

## Supplementary Materials

# Boswellianols A–I, Structurally Diverse Diterpenoids from the Oleo-gum Resin of *Boswellia carterii* and Their TGF- $\beta$ Inhibition Activity

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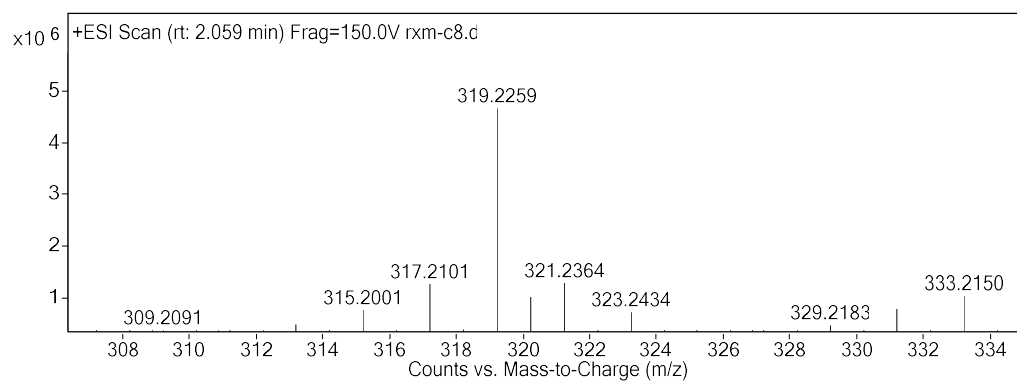
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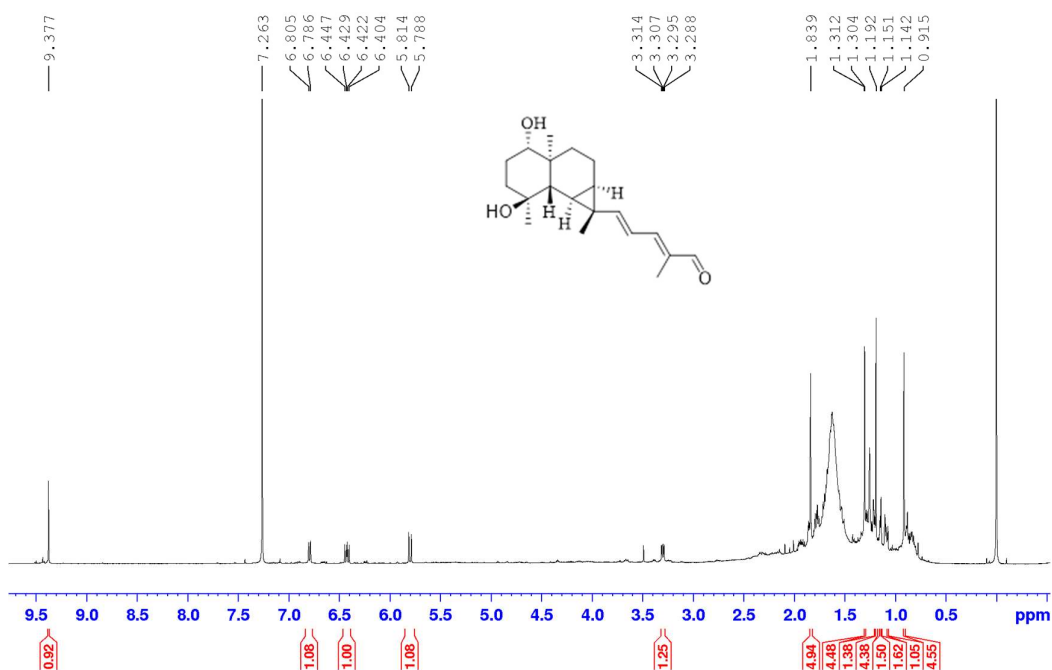
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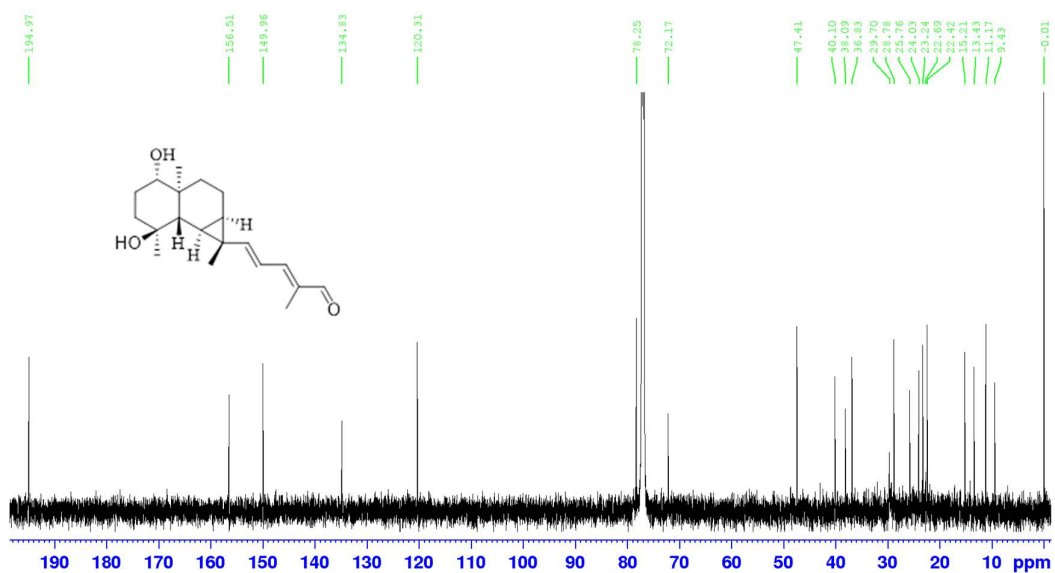


Formular	Score	Mass	Mass (MGF)	m/z (Calc)	Diff (ppm)	Ion Formular	m/z
C <sub>20</sub> H <sub>30</sub> O <sub>3</sub>	99.84	318.2191	319.2268	319.2268	1.17	C <sub>20</sub> H <sub>31</sub> O <sub>3</sub>	319.2259

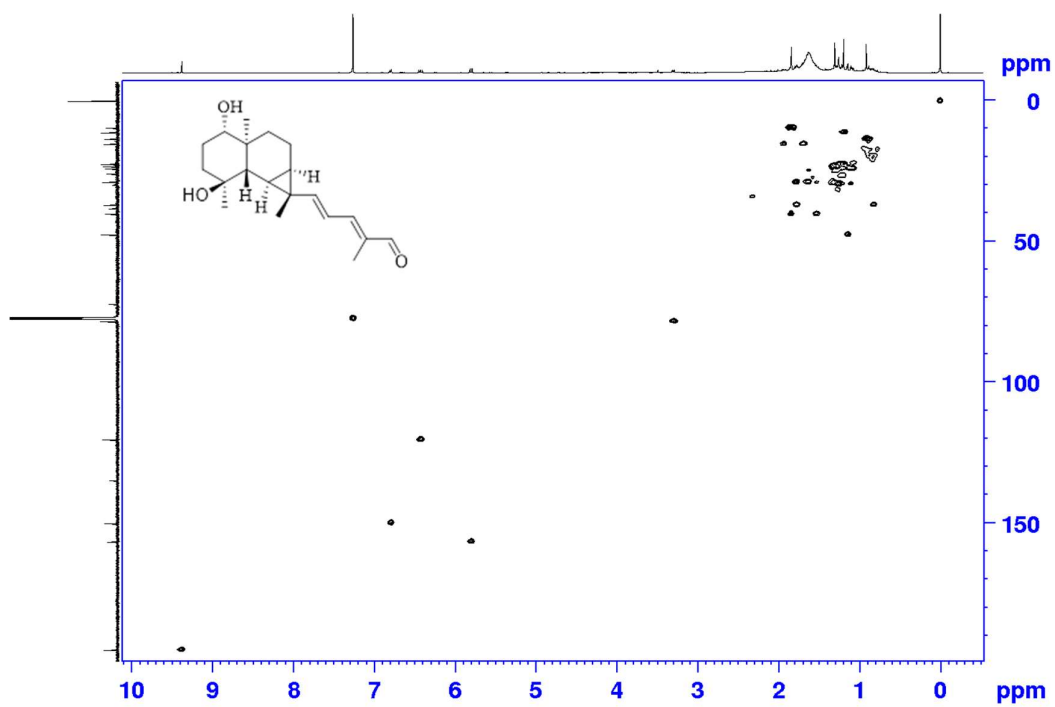
**FigureS1.** HRESIMS spectrum of compound **1**.



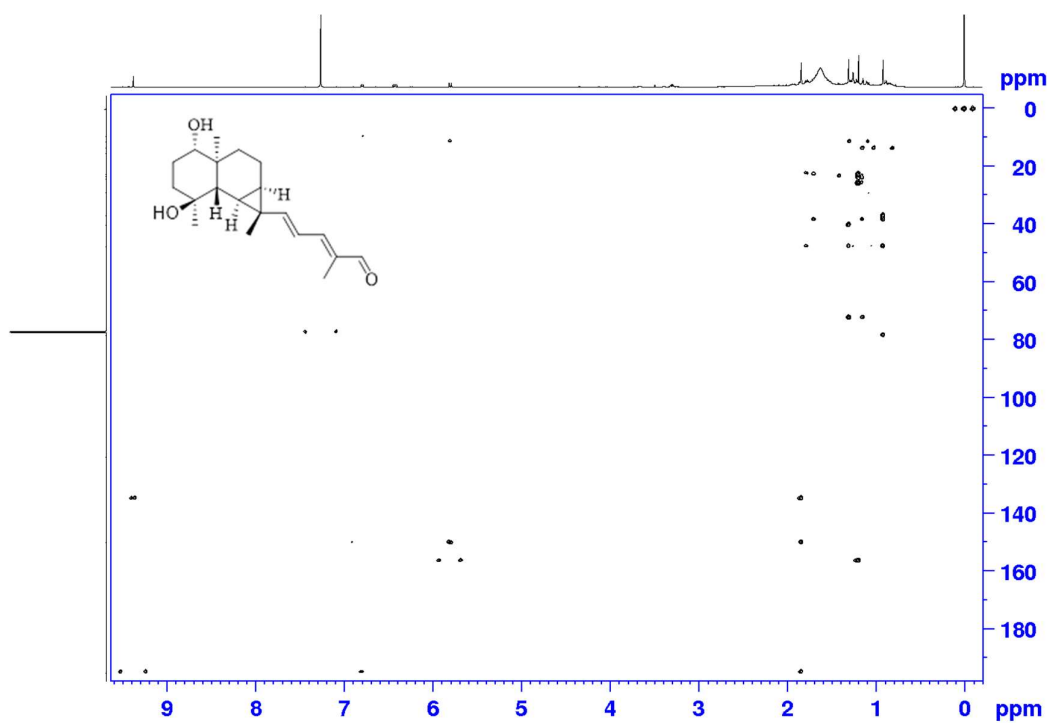
**FigureS2.** <sup>1</sup>H NMR spectrum of compound **1**



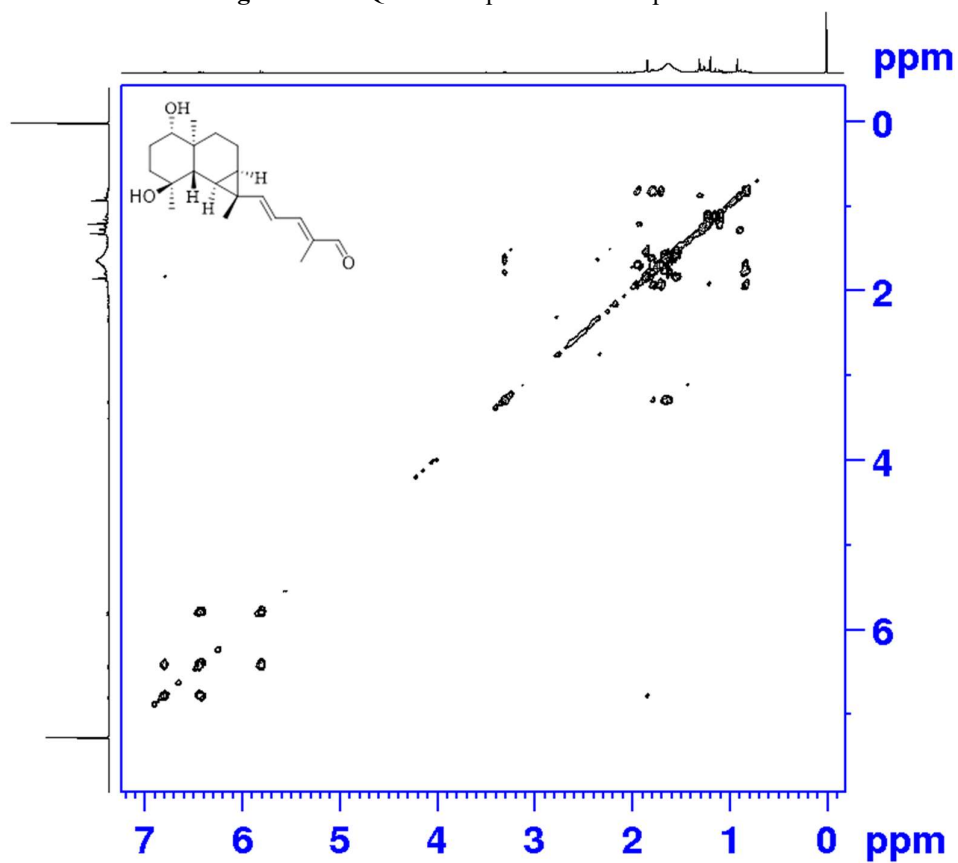
FigureS3.<sup>13</sup>C-NMR spectrum of compound 1



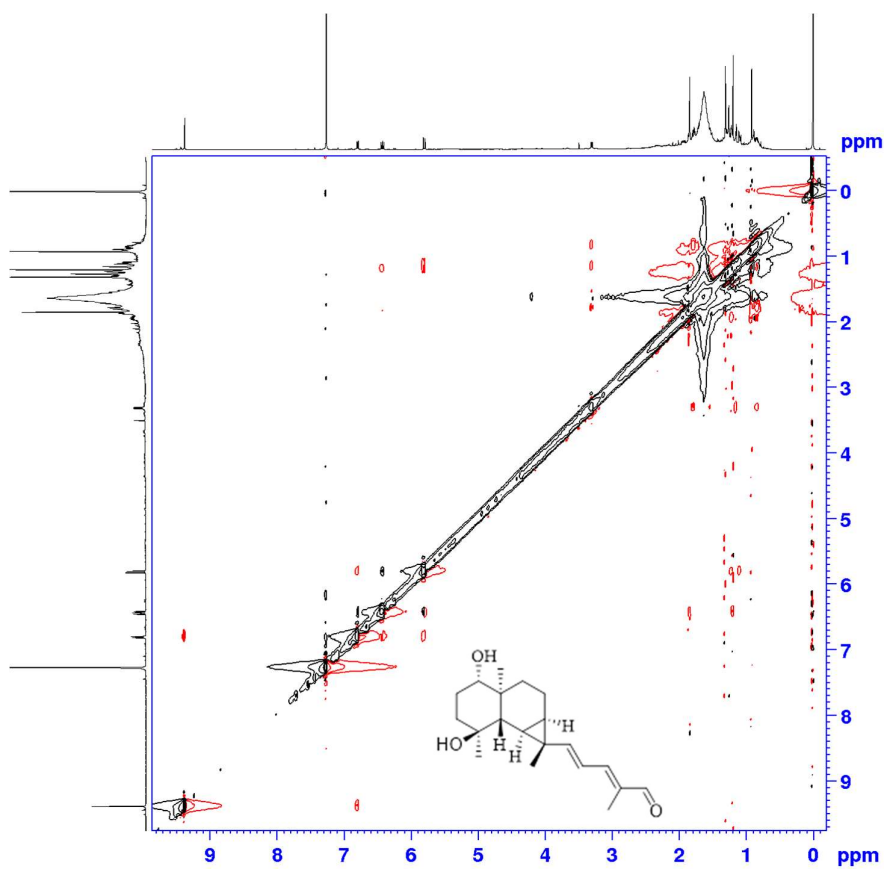
FigureS4.HSQC NMR spectrum of compound 1



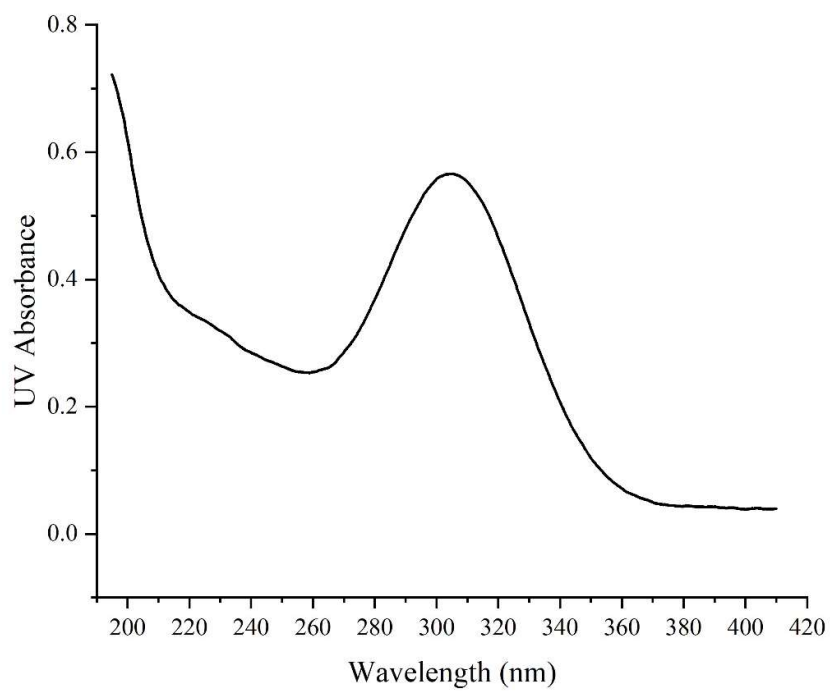
FigureS5.HMQC NMR spectrum of compound 1



FigureS6. $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound 1

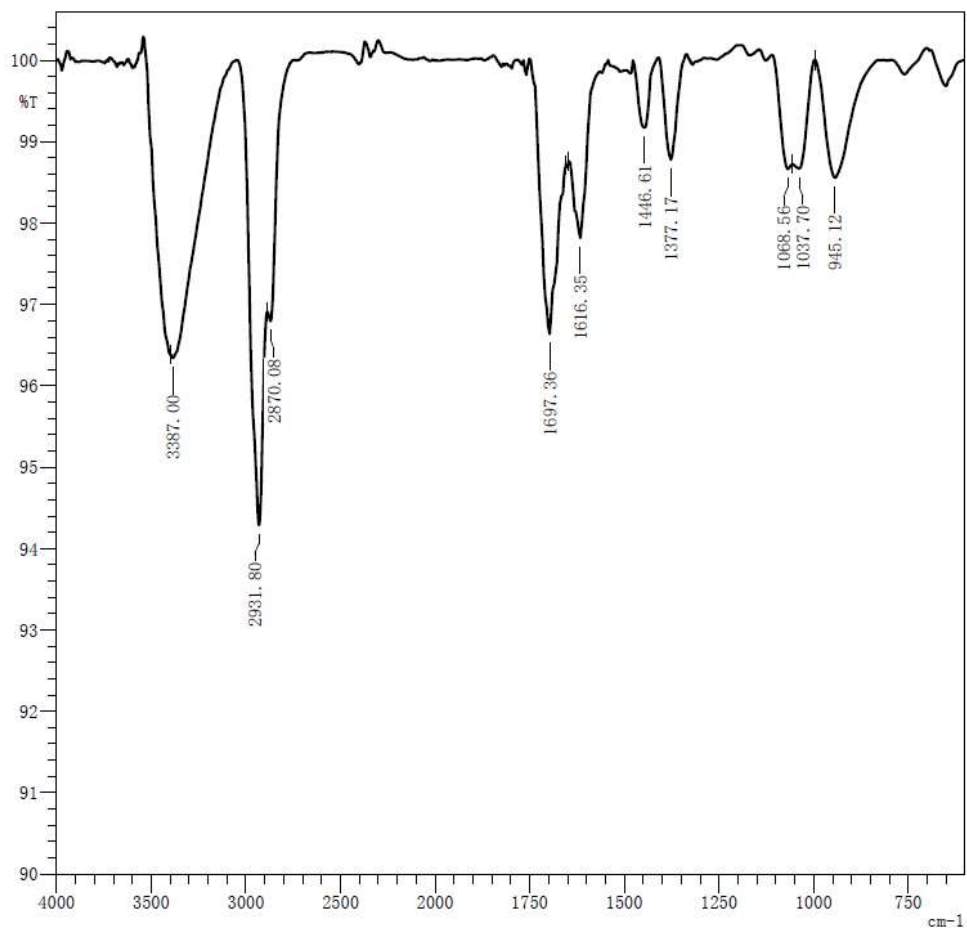


**FigureS7.**NOESY spectrum of compound **1**

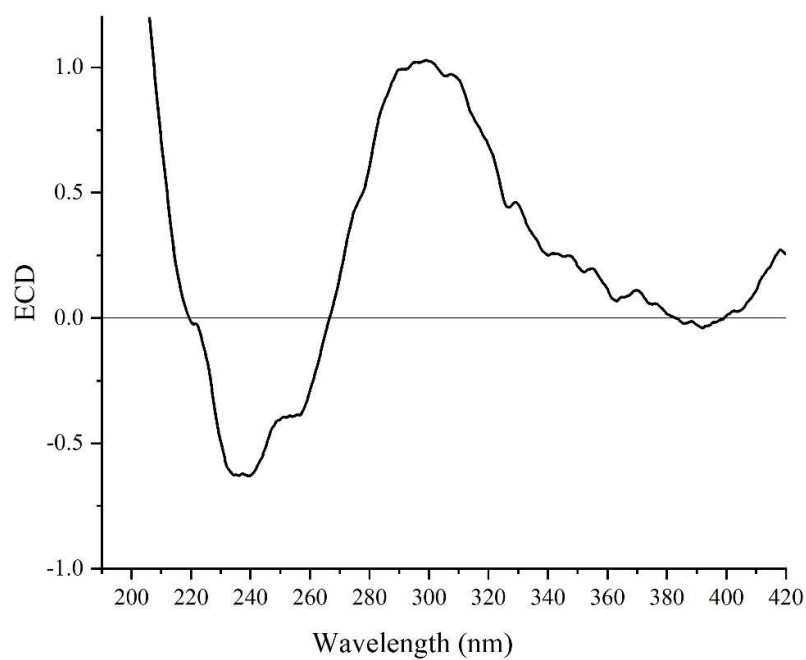


**FigureS8.** The UV spectrum of compound **1**

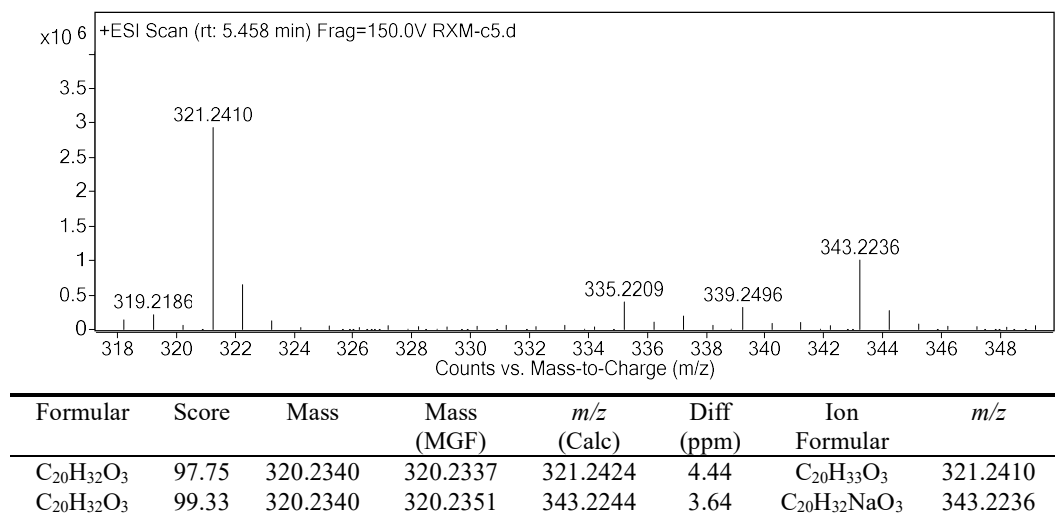




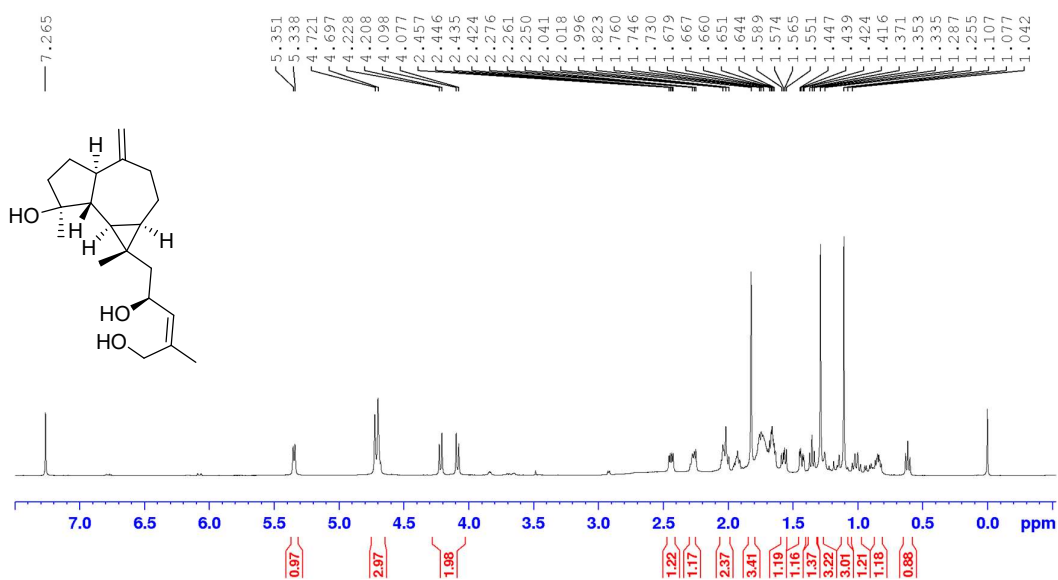
**FigureS9.**The IR spectrum of compound **1**.



