Electronic Supplementary Information of *New Journal of Chemistry*

Sesquiterpenoids isolated from the rhizome of Curcuma phaeocaulis Valeton: antitumor activity, in silico molecular docking and molecular dynamics study

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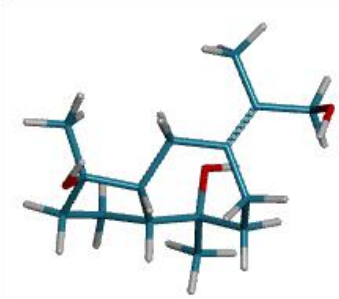
Table S1. Cartesian Coordinates and Equilibrium Populations of Low-energy Conformers of 1*S*, 4S, 5*S*, 10*R* in CH_3OH of Compound **1.**

Compound **1** conformer 1				Compound **1** conformer 2			
C	-0.542352792	-1.305018108	-0.16767212	C	-0.900050662	-1.414756852	-0.45976036
C	-0.903487757	0.040473604	0.555036837	C	-1.046634197	-0.360861729	0.701750757
C	-0.303969562	1.347577163	0.026940351	C	-0.163134445	0.888609579	0.706621669
C	1.2039931	1.347486173	0.073035989	C	1.334450079	0.66567024	0.661618952
C	1.831060986	0.811714949	-1.184173158	C	1.793231828	-0.755792498	0.492489505
C	1.66466857	-0.707159242	-1.357735497	C	1.593158226	-1.30336658	-0.930231339
C	0.23694132	-1.277526573	-1.499536418	C	0.17567965	-1.178134856	-1.528210392
C	-1.887650595	-2.075052109	-0.261085084	C	-2.329148104	-1.603467626	-1.014092219
C	-2.78889837	-1.424121943	0.785986148	C	-3.226602393	-1.26770086	0.173163421
C	-2.444795646	0.065407569	0.677943228	C	-2.571524756	-0.023954643	0.772807629
C	1.900042533	1.730893977	1.160751258	C	2.160481595	1.729428647	0.727412315
C	3.403704905	1.703431026	1.213025442	C	3.655545056	1.63386361	0.642606651
C	1.266308503	2.173367245	2.455214876	C	1.621413097	3.132111699	0.894477748
C	0.374468194	-2.715280995	-2.024376756	C	0.04340758	-2.198269315	-2.665082024
H	0.115601243	-1.86207369	0.511546888	H	-0.613544116	-2.364974972	0.012755986
H	-0.551196938	-0.066514041	1.590766727	H	-0.849331731	-0.899169074	1.637979558
O	-0.53128705	-0.506362471	-2.448900249	O	-0.040905607	0.144693471	-2.072924101
O	-2.75979655	0.7904167	1.886585779	O	-3.018392676	0.101954738	2.139617925
C	-3.155371093	0.720653125	-0.502793282	C	-2.974089326	1.231843618	0.001566003
O	3.826179136	0.404032804	1.699337753	O	4.292270165	1.968091795	1.901486861
H	-0.714639926	2.169405014	0.624266737	H	-0.431282348	1.541341252	-0.129336643
H	-0.622523449	1.504831381	-1.007344177	H	-0.408341328	1.457990138	1.618365948
H	2.903324297	1.022309922	-1.225519813	H	2.847913614	-0.87024898	0.757558665
H	1.373066776	1.309830971	-2.049524847	H	1.238605148	-1.392965493	1.193367774
H	2.218922967	-0.989716793	-2.264267307	H	1.86665299	-2.366791162	-0.923454112
H	2.15280318	-1.224186325	-0.520889383	H	2.29140339	-0.802444911	-1.615864639
H	-2.322816723	-1.947855405	-1.258753542	H	-2.496426189	-2.615710993	-1.394837998
H	-1.761382842	-3.149161284	-0.094332674	H	-2.513683143	-0.905269155	-1.83912564
H	-3.855684561	-1.624464468	0.63095657	H	-3.185059997	-2.075227175	0.916630252
H	-2.515712418	-1.766157242	1.793012766	H	-4.275099985	-1.099284074	-0.096188926
H	3.754536223	2.483527108	1.904988926	H	4.035420323	2.378704962	-0.067733677
H	3.855468634	1.899641302	0.232816707	H	3.993889786	0.649157468	0.300366647
H	0.182701243	2.049506165	2.479054928	H	1.001046191	3.427254358	0.037301002
H	1.687444122	1.59657966	3.289219697	H	2.437051073	3.854927875	0.984207737
H	1.496756099	3.228052785	2.659090974	H	0.98973302	3.230260755	1.785898518
H	0.926799983	-2.713919493	-2.971241985	H	0.06030914	-3.222847061	-2.277907798
H	-0.604880278	-3.166903587	-2.200175349	H	0.880990966	-2.086283208	-3.365079419
H	0.92513322	-3.33925694	-1.311372662	H	-0.888795792	-2.046610242	-3.216475314
H	-0.067514815	-0.5478094	-3.296031805	H	0.575804563	0.254474952	-2.808626008
H	-3.71932695	0.897796563	1.919366069	H	-2.675963003	0.936608093	2.48589638

