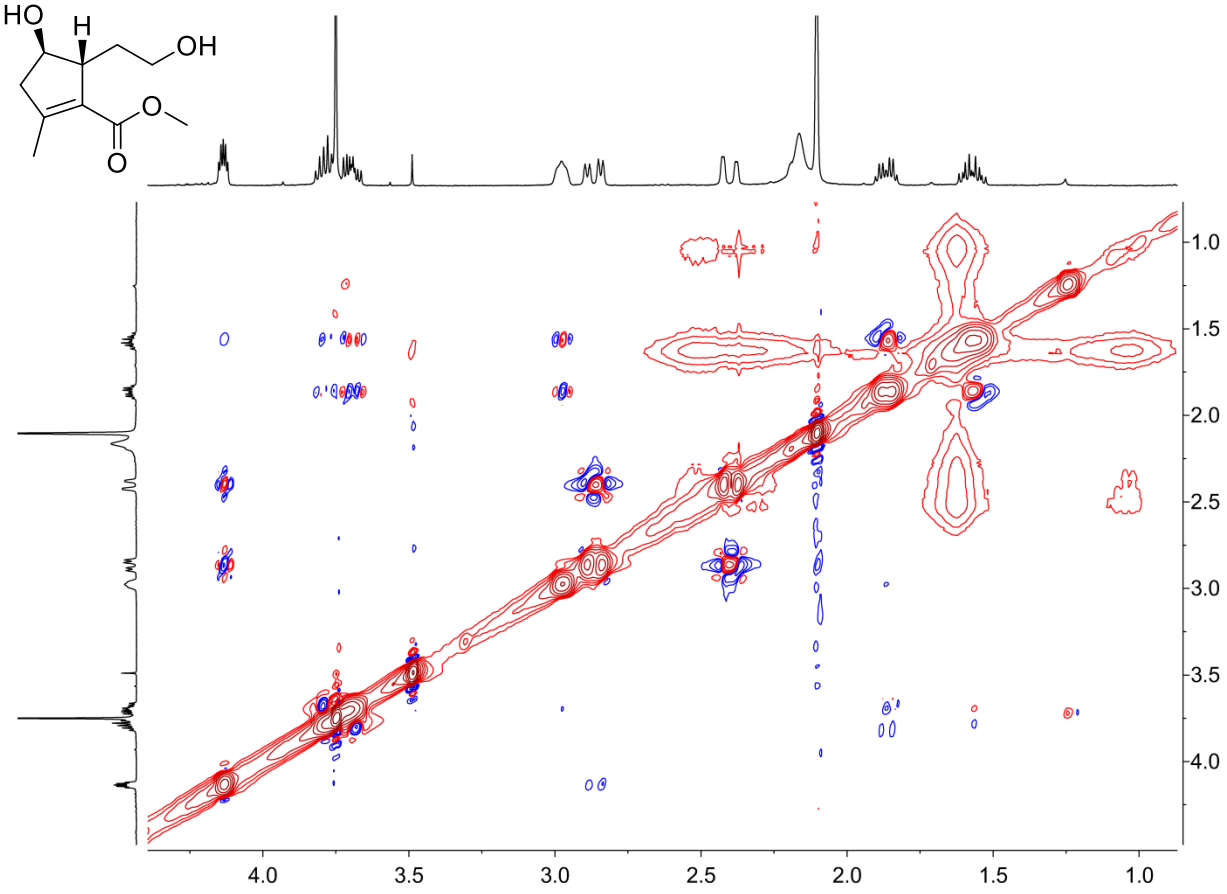

Figure S115. NOESY spectrum (400 MHz, chloroform-*d*) of compound **5**

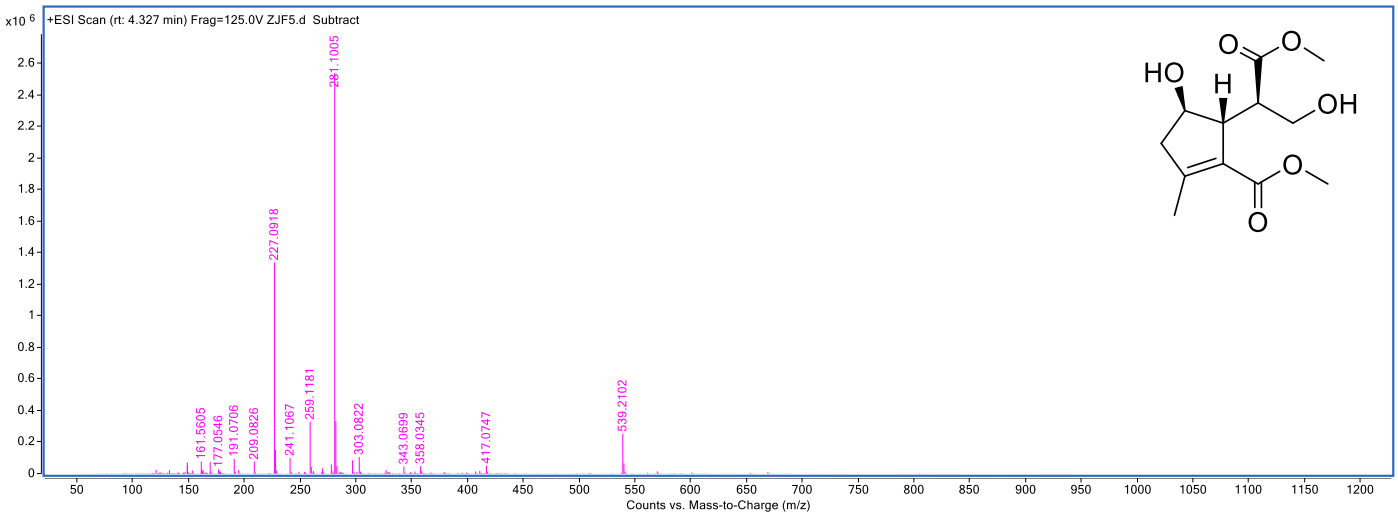

Figure S116. (+)-HR-ESI-MS spectrum of **6**

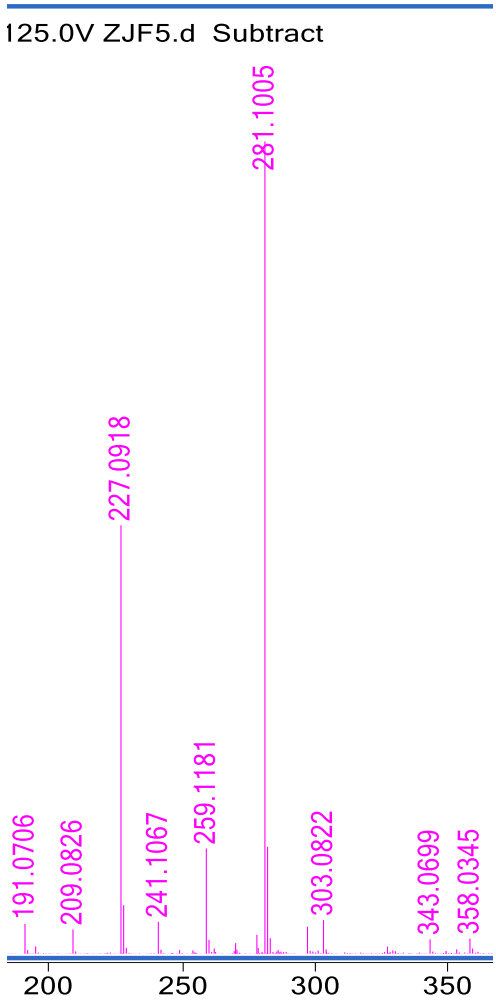

Figure S117. (+)-HR-ESI-MS spectrum of **6** (amplified)

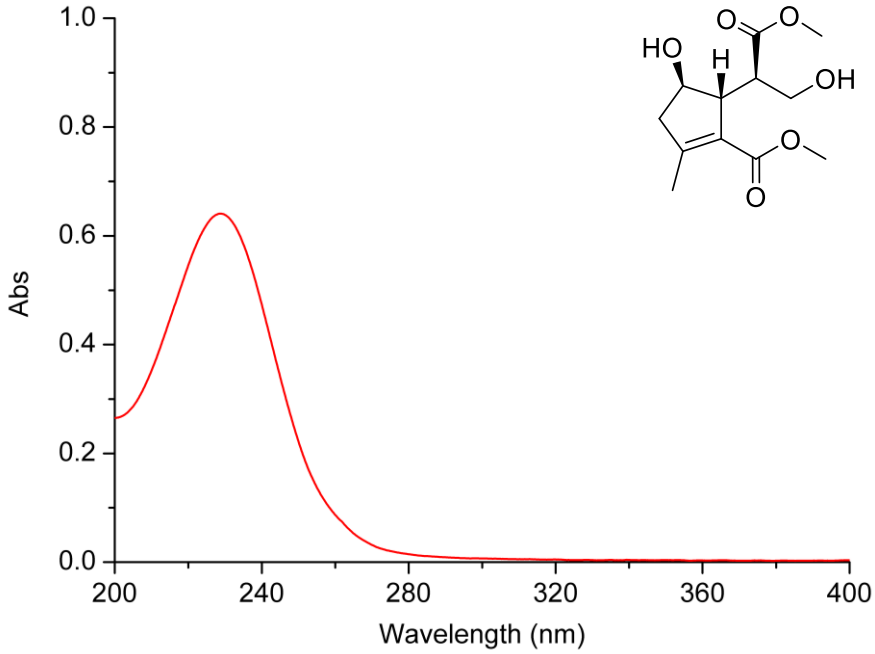

Figure S118. UV spectrum of compound **6**

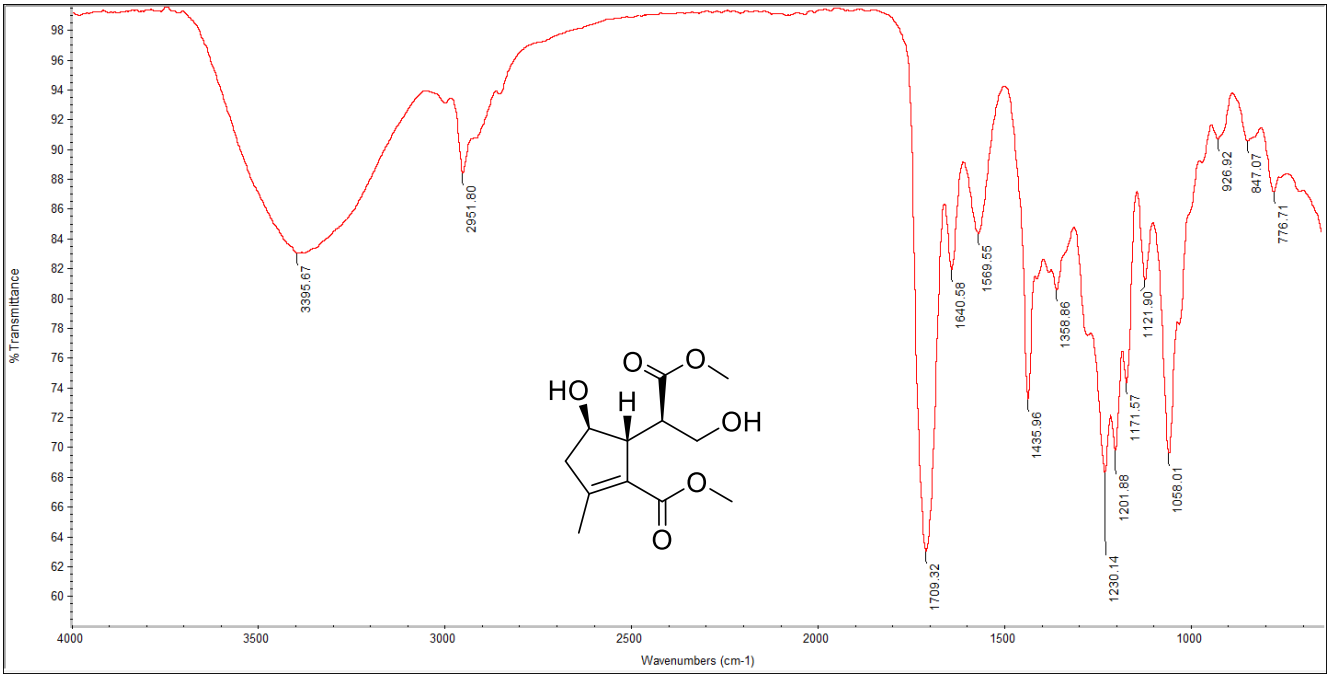

Figure S119. IR spectrum of compound **6**

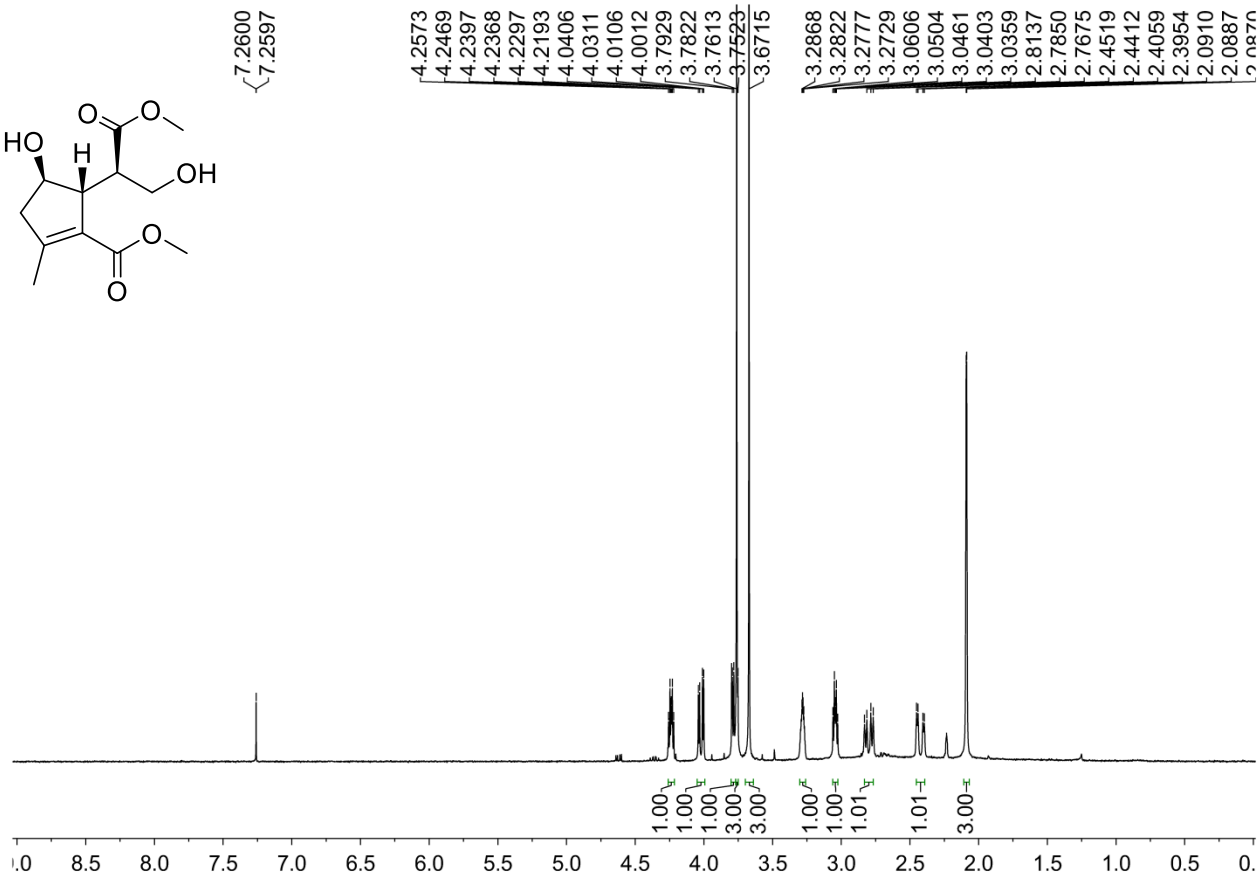

Figure S120. ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of compound **6**

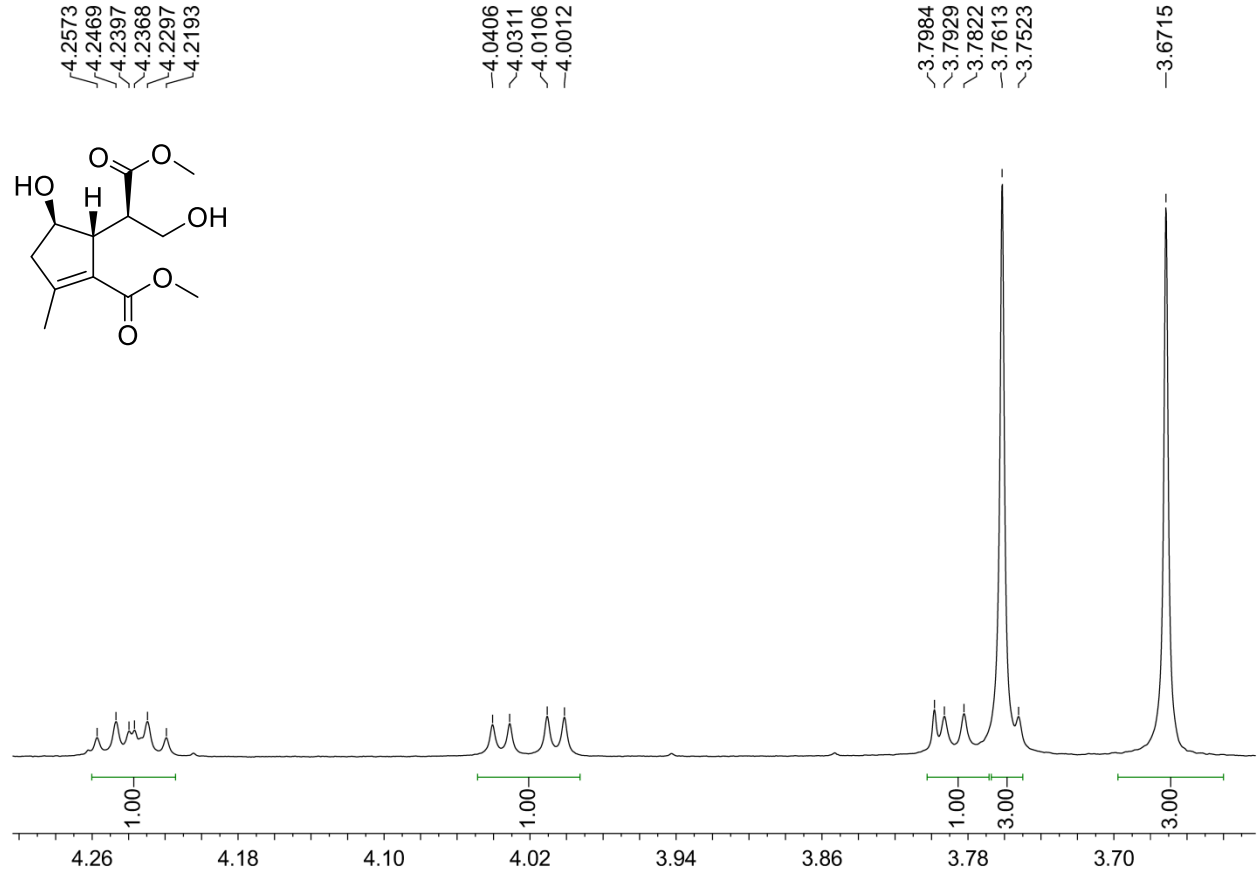

Figure S121. ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of compound **6** (amplified)