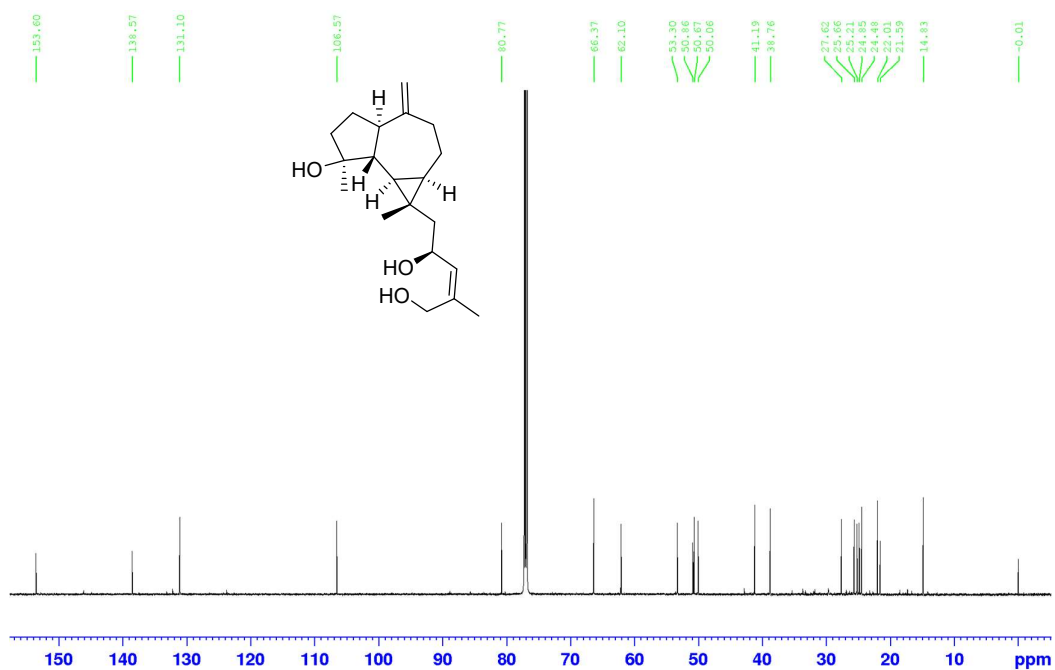
**FigureS10.** The ECD spectrum of compound **1**



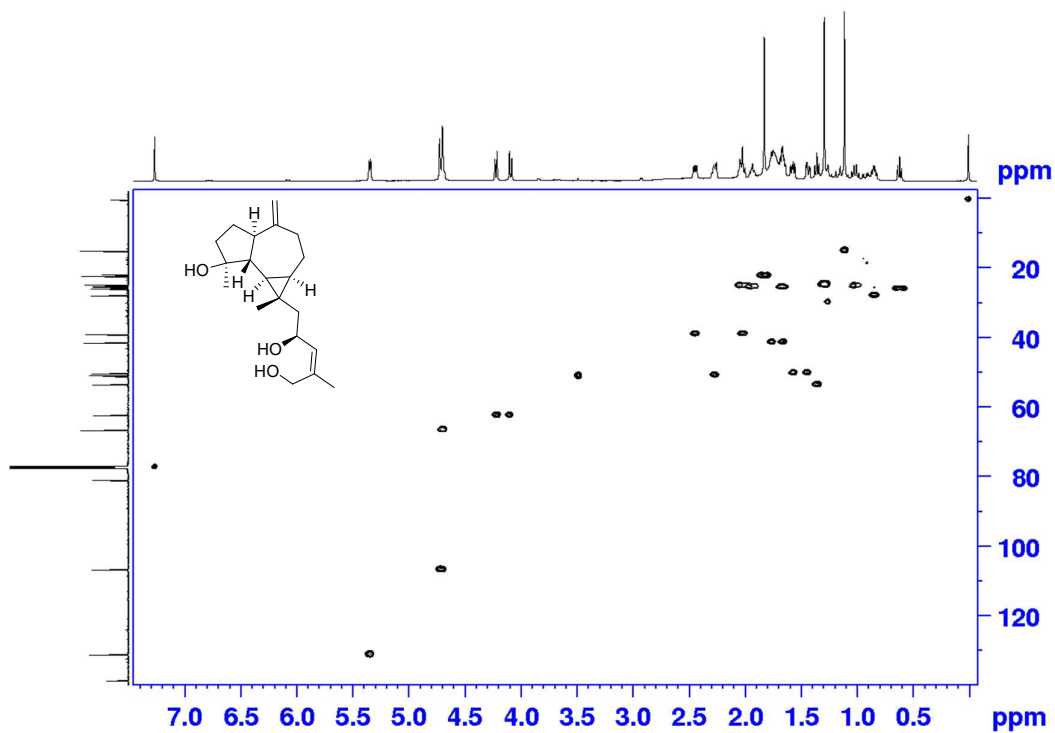
**FigureS11.** HRESIMS spectrum of compound **2**



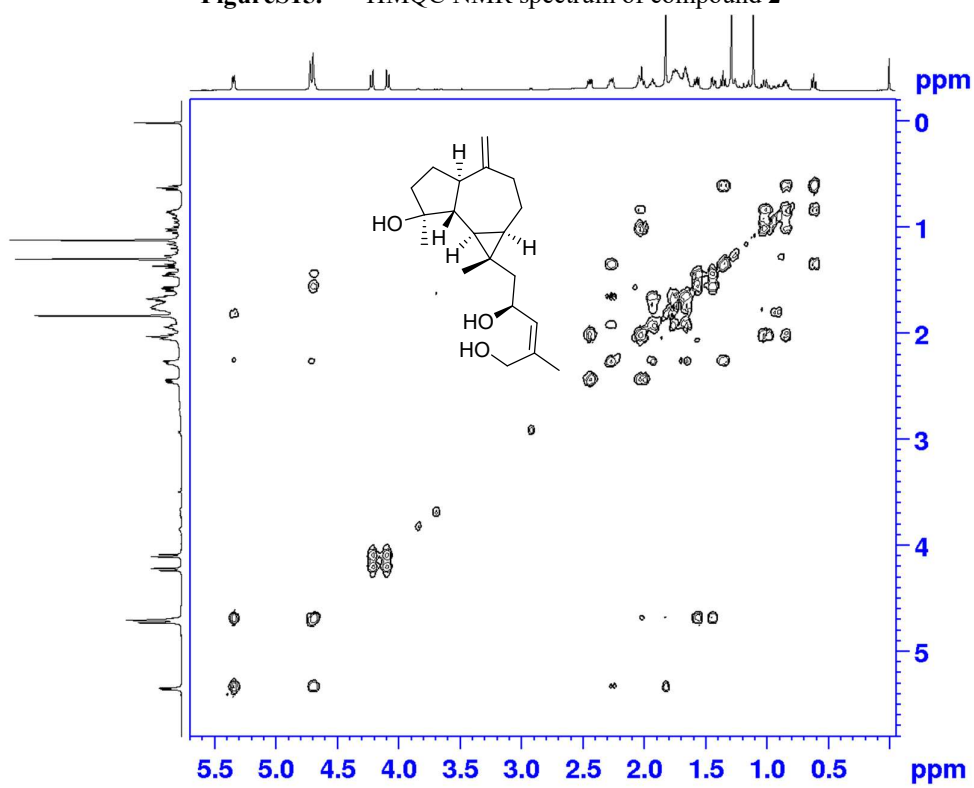
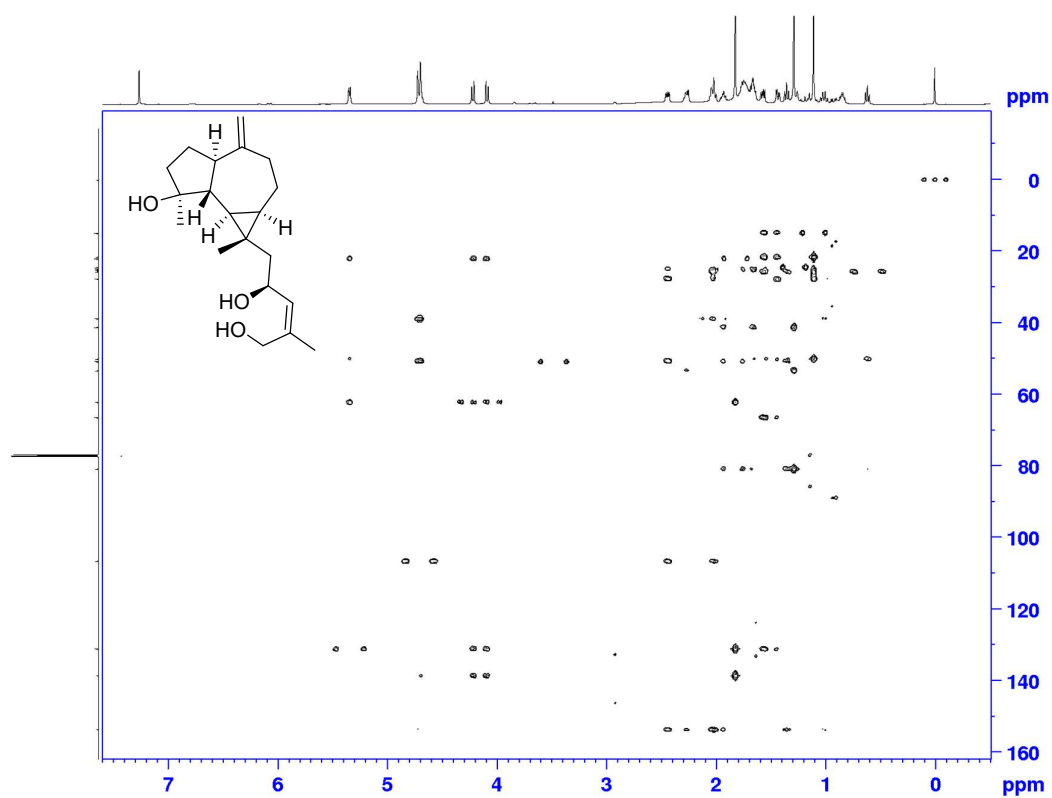
**FigureS12.** <sup>1</sup>H NMR spectrum of compound **2**.

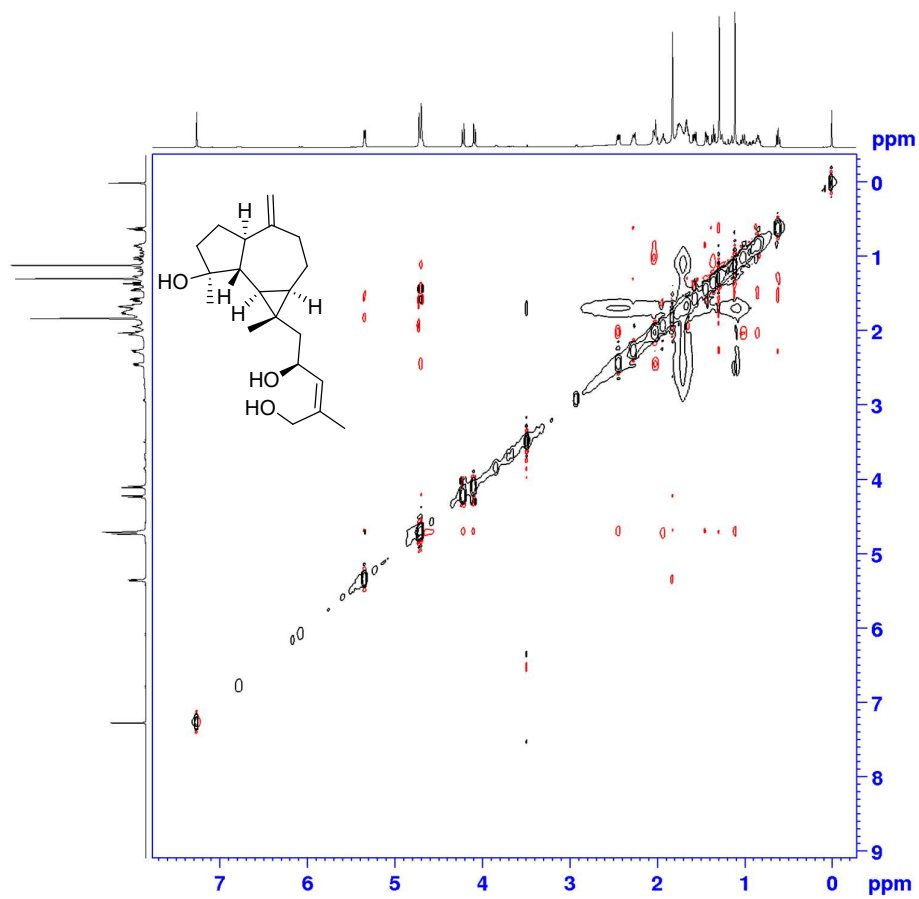


FigureS13.  $^{13}\text{C}$  NMR spectrum of compound 2

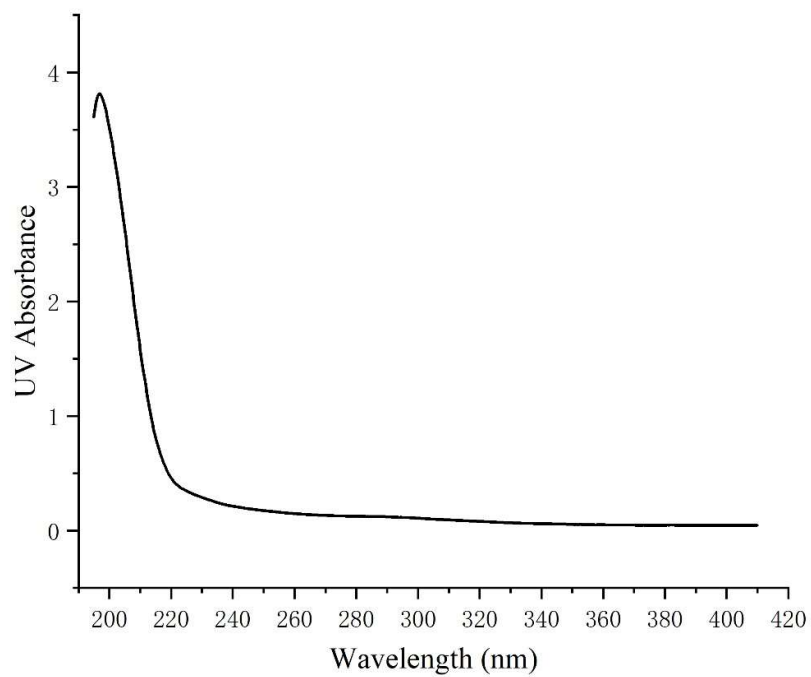


FigureS14. HSQC NMR spectrum of compound 2

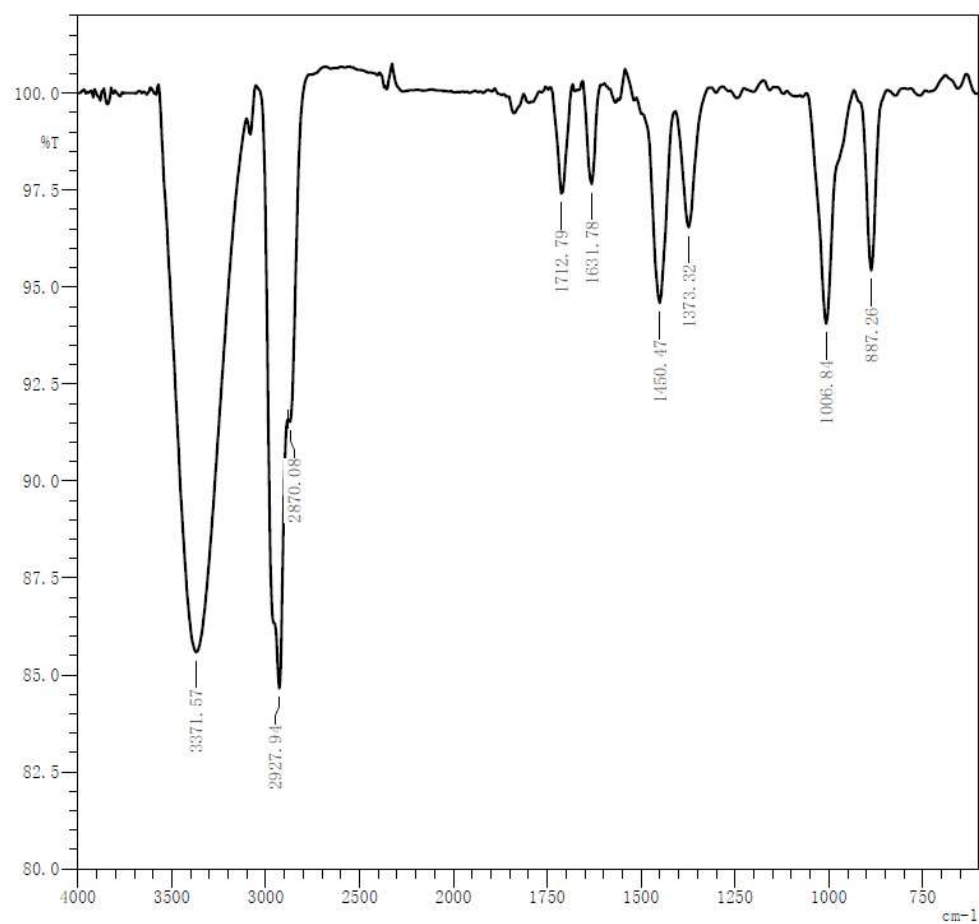




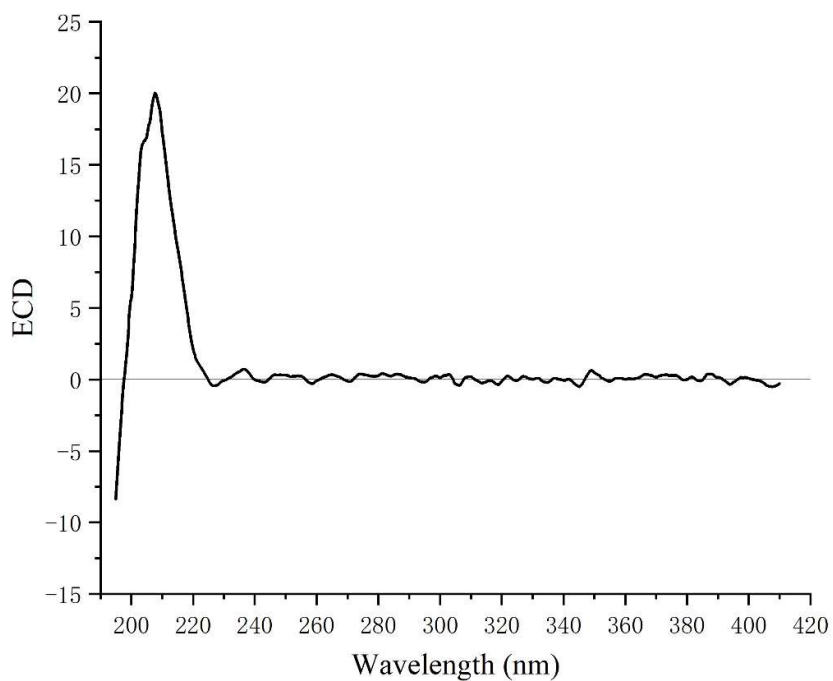
**FigureS17.** NOESY NMR spectrum of compound 2



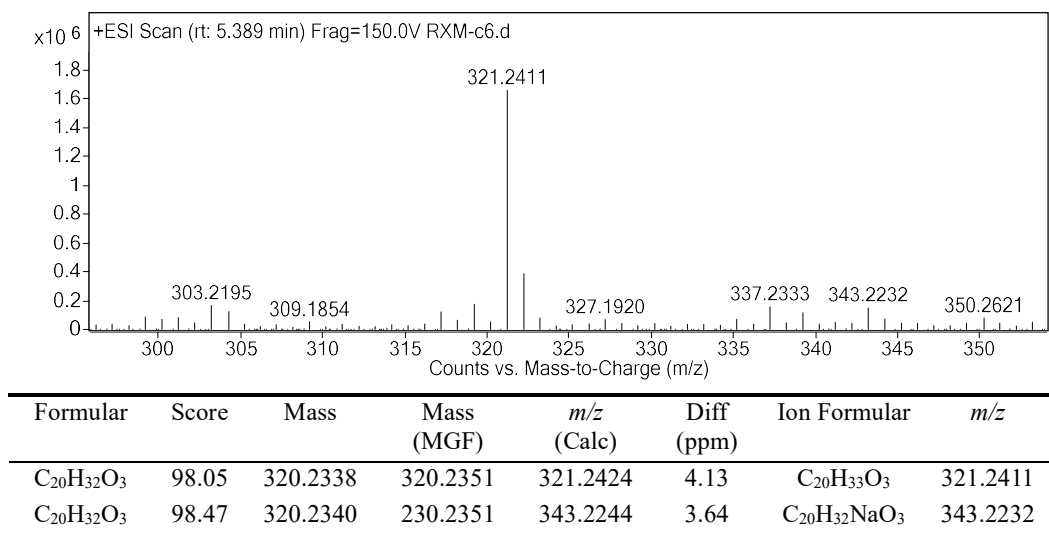
**FigureS18.** UV spectrum of compound 2.



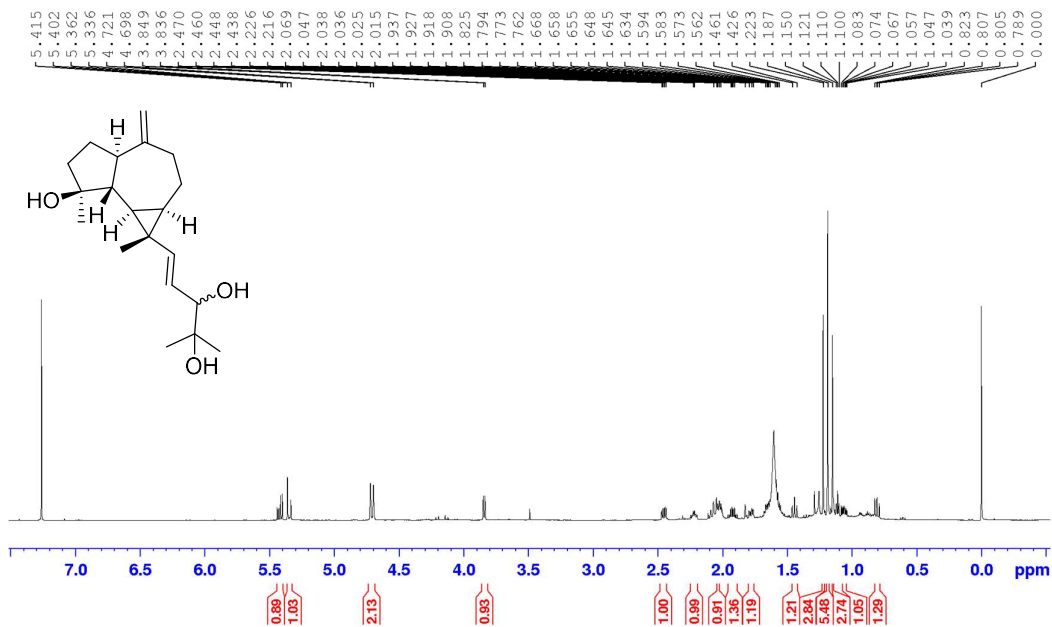
**FigureS19.** IR spectrum of compound 2.