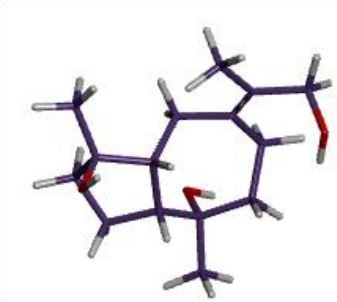
H	-4.240992621	0.613561075	-0.386895764	H	-2.562383213	2.132860194	0.469180897
H	-2.86203731	0.258010984	-1.449385026	H	-4.065926623	1.317128702	-0.00768163
H	-2.917139878	1.787149511	-0.555360045	H	-2.617126974	1.20020764	-1.032262971
H	4.775532891	0.454883335	1.870422291	H	3.903989125	1.385947675	2.567746412
Compound **1** conformer 3				Compound **1** conformer 4			
C	-0.785456754	-1.370015547	-0.318744898	C	-0.933246317	-1.398728157	-0.439606496
C	-0.842967057	-0.035465717	0.499782726	C	-1.129401861	-0.35182524	0.720054155
C	-0.249992869	1.213520092	-0.188507265	C	-0.179235021	0.842838725	0.826363072
C	1.257381096	1.243631658	-0.083945622	C	1.300673546	0.535066844	0.93431084
C	1.974361995	0.437546683	-1.128508477	C	1.696760644	-0.904958864	0.765584342
C	1.671582643	-1.069230885	-1.057851562	C	1.593509616	-1.405792115	-0.685944728
C	0.249366811	-1.51923423	-1.453761722	C	0.243459431	-1.202379051	-1.40428665
C	-2.244559964	-1.637843847	-0.807527844	C	-2.313703883	-1.507125842	-1.123467771
C	-3.048212257	-0.400859853	-0.400046959	C	-3.298154404	-1.125345623	-0.022504889
C	-2.350003145	0.093715084	0.858987717	C	-2.63142671	0.073778348	0.651055269
C	1.866833538	1.906586579	0.920315666	C	2.166021207	1.551762136	1.120220759
C	3.359144413	1.961115635	1.096475115	C	3.653452549	1.392108021	1.200379935
C	1.103540724	2.634502983	2.00663028	C	1.682544536	2.981630065	1.214659369
C	0.318318468	-3.000618485	-1.852743892	C	0.164410553	-2.198847561	-2.567333051
H	-0.515626248	-2.15655519	0.395265751	H	-0.737164628	-2.367500142	0.040786023
H	-0.288088699	-0.161577566	1.440632253	H	-1.05465788	-0.909842361	1.66258055
O	-0.222063673	-0.757090865	-2.588216784	O	0.140885039	0.136747878	-1.942776663
O	-2.652087596	-0.893533976	1.881056248	O	-3.197211892	0.216763475	1.97099216
C	-2.828839731	1.456203578	1.337749114	C	-2.886353416	1.356182724	-0.139170821
O	3.803735474	1.087605167	2.164878733	O	4.23179007	1.929616265	-0.017788411
H	-0.655939662	2.108568214	0.28688115	H	-0.480371488	1.424975263	1.71283379
H	-0.547229359	1.237152131	-1.242245768	H	-0.323160482	1.51133508	-0.027266327
H	3.057868186	0.554494633	-1.053954524	H	1.054666586	-1.530746632	1.39894703
H	1.684202783	0.800630019	-2.12389695	H	2.719409057	-1.08331609	1.106290448
H	1.887723257	-1.445878142	-0.048414947	H	1.81726917	-2.480748141	-0.68292085
H	2.376293676	-1.572015843	-1.735168005	H	2.372767529	-0.924375517	-1.293629652
H	-2.287294753	-1.807121925	-1.885584076	H	-2.499294455	-2.508456038	-1.524298057
H	-2.646531899	-2.528990343	-0.316183965	H	-2.384837074	-0.800536169	-1.959082019
H	-4.111462766	-0.601215406	-0.226067399	H	-3.376674952	-1.938778473	0.711624886
H	-2.970291507	0.380566042	-1.166255905	H	-4.304507581	-0.89307959	-0.388018538
H	3.656966583	2.967687845	1.414042282	H	4.033948435	1.963520354	2.06189214
H	3.904252776	1.730603847	0.174720535	H	3.959727831	0.348206316	1.326080463
H	0.794346199	3.63625222	1.677558821	H	1.159850829	3.296002026	0.301980126
H	1.739790726	2.76448176	2.887654133	H	2.521023057	3.666660971	1.368002924
H	0.204022568	2.101590955	2.326218668	H	0.97615335	3.119947263	2.04346925
H	0.760129917	-3.596038433	-1.045823121	H	0.097800742	-3.228555788	-2.199488427
H	0.94652554	-3.118191538	-2.743723937	H	1.065876186	-2.117206663	-3.187466807
H	-0.676232624	-3.398746324	-2.074896806	H	-0.706206549	-1.992562438	-3.19608773
H	0.399356156	-0.904970621	-3.313307201	H	0.842792822	0.233501008	-2.5996417
H	-2.149887322	-0.650430784	2.670215347	H	-2.858186856	1.03803844	2.350574251