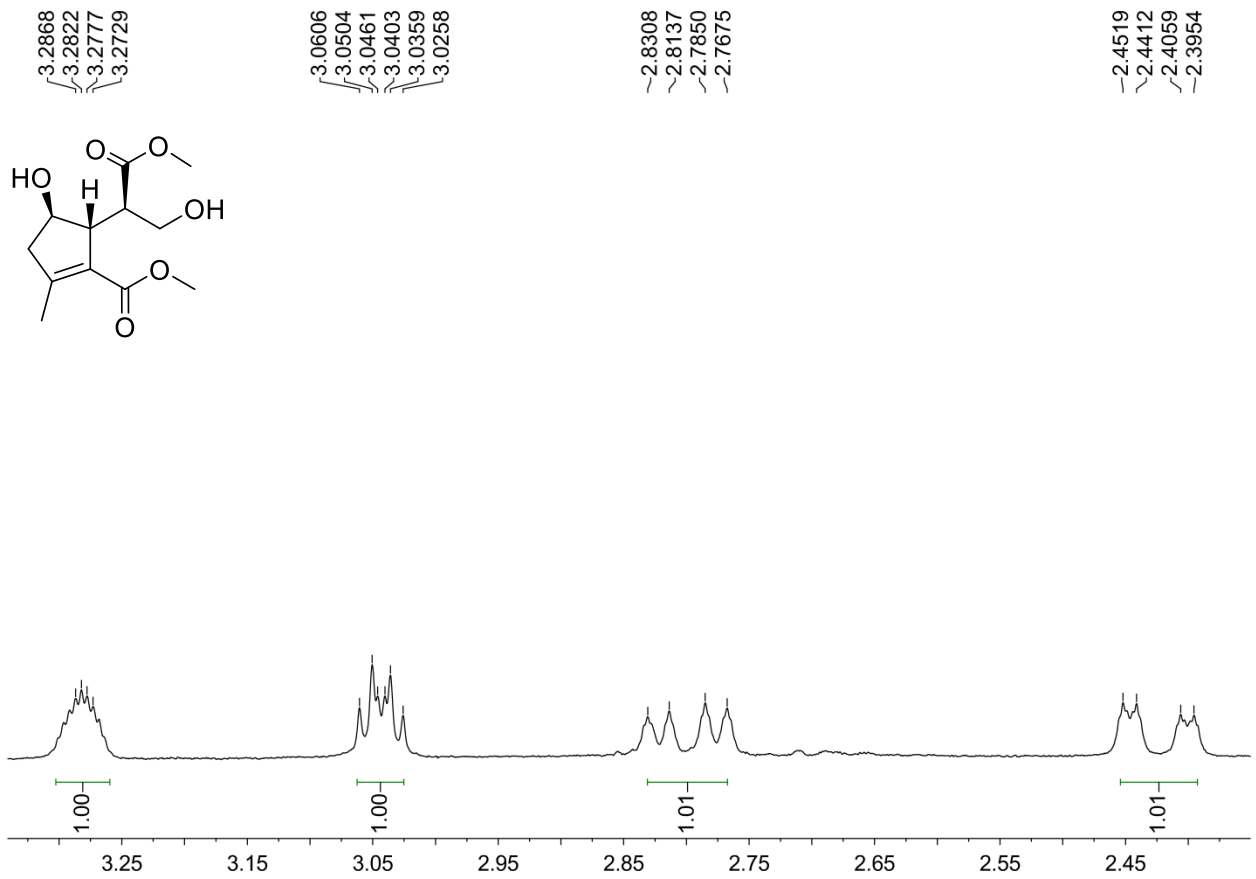

Figure S122. ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of compound **6** (amplified)

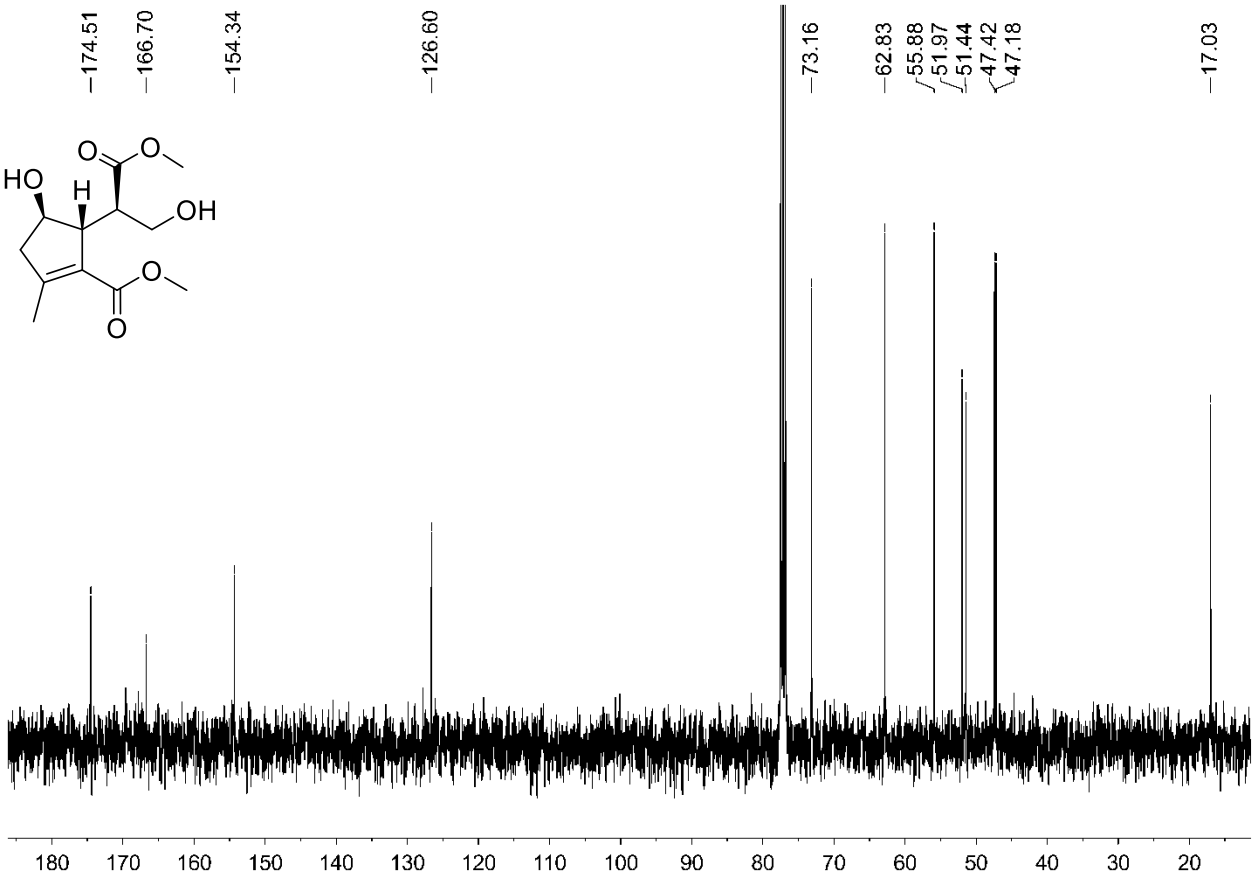

Figure S123. ^{13}C NMR (100 MHz, chloroform-*d*) spectrum of compound **6**

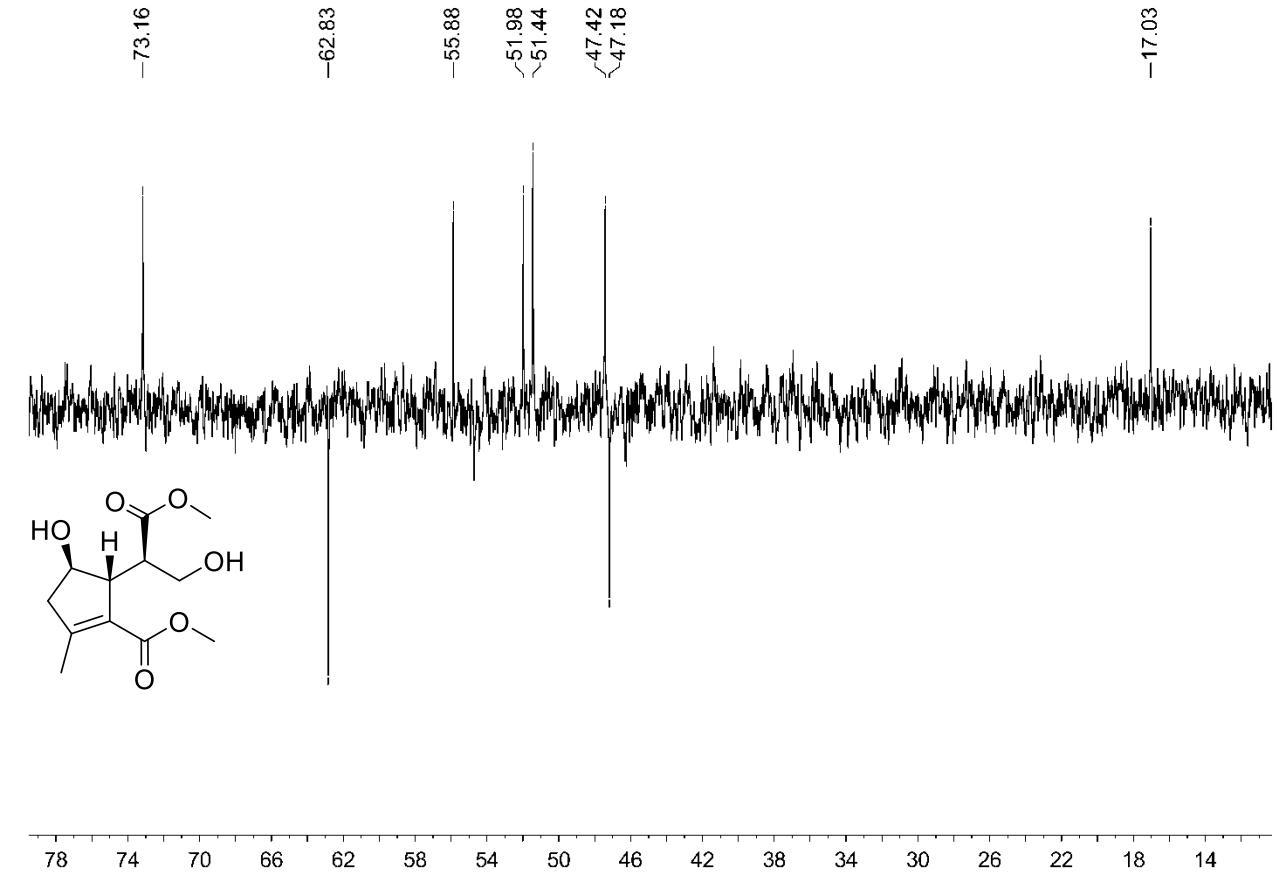

Figure S124. DEPT135 (100 MHz, chloroform-*d*) spectrum of compound **6**

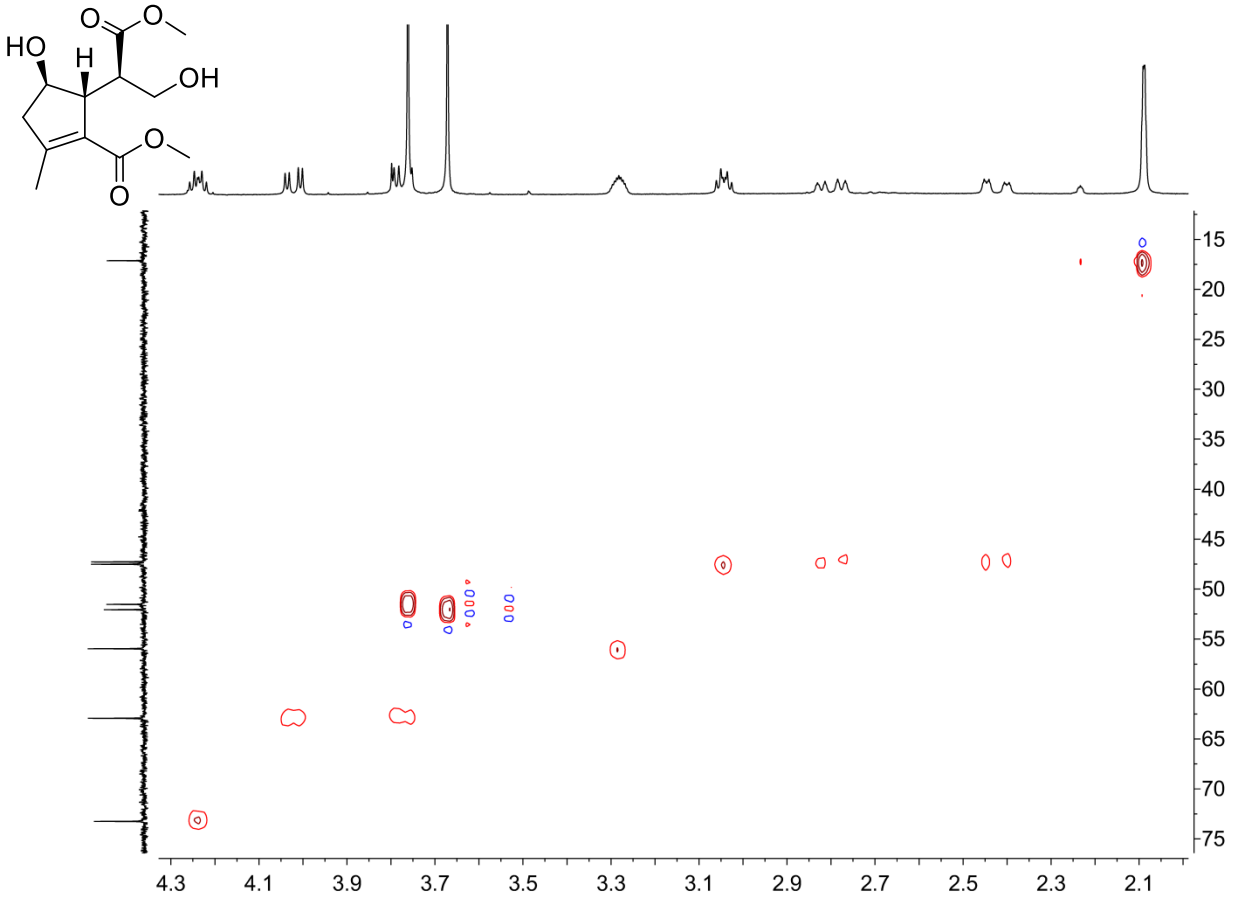

Figure S125. HSQC spectrum (chloroform-*d*) of compound **6** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

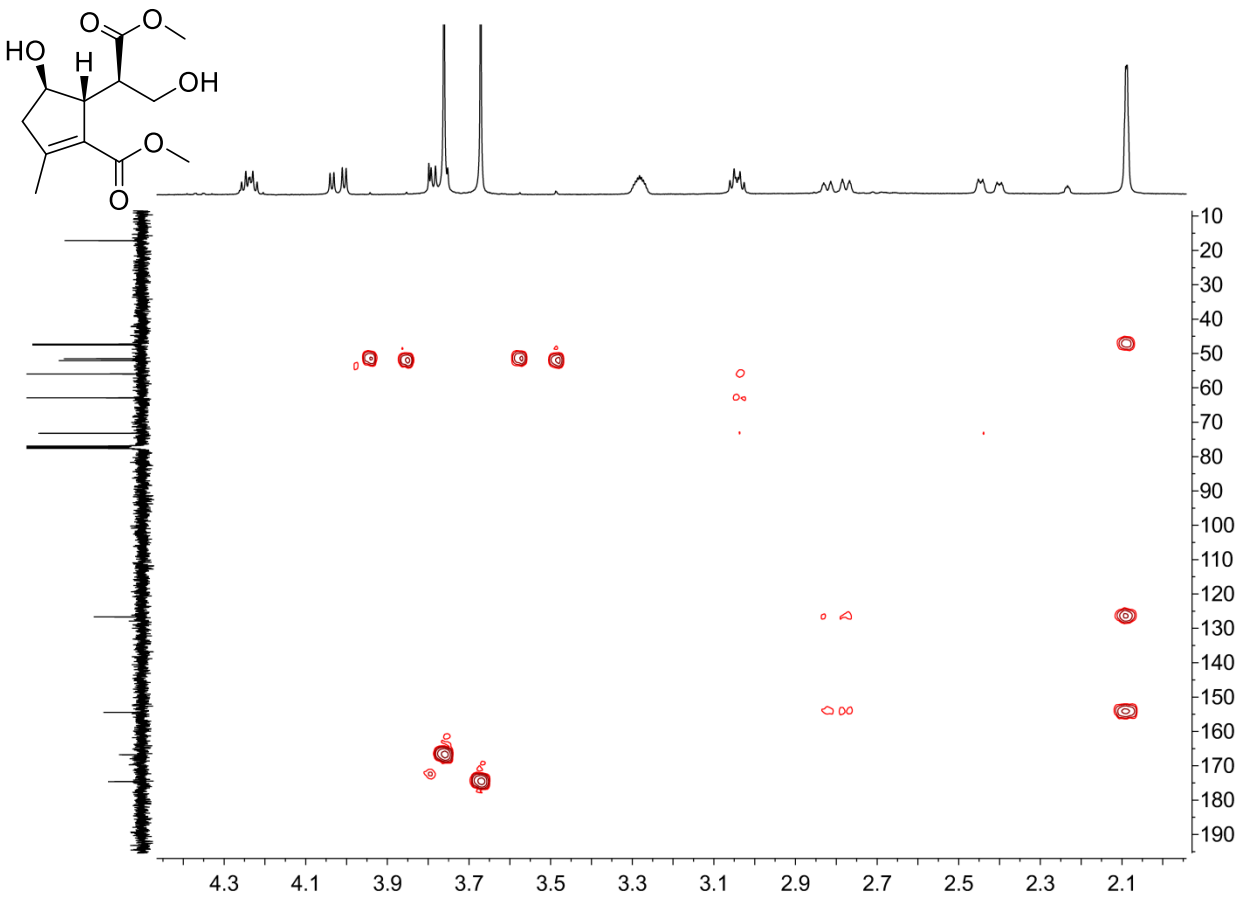

Figure S126. HMBC spectrum (chloroform-*d*) of compound **6** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