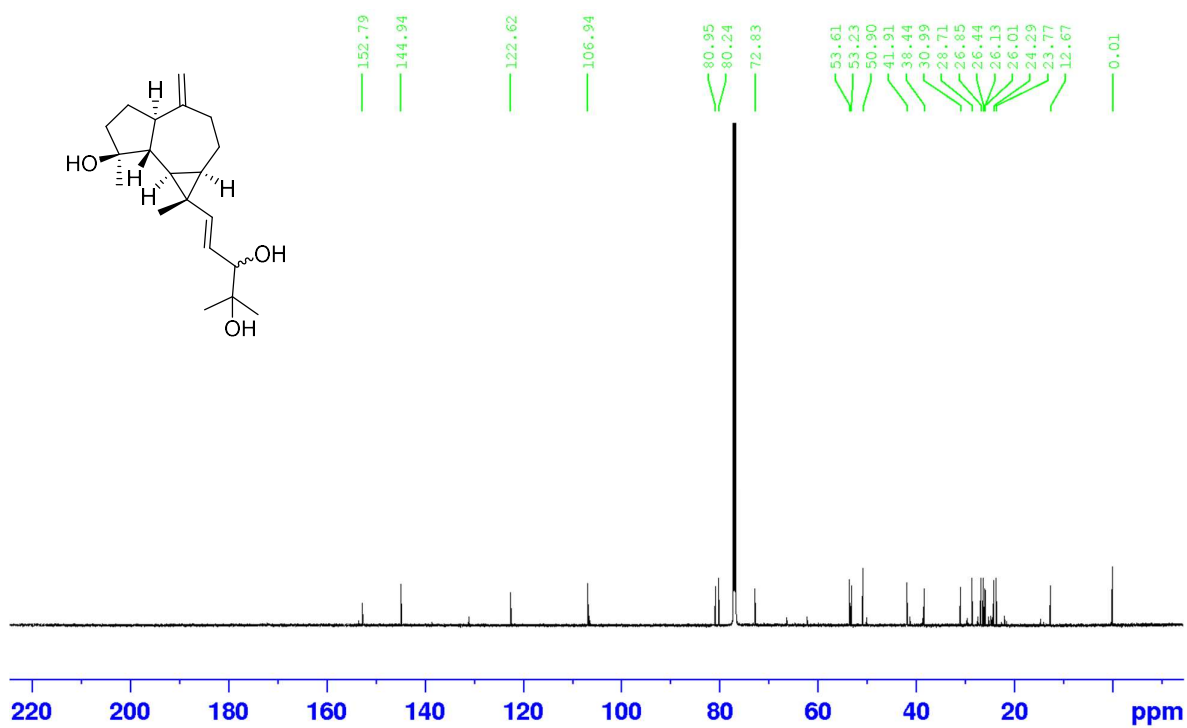
**FigureS20.** ECD spectrum of compound 2.



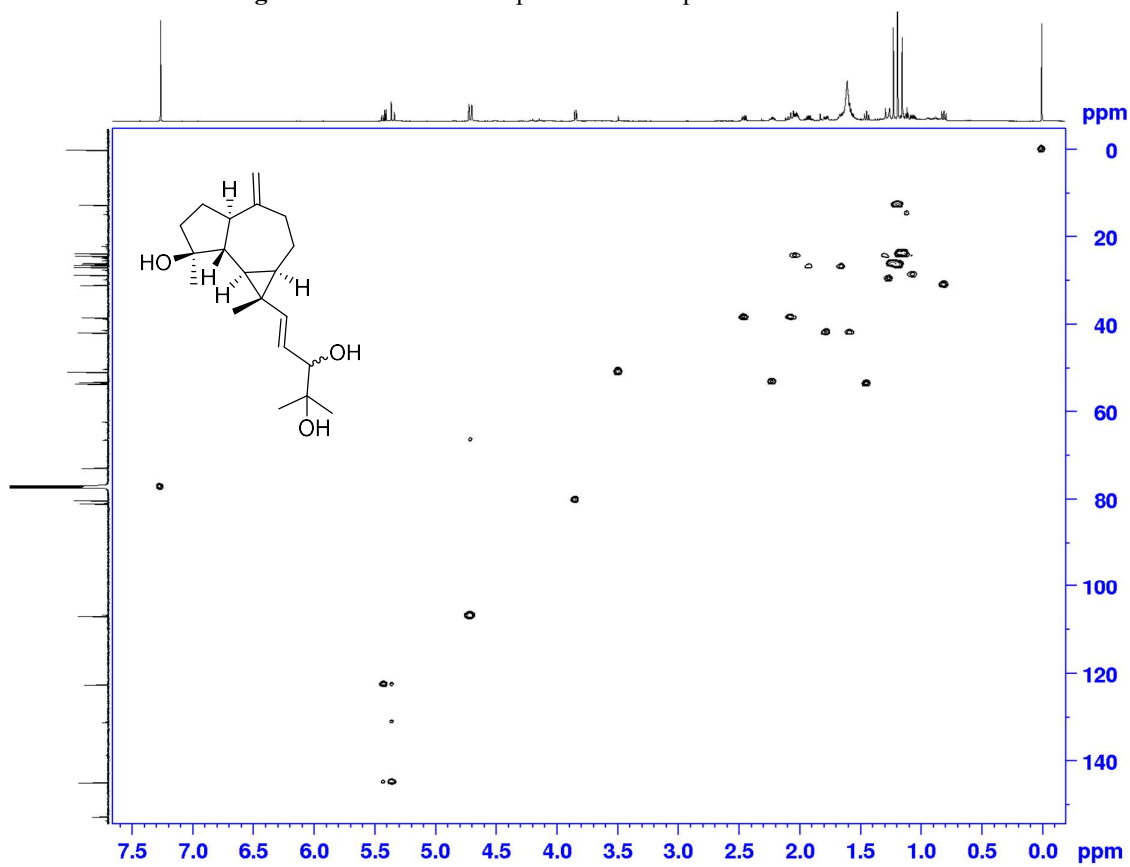
**FigureS21.** HRESIMS spectrum of compound **3**.



**FigureS22.** <sup>1</sup>H NMR spectrum of compound **3**

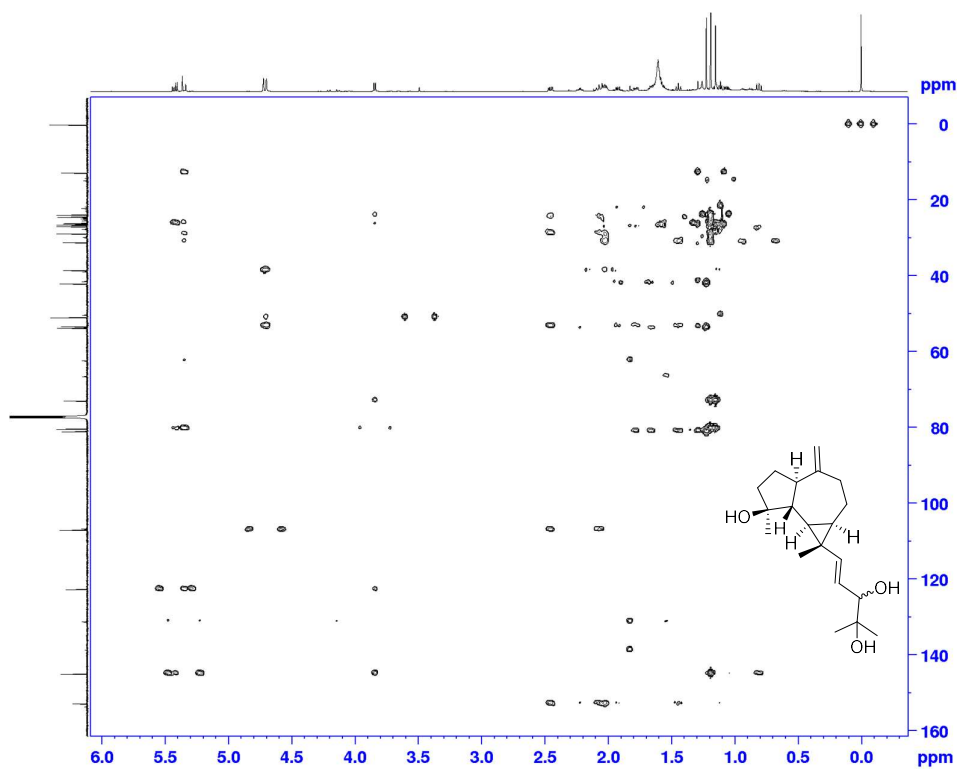


FigureS23. <sup>13</sup>C NMR spectrum of compound 3

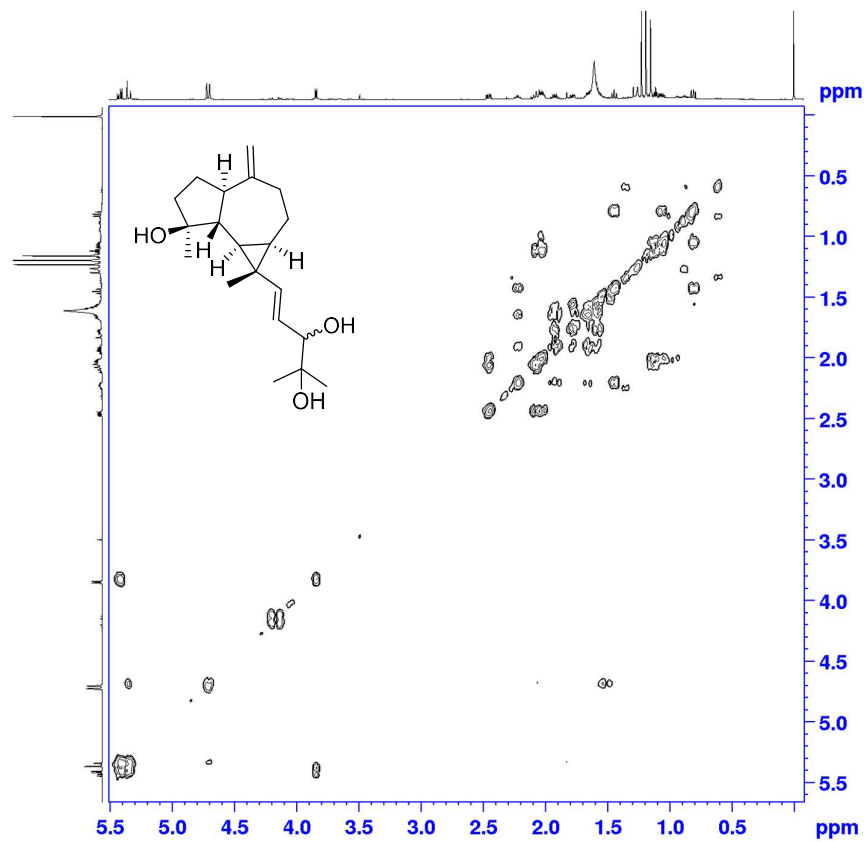


FigureS24. HSQC NMR spectrum of compound 3

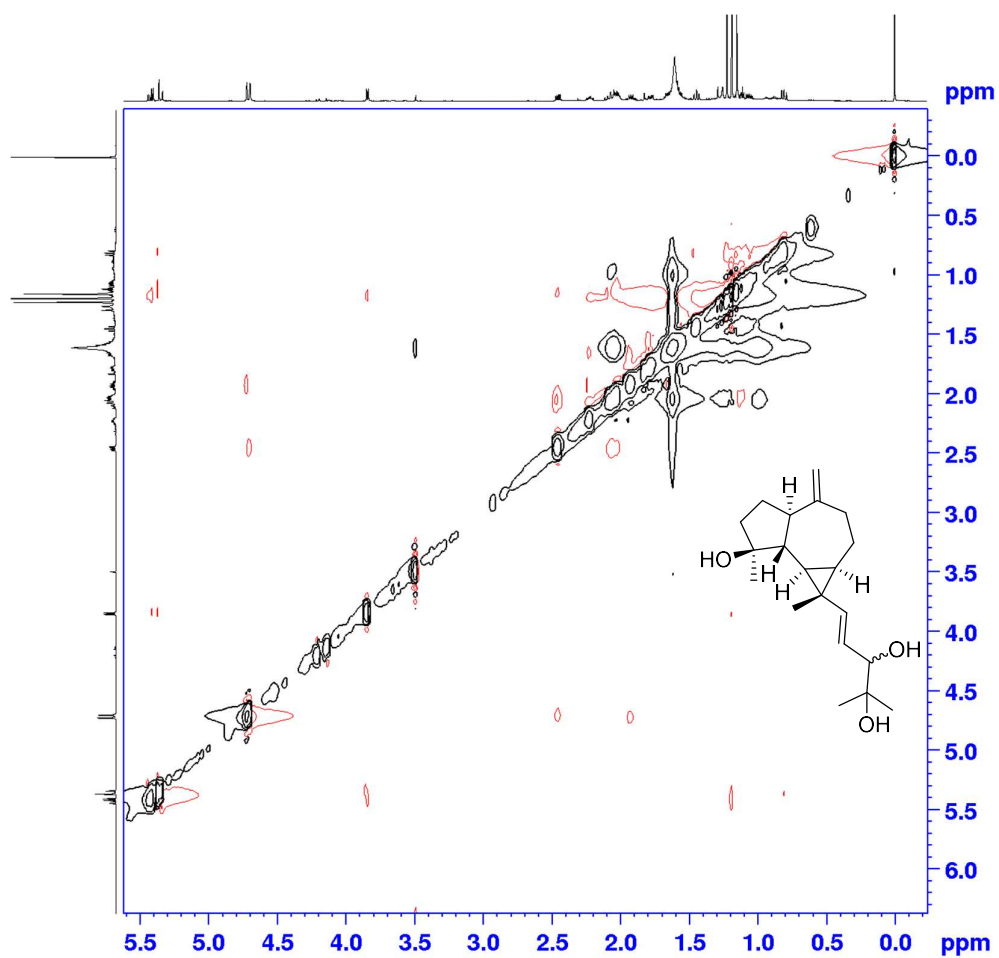




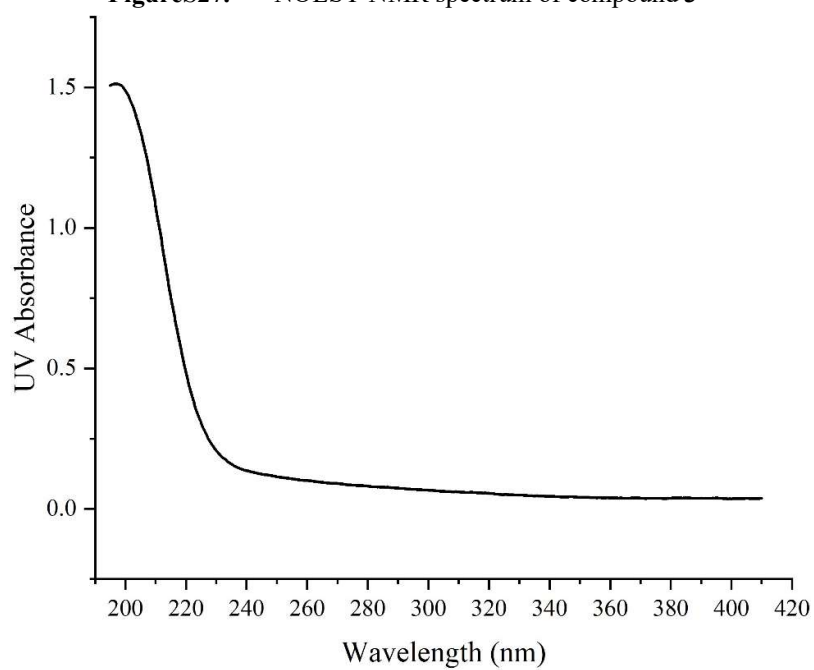
FigureS25. HMBC NMR spectrum of compound 3



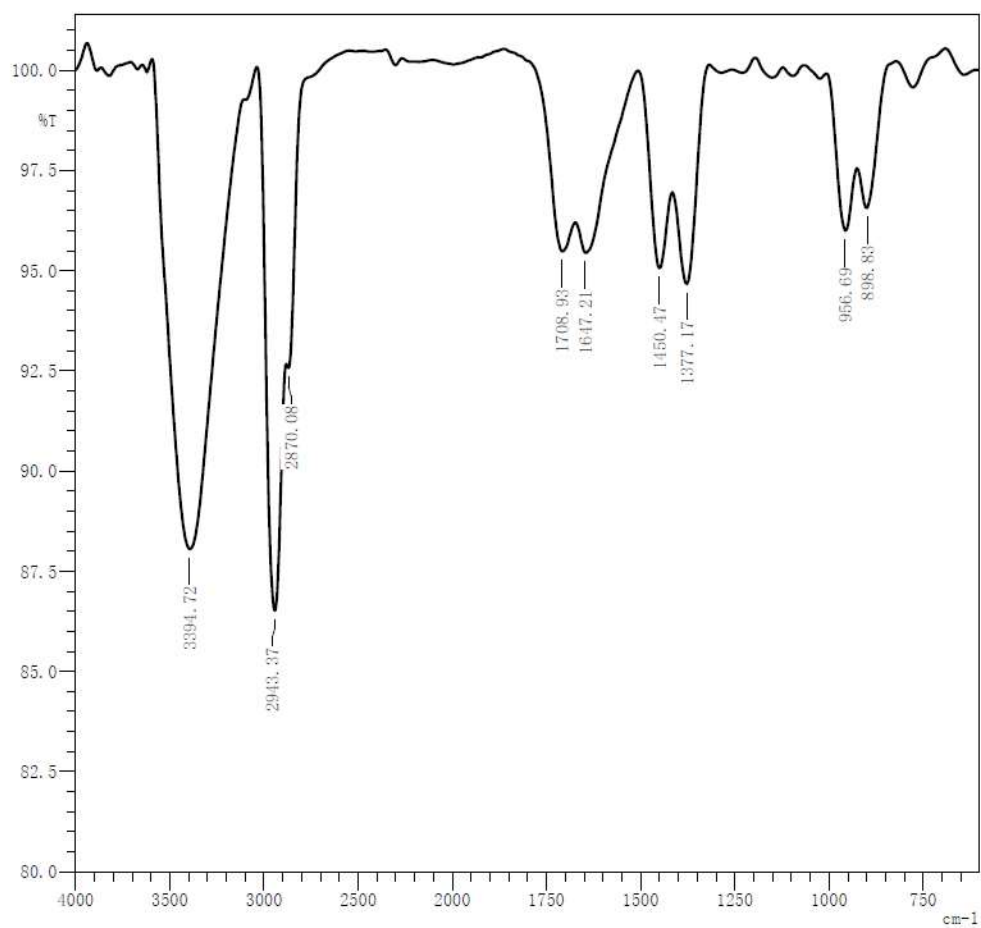
FigureS26.  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of compound 3



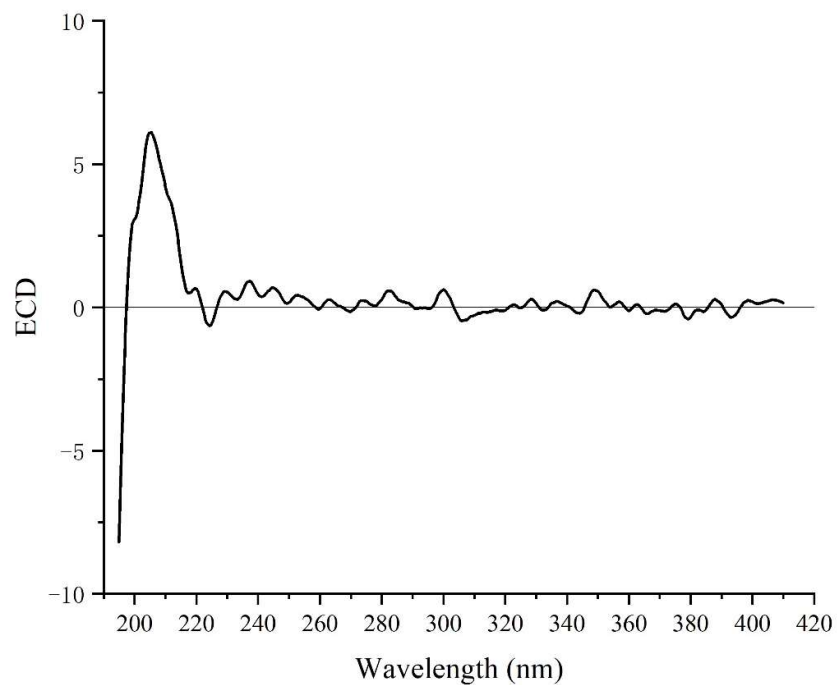
**FigureS27.** NOESY NMR spectrum of compound **3**



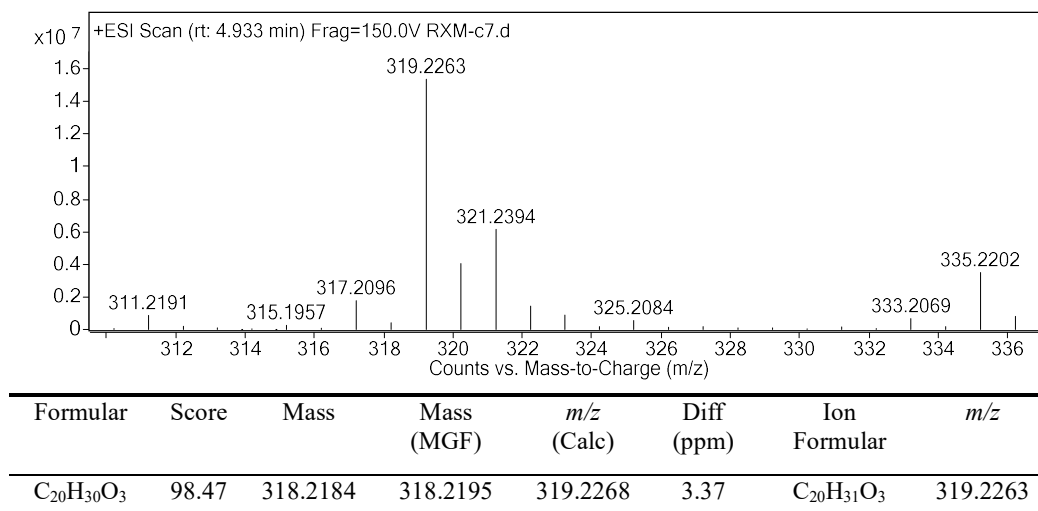
**FigureS28.** UV spectrum of compound **3**



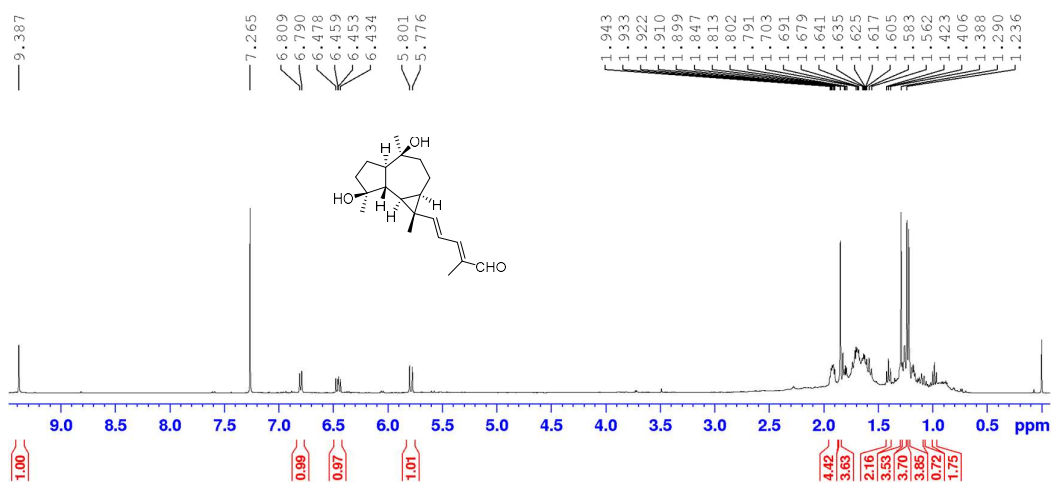
**FigureS29.** IR spectrum of compound **3**.