H	-2.773828876	2.209795828	0.547023576	H	-3.965668987	1.503278807	-0.25210416
H	-2.237327984	1.806378204	2.192722028	H	-2.433148248	1.313323136	-1.134333471
H	-3.873924472	1.373984792	1.65432611	H	-2.472775276	2.228693028	0.378397917
H	3.464105689	0.20701157	1.957241379	H	5.18459517	2.000730322	0.122137522
Compound **1** conformer 5							
C	-0.589687068	-1.266253629	-0.16822939	H	2.912547542	0.933103283	-1.294856751
C	-0.897851518	0.093827599	0.550886181	H	1.379097496	1.276189352	-2.083855364
C	-0.257607912	1.376688544	0.010647717	H	2.13506318	-1.05123442	-2.325459672
C	1.2497891	1.313129678	0.040403206	H	2.102102892	-1.291151676	-0.582136025
C	1.835416348	0.758157027	-1.229736129	H	-1.867846846	-3.067895016	-0.046016434
C	1.612228762	-0.752837864	-1.405482652	H	-2.41067809	-1.865184412	-1.21732717
C	0.162446438	-1.272763731	-1.51559269	H	-3.900711586	-1.469098304	0.687135612
C	-1.961314684	-1.992691299	-0.225904117	H	-2.551539296	-1.638053614	1.833381085
C	-2.826839117	-1.300528942	0.825217514	H	3.939234147	1.553753314	0.208898057
C	-2.44221214	0.171040313	0.691707668	H	3.884243067	2.355497224	1.785684656
C	1.968485508	1.656237881	1.128293422	H	1.637125875	3.187094834	2.606383998
C	3.467483478	1.52927631	1.197643011	H	1.76486717	1.557977879	3.260047024
C	1.361418268	2.139740955	2.421631896	H	0.273883079	2.061241761	2.45633955
C	0.238174908	-2.716264561	-2.037313931	H	0.778610332	-3.35734755	-1.331699058
H	0.064733549	-1.837964439	0.50223812	H	0.773335326	-2.738143038	-2.993757737
H	-0.539324944	-0.02086196	1.583338036	H	-0.759785362	-3.132865559	-2.193943271
O	-0.5953283	-0.476776451	-2.452443628	H	-0.154135689	-0.542698667	-3.310027669
O	-2.821843174	0.848502187	1.907722716	H	-2.680597675	1.795095296	1.775197783
C	-3.13595772	0.833884241	-0.494207528	H	-2.821421289	0.38250046	-1.439373949
O	3.871636098	0.330529457	1.906284649	H	-4.22157525	0.730304899	-0.392583285
H	-0.58451064	1.546110216	-1.018903457	H	-2.894048619	1.901955712	-0.540014915
H	-0.623633265	2.220211401	0.609394514	H	3.442527619	-0.411434689	1.460388408