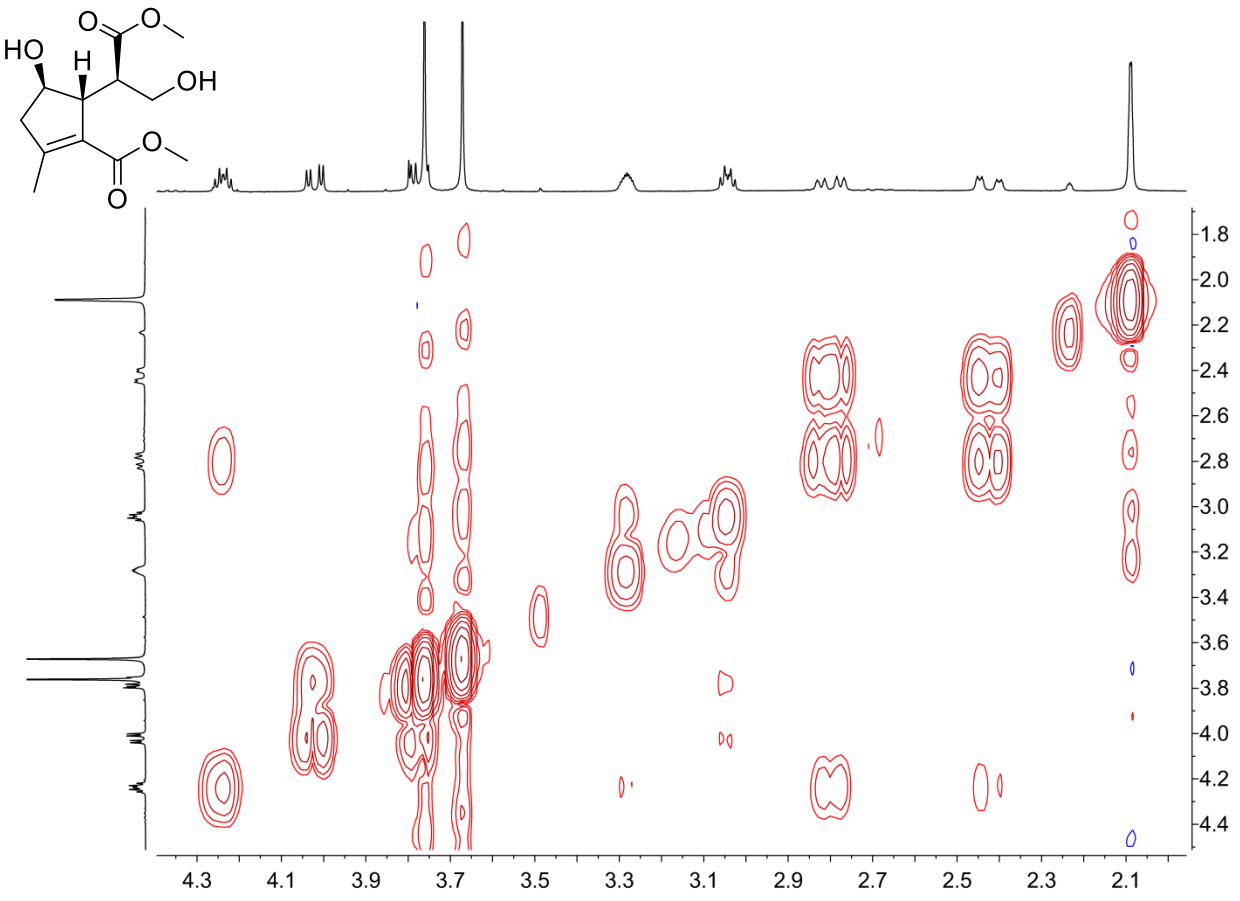

Figure S127. ^{1}H–^{1}H COSY spectrum (400 MHz, chloroform-*d*) of compound **6**

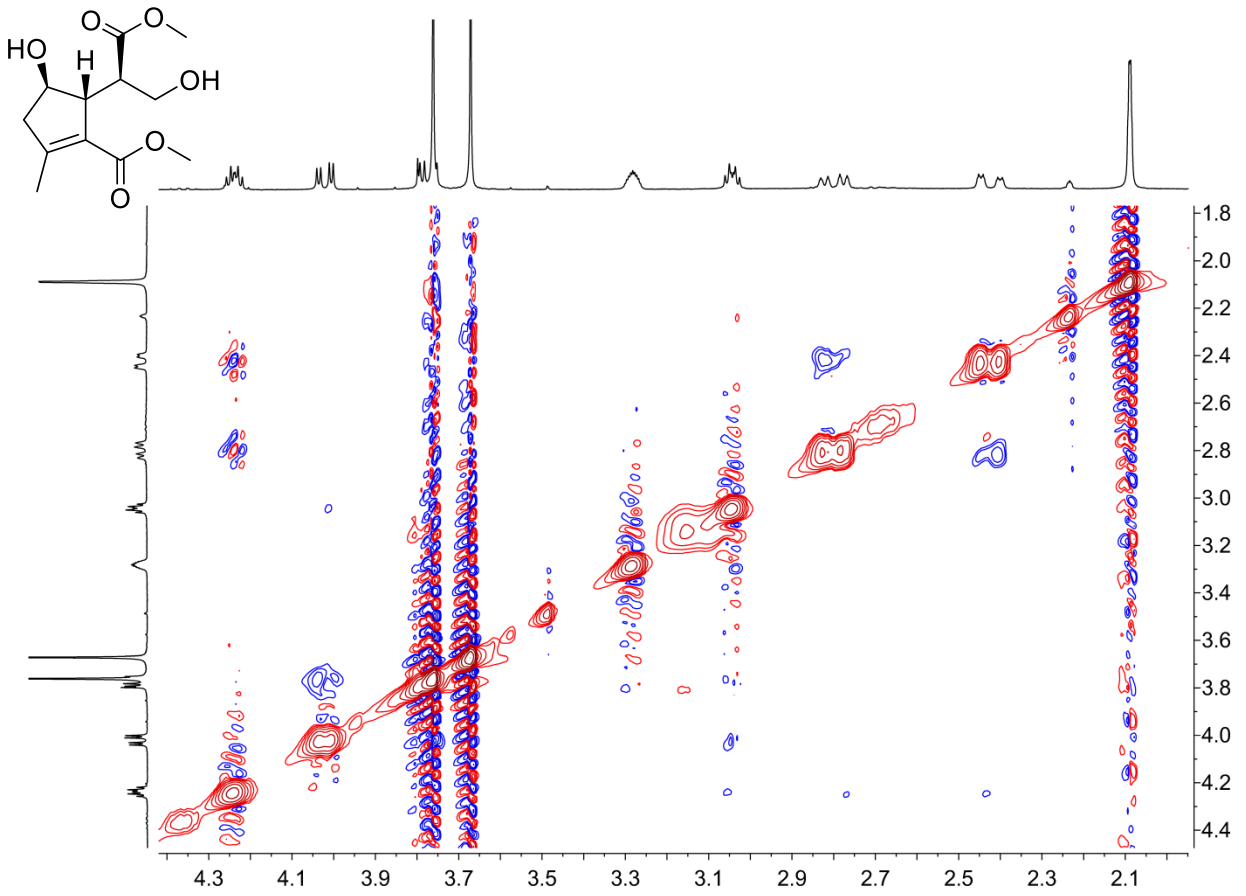

Figure S128. NOESY spectrum (400 MHz, chloroform-*d*) of compound **6**

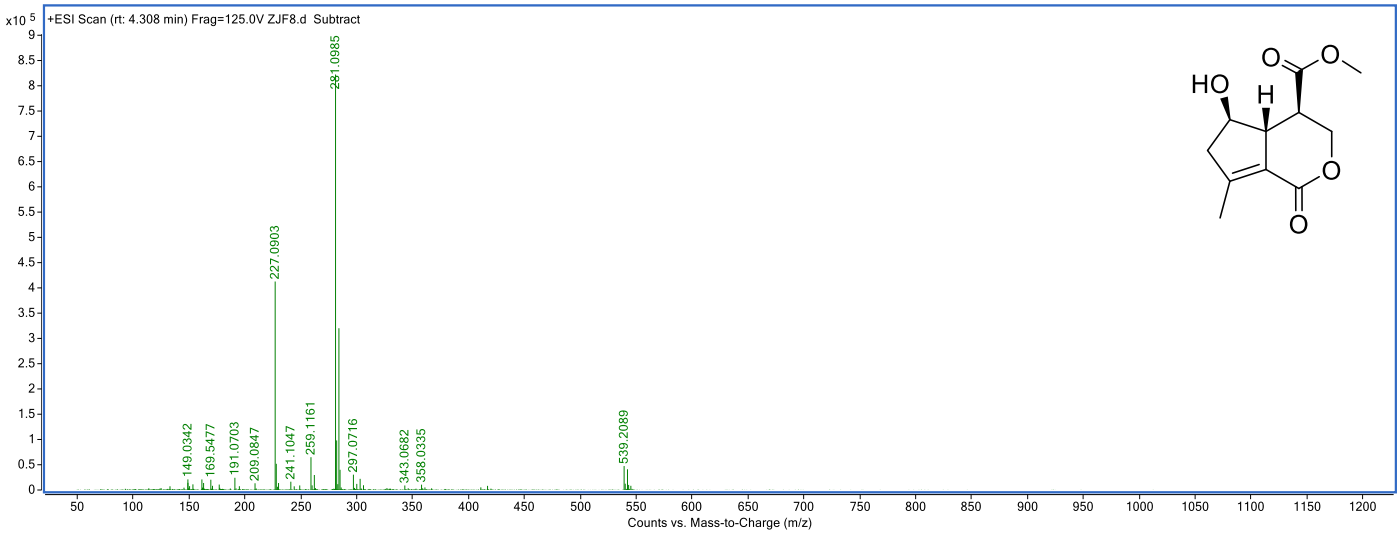

Figure S129. (+)-HR-ESI-MS spectrum of **6a**

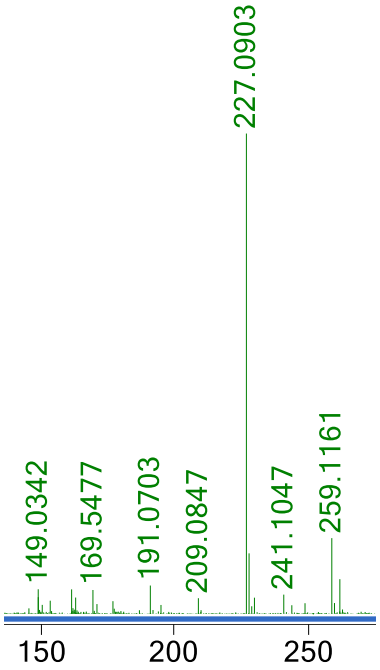

Figure S130. (+)-HR-ESI-MS spectrum of **6a** (amplified)

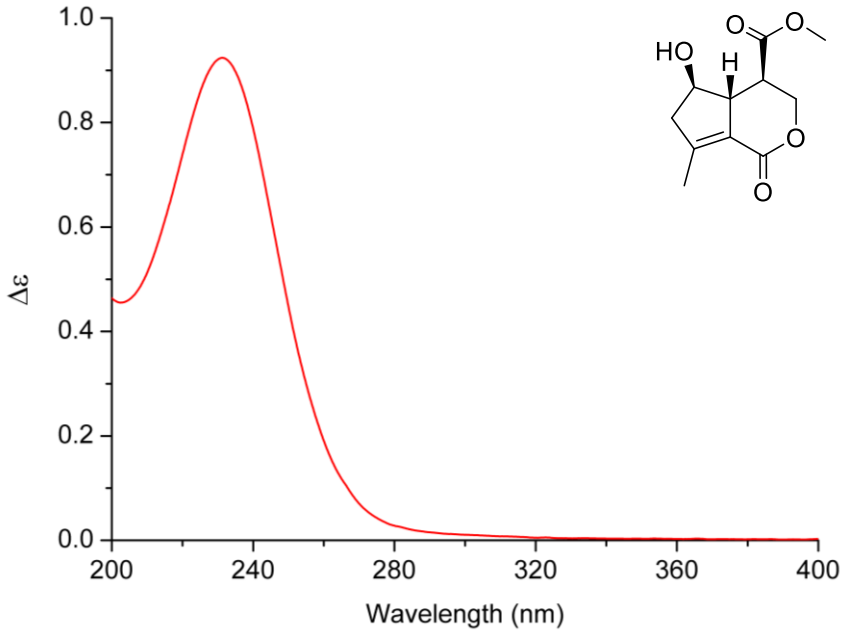

Figure S131. UV spectrum of compound **6a**

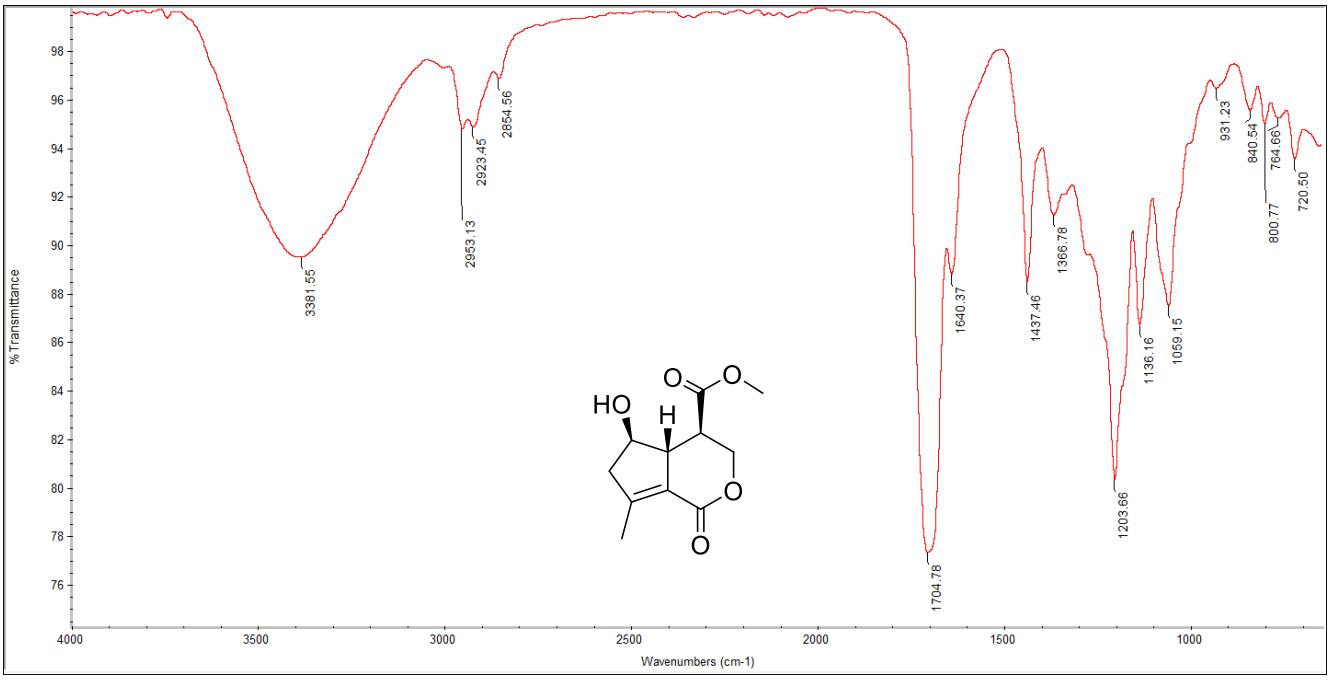

Figure S132. IR spectrum of compound **6a**

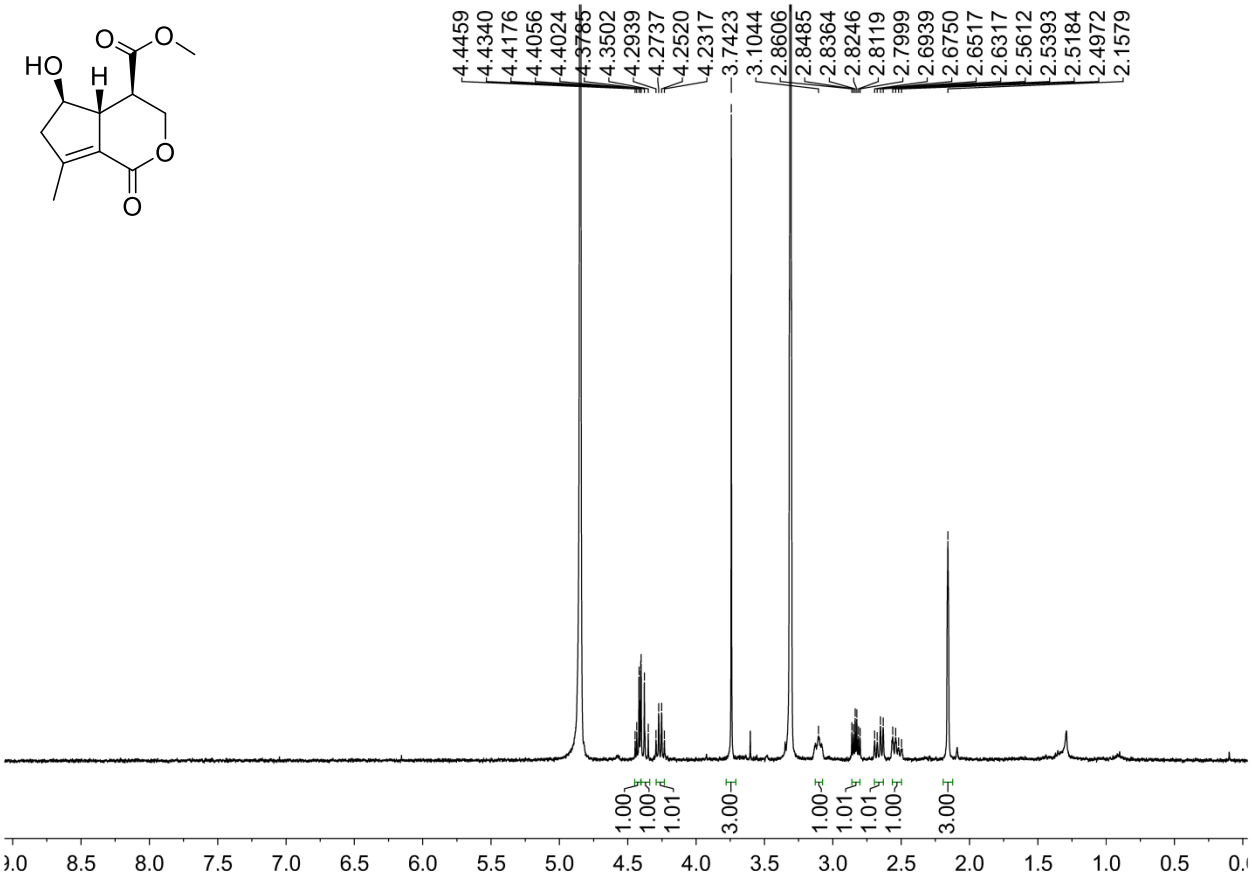

Figure S133. ^{1}H NMR (400 MHz, methanol-d_4) spectrum of compound **6a**

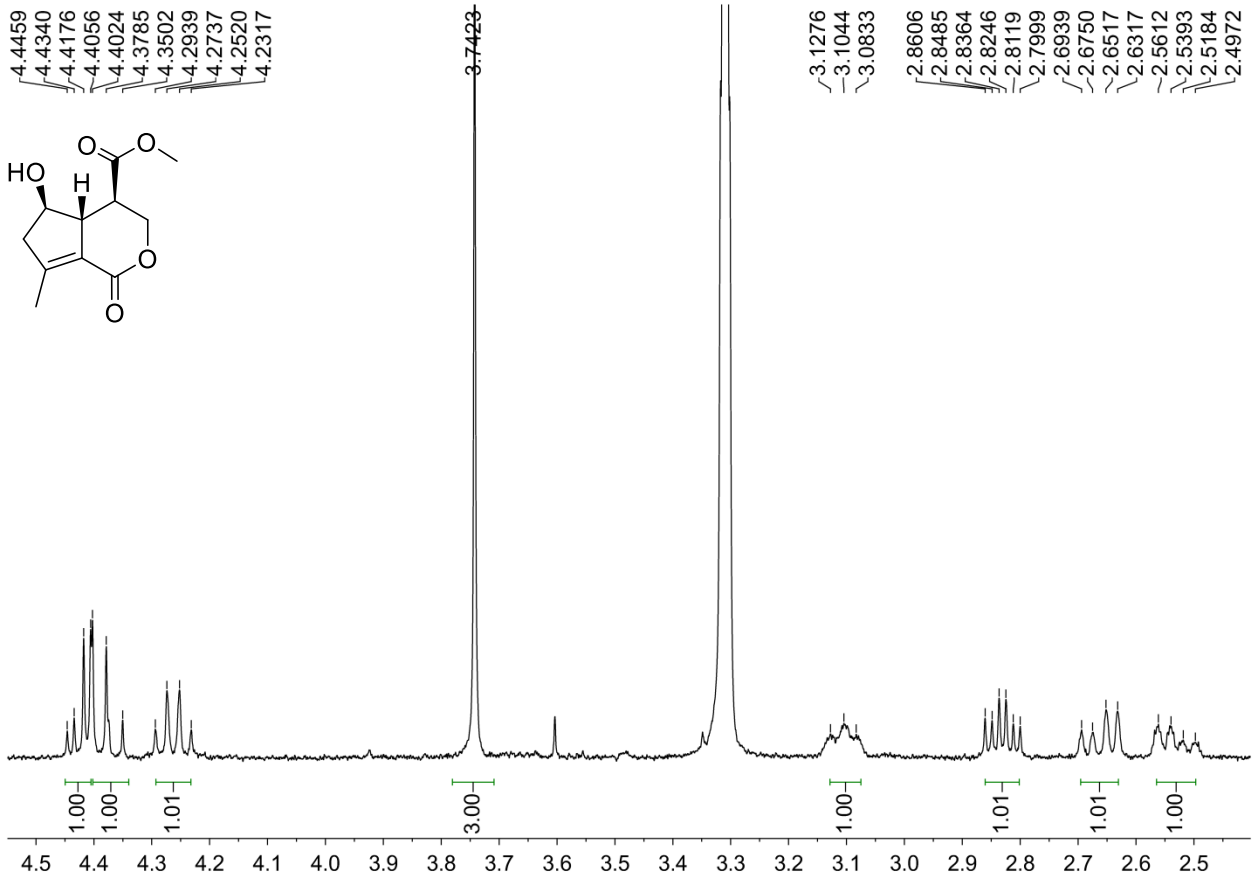

Figure S134. ^{1}H NMR (400 MHz, methanol-d_4) spectrum of compound **6a** (amplified)