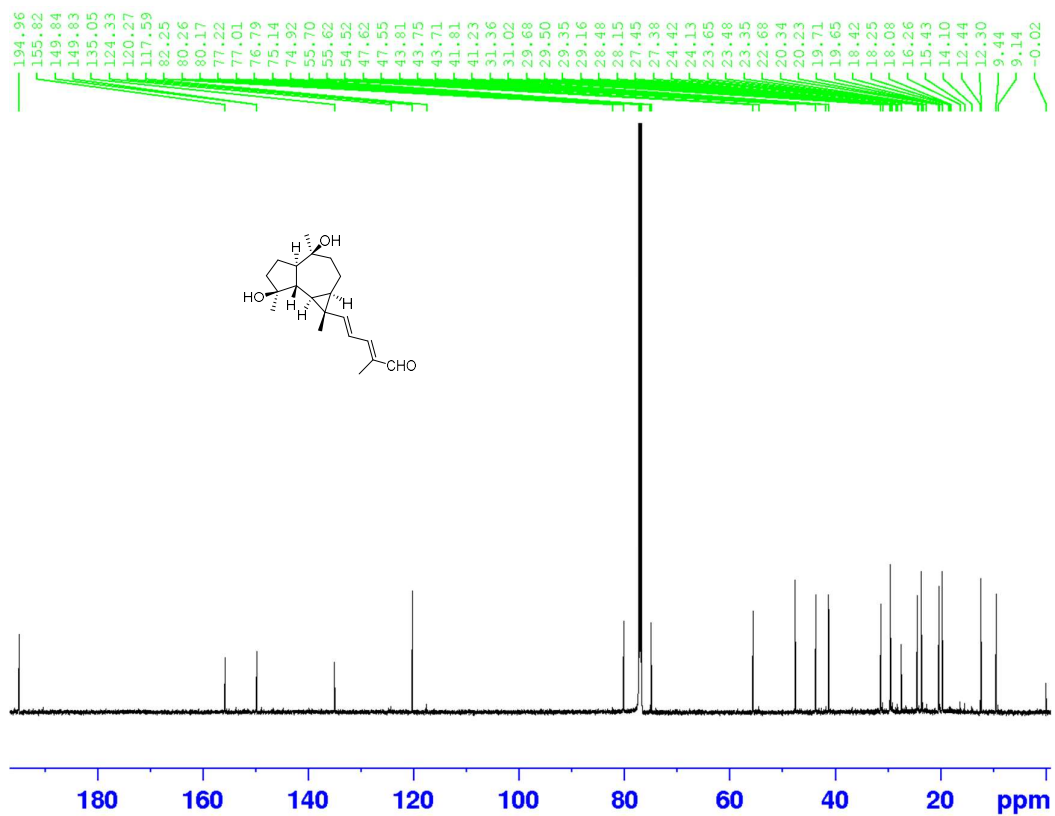
**FigureS30.** ECD spectrum of compound **3**



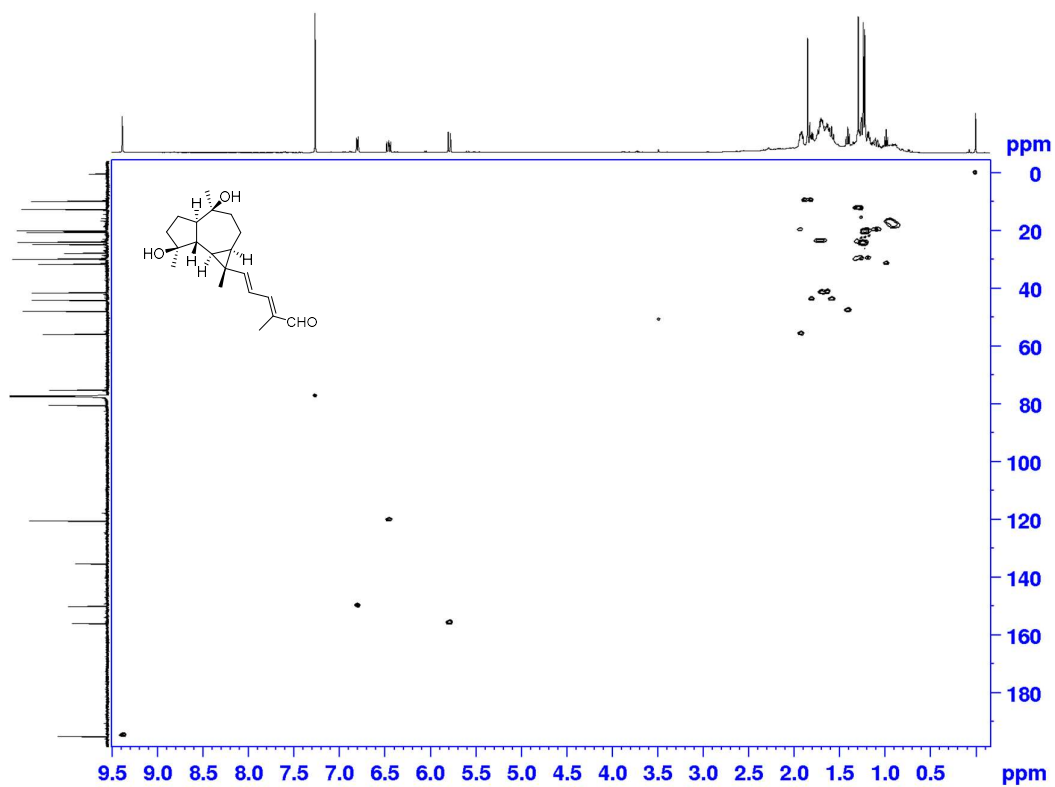
**FigureS31.** HRESIMS spectrum of compound 4.



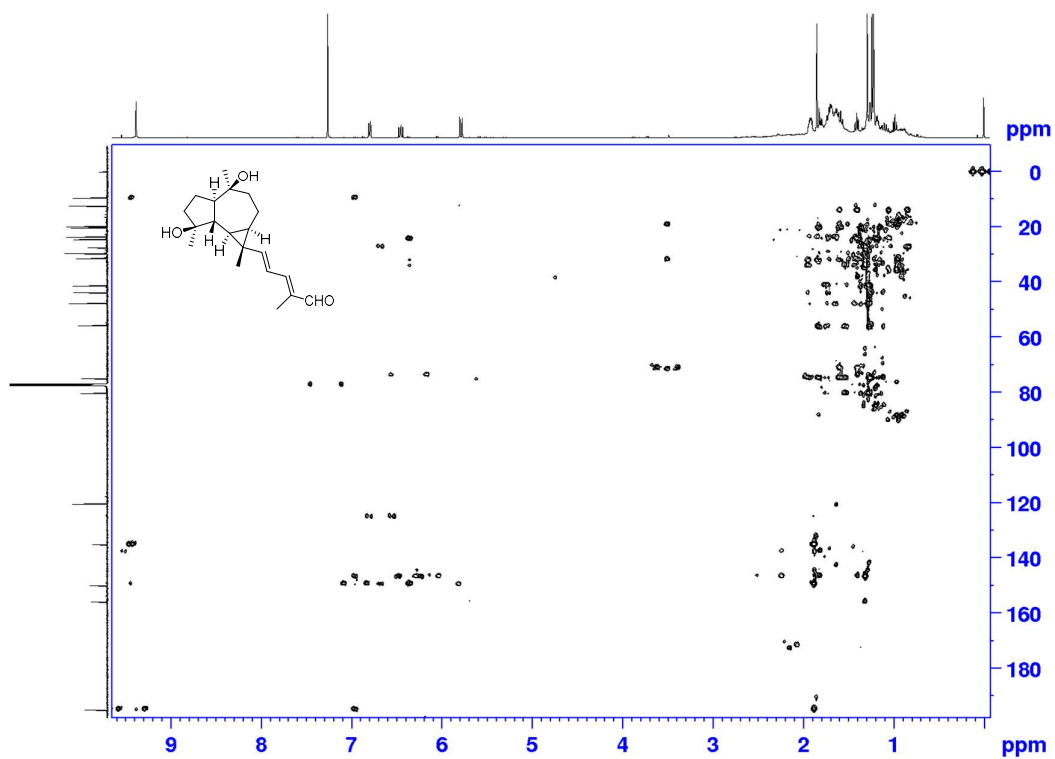
**FigureS32.** <sup>1</sup>H NMR spectrum of compound 4



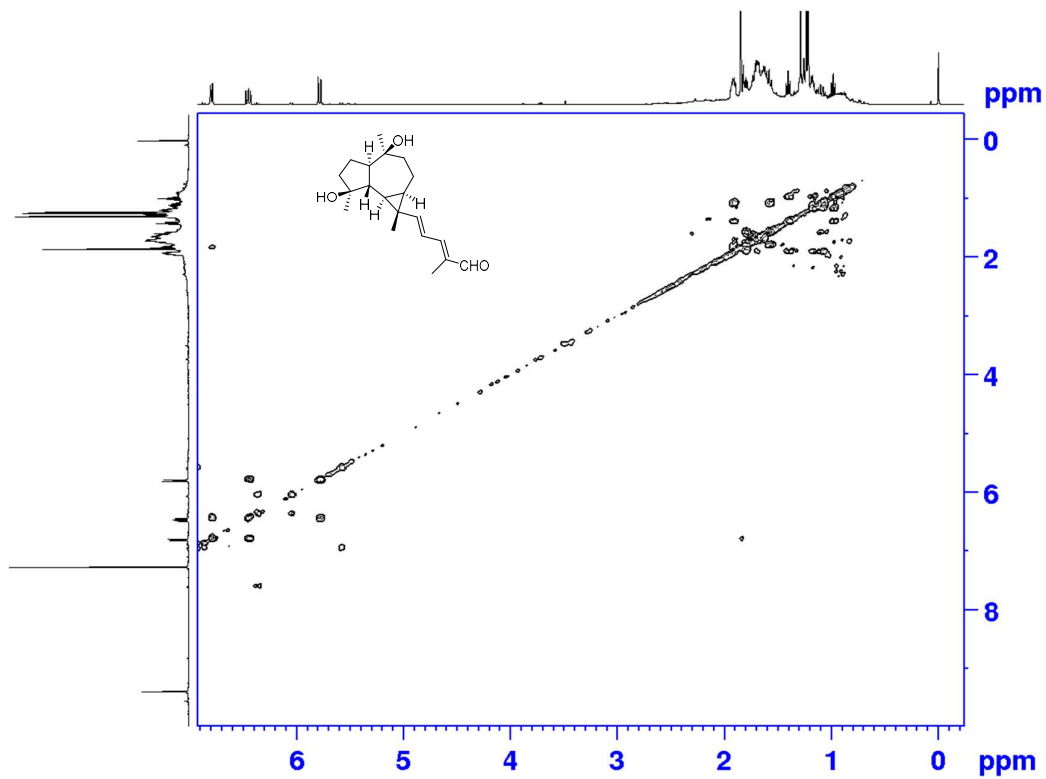
FigureS33. <sup>13</sup>C-NMR spectrum of Compound 4



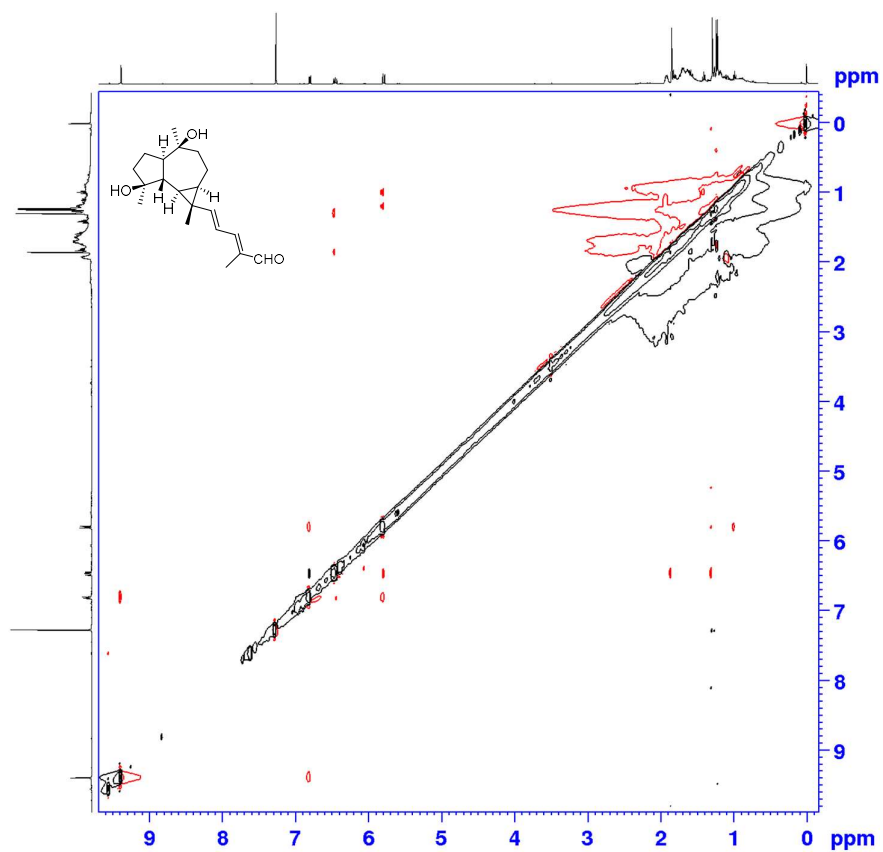
FigureS34. HSQC NMR spectrum of compound 4



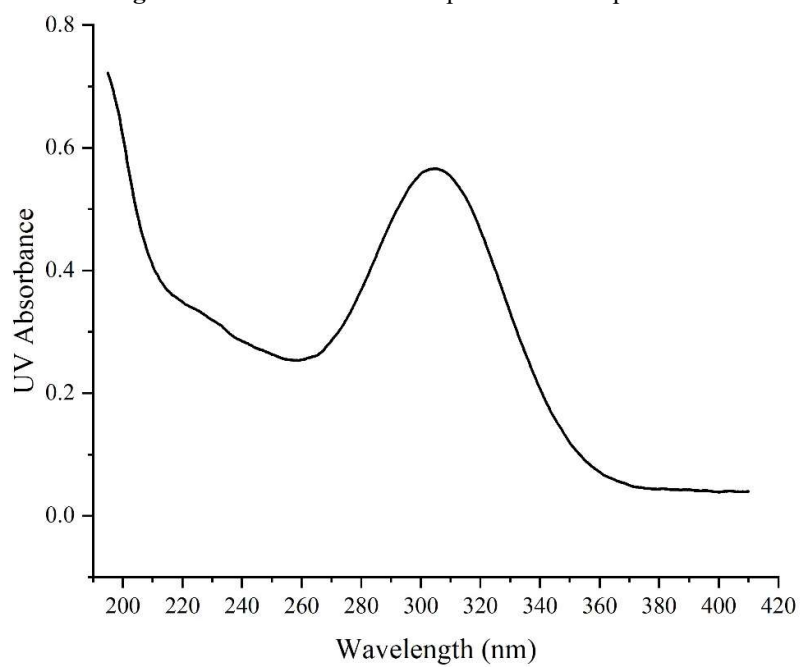
FigureS35. HMBC NMR spectrum of compound 4



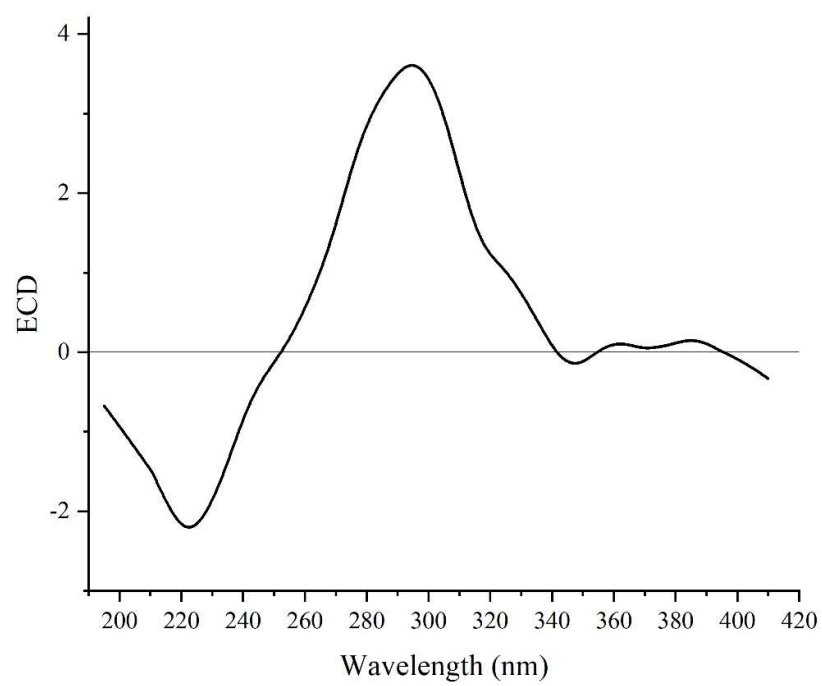
FigureS36.  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of compound 4



**FigureS37.** NOESY NMR spectrum of compound **4**

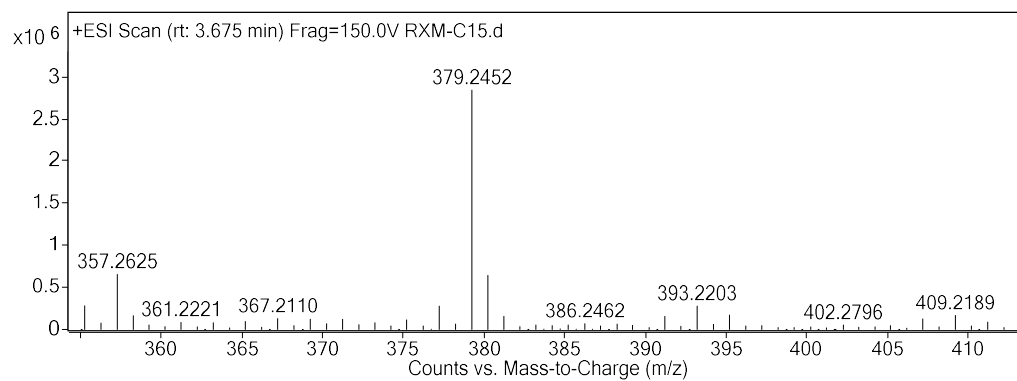


**FigureS38.** UV spectrum of compound **4**



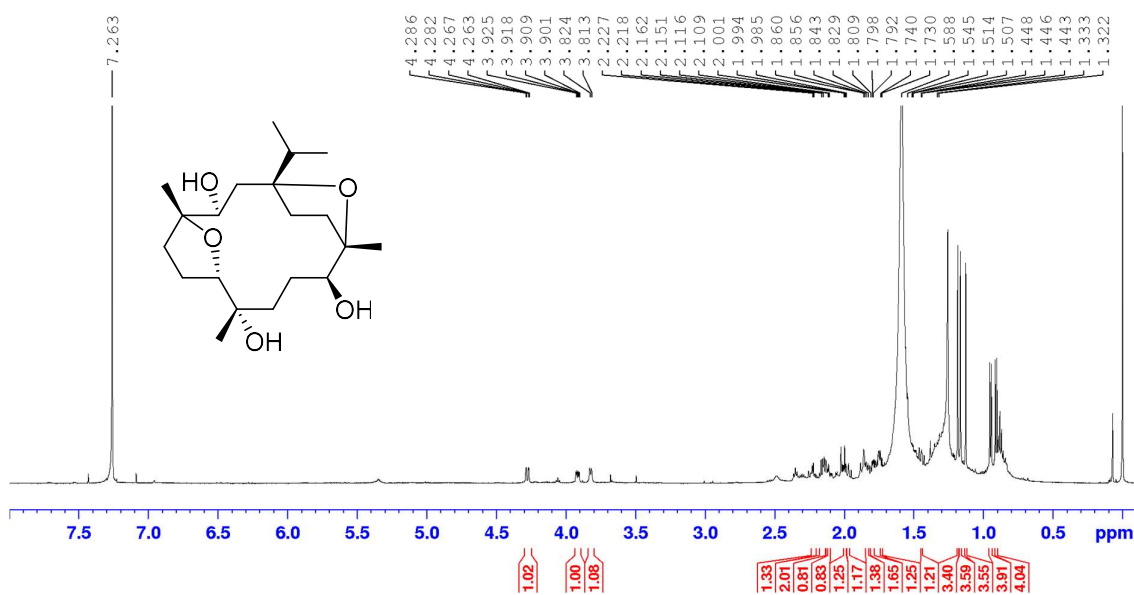
**FigureS39.** ECD spectrum of compound **4**



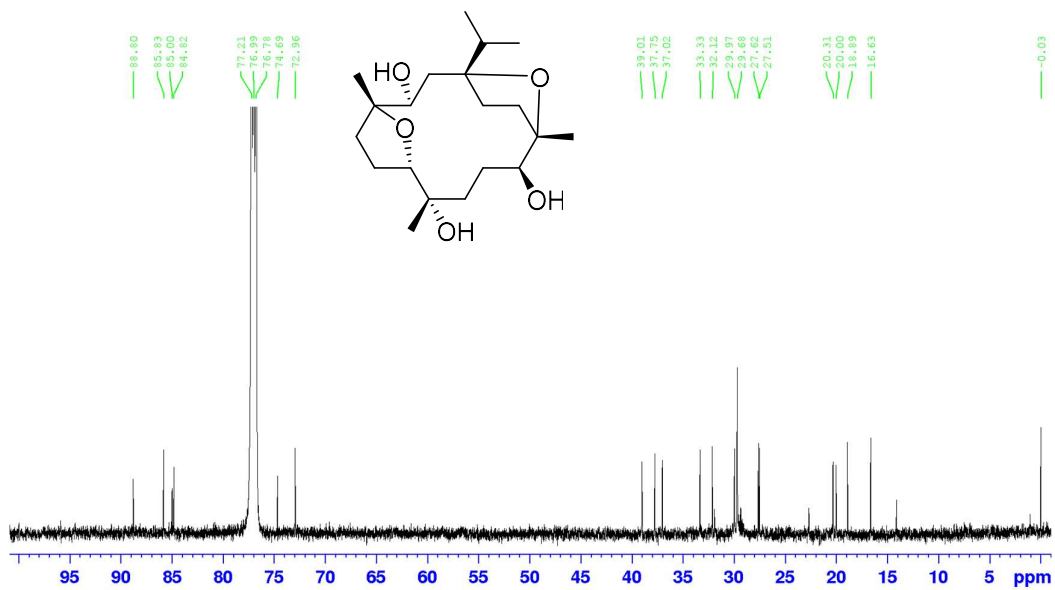


Formular	Score	Mass	Mass (MGF)	<i>m/z</i> (Calc)	Diff (ppm)	Ion Formular	<i>m/z</i>
C <sub>20</sub> H <sub>36</sub> O <sub>5</sub>	98.90	356.2552	356.2563	357.2636	2.95	C <sub>20</sub> H <sub>37</sub> O <sub>5</sub>	357.2625
C <sub>20</sub> H <sub>36</sub> O <sub>5</sub>	99.91	356.2560	356.2563	379.2455	0.83	C <sub>20</sub> H <sub>36</sub> NaO <sub>5</sub>	379.2452

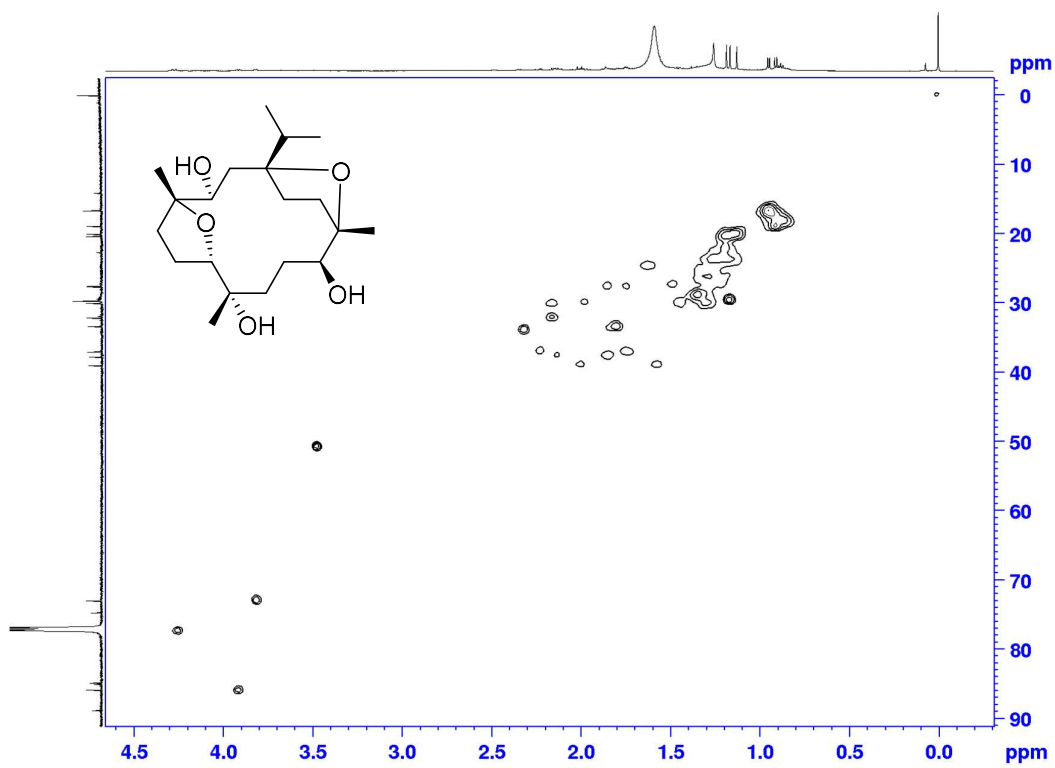
**FigureS40.** HRESIMS spectrum of compound **5**.