conformer 1

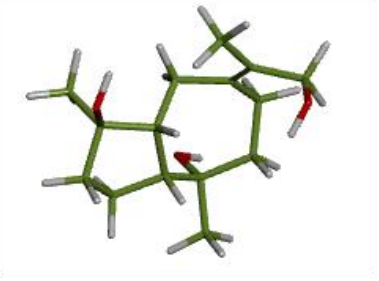


conformer 2



conformer 3

conformer 4



conformer 5

The optimized conformers of (1*S*, 4*S*, 5*S*, 10*R*)-**1**

Table S2. Free Energy Summary of Conformer set of Compound **1**

	Conformer No.	Energy (a.u.)	Relative Energy (kcal/mol)	Equilibrium Mole Fraction
1*S*, 4*S*, 5*S*, 10*R*	1	-509883.135239208	0.02974544698	45.94%
	2	-509881.239573289	1.92541136587	1.87%
	3	-509881.239060502	1.92592415347	1.87%
	4	-509880.895126919	2.26985773561	1.04%
	5	-509883.164984655	0.00000000000	48.30%

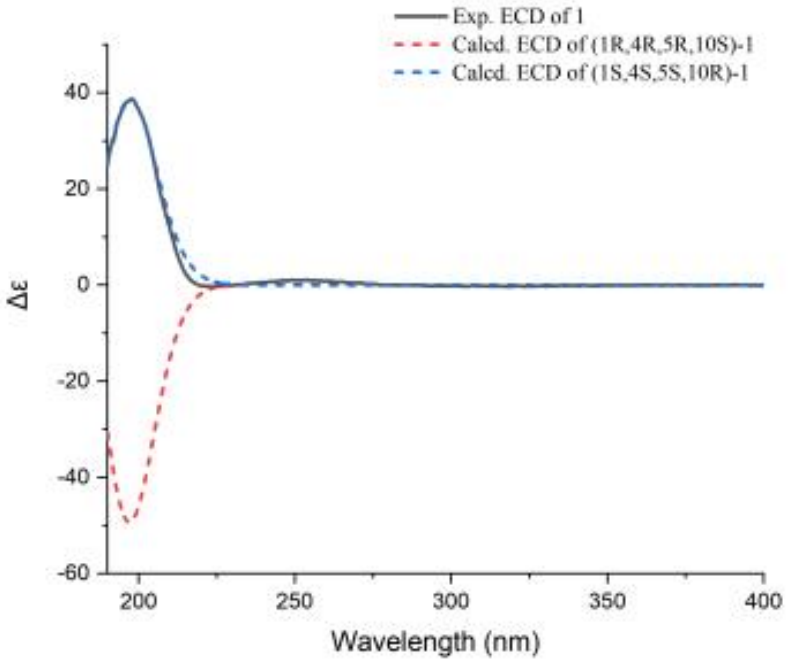


Figure S1. The Experimental ECD Spectrum of **1** (black), and the Calculated ECD Spectra of (1*R*, 4*R*, 5*R*, 10*S*)-**1** (dash red) and (1*S*, 5*S*, 6*S*, 10*R*)-**1** (dash blue)