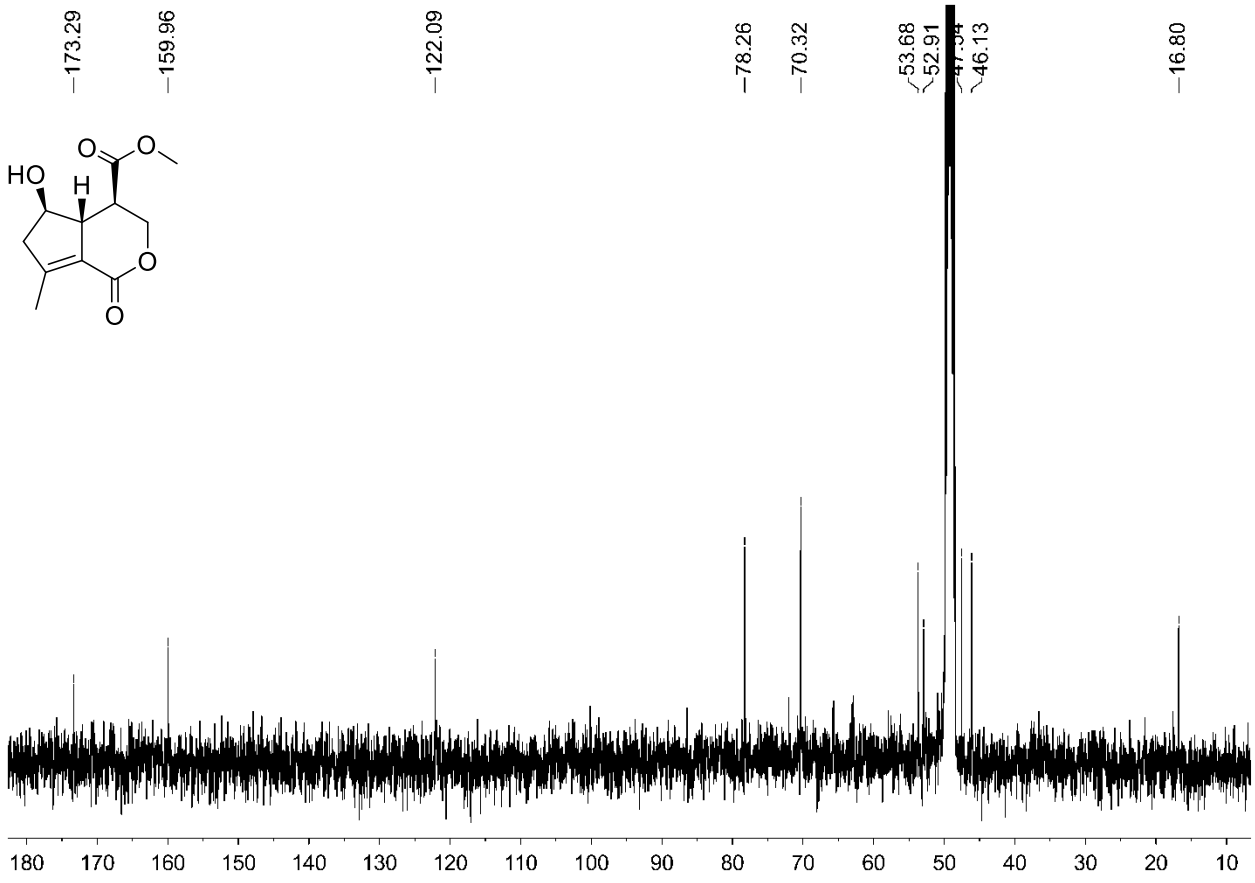

Figure S135. ^{13}C NMR (100 MHz, methanol-d_4) spectrum of compound **6a**

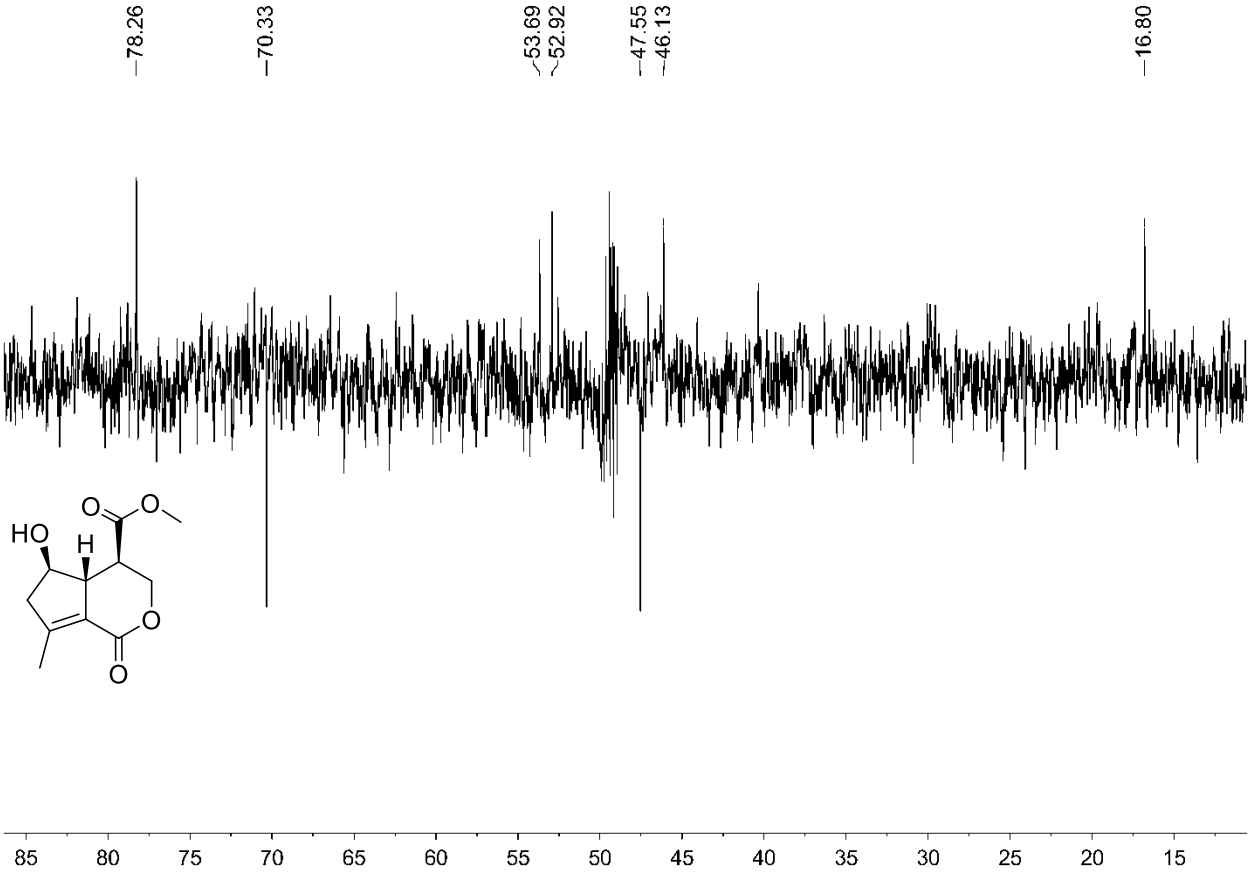

Figure S136. DEPT135 (100 MHz, methanol-d_4) spectrum of compound **6a**

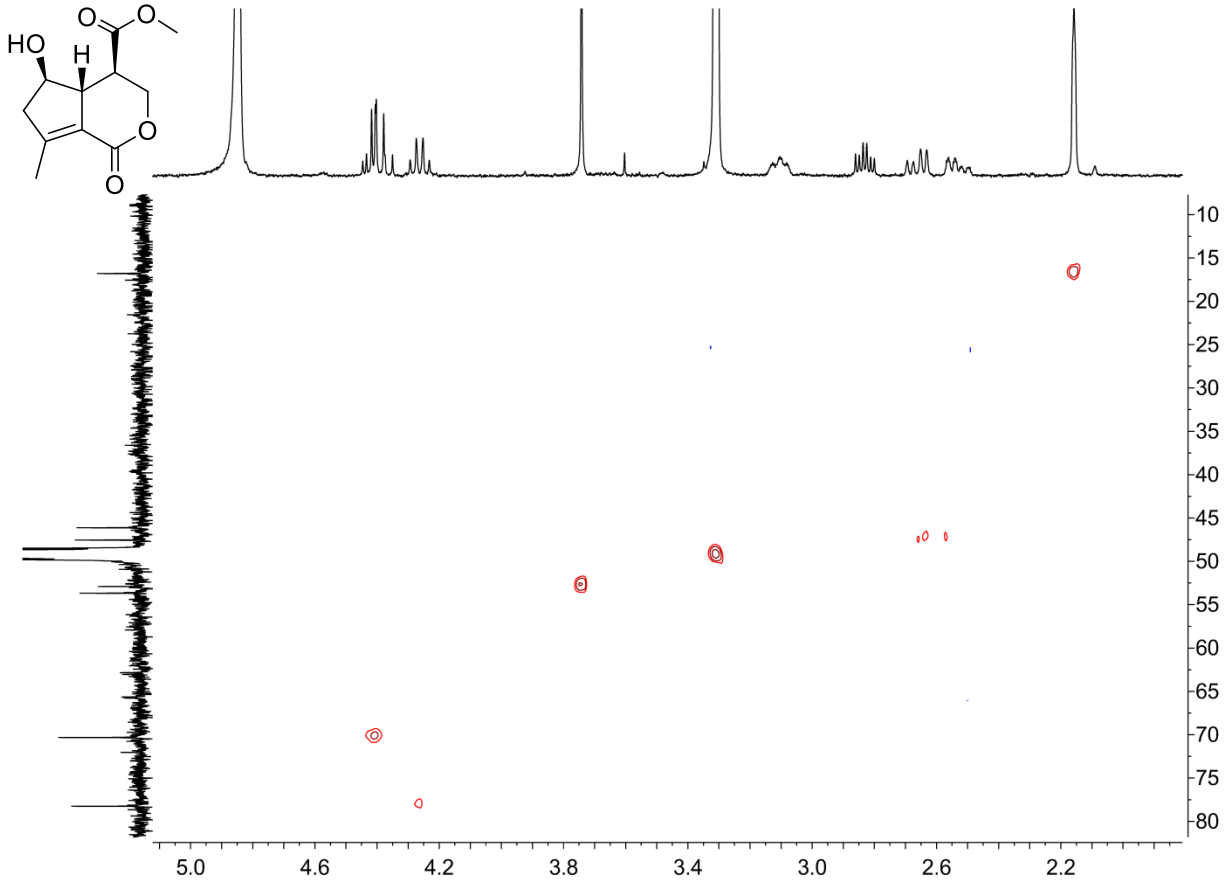

Figure S137. HSQC spectrum (methanol-d_4) of compound **6a** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

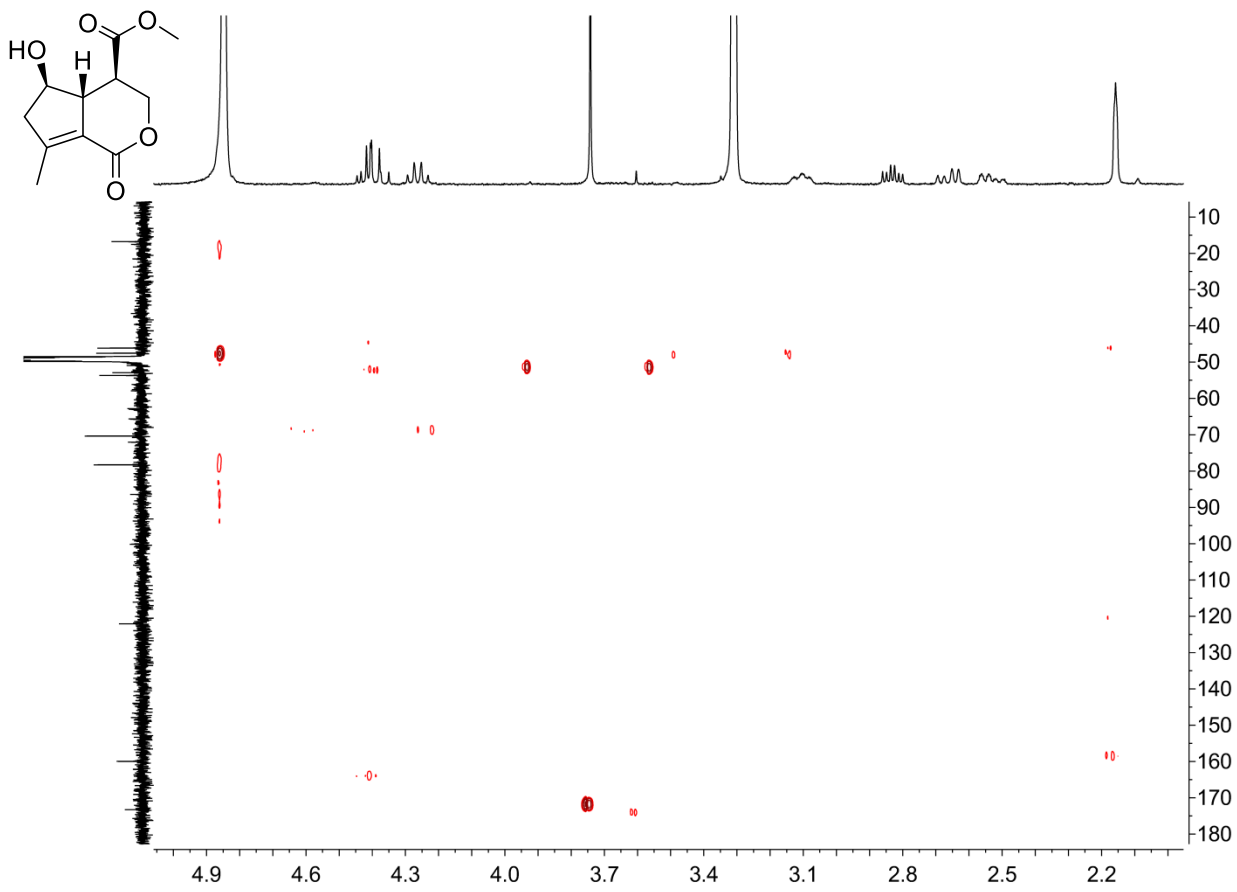

Figure S138. HMBC spectrum (methanol-d_4) of compound **6a** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

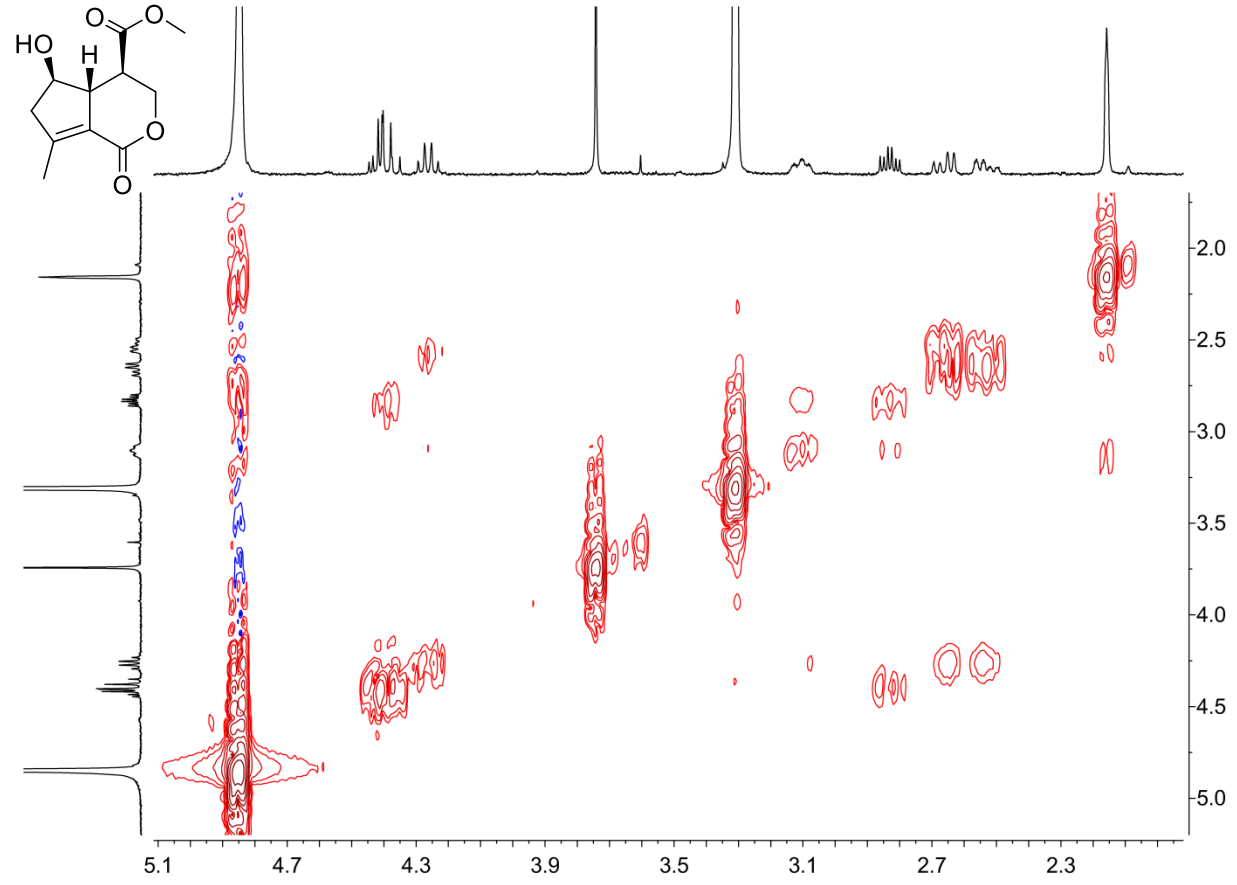

Figure S139. ^{1}H–^{1}H COSY spectrum (400 MHz, methanol-d_4) of compound **6a**