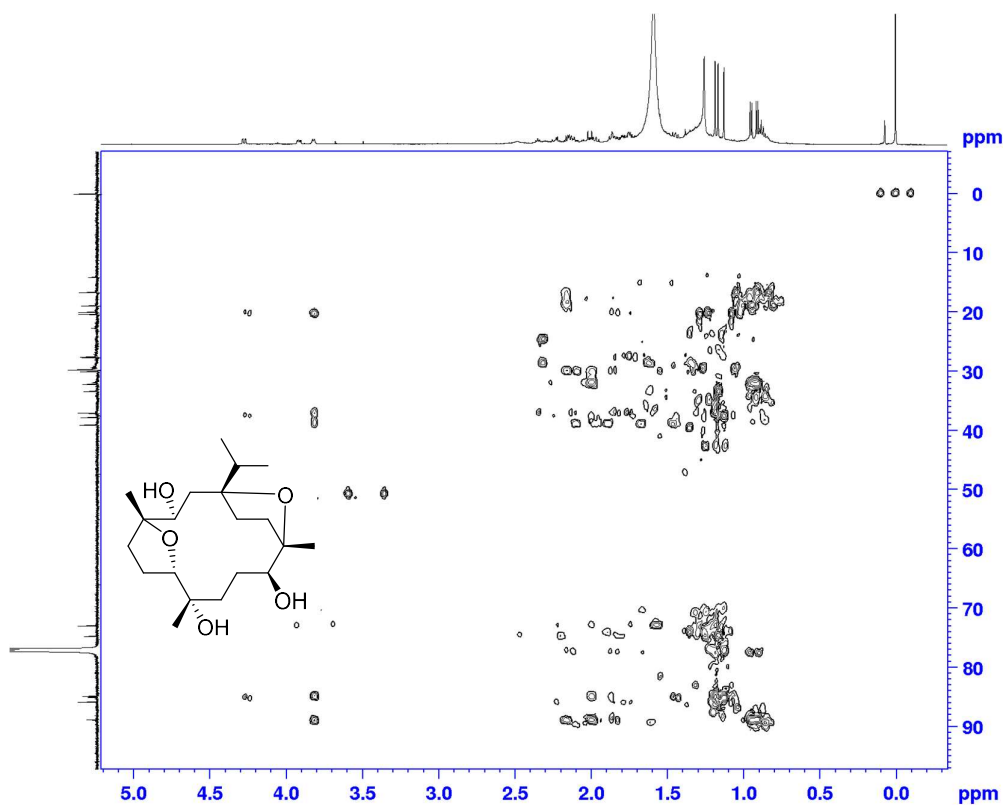
**FigureS41.** <sup>1</sup>H NMR spectrum of compound **5**



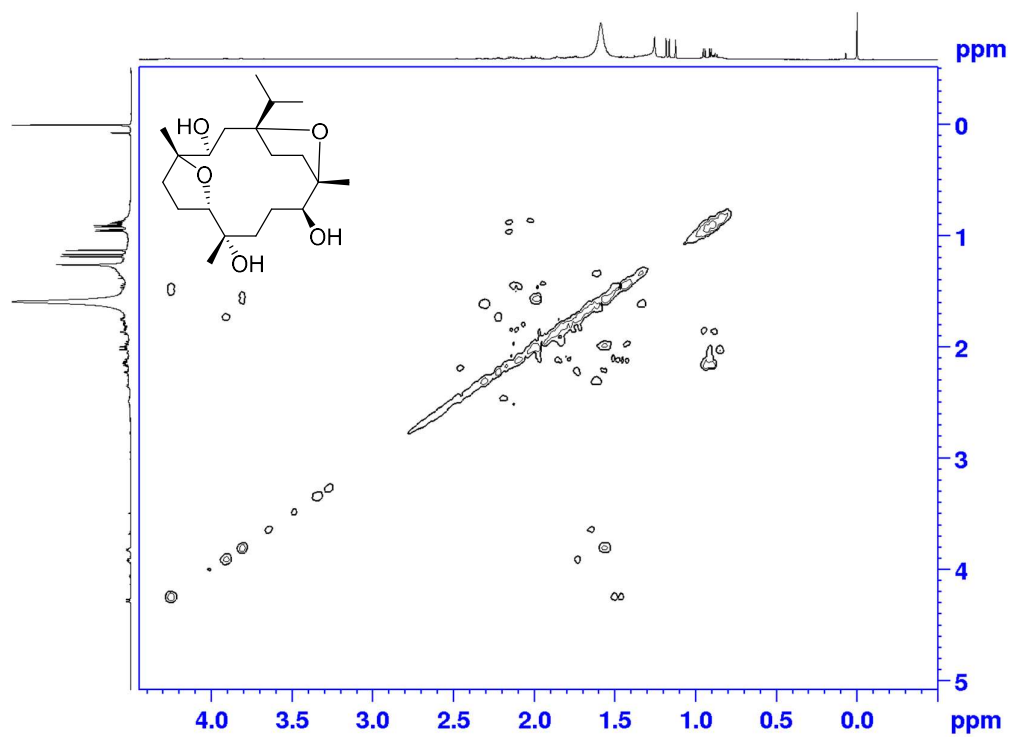
FigureS42.  $^{13}\text{C}$  NMR spectrum of compound 5



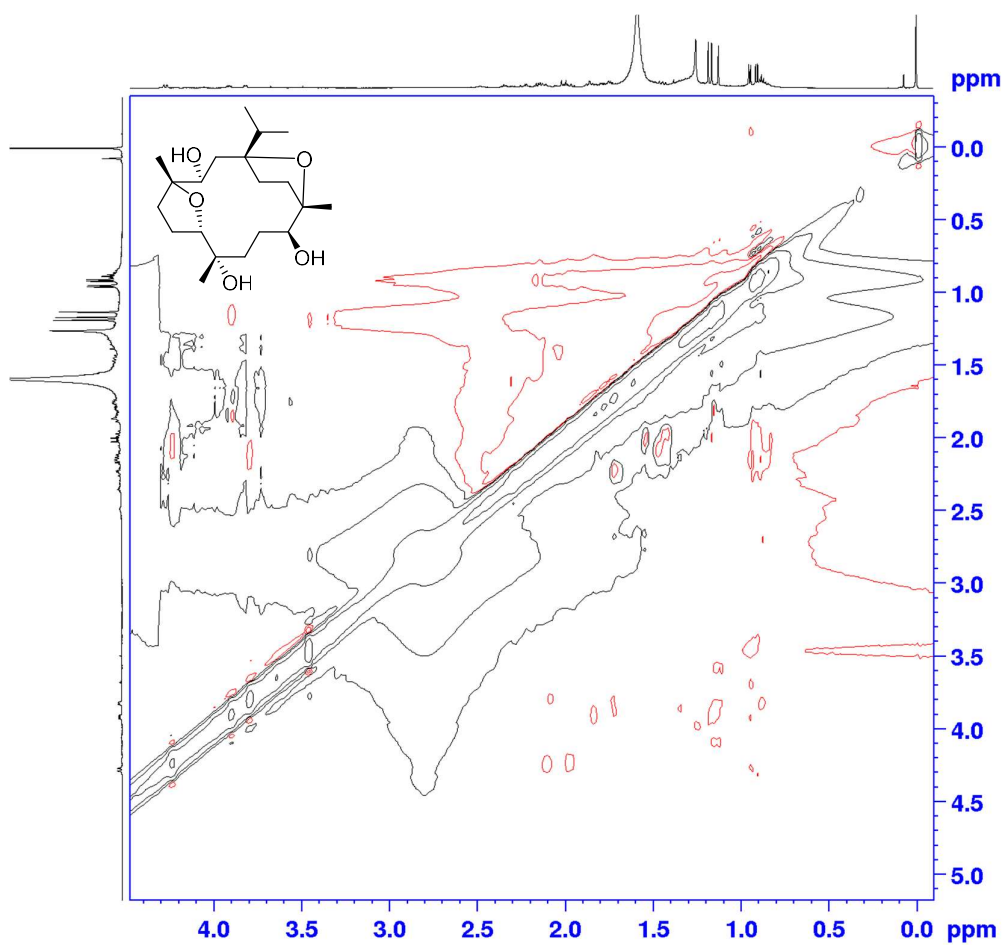
FigureS43. HSQC NMR spectrum of compound 5



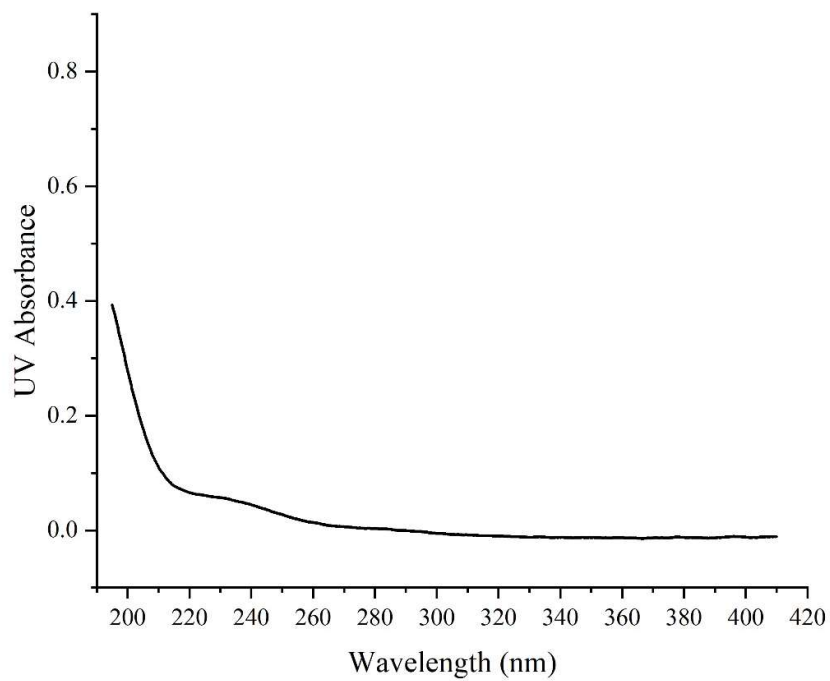
FigureS44. HMBC NMR spectrum of compound 5



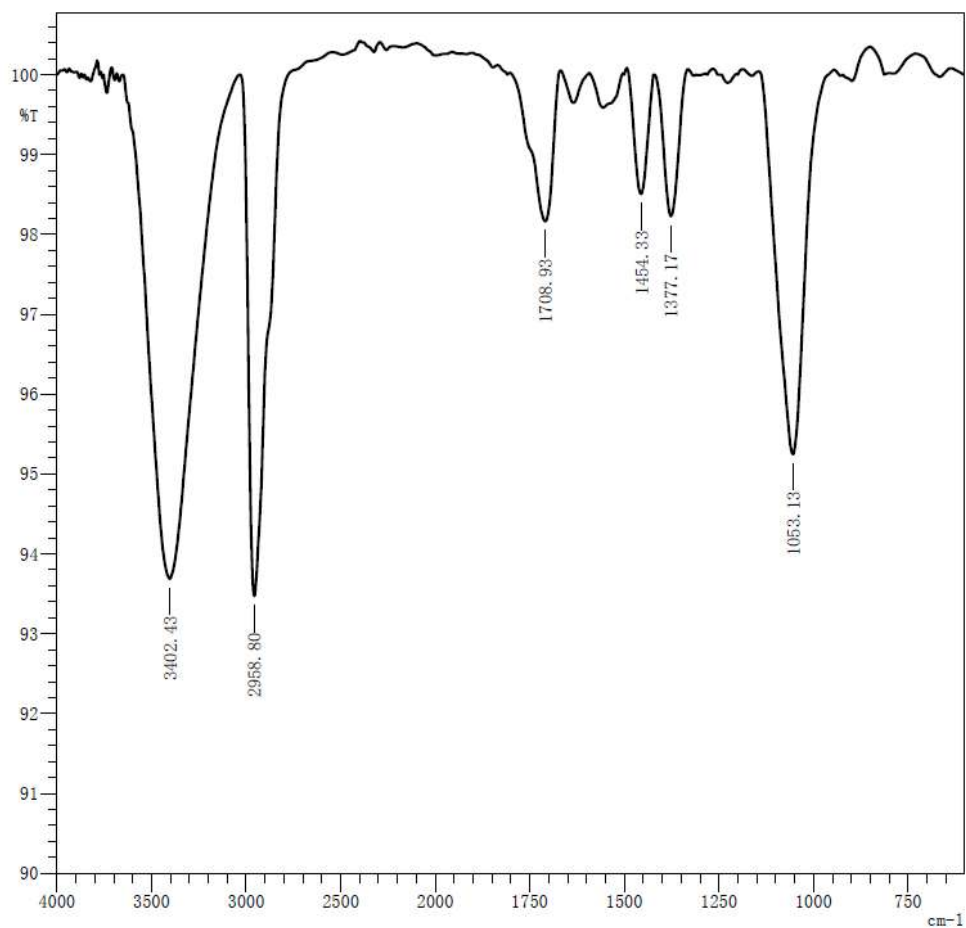
FigureS45.  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of compound 5



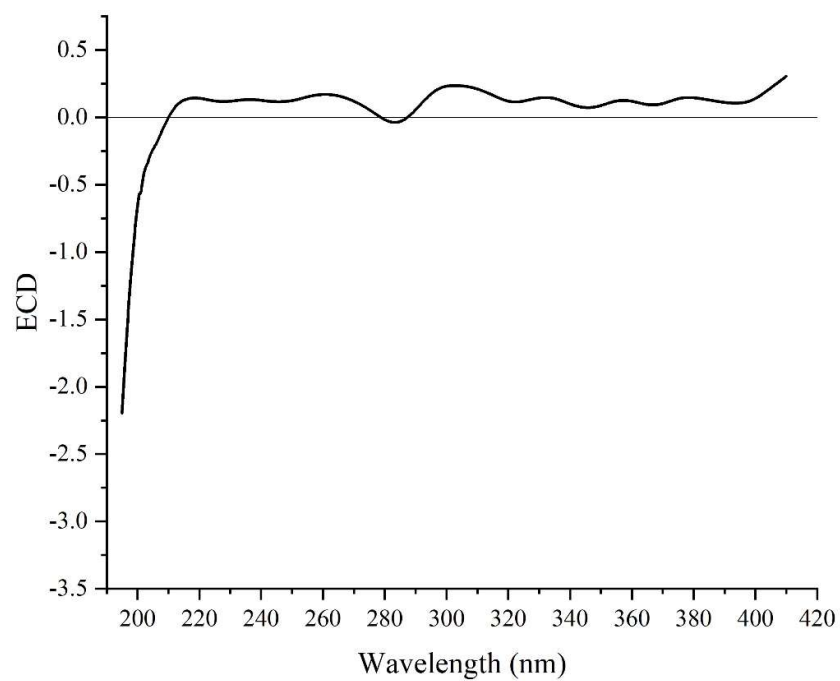
**FigureS46.** NOESY NMR spectrum of compound 5.



**FigureS47.** UV spectrum of compound 5



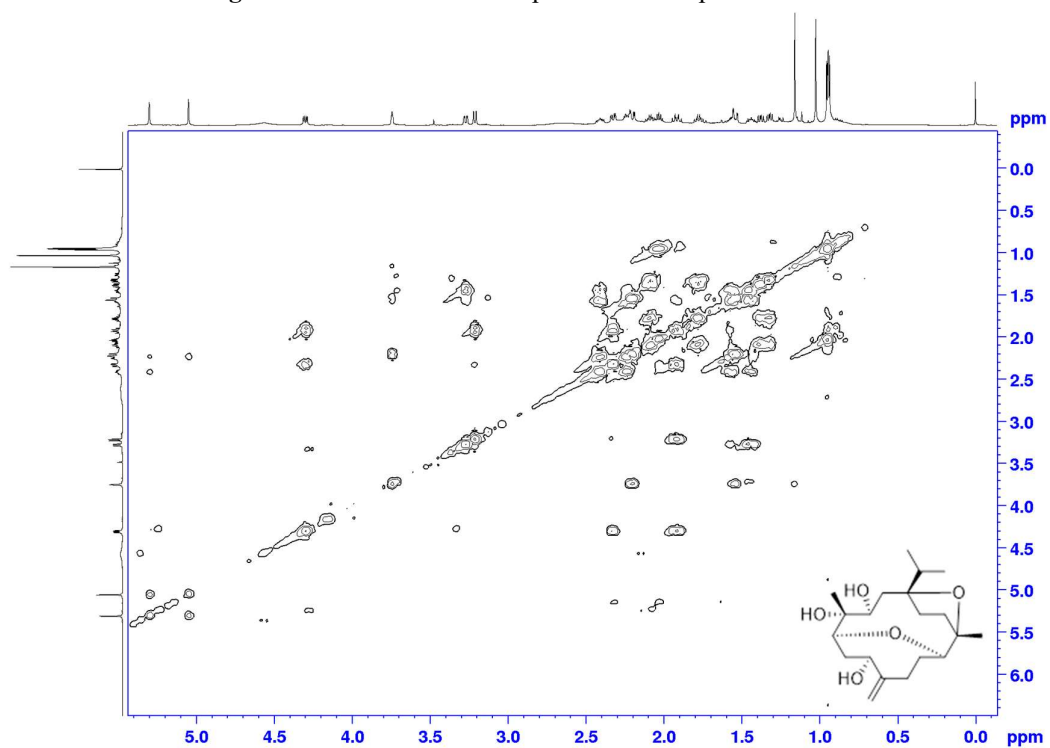
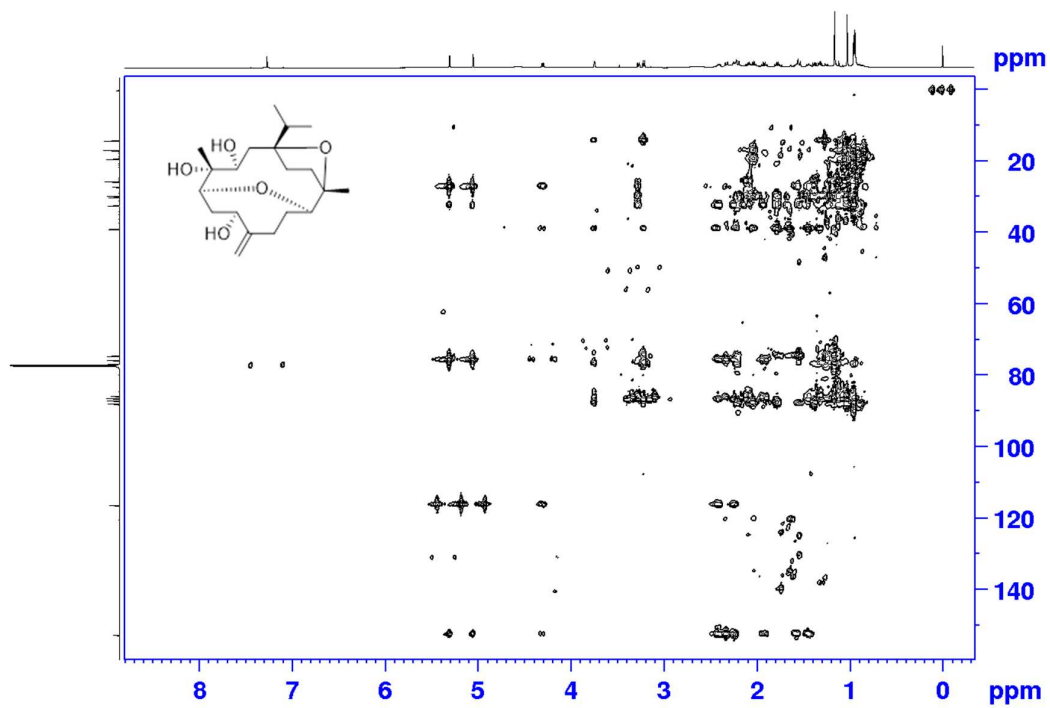
**FigureS48.** IR spectrum of compound **5**.



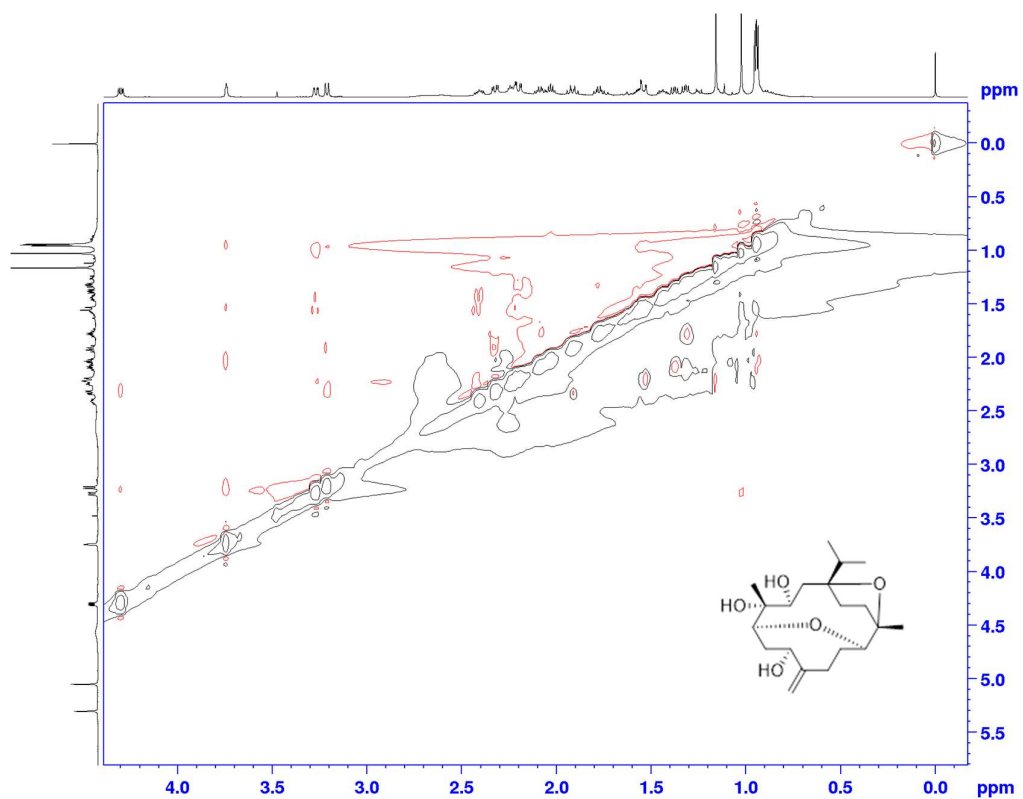
**FigureS49.** ECD spectrum of compound **5**



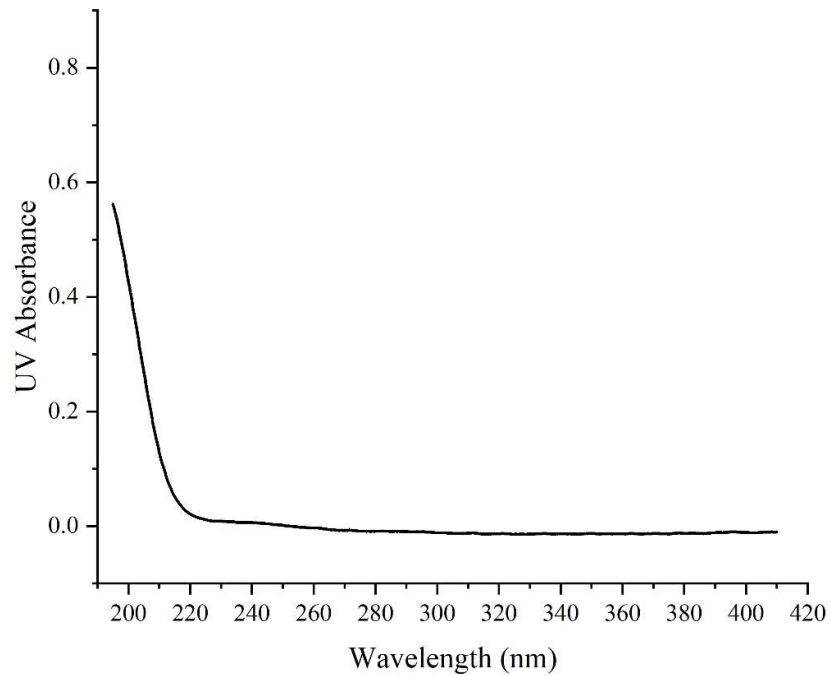




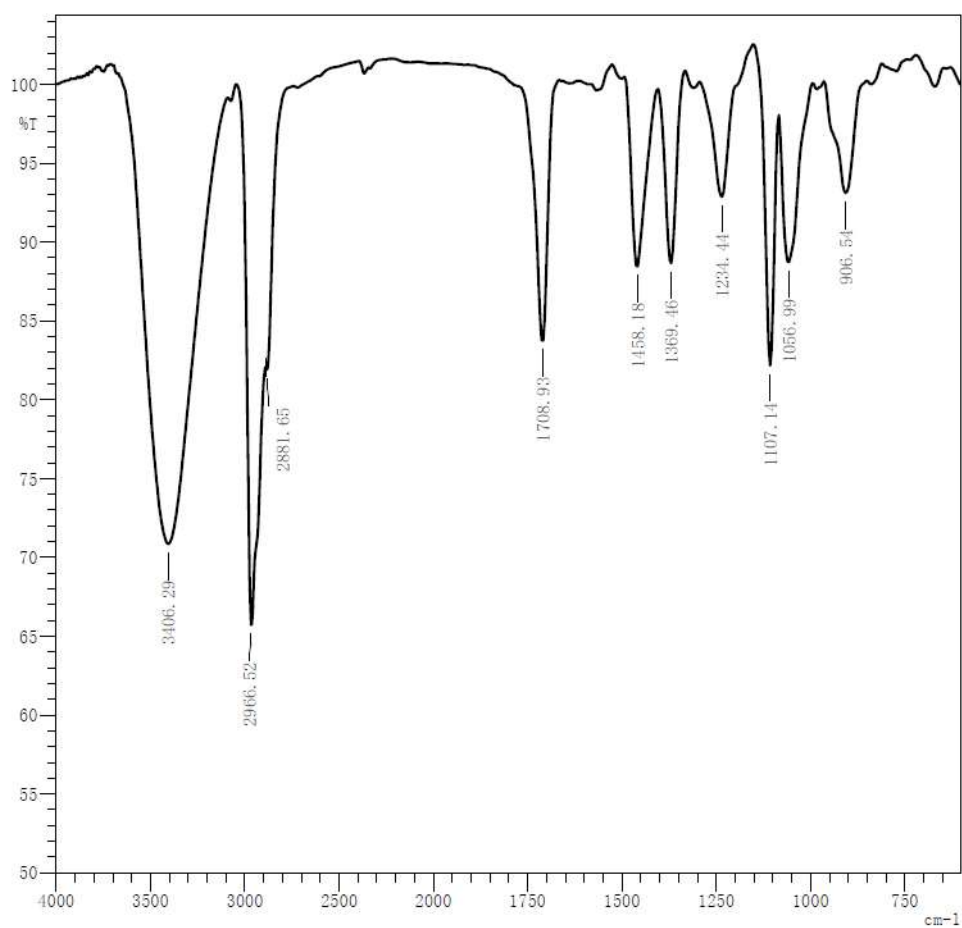




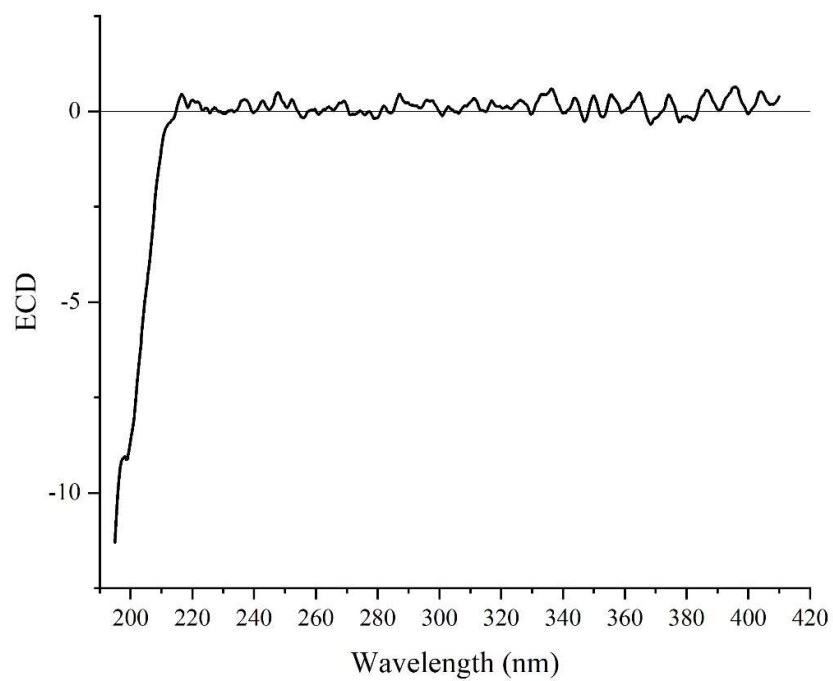
**FigureS56.** NOESY NMR spectrum of compound **6**