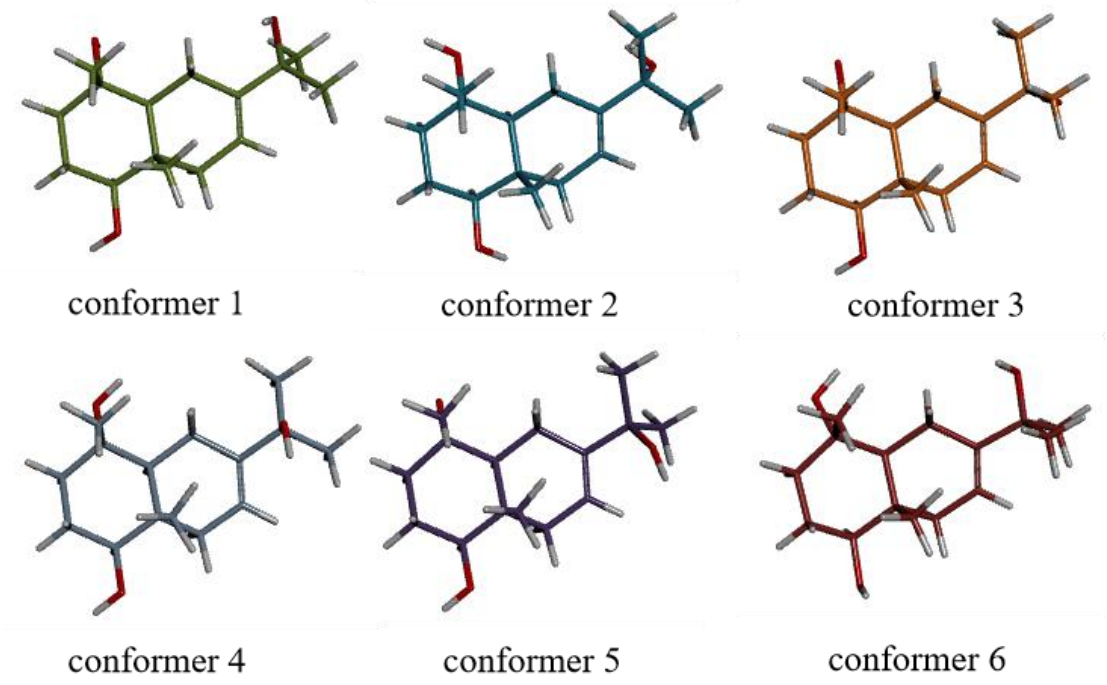
Table S3. Cartesian Coordinates and Equilibrium Populations of Low-energy Conformers of $1S,4S,5S,10S$ in CH_3OH of Compound **19**

Compound **19** conformer 1				Compound **19** conformer 2			
C	-3.152444643	-1.44660071	0.010810918	C	-3.143030241	-1.499052726	0.052565127
C	-3.250069877	-0.033563936	-0.561438193	C	-3.316678195	-0.032827621	-0.337981954
C	-2.118837381	0.882890144	-0.076041897	C	-2.175762477	0.858751814	0.170948733