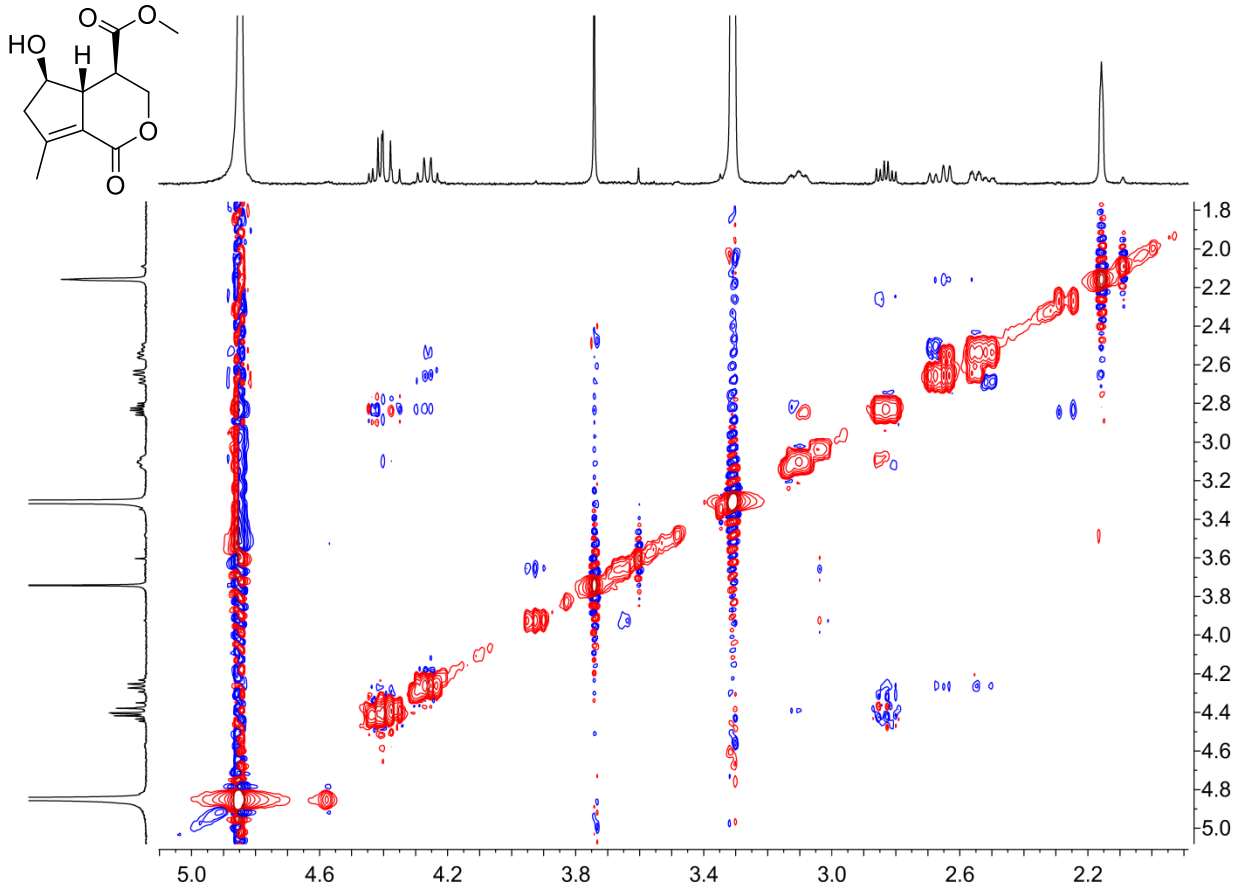

Figure S140. NOESY spectrum (400 MHz, methanol-d_4) of compound **6a**

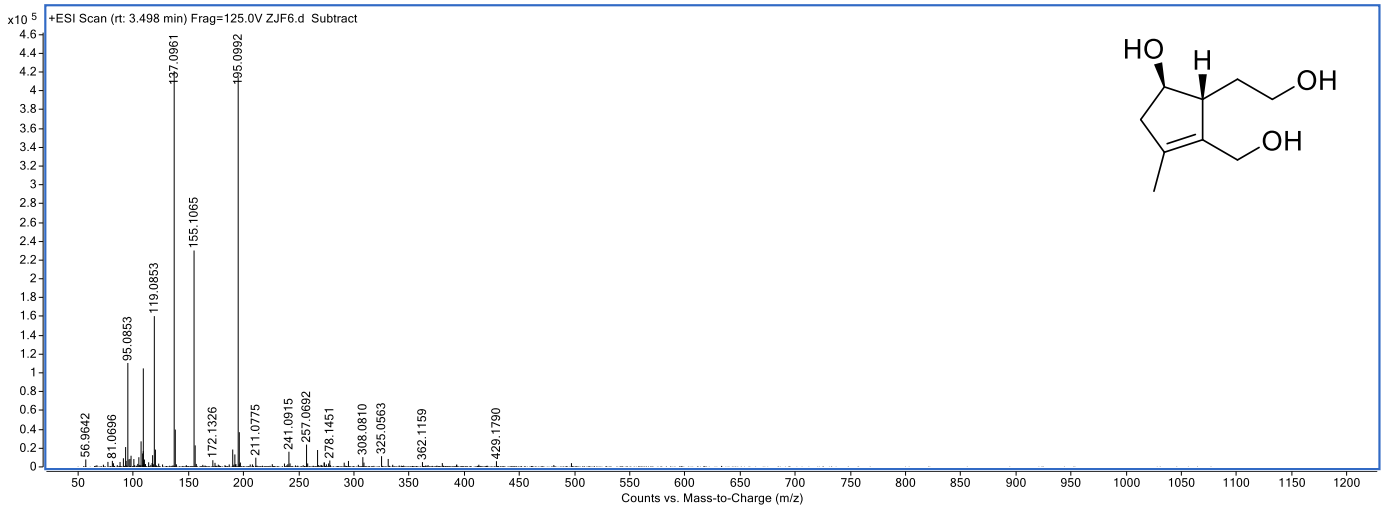

Figure S141. (+)-HR-ESI-MS spectrum of **7**

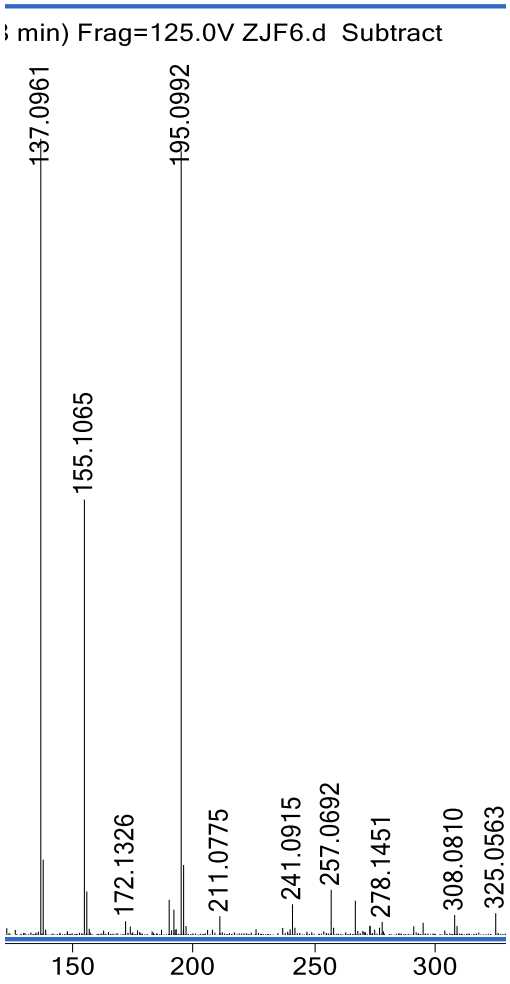

Figure S142. (+)-HR-ESI-MS spectrum of **7** (amplified)

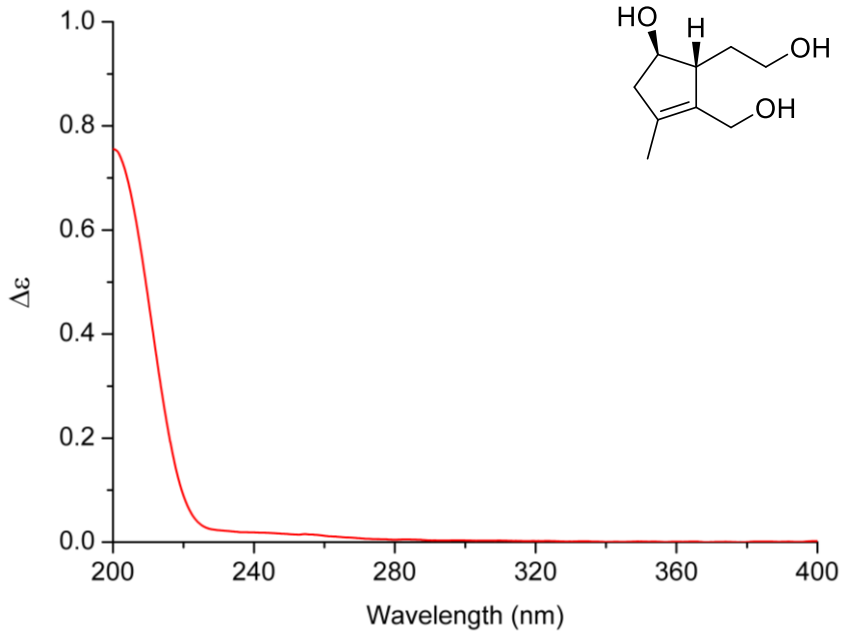

Figure S143. UV spectrum of compound **7**

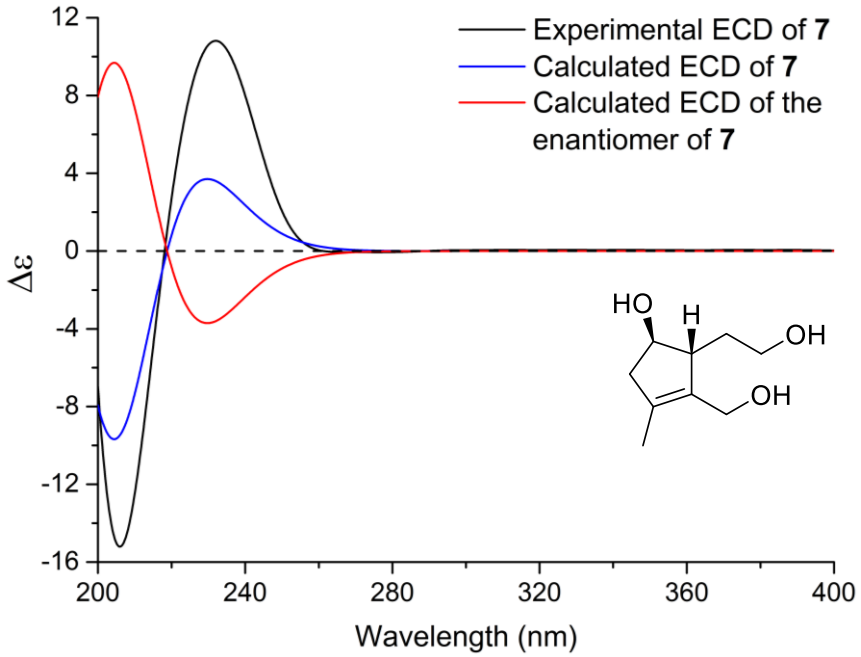

Figure S144. Experimental ECD spectrum of **7** and the calculated ECD spectra for **7** and its enantiomer.

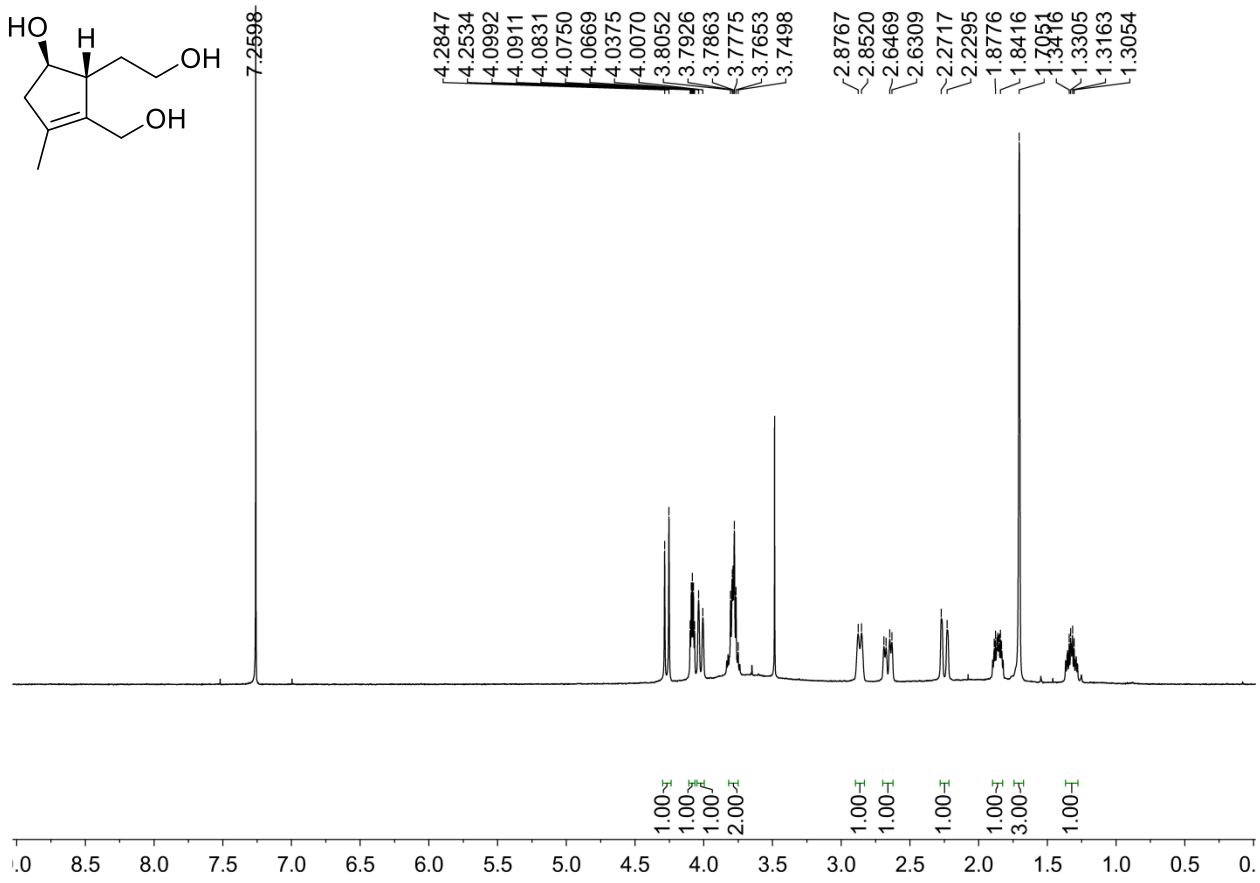

Figure S145. ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of compound **7**

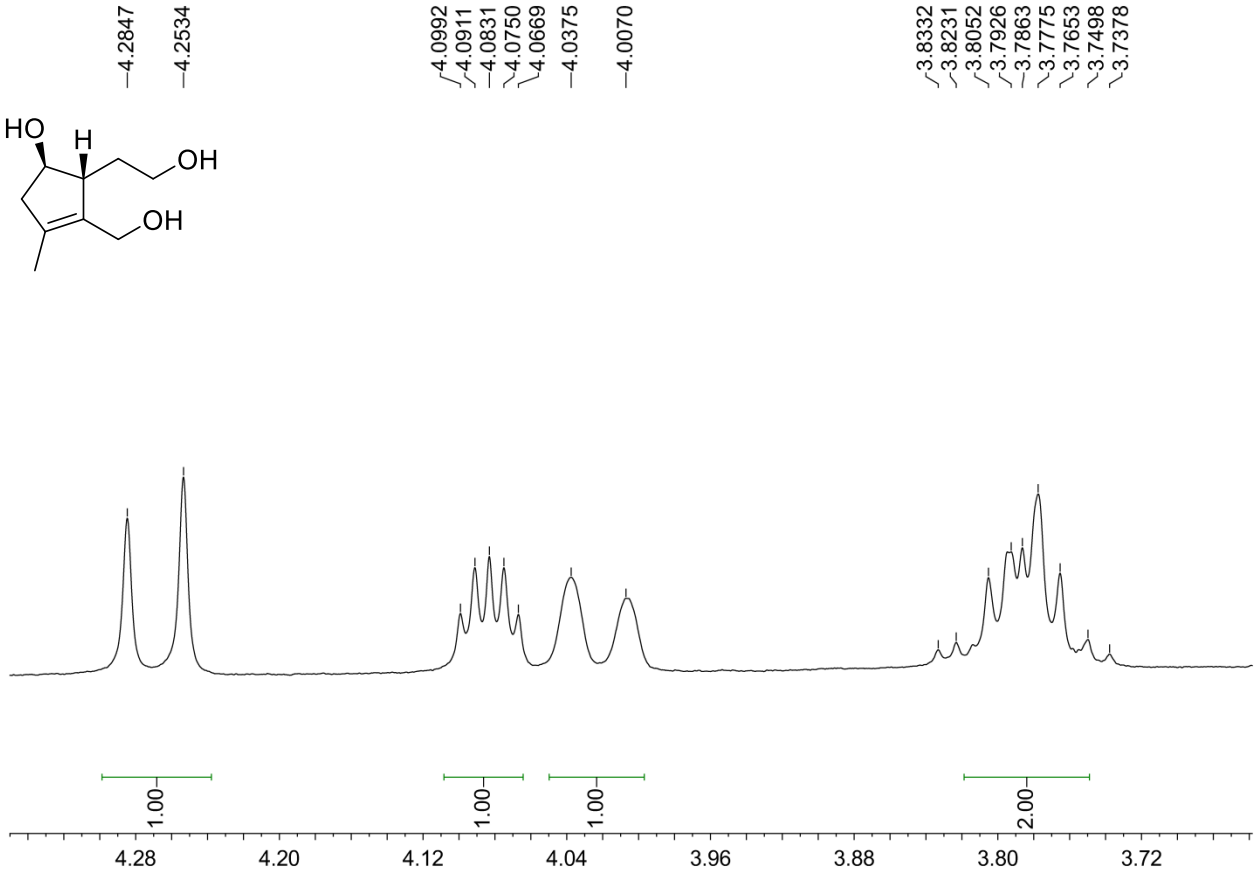

Figure S146. [1]H NMR (400 MHz, chloroform-*d*) spectrum of compound **7** (amplified)

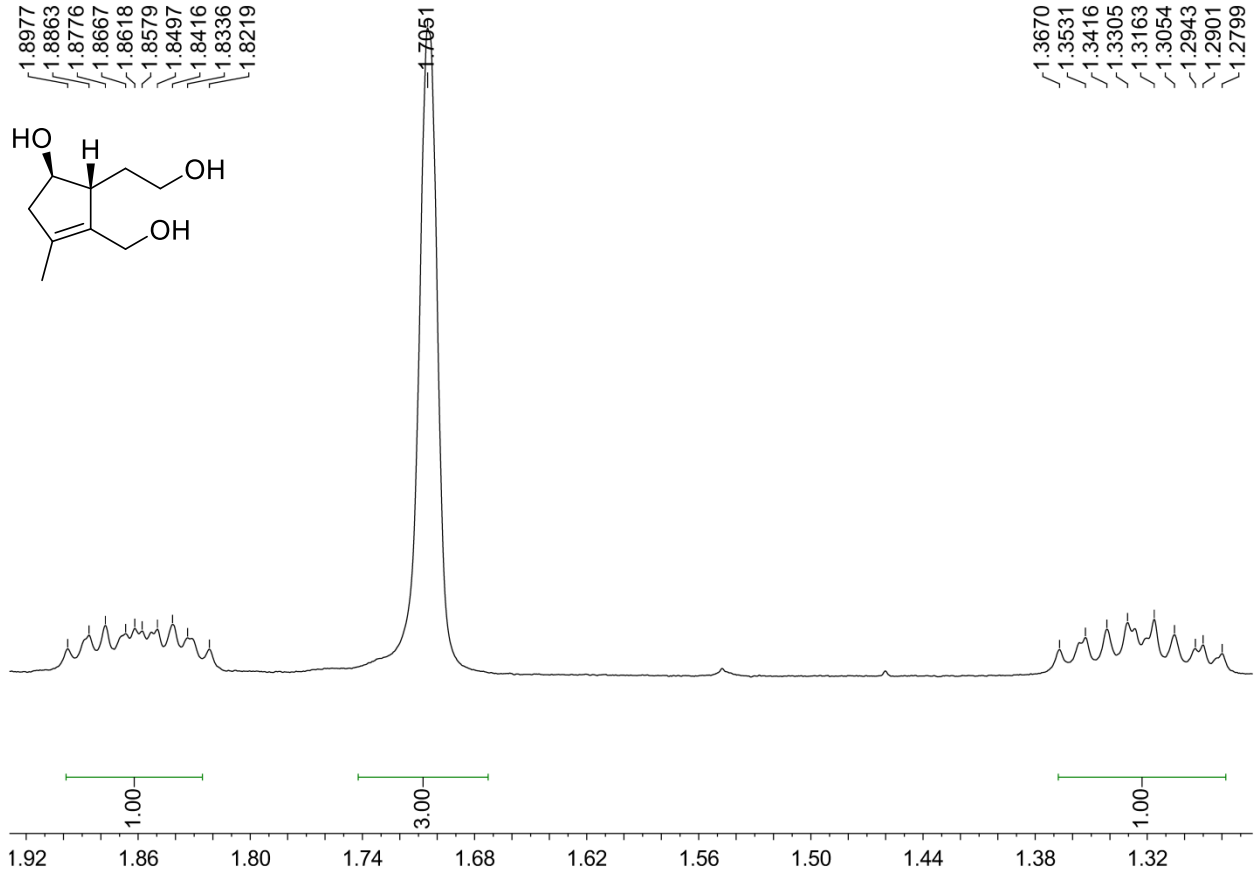

Figure S147. [1]H NMR (400 MHz, chloroform-*d*) spectrum of compound **7** (amplified)