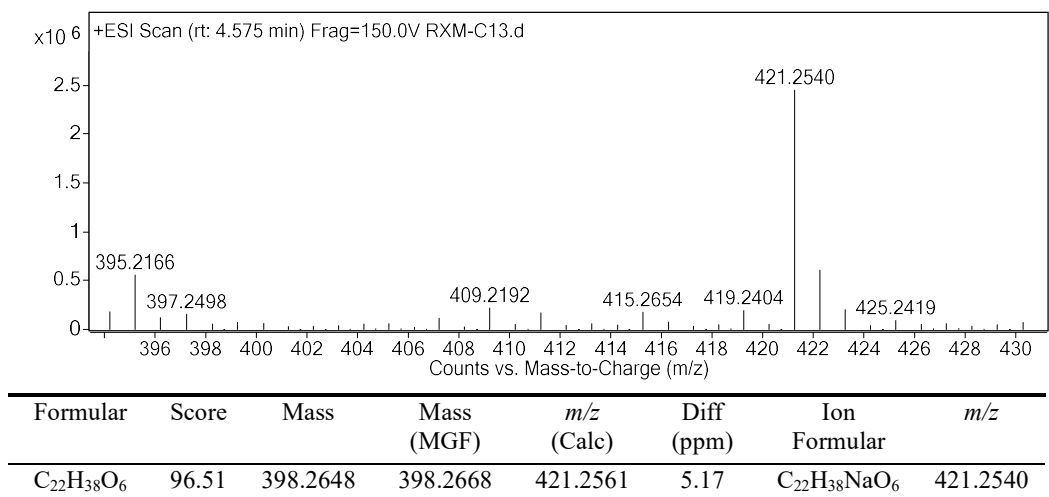
**FigureS57.** UV spectrum of compound **6**



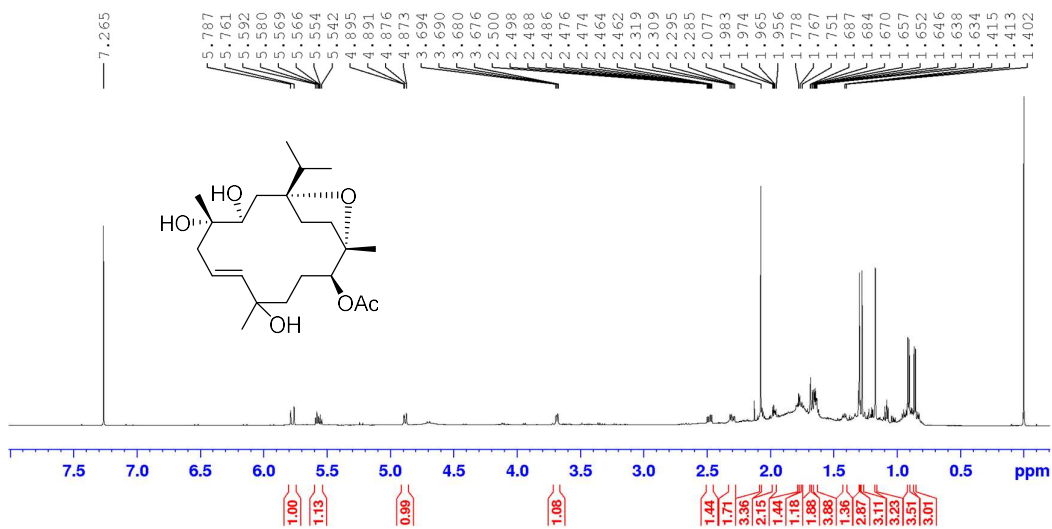
**FigureS58.** IR spectrum of compound 6



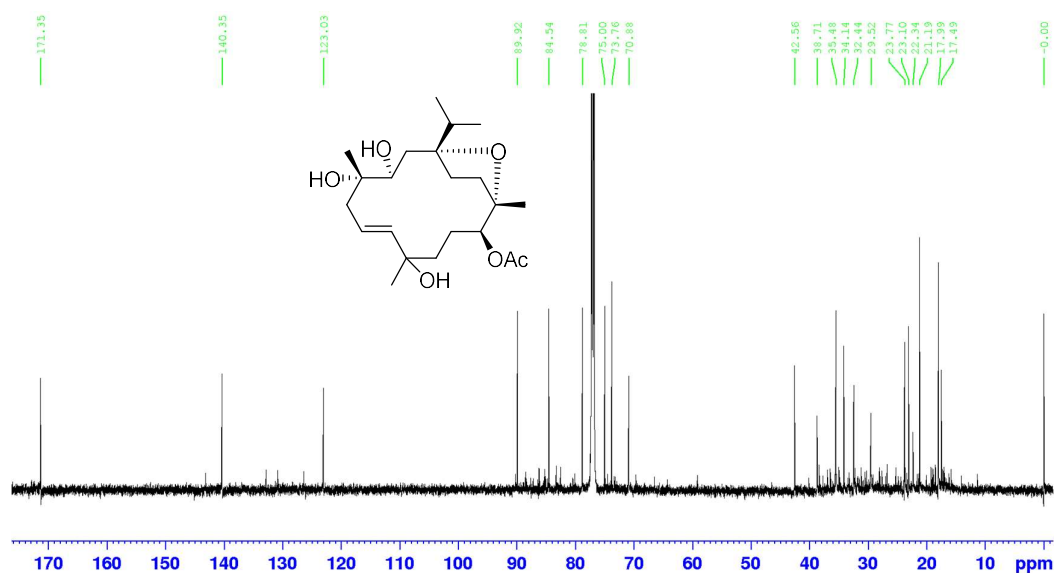
**FigureS59.** ECD spectrum of compound 6.



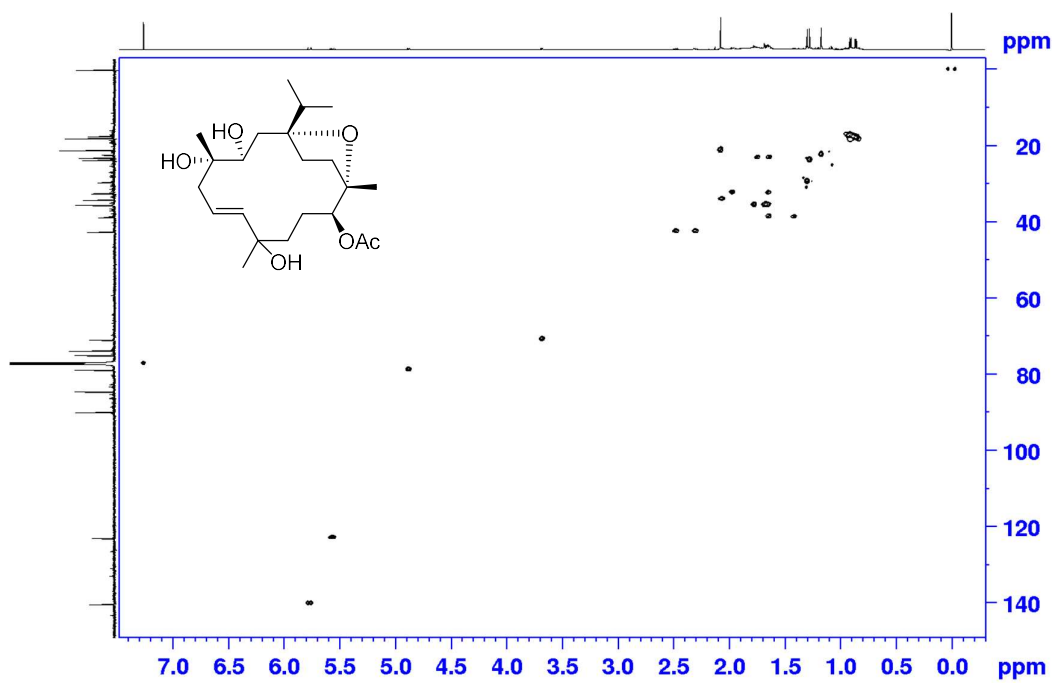
**FigureS60.** HRESIMS spectrum of compound 7.



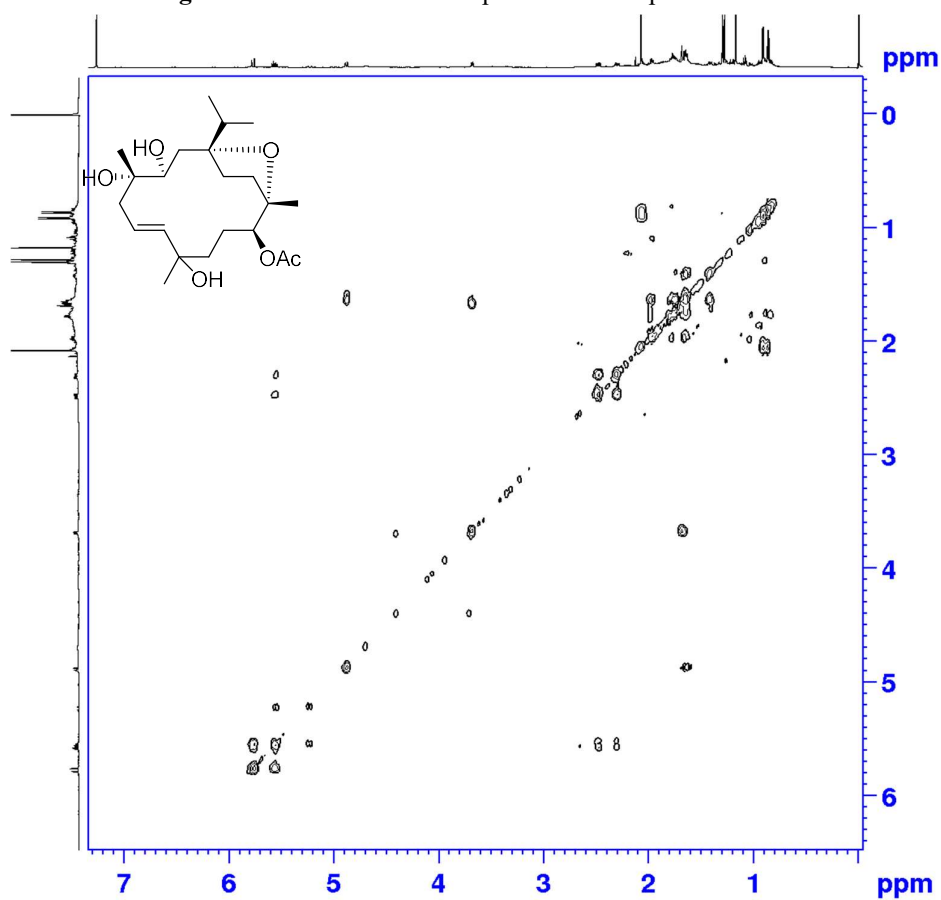
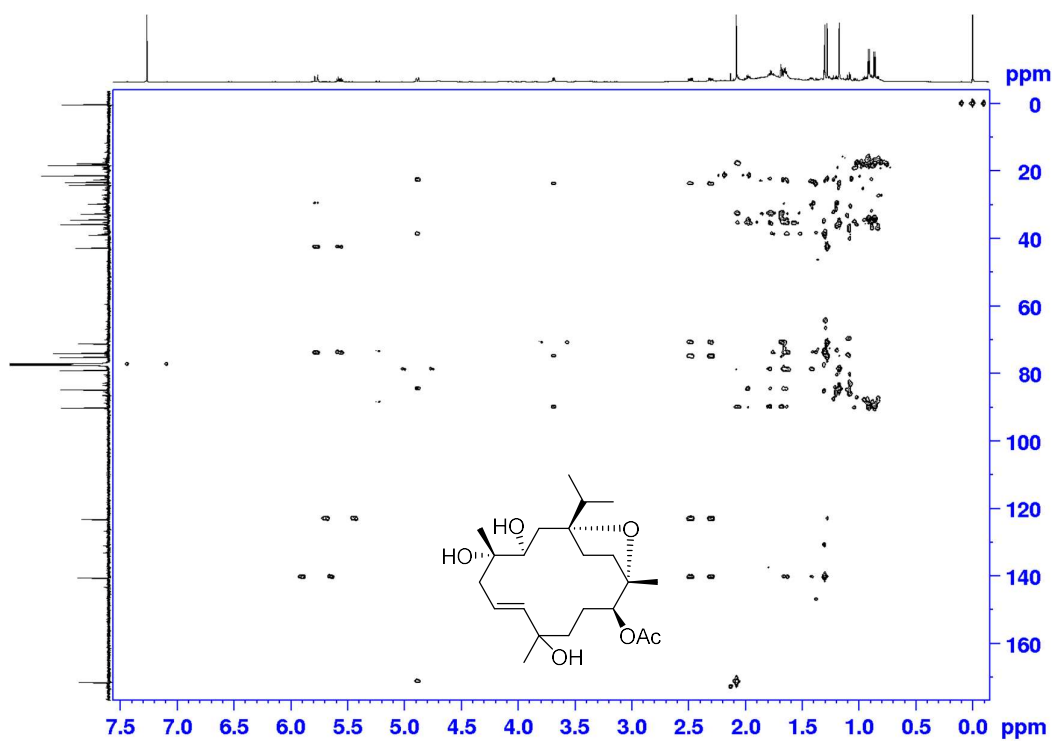
**FigureS61.** <sup>1</sup>H NMR spectrum of compound 7

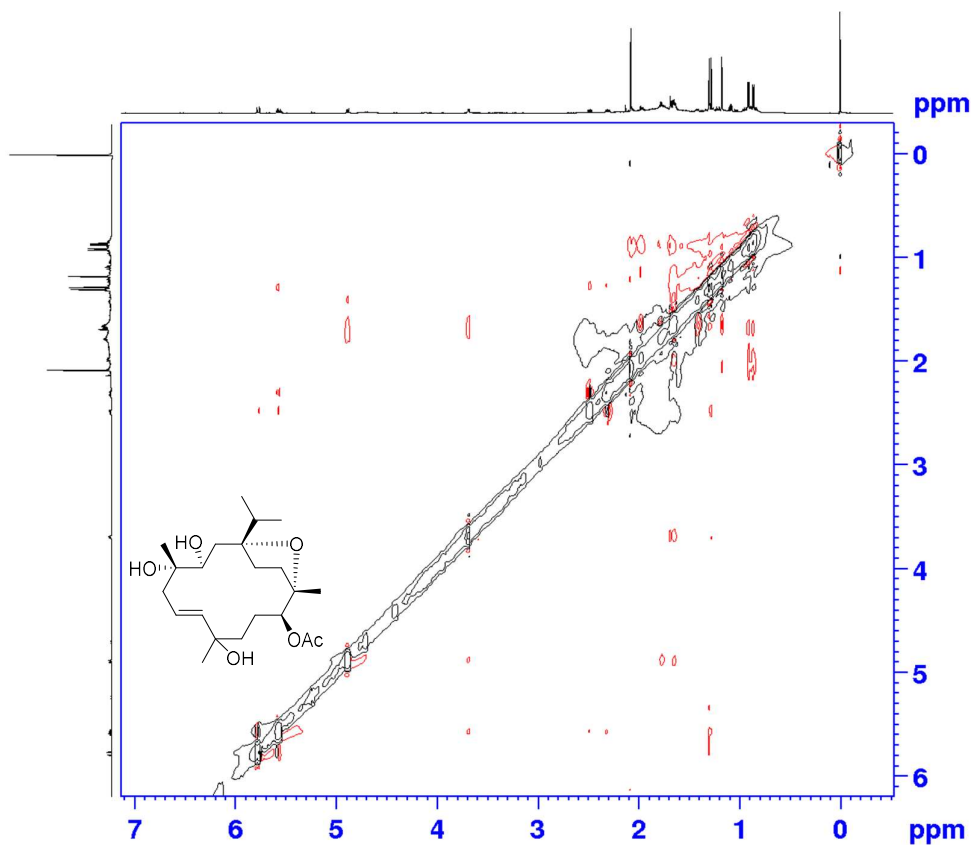


FigureS62.  $^{13}\text{C}$  NMR spectrum of compound 7

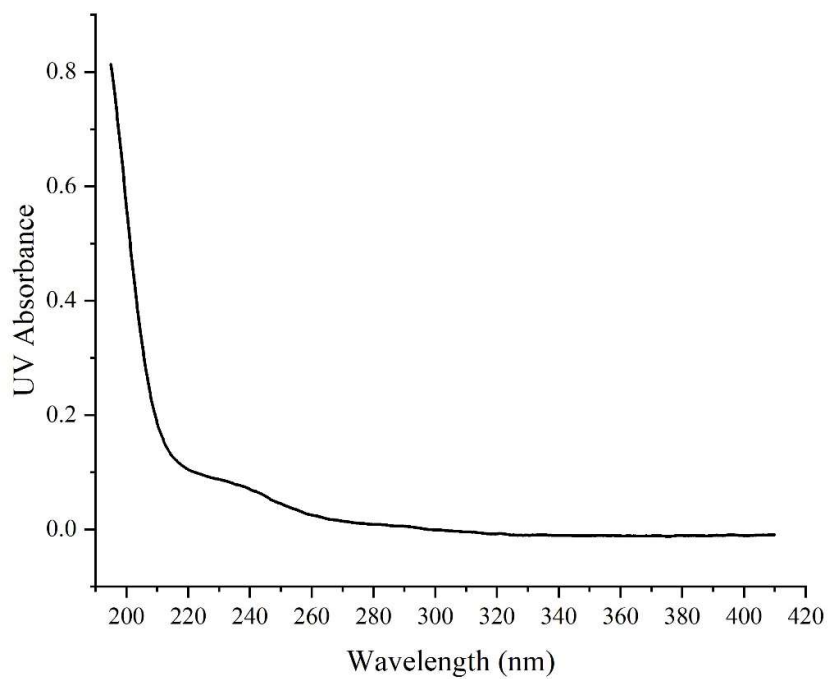


FigureS63. HSQC NMR spectrum of compound 7

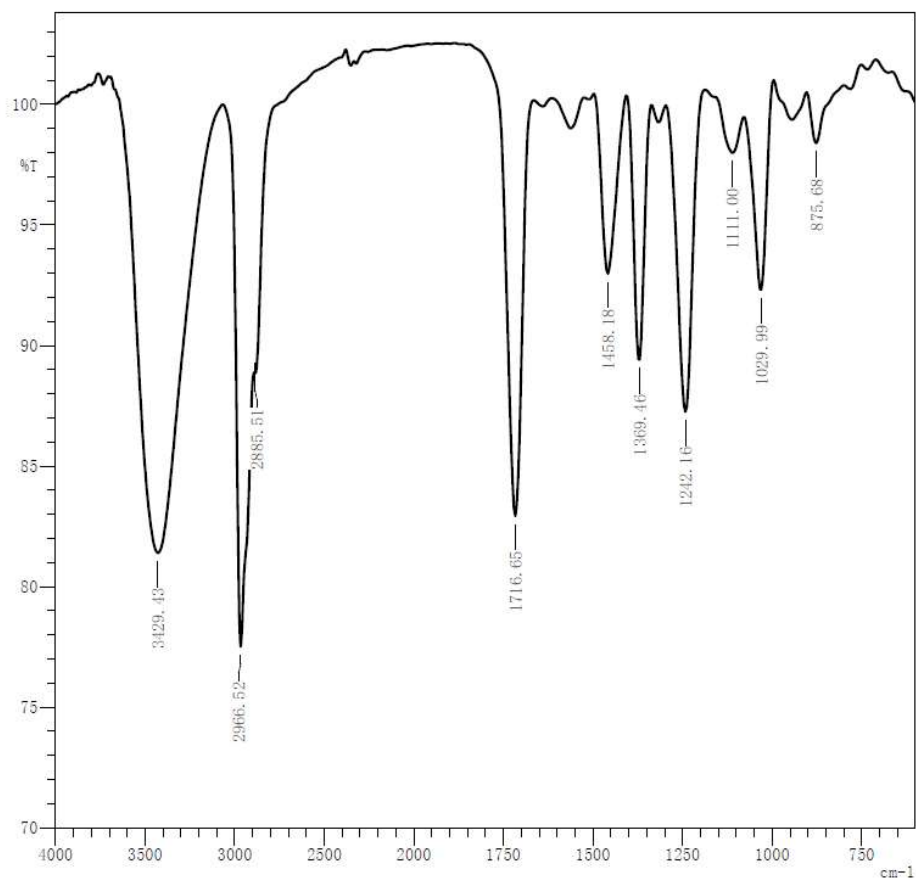




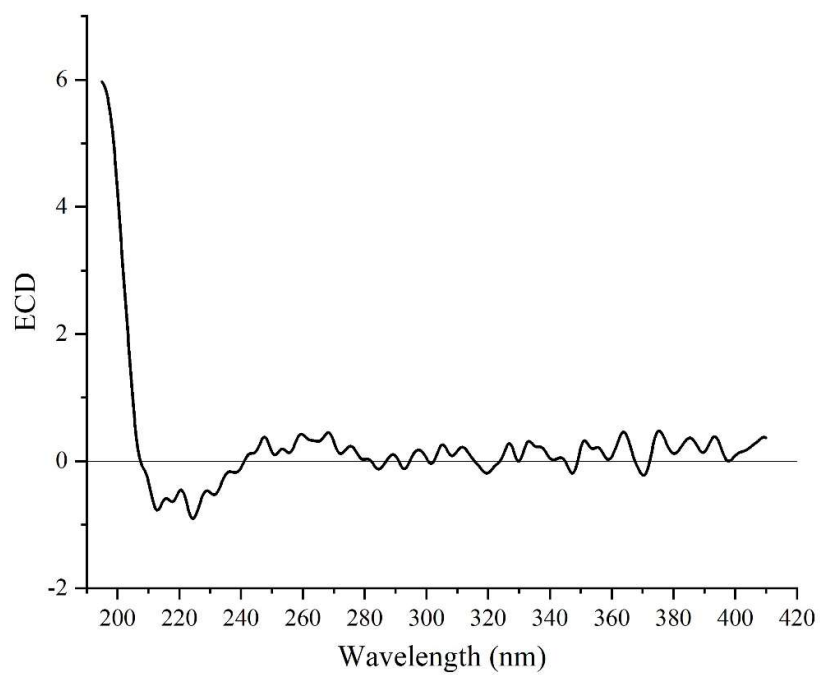
**FigureS66.** NOESY NMR spectrum of compound 7