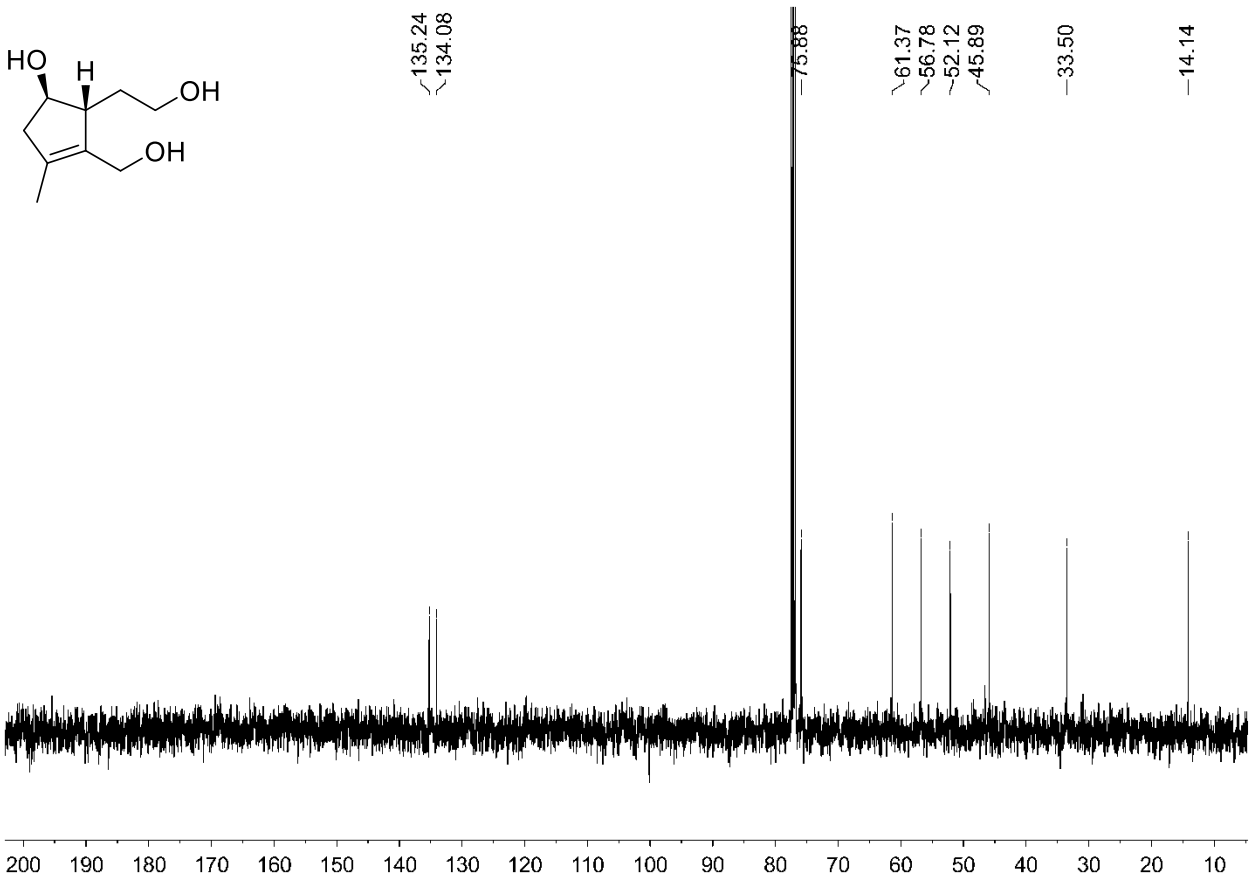

Figure S148. ^{13}C NMR (100 MHz, chloroform-*d*) spectrum of compound **7**

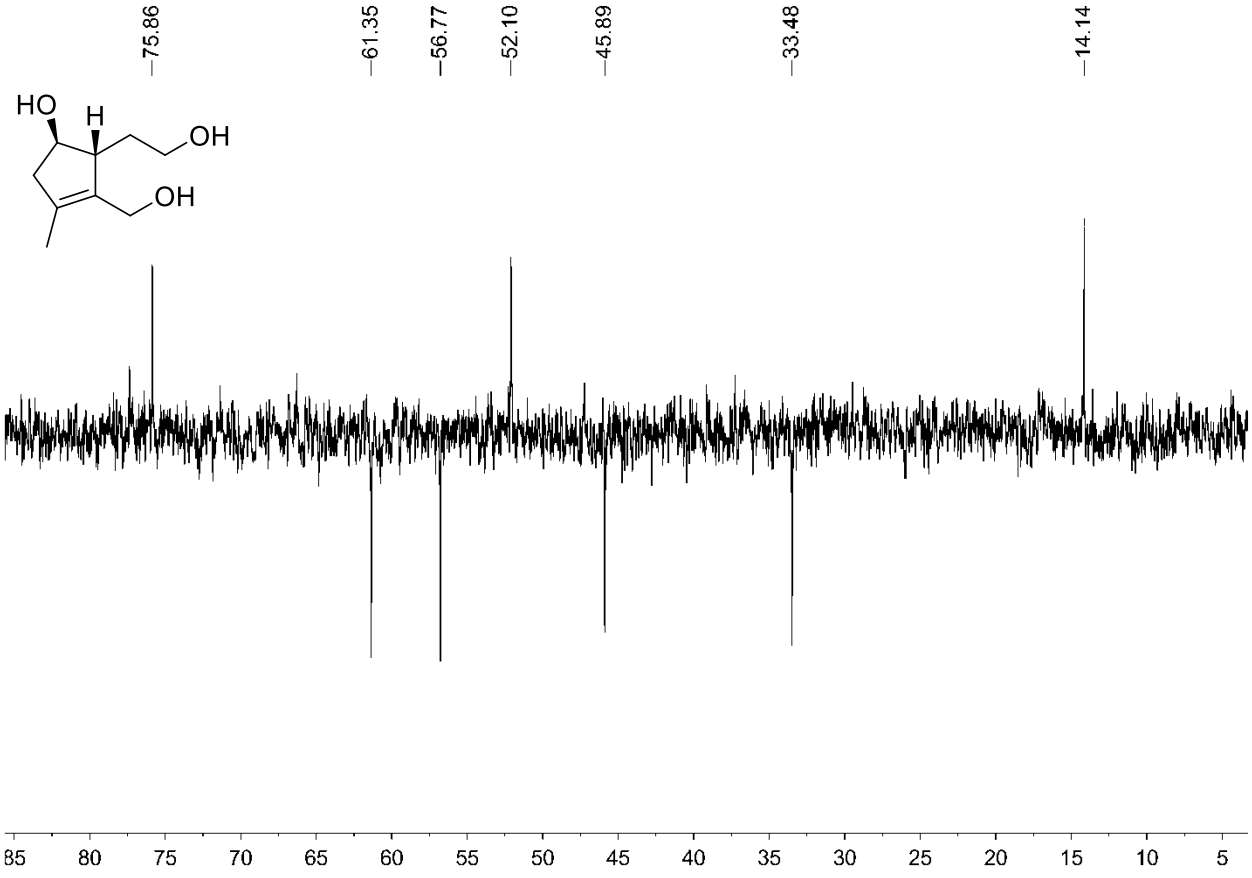

Figure S149. DEPT135 (100 MHz, chloroform-*d*) spectrum of compound **7**

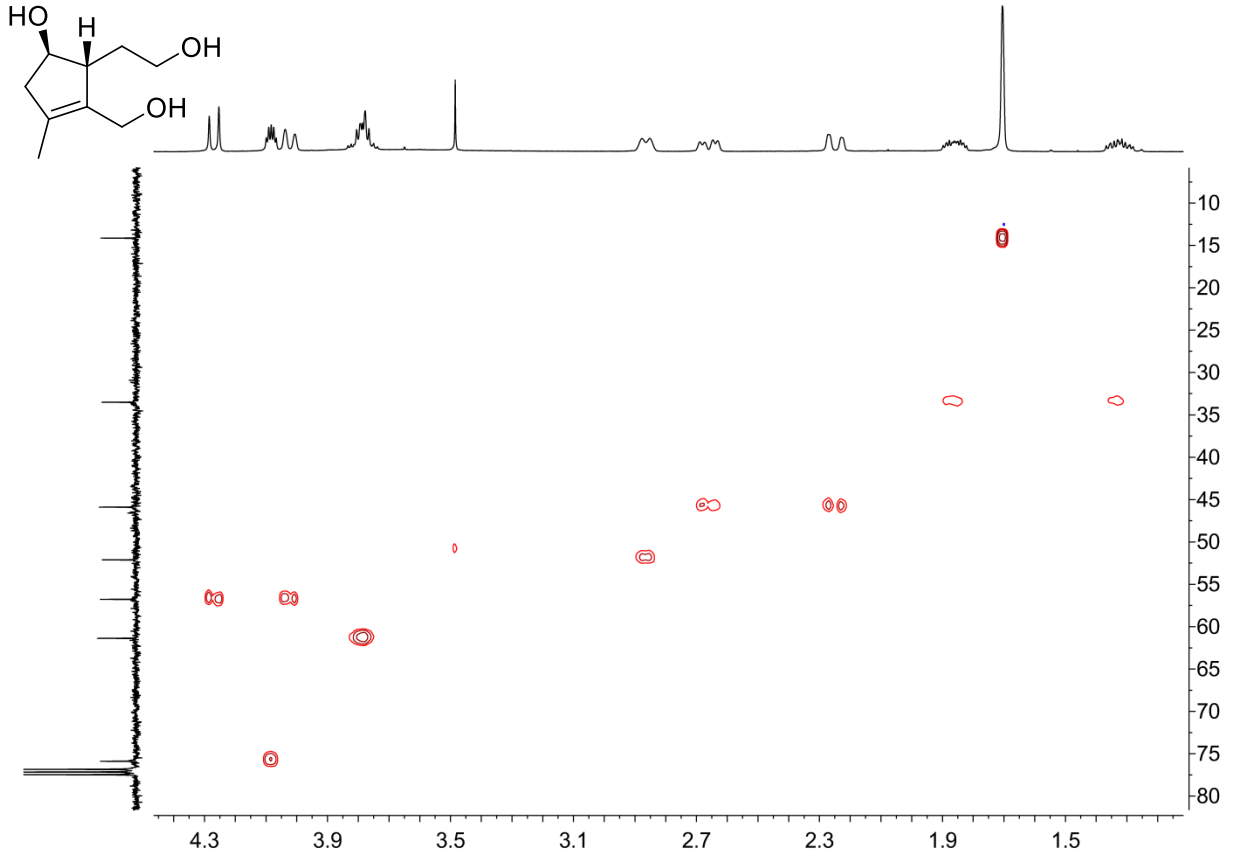

Figure S150. HSQC spectrum (chloroform-*d*) of compound **7** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

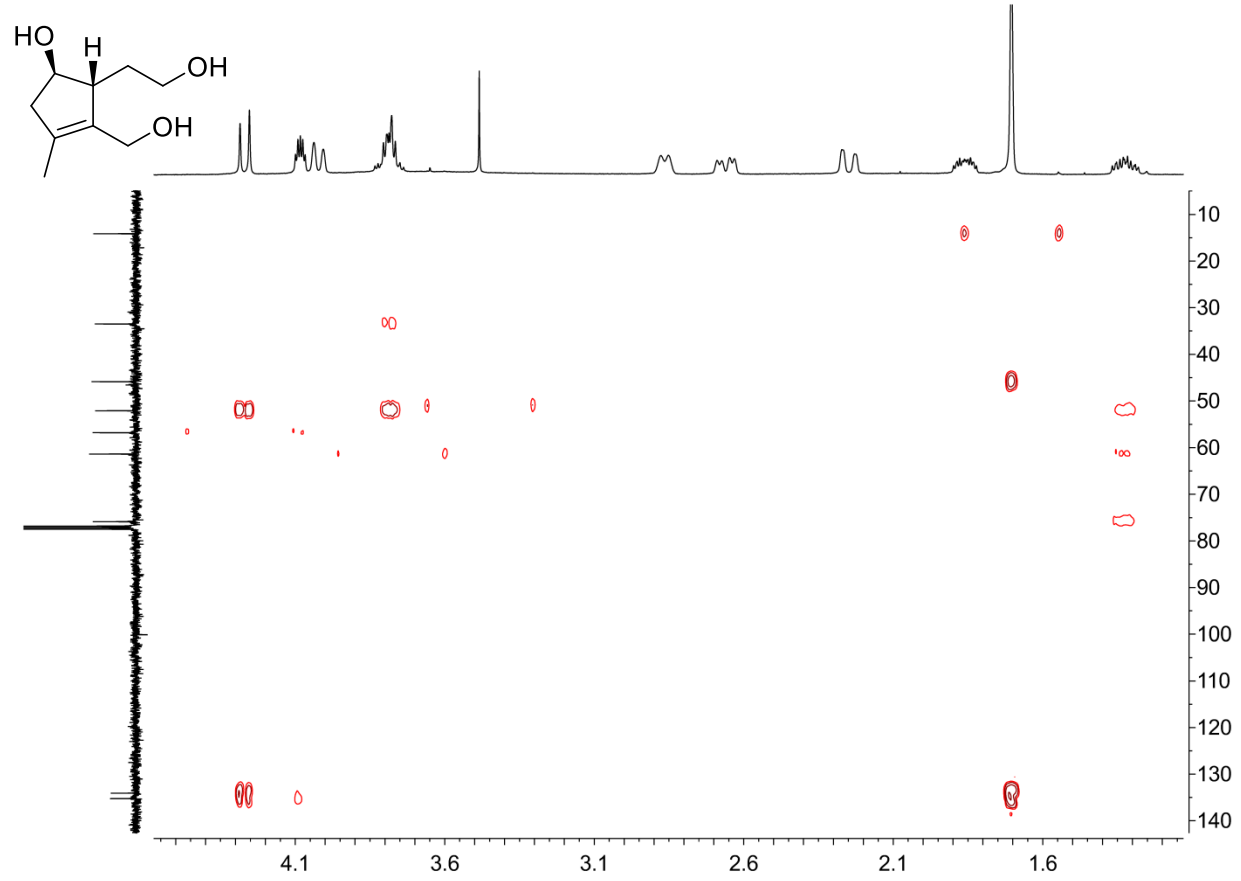

Figure S151. HMBC spectrum (chloroform-*d*) of compound **7** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

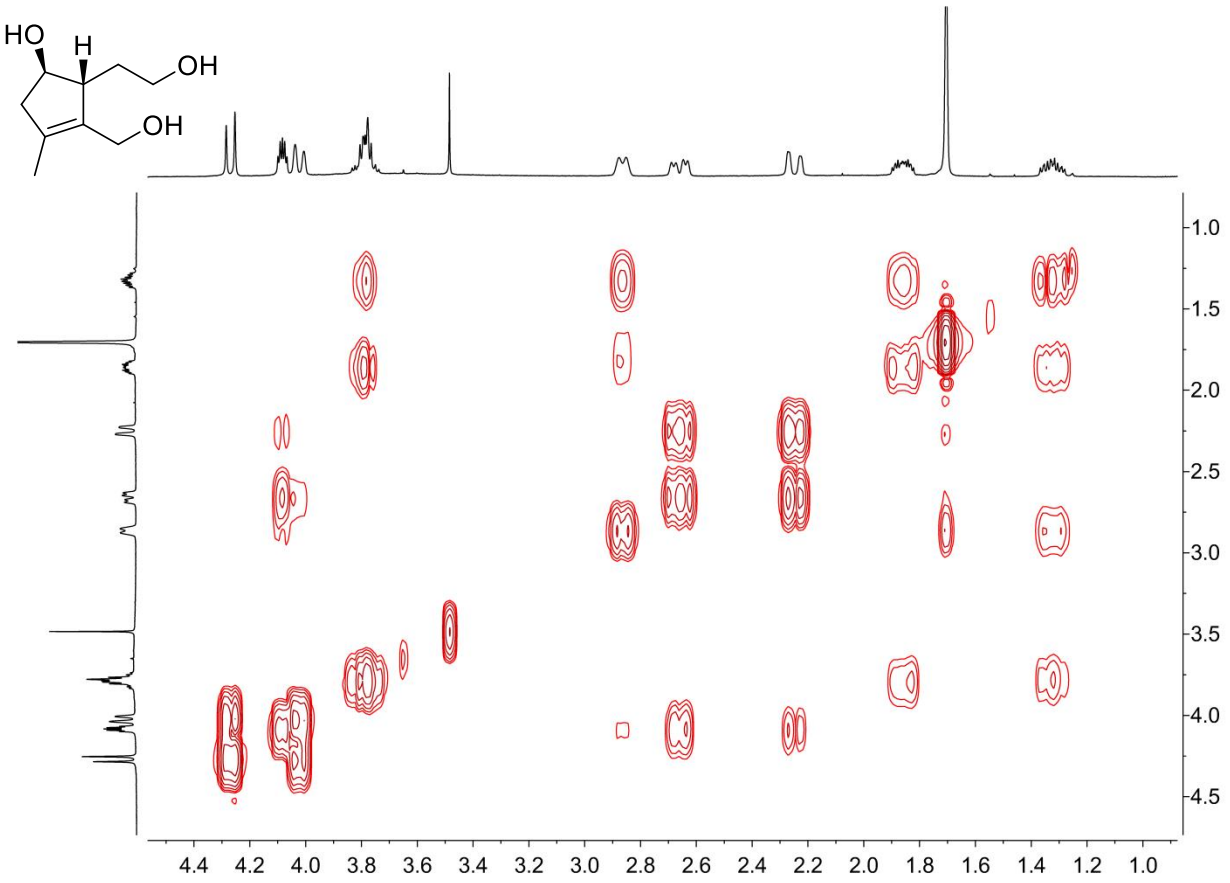

Figure S152. $^{1}H–^{1}H$ COSY spectrum (400 MHz, chloroform-*d*) of compound **7**

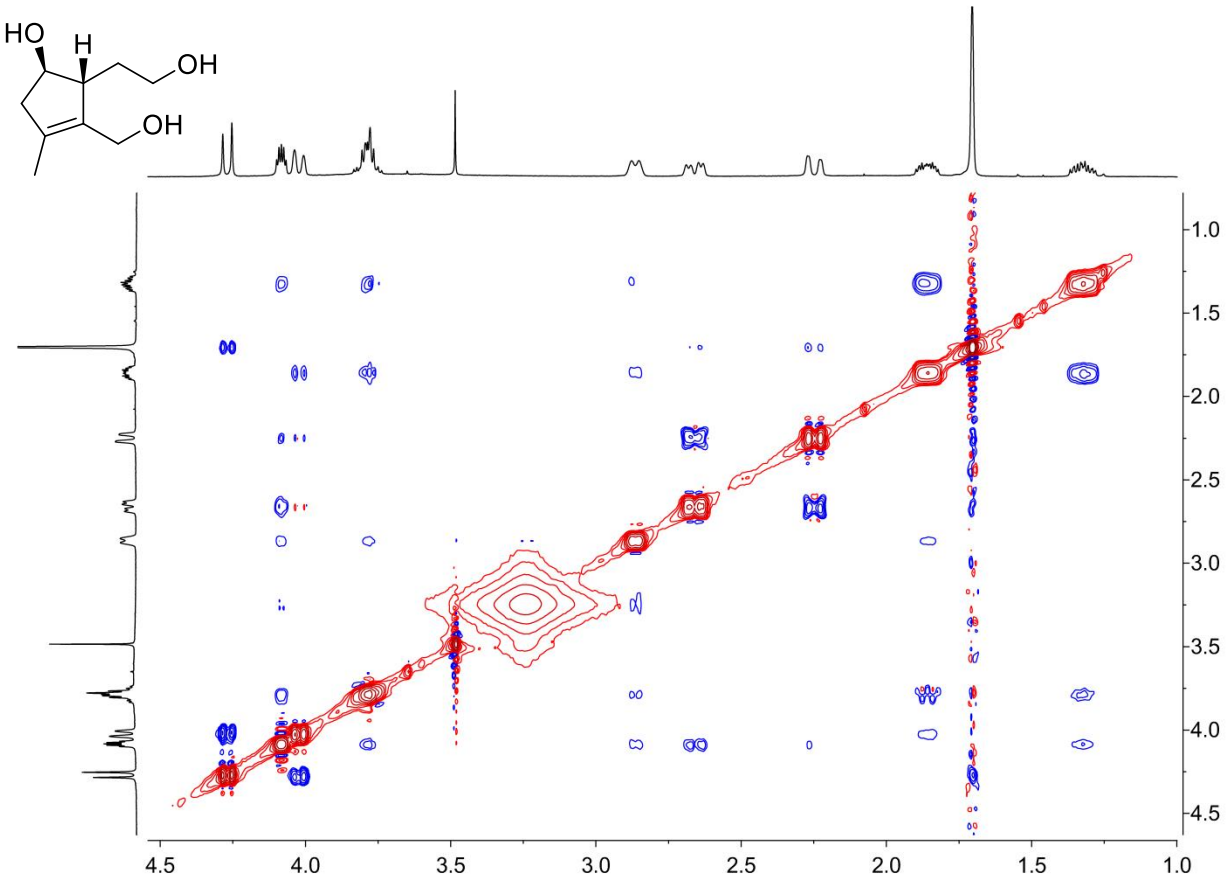

Figure S153. NOESY spectrum (400 MHz, chloroform-*d*) of compound **7**

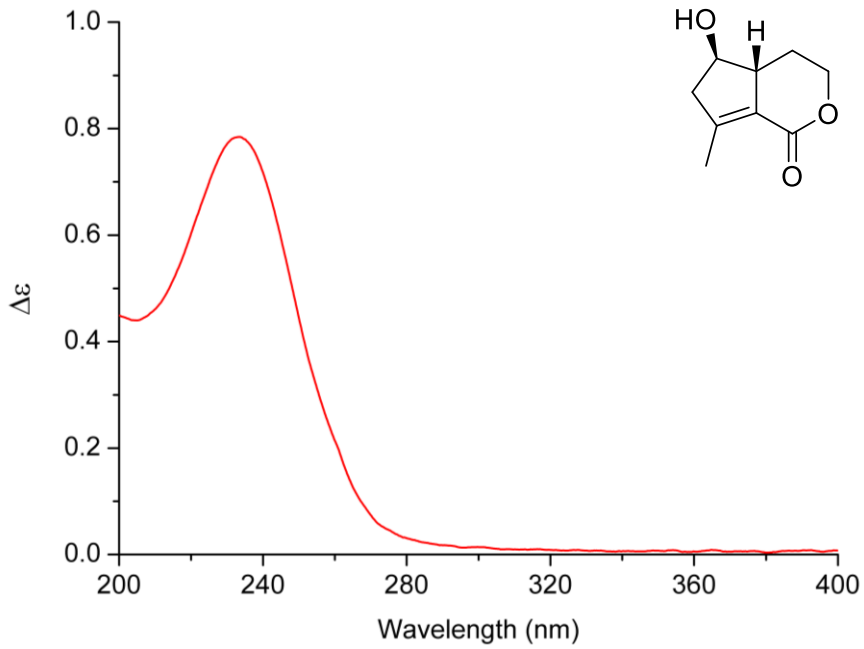

Figure S154. UV spectrum of compound **8**

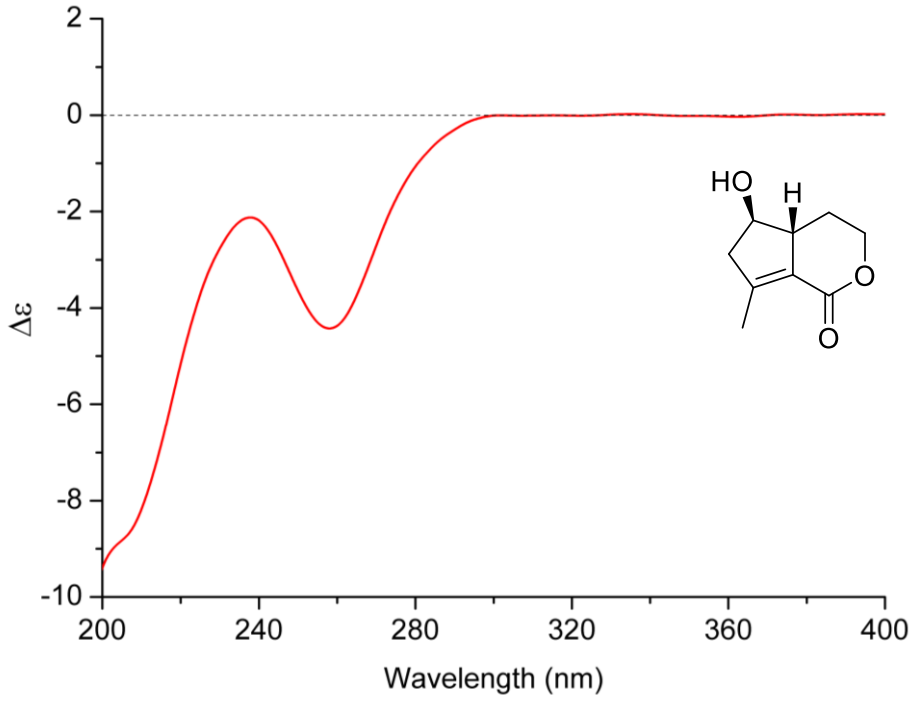

Figure S155. Experimental ECD spectrum of compound **8**

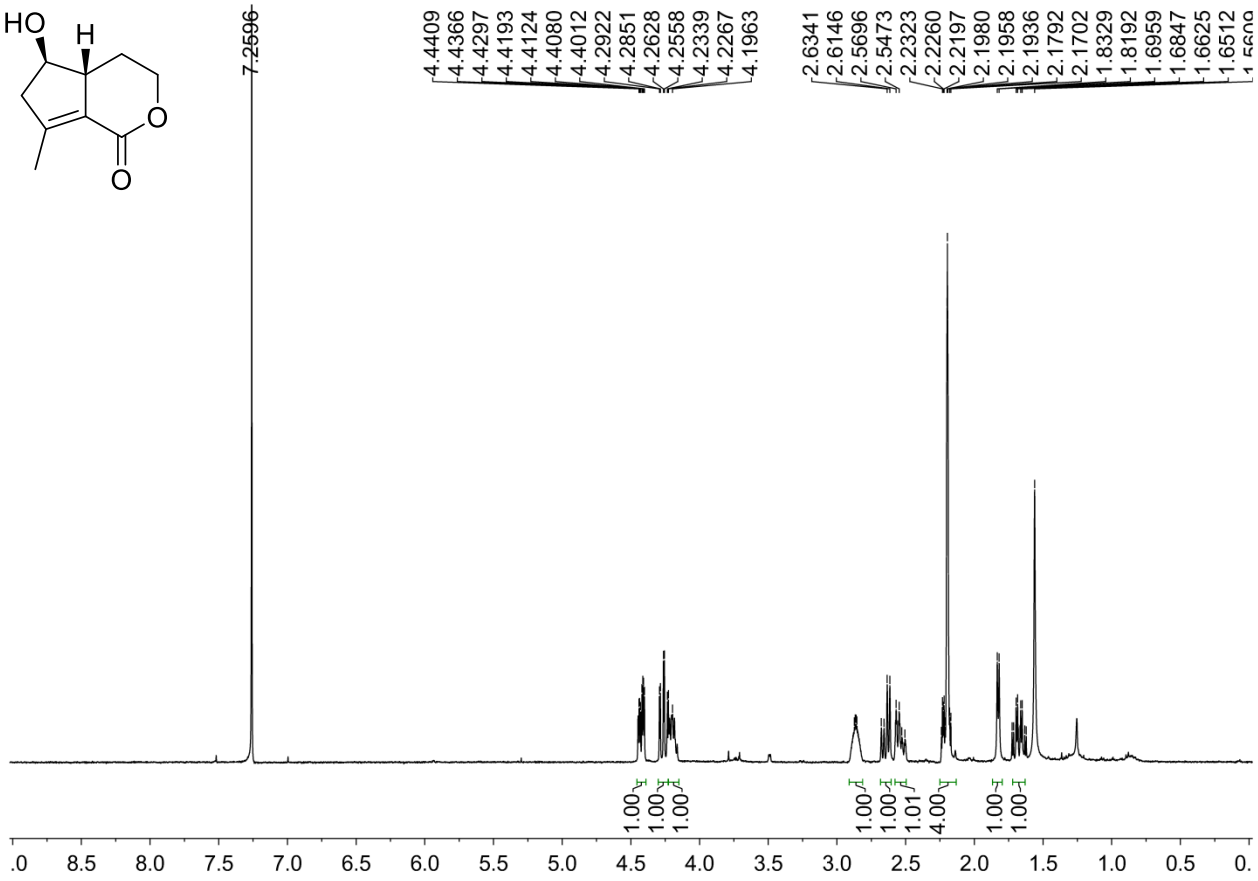

Figure S156. ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of compound **8**

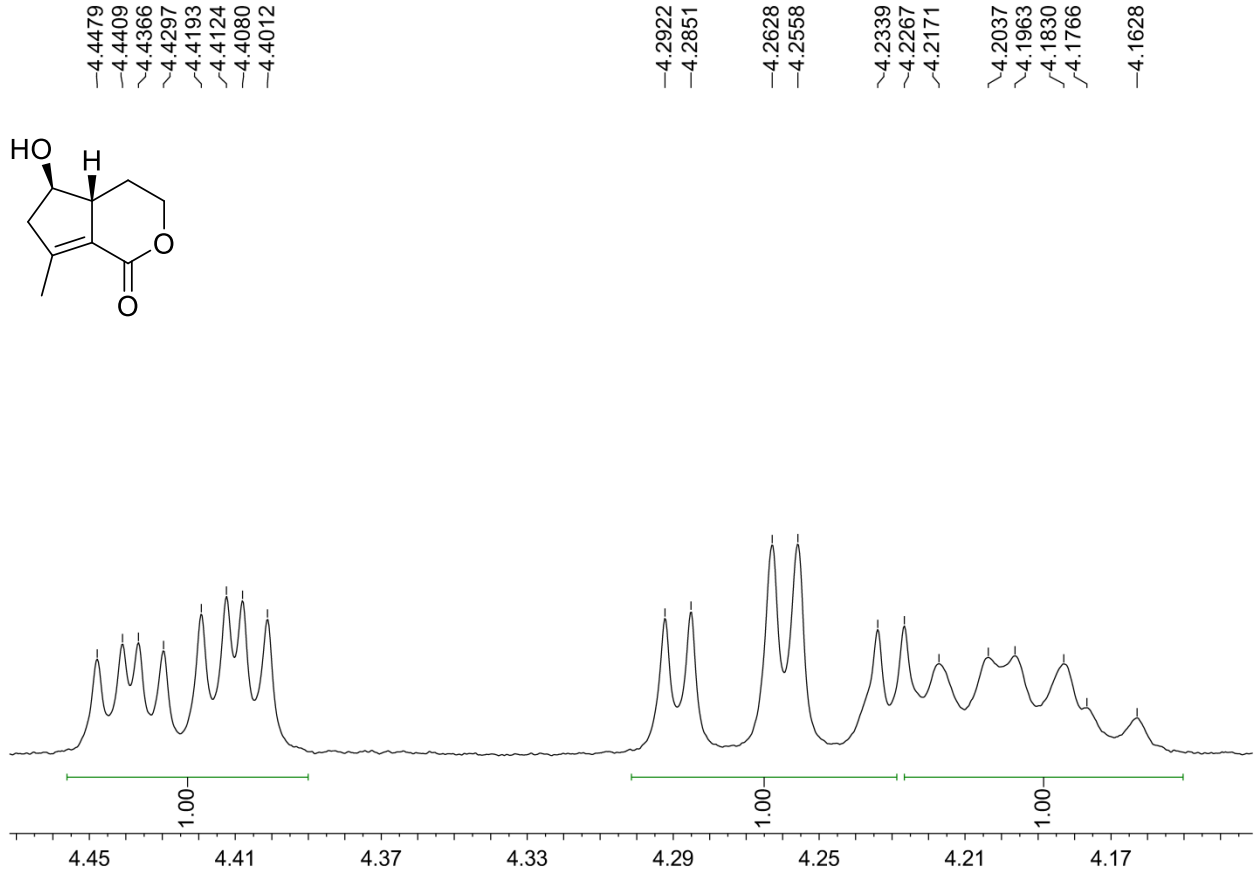

Figure S157. ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of compound **8** (amplified)

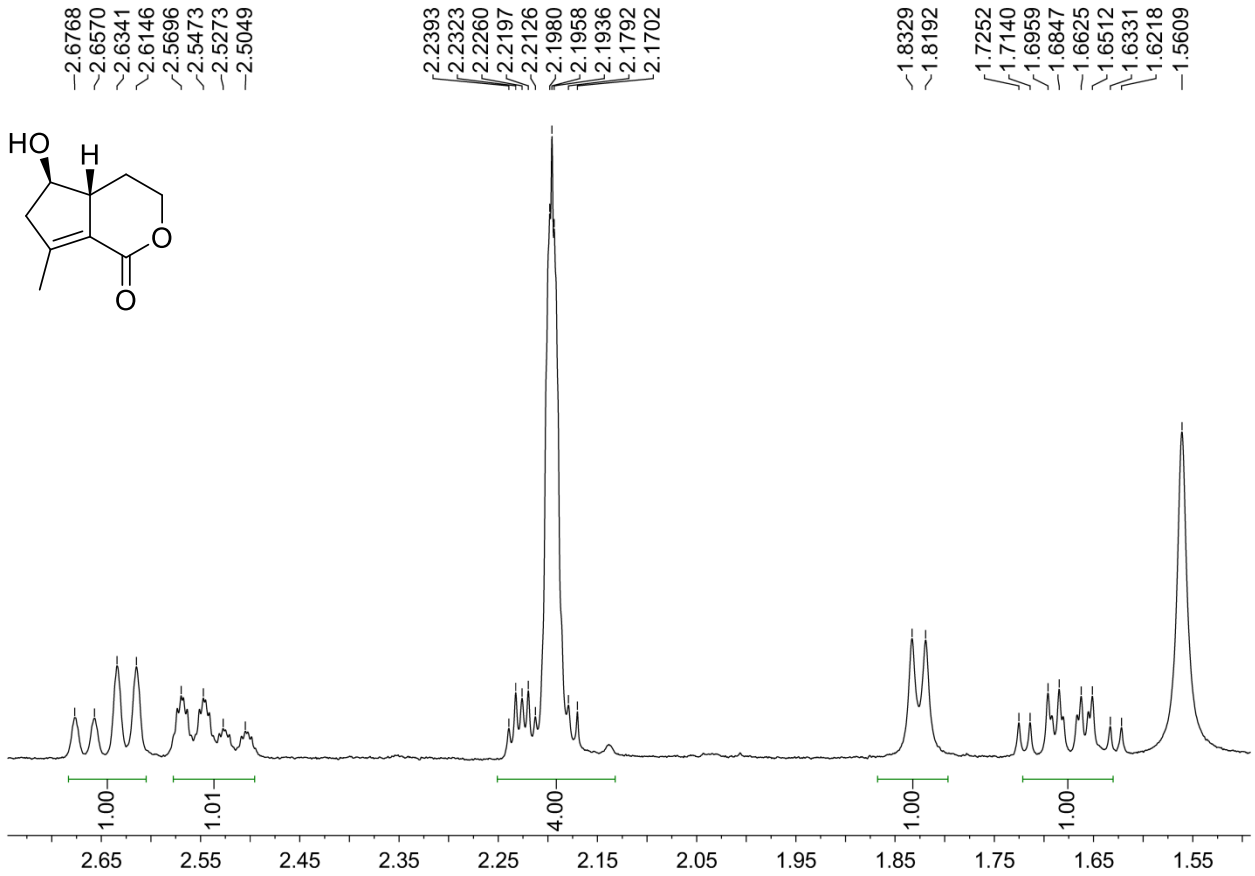

Figure S158. ^{1}H NMR (400 MHz, chloroform-*d*) spectrum of compound **8** (amplified)