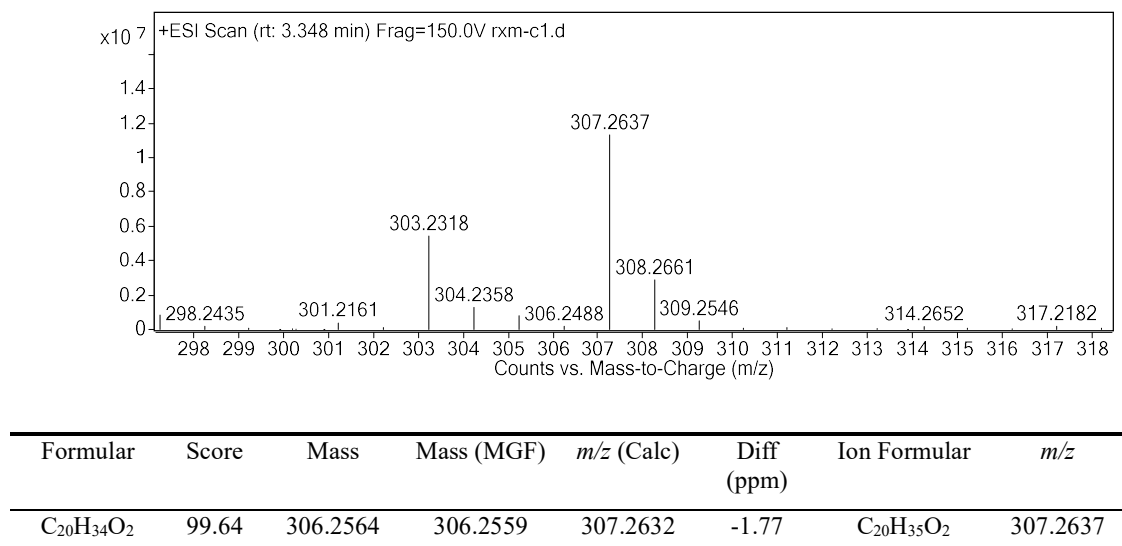
**FigureS67.** UV spectrum of compound 7



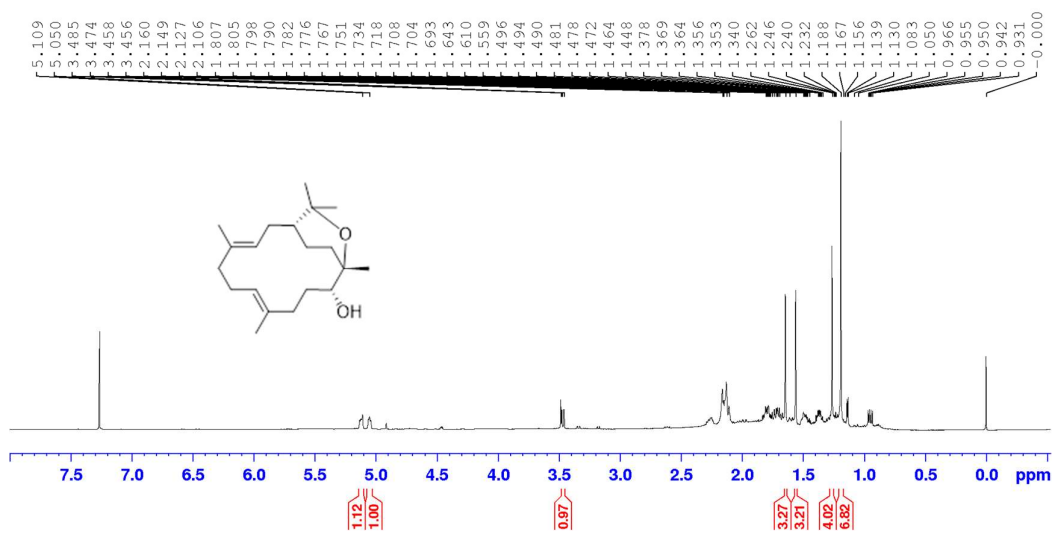
**FigureS68.** IR spectrum of compound 7



**FigureS69.** ECD spectrum of compound 7



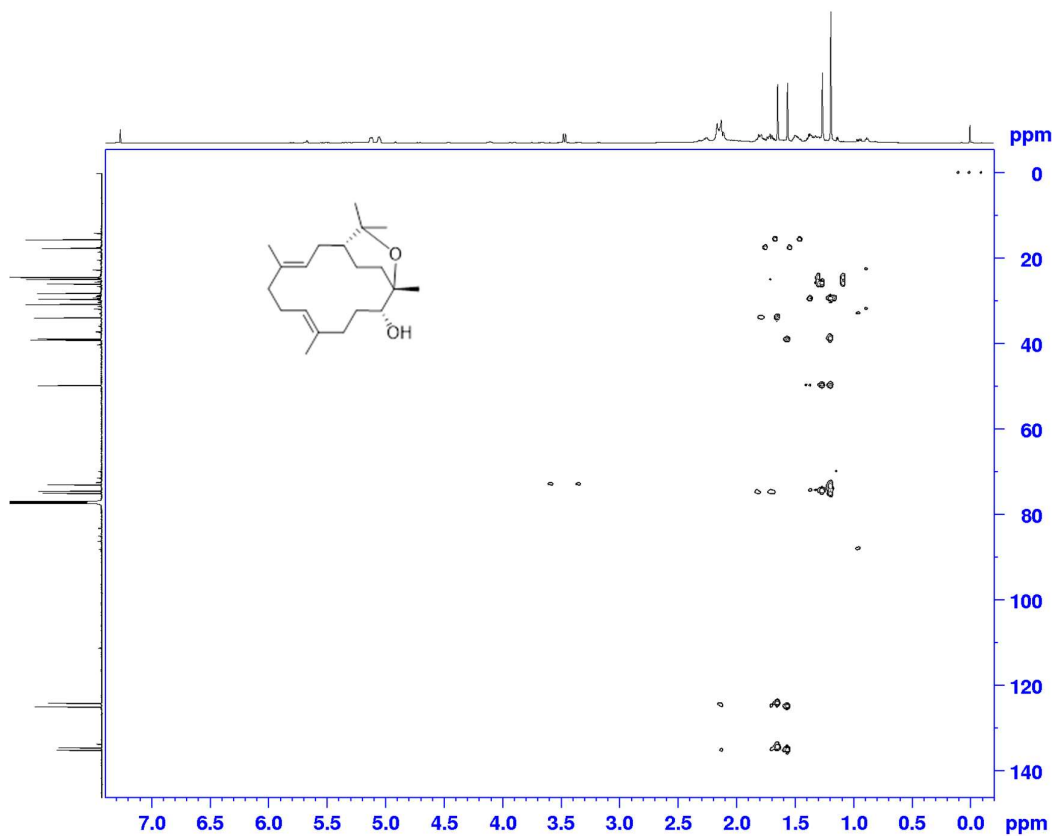
**FigureS70.** HRESIMS spectrum of compound **8**.



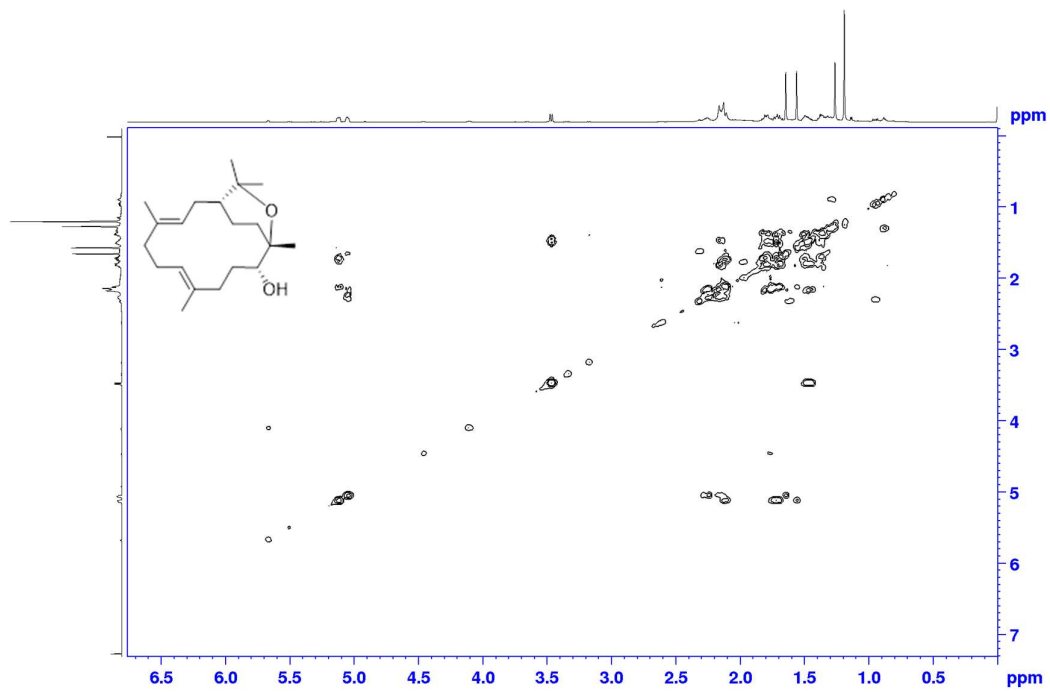
**FigureS71.** <sup>1</sup>H NMR spectrum of compound **8**



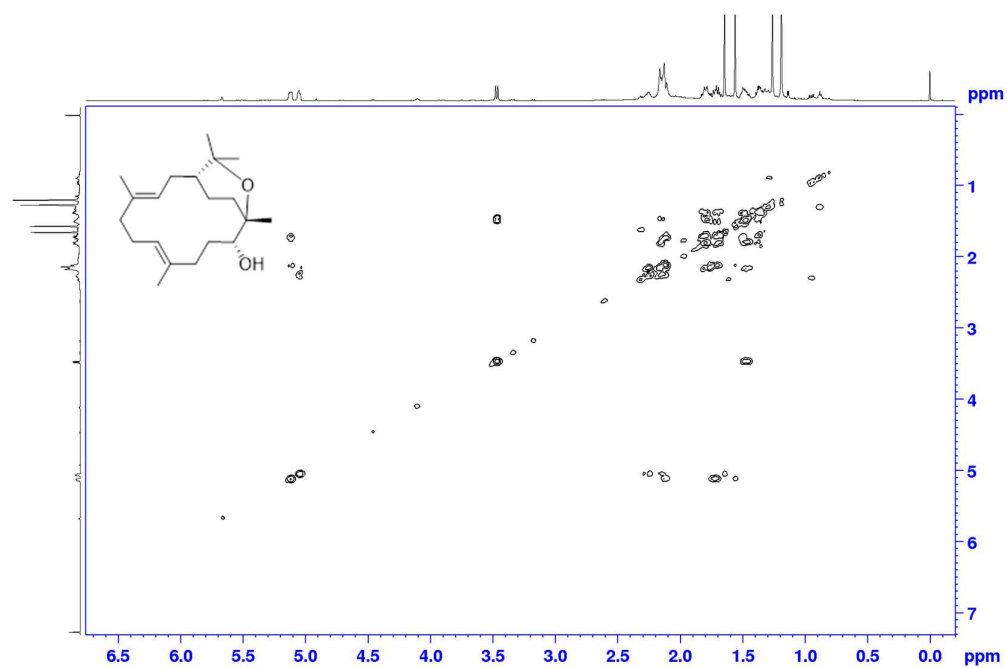




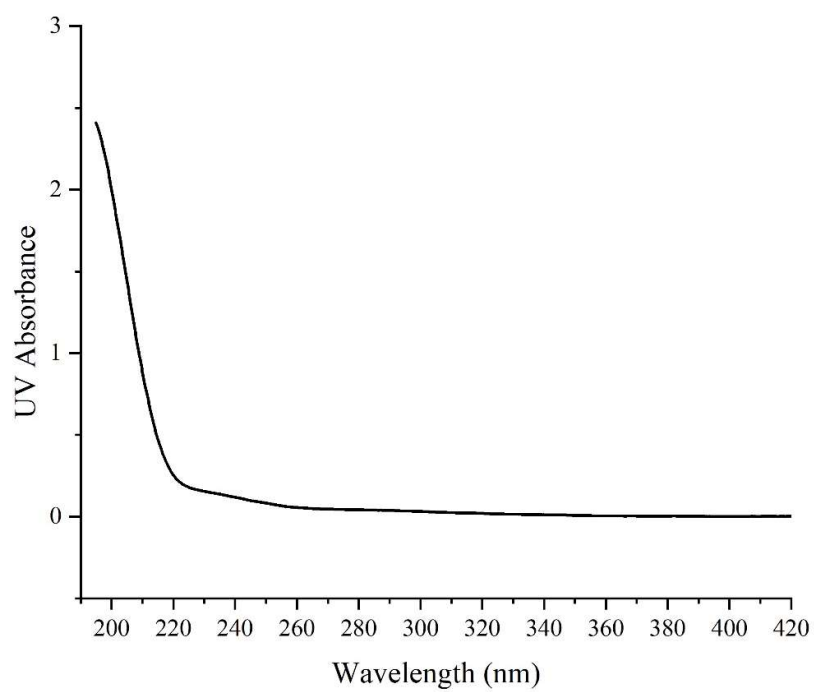
FigureS74. HMBC NMR spectrum of compound **8**



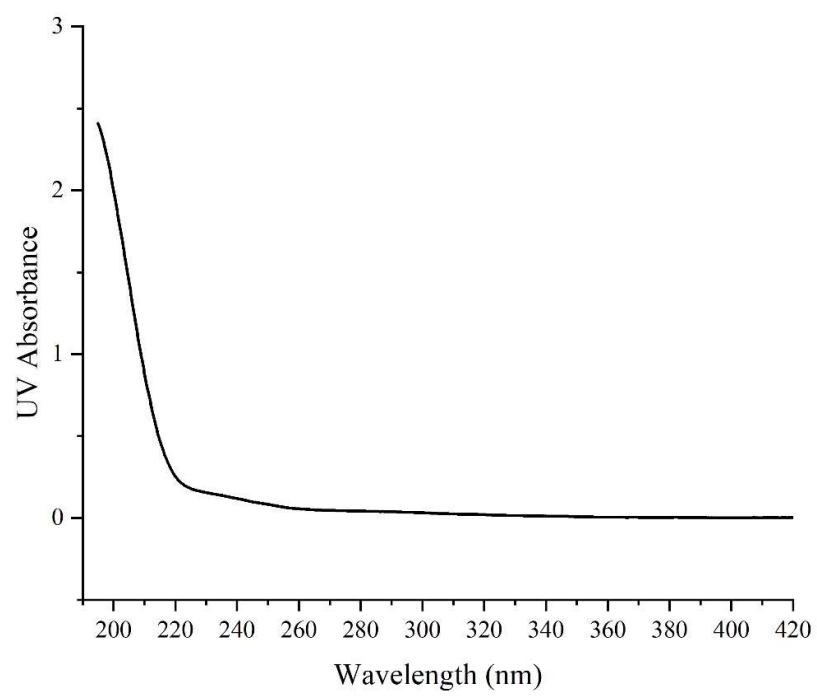
FigureS75.  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of compound **8**



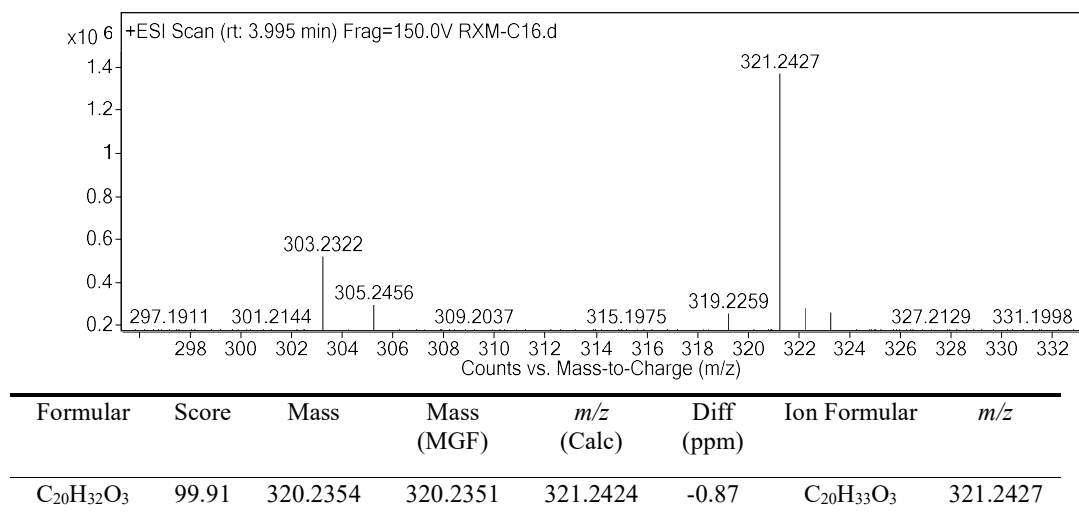
**FigureS76.** NOESY NMR spectrum of compound **8**



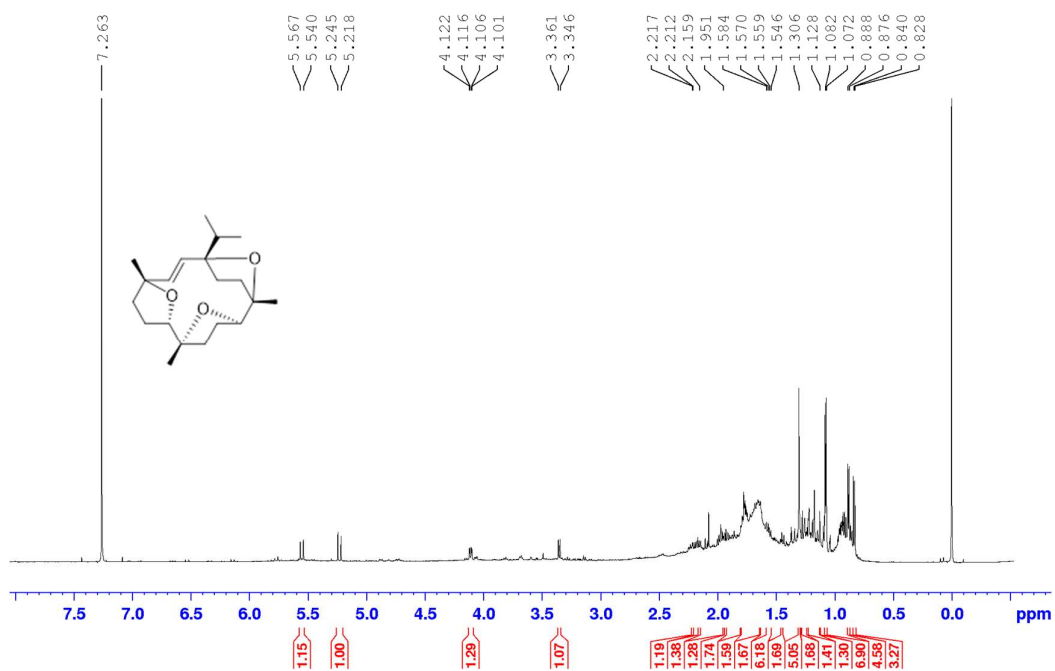
**FigureS77.** UV spectrum of compound **8**



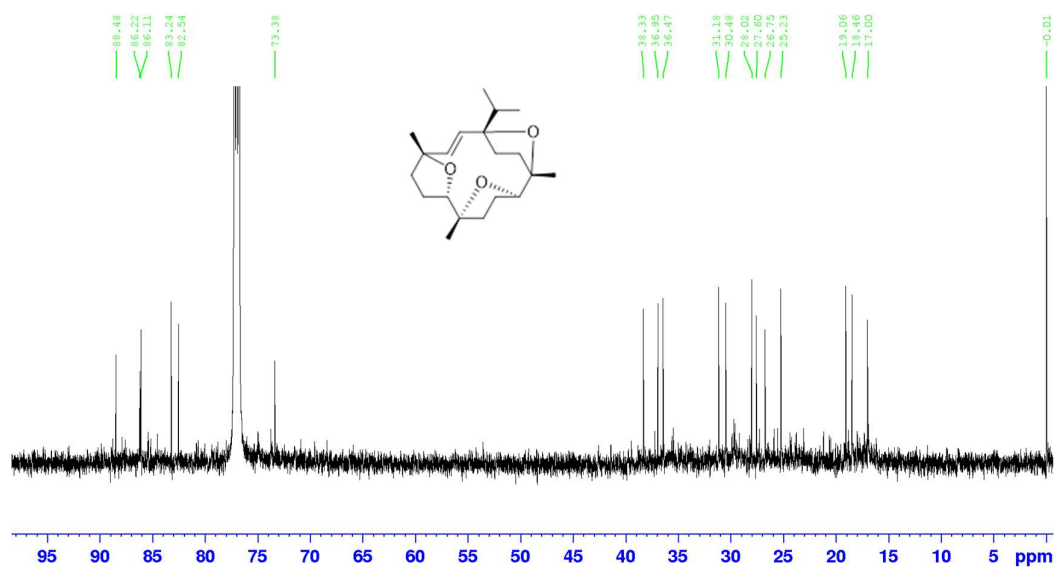
**FigureS78.** ECD spectrum of compound **8**



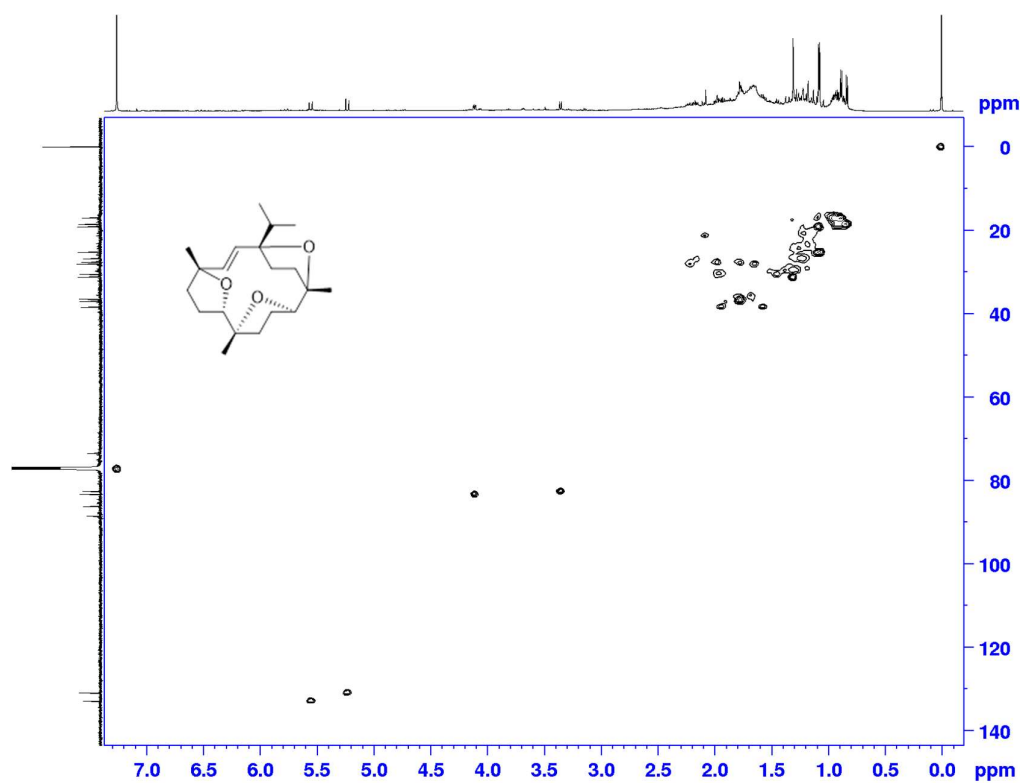
**FigureS79.** HRESIMS spectrum of compound **9**.



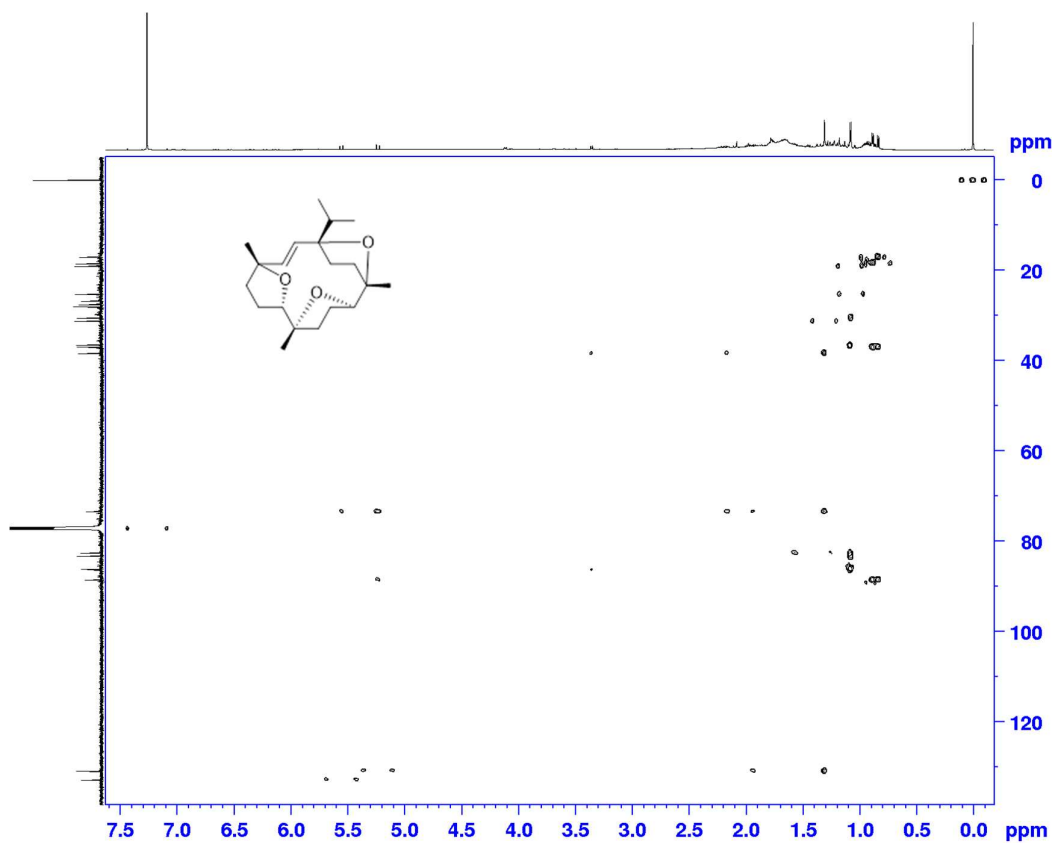
**FigureS80.** <sup>1</sup>H NMR spectrum of compound **9**



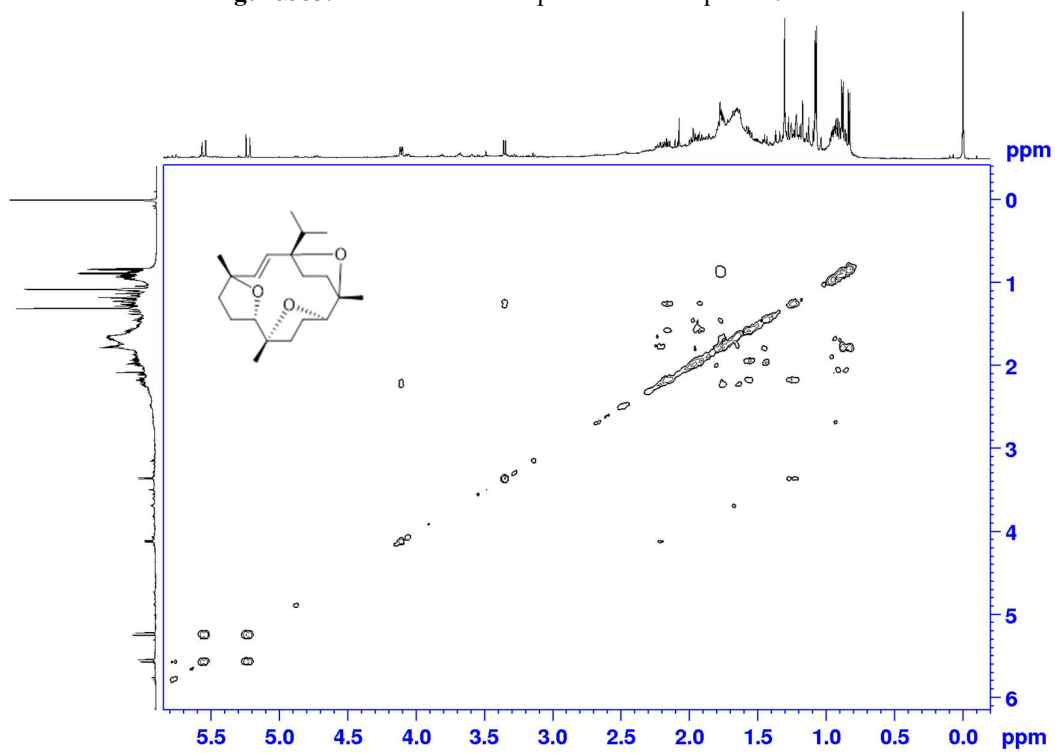
FigureS81. <sup>13</sup>C NMR spectrum of compound 9



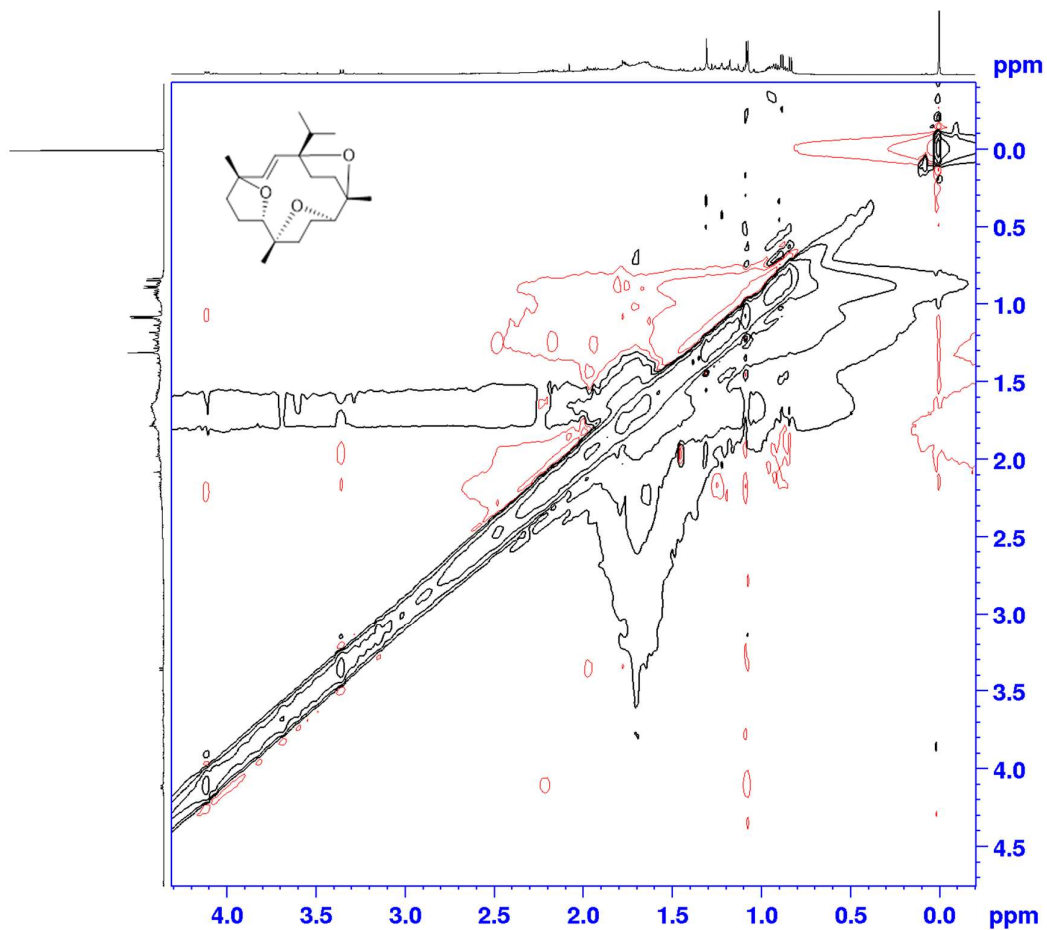
FigureS82. HSQC NMR spectrum of compound 9



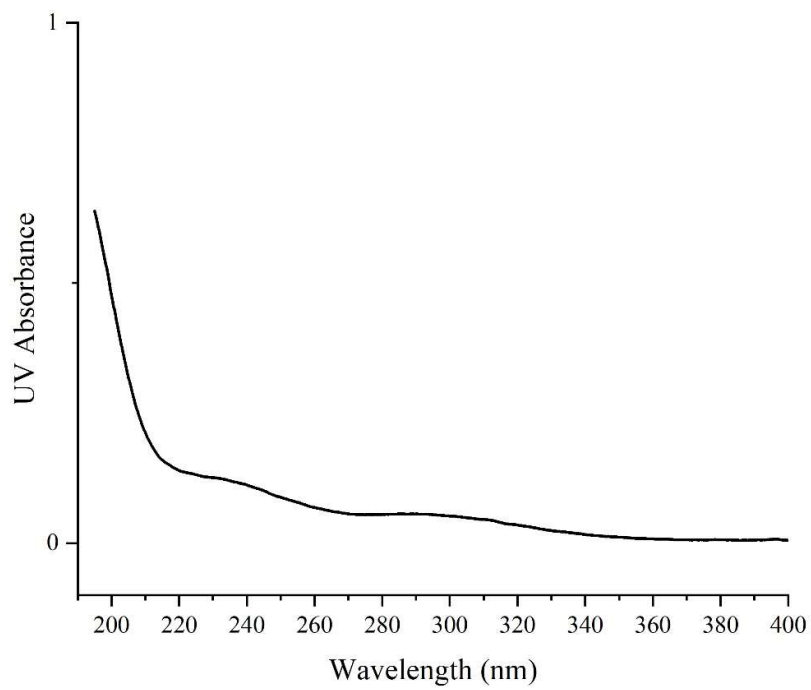
FigureS83. HMBC NMR spectrum of compound 9



FigureS84.  $^1\text{H}$ - $^1\text{H}$  COSY NMR spectrum of compound 9

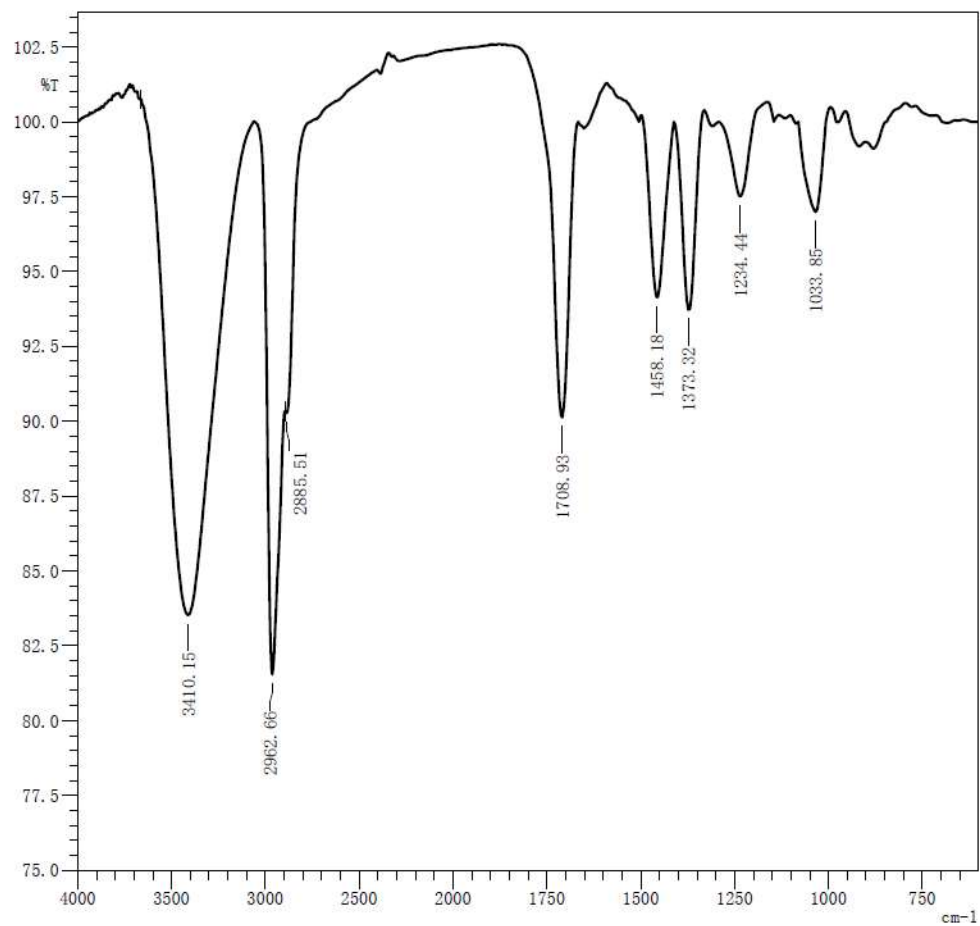


**FigureS85.** NOESY NMR spectrum of compound **9**

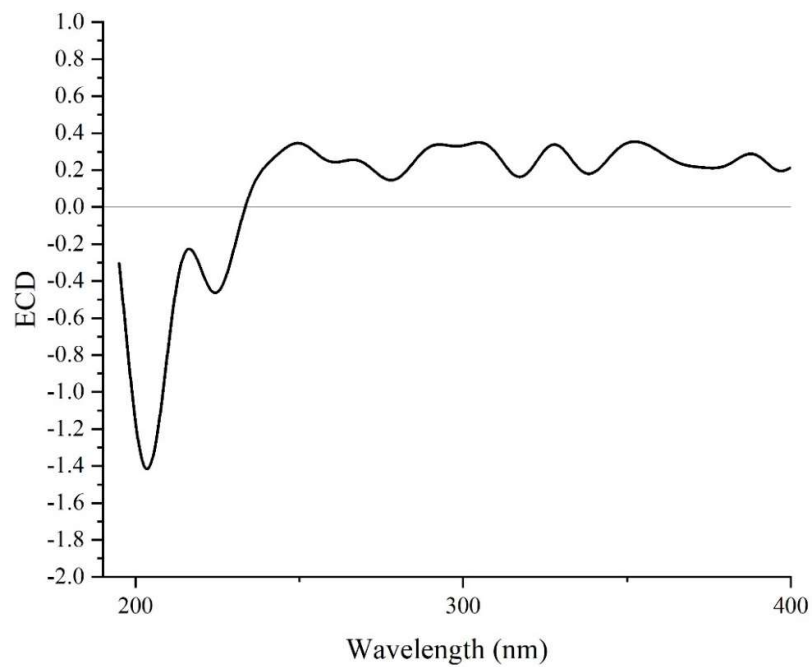


**FigureS86.** UV spectrum of compound **9**





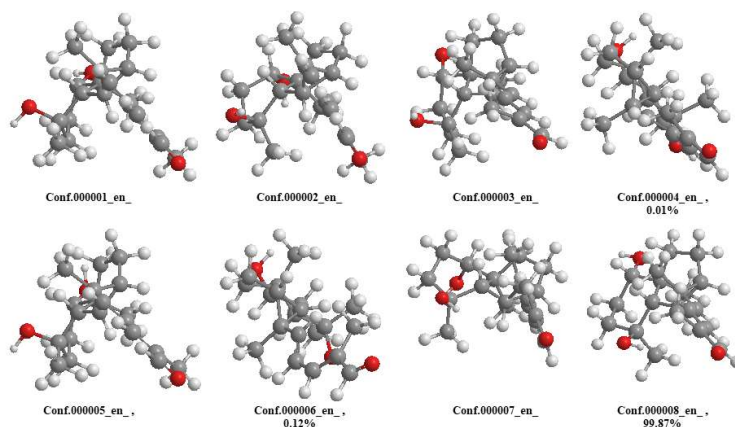
**FigureS87.** IR spectrum of compound **9**



**FigureS88.** ECD spectrum of compound **9**



**FigureS89.** Western blot of TGF-β/Smad signal molecules for screening isolated compounds **1**, **5**, **7**, **9**, **10**, and **11** at 25 μM. GAPDH was used as an invariant control for equal loading.



**FigureS90.** DFT computational optimized conformations of (1*R*,4*R*,5*R*,6*S*,7*S*,10*R*,13*R*)-**1**.

**TableS1.** Gibbs free energies<sup>a</sup> and equilibrium populations<sup>b</sup> of low-energy conformers of compound **1**.

Conformers	ΔG (a.u.)	P (%) / 100	G (a.u.)
Conf.000001_en	0.01365	0.0	-1005.373905
Conf.000002_en	0.01278	0.0	-1005.374774
Conf.000003_en	0.01159	0.0	-1005.375966
Conf.000004_en	0.00892	0.01	-1005.378635
Conf.000005_en	0.01303	0.0	-1005.374527
Conf.000006_en	0.00632	0.12	-1005.381236
Conf.000007_en	0.01335	0.0	-1005.374209
Conf.000008_en	0.00000	99.87	-1005.387556

<sup>a</sup>wB97M-V/def2-TZVP, in a.u.

<sup>b</sup>From ΔG values at 298.15 K.

**TableS2.** Cartesian coordinates for the low-energy reoptimized random research conformers of compound **1** at B3LYP-D3(BJ)/6-31G\* level of theory in methanol.

Conf.000004 en		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-6.411856	0.643691	-7.962031
1	6	0	-5.525125	-1.754469	-6.61434
2	6	0	-4.710425	-1.280432	-3.861802
3	6	0	-6.888961	0.100888	-2.486629
4	6	0	-7.898505	2.546685	-3.759552
5	6	0	-8.577284	1.933163	-6.543176
6	6	0	-6.355031	0.490205	0.307909
7	6	0	-7.92659	2.352141	1.807486
8	6	0	-9.959718	3.892998	0.470934
9	6	0	-10.349893	3.250761	-2.342567
10	6	0	-8.112397	-0.470267	2.34249
11	6	0	-2.121746	0.017988	-3.766268
12	8	0	-4.530285	-3.642302	-2.548362
13	8	0	-9.501172	4.066444	-7.870721
14	6	0	-6.050938	4.793809	-3.630494
15	1	0	-8.450024	-1.265909	-2.649891
16	1	0	-6.889531	3.417199	3.247378
17	1	0	-4.359361	0.431608	0.815324
18	6	0	-10.512234	-1.919817	1.714253
19	6	0	-4.736581	-2.719183	4.790306
20	6	0	-6.918348	-1.394937	4.725362
21	6	0	-3.447658	-3.74502	6.985429
22	6	0	-3.614927	-3.074276	9.461894
23	6	0	-5.229333	-1.01637	10.550219
24	1	0	-10.18096	0.60014	-6.49861
25	6	0	-1.993241	-4.492541	11.239295
26	8	0	-1.87027	-4.110906	13.495146
27	1	0	-4.824511	1.982278	-8.175783
28	1	0	-7.060699	0.201689	-9.889024
29	1	0	-3.960591	-2.647516	-7.666722
30	1	0	-7.080753	-3.139139	-6.559646
31	1	0	-11.78264	3.74467	1.473392
32	1	0	-9.404272	5.893708	0.622756
33	1	0	-11.676206	1.656872	-2.540834
34	1	0	-11.247056	4.855031	-3.314666
35	1	0	-2.032283	1.719866	-4.945271
36	1	0	-1.593196	0.542731	-1.828947
37	1	0	-0.674389	-1.300098	-4.48212
38	1	0	-3.188275	-4.613721	-3.317045
39	1	0	-8.105458	5.212925	-8.137418
40	1	0	-4.492665	4.638878	-4.993695
41	1	0	-7.054635	6.573094	-4.02487
42	1	0	-5.196473	4.968802	-1.746843
43	1	0	-10.050118	-3.885189	1.207493
44	1	0	-11.778774	-1.966563	3.367055
45	1	0	-11.575701	-1.082003	0.145692
46	1	0	-3.860911	-3.1486	2.962524
47	1	0	-7.993461	-1.058485	6.459102
48	1	0	-2.083687	-5.246966	6.554576
49	1	0	-5.270897	0.654982	9.310925

50	1	0	-7.200834	-1.647773	10.803662
51	1	0	-4.505524	-0.488663	12.423782
52	1	0	-0.825166	-6.009507	10.327543

Conf.000006 en		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-6.307867	1.007363	-7.979236
1	6	0	-5.054885	-1.262709	-6.708538
2	6	0	-4.36177	-0.777332	-3.93397
3	6	0	-6.751436	0.215602	-2.549649
4	6	0	-8.161057	2.49197	-3.757134
5	6	0	-8.68492	1.858509	-6.570278
6	6	0	-6.309606	0.626353	0.263946
7	6	0	-8.209828	2.073268	1.789611
8	6	0	-10.479337	3.268742	0.478785
9	6	0	-10.717493	2.697725	-2.363956
10	6	0	-7.900335	-0.763628	2.26809
11	6	0	-2.000692	0.892483	-3.74315
12	8	0	-3.781627	-3.210435	-2.912359
13	8	0	-9.951081	3.842799	-7.845561
14	6	0	-6.739013	5.01825	-3.52898
15	1	0	-8.056365	-1.38938	-2.76314
16	1	0	-7.433216	3.250445	3.30224
17	1	0	-4.338248	0.92358	0.806975
18	6	0	-9.935483	-2.607597	1.479381
19	6	0	-6.695838	-3.556795	5.949939
20	6	0	-6.453109	-1.415551	4.565578
21	6	0	-5.289784	-4.283958	8.186233
22	6	0	-3.292583	-3.166178	9.36529
23	6	0	-1.973109	-0.781128	8.589694
24	1	0	-10.031237	0.265224	-6.591806
25	6	0	-2.322738	-4.464619	11.637973
26	8	0	-0.555911	-3.749355	12.910681
27	1	0	-4.966657	2.601933	-8.11097
28	1	0	-6.840462	0.538094	-9.935243
29	1	0	-3.352026	-1.856092	-7.747344
30	1	0	-6.358492	-2.887062	-6.735073
31	1	0	-12.248412	2.749644	1.451316
32	1	0	-10.290236	5.326672	0.727562
33	1	0	-11.746929	0.911116	-2.659391
34	1	0	-11.86623	4.166488	-3.283487
35	1	0	-0.394381	-0.155775	-4.543328
36	1	0	-2.191484	2.6799	-4.776912
37	1	0	-1.529662	1.360048	-1.771783
38	1	0	-3.417819	-3.00793	-1.133579
39	1	0	-8.746269	5.181539	-8.144554
40	1	0	-5.124793	5.154628	-4.827164
41	1	0	-8.020622	6.601723	-3.950485
42	1	0	-6.00068	5.313714	-1.610918
43	1	0	-9.104175	-4.434211	0.924526
44	1	0	-11.255007	-2.946218	3.051944
45	1	0	-11.053515	-1.917937	-0.119174
46	1	0	-8.121228	-4.929274	5.355816
47	1	0	-5.064921	-0.001276	5.134575

48	1	0	-5.948069	-6.046737	9.05679
49	1	0	-3.228924	0.876391	8.742401
50	1	0	-0.33734	-0.471505	9.829445
51	1	0	-1.315389	-0.877617	6.614597
52	1	0	-3.371333	-6.238862	12.134952

Conf.000008 en		Standard Orientation (A.U.)			
Center number	Atomic number	Atomic Type	X	Y	Z
0	6	0	-10.679822	-0.121417	-7.163672
1	6	0	-11.355287	-1.751796	-4.878877
2	6	0	-9.052642	-2.409205	-3.241351
3	6	0	-7.655709	0.084631	-2.573223
4	6	0	-6.963446	1.872678	-4.802052
5	6	0	-9.380174	2.33457	-6.367644
6	6	0	-5.40315	-0.33539	-0.828248
7	6	0	-3.517448	1.745702	-0.448641
8	6	0	-3.780243	4.205015	-1.921266
9	6	0	-6.151051	4.403685	-3.593212
10	6	0	-5.220185	0.97833	1.762901
11	6	0	-7.447193	-4.463447	-4.505852
12	8	0	-10.080674	-3.408003	-0.950762
13	8	0	-8.727253	3.854347	-8.473299
14	6	0	-4.816853	0.883703	-6.496427
15	1	0	-9.111014	1.108825	-1.49846
16	1	0	-1.552335	1.142943	-0.222925
17	1	0	-4.607035	-2.241766	-0.866353
18	6	0	-7.304229	2.712179	2.668864
19	6	0	-4.502254	-0.597275	6.228495
20	6	0	-3.961207	-0.547086	3.729201
21	6	0	-3.141013	-2.156034	8.003549
22	6	0	-3.559186	-2.280134	10.53686
23	6	0	-5.544735	-0.797345	11.927626
24	1	0	-10.713656	3.370438	-5.120191
25	6	0	-1.933785	-3.991191	12.014819
26	8	0	-2.065362	-4.306033	14.28223
27	1	0	-9.445164	-1.151222	-8.48592
28	1	0	-12.413009	0.343156	-8.228297
29	1	0	-12.305846	-3.507941	-5.46409
30	1	0	-12.697573	-0.731946	-3.654932
31	1	0	-3.682604	5.844416	-0.637141
32	1	0	-2.098928	4.34828	-3.139596
33	1	0	-7.760835	5.126756	-2.48576
34	1	0	-5.824398	5.795808	-5.101412
35	1	0	-5.73682	-4.904363	-3.407005
36	1	0	-8.584408	-6.199469	-4.621457
37	1	0	-6.838547	-3.951538	-6.42032
38	1	0	-8.6947	-3.763238	0.184926
39	1	0	-10.238302	4.163321	-9.447036
40	1	0	-3.233013	0.155591	-5.367729
41	1	0	-5.435578	-0.638055	-7.761082
42	1	0	-4.11139	2.416875	-7.70504
43	1	0	-8.036534	3.922738	1.159759
44	1	0	-8.901192	1.612736	3.42836
45	1	0	-6.603714	3.964059	4.176045

46	1	0	-6.019962	0.587592	6.972845
47	1	0	-2.42314	-1.765502	3.055406
48	1	0	-1.624621	-3.337191	7.223852
49	1	0	-5.259853	1.255239	11.713603
50	1	0	-7.458531	-1.234199	11.230466
51	1	0	-5.460392	-1.263529	13.948515
52	1	0	-0.495755	-5.0355	10.856843