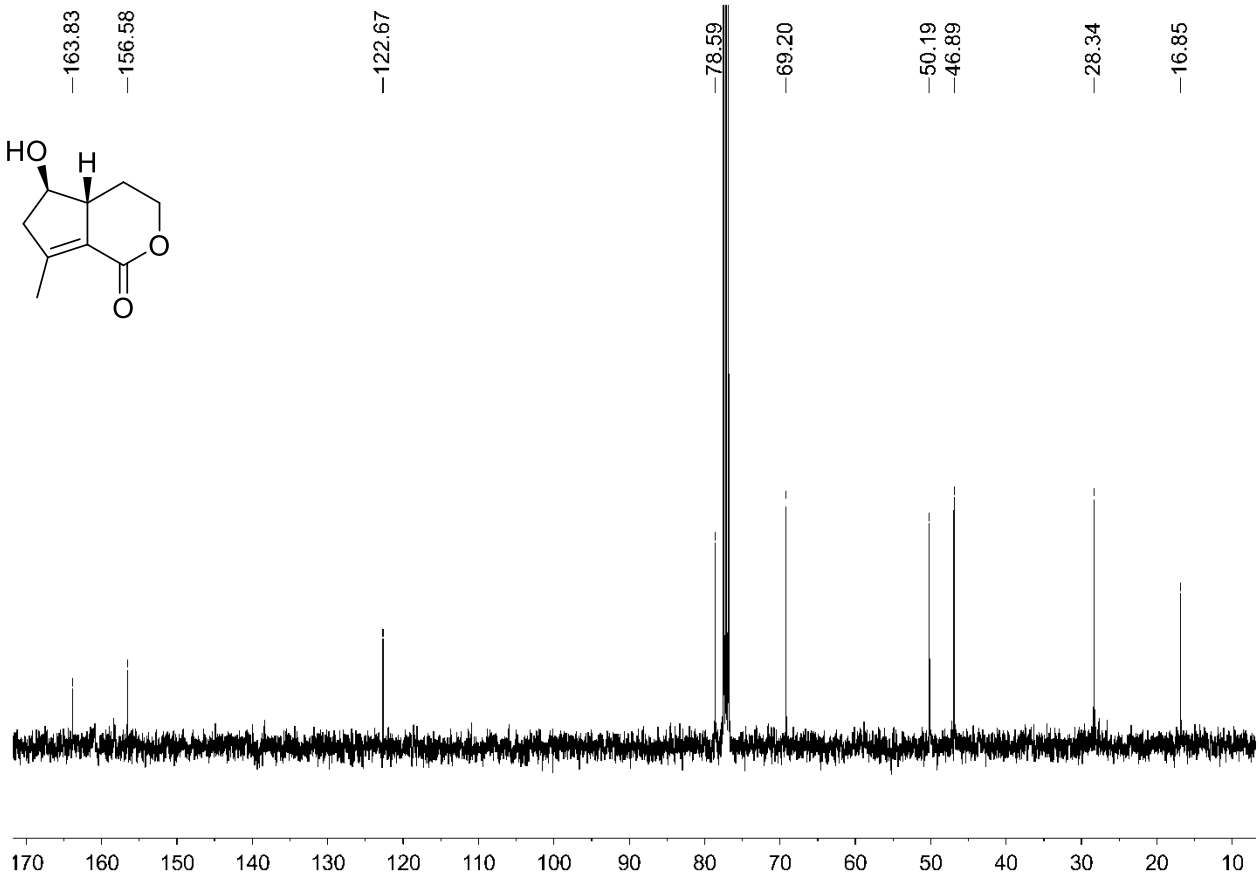

Figure S159. ^{13}C NMR (100 MHz, chloroform-*d*) spectrum of compound **8**

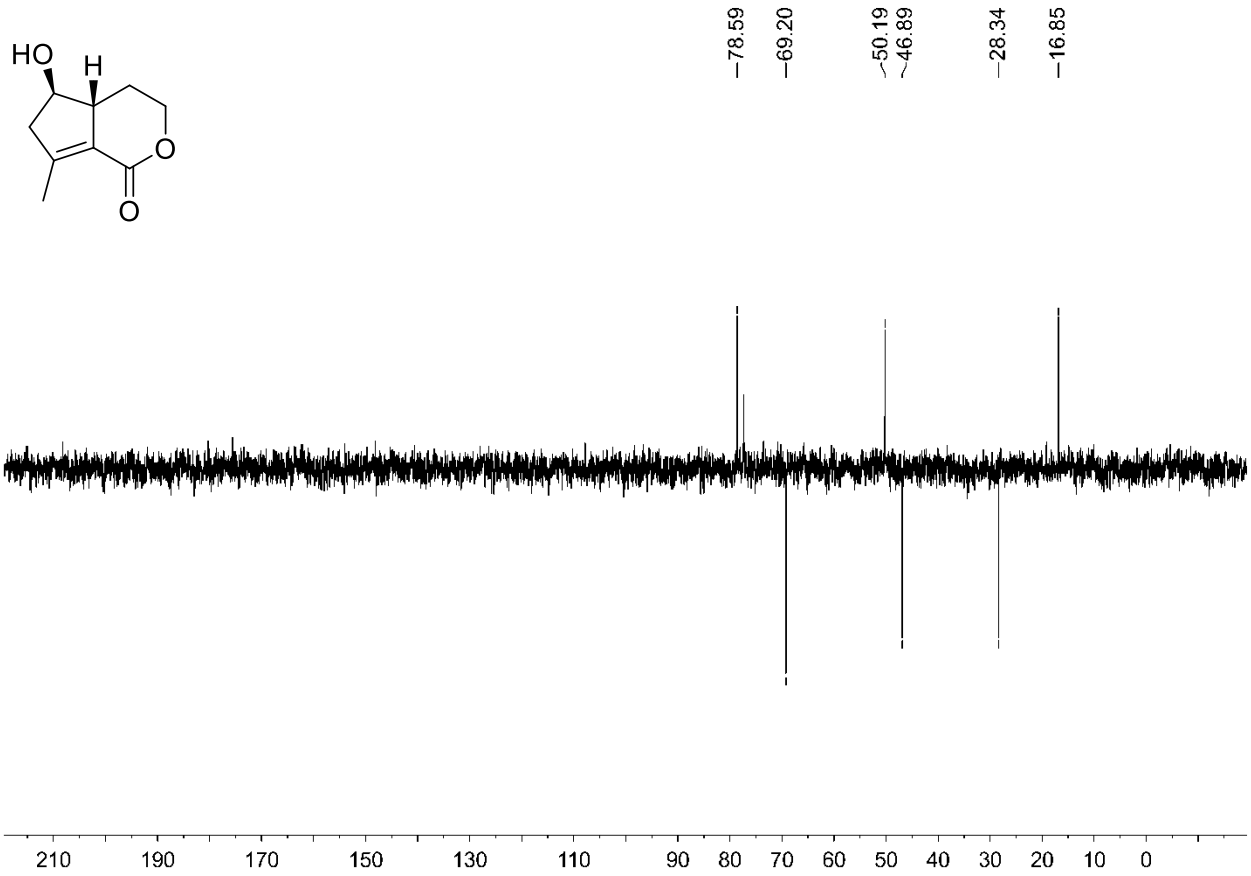

Figure S160. DEPT135 (100 MHz, chloroform-*d*) spectrum of compound **8**

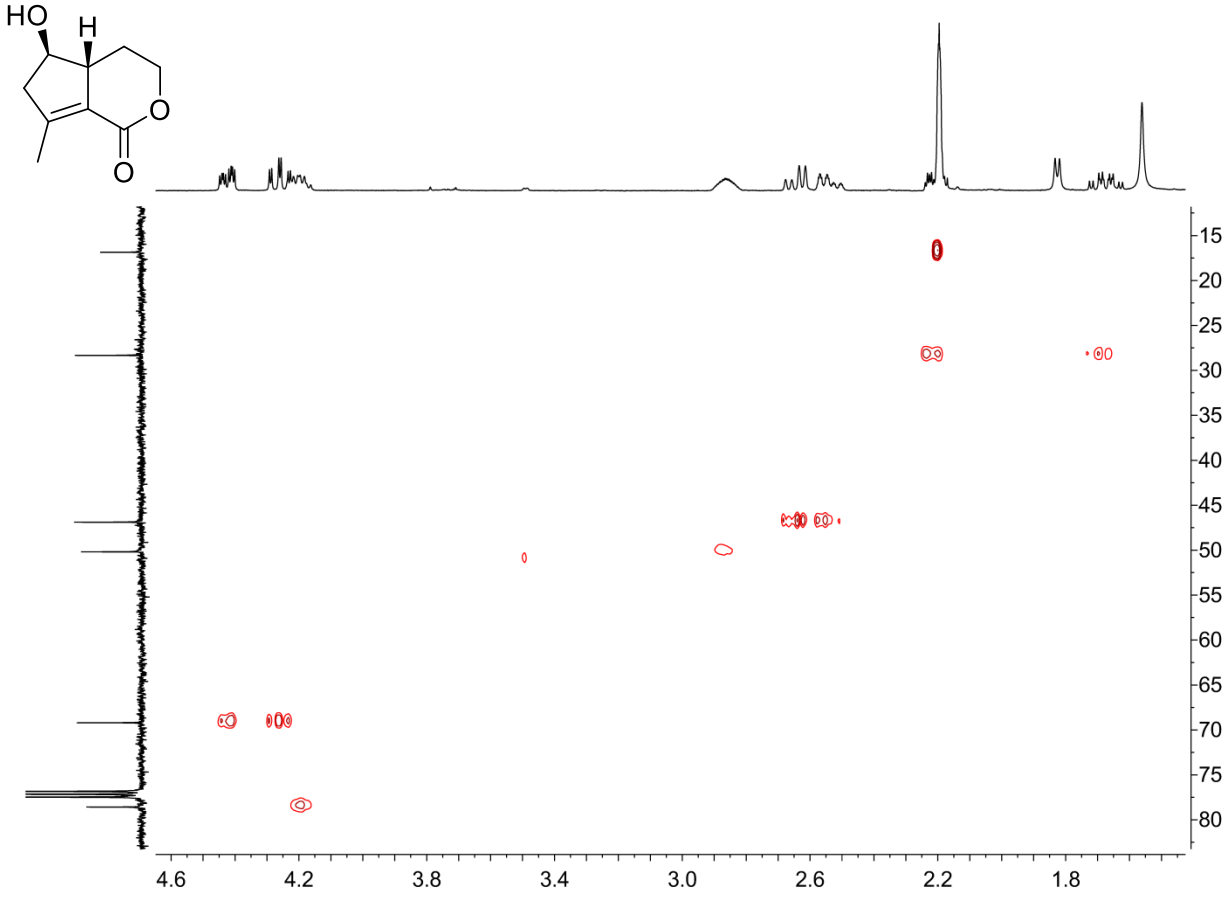

Figure S161. HSQC spectrum (chloroform-*d*) of compound **8** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

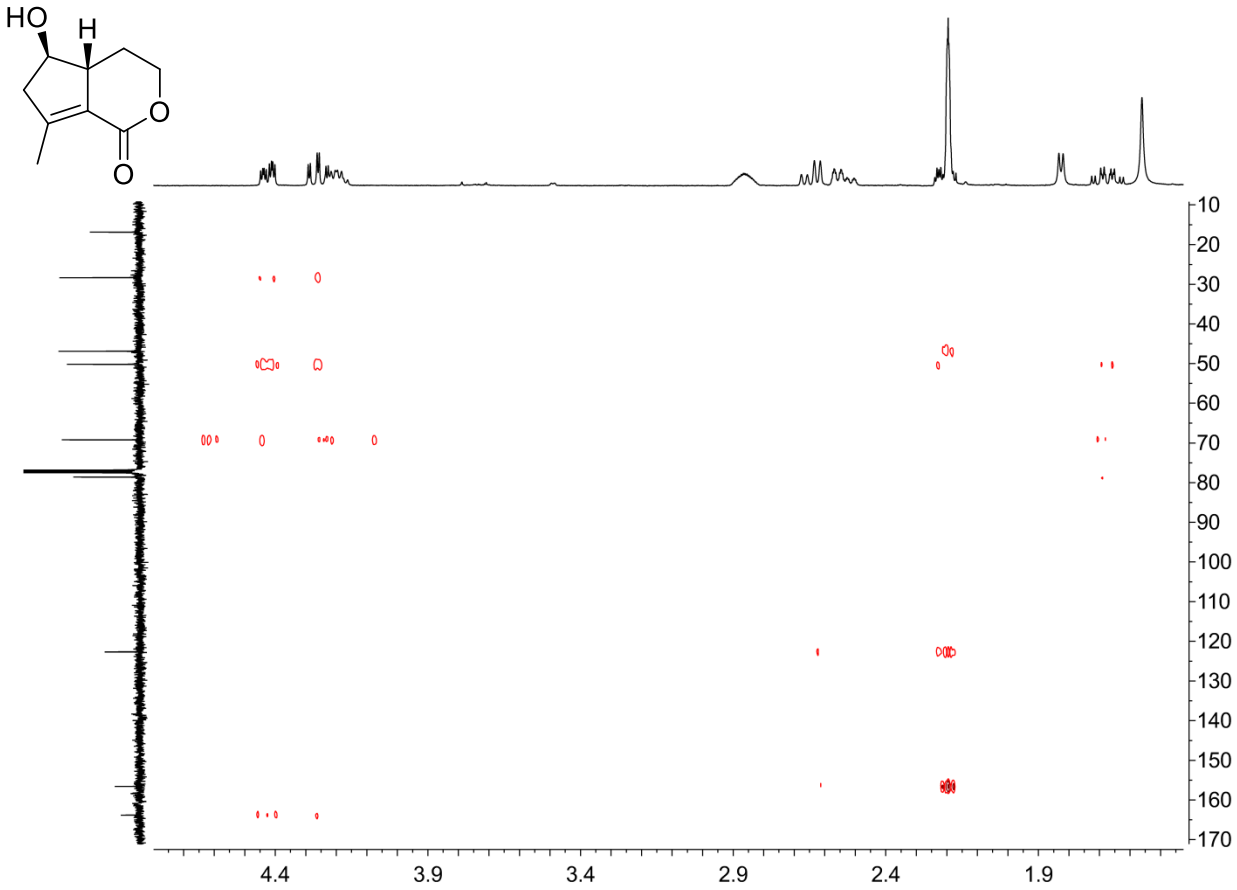

Figure S162. HMBC spectrum (chloroform-*d*) of compound **8** (^{1}H: 400 MHz, ^{13}C: 100 MHz)

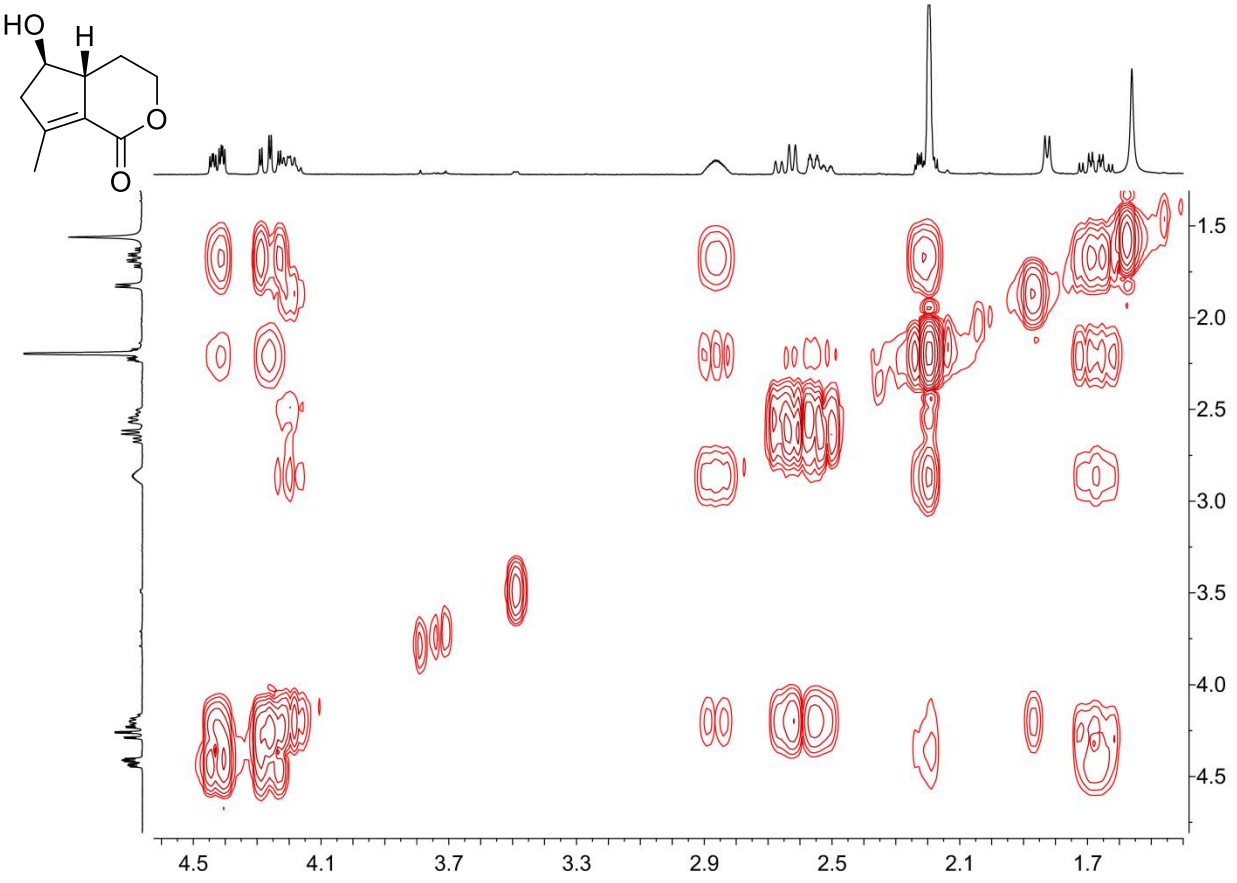

Figure S163. ^{1}H–^{1}H COSY spectrum (400 MHz, chloroform-*d*) of compound **8**

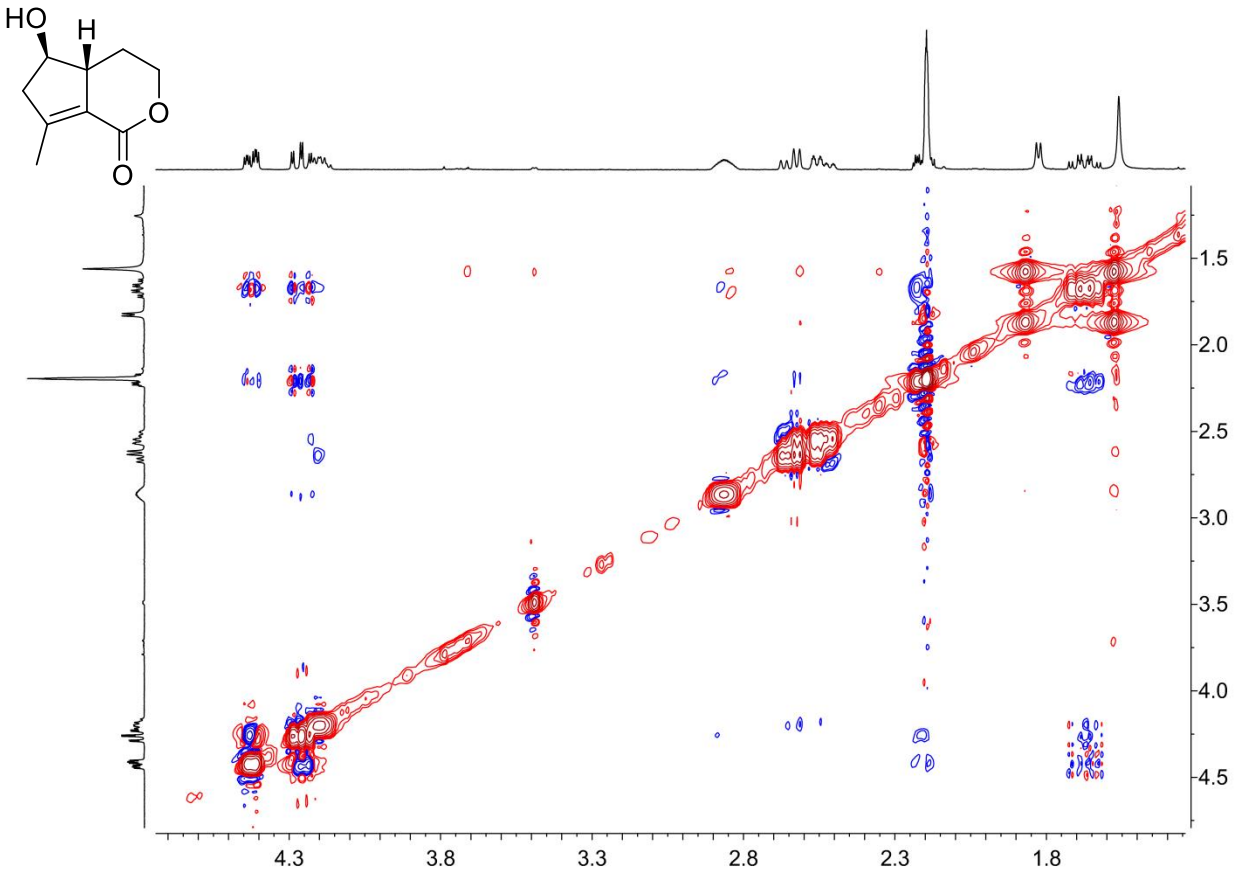

Figure S164. NOESY spectrum (400 MHz, chloroform-*d*) of compound **8**

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