C	-0.747331274	0.192058557	-0.318584264	C	-0.817151055	0.261624674	-0.268416879
C	-0.610665539	-1.288497287	0.136015065	C	-0.604413036	-1.252866917	0.005049344
C	-1.823254055	-2.07220173	-0.394145641	C	-1.837350312	-2.024123213	-0.518565939
C	0.434673501	1.021845642	0.1838253	C	0.380355164	1.075889403	0.226733735
C	1.764947193	0.394093682	-0.150246111	C	1.698697392	0.535115014	-0.269552246
C	1.843382656	-0.902848404	-0.467671076	C	1.782853615	-0.712586549	-0.740659221
C	0.66727756	-1.83334827	-0.537298578	C	0.628240856	-1.668599191	-0.82605382
C	2.979990723	1.316530798	-0.111387468	C	2.895916737	1.482060501	-0.2005113
C	2.952364142	2.291337533	-1.290774404	C	4.205097469	0.857078523	-0.663409206
C	4.316243442	0.574871276	-0.09154775	C	3.060270122	2.034712642	1.21954813
O	2.896405027	2.154575471	1.073196911	O	2.677877905	2.589090977	-1.123257889
O	-1.714422496	-3.435666107	0.047492402	O	-1.775150194	-3.43149787	-0.238294324
C	-2.377743786	1.360188456	1.349218256	C	-2.332516414	1.141182016	1.665714261
C	-0.456199663	-1.456123872	1.655701616	C	-0.318783212	-1.588137327	1.476661127
H	-1.766046243	-2.045294472	-1.497917847	H	-1.869685286	-1.875494628	-1.613439765
H	-0.661308026	0.153967885	-1.420025071	H	-0.833104767	0.356152551	-1.367340272
O	-2.150164243	2.106815297	-0.855324061	O	-2.236784053	2.131435382	-0.52895257
H	-3.972789384	-2.062535313	-0.381172275	H	-3.160147929	-1.625573873	1.142428509
H	-3.252797076	-1.442455101	1.103496092	H	-3.971442859	-2.094101409	-0.350109353
H	-3.190719918	-0.095141761	-1.658554628	H	-3.335929209	0.044875724	-1.433704396
H	-4.215400295	0.425498592	-0.315808119	H	-4.273446816	0.357287812	0.03367471
H	0.373447471	2.028709221	-0.242867046	H	0.394472436	1.101143103	1.325034936
H	0.369430822	1.163284416	1.270843466	H	0.247041824	2.118200272	-0.088768608
H	2.806452198	-1.344743329	-0.714395565	H	2.733865038	-1.094806063	-1.103740917
H	0.455963319	-2.059696153	-1.59550975	H	0.97390421	-2.66266332	-0.505943314
H	0.937977943	-2.794342979	-0.080809828	H	0.340131333	-1.778920496	-1.885105602
H	2.027295725	2.874247506	-1.303926554	H	4.138062634	0.517443235	-1.701368079
H	3.032047627	1.739798906	-2.231976445	H	4.479427123	0.008421066	-0.030780291
H	3.796732054	2.985494148	-1.218207445	H	4.998531126	1.607608201	-0.598135666
H	4.477380933	0.010366929	-1.014870094	H	2.176215309	2.60035308	1.531851426
H	4.366958356	-0.119518936	0.754287087	H	3.210171317	1.215765211	1.931664458
H	5.124579425	1.306168081	0.004985558	H	3.928462031	2.700555985	1.260539414
H	2.887593013	1.566227166	1.840264126	H	1.970402254	3.142433245	-0.768920089
H	-2.438653786	-3.927651421	-0.358931613	H	-1.001244369	-3.795299497	-0.686408584
H	-1.583592399	2.02633406	1.696653734	H	-3.274618342	1.680330379	1.82443694
H	-2.463545718	0.529931901	2.050829302	H	-1.517971855	1.764579808	2.043791974
H	-3.321546599	1.915267426	1.366131222	H	-2.3777691	0.22862036	2.263199912
H	0.430487589	-0.923864836	2.012344111	H	-0.106891101	-2.65709947	1.572361483
H	-0.327779404	-2.514794775	1.897205361	H	-1.153444729	-1.35900098	2.141450675
H	-1.317328975	-1.08922085	2.216716648	H	0.559646857	-1.041955213	1.832943531
H	-2.026989935	1.86560715	-1.783585452	H	-3.0713272	2.552895387	-0.284178144
Compound **19** conformer 3				Compound **19** conformer 4			
C	-3.148837386	-1.456201627	0.058899335	C	-4.446350845	-0.997456628	-2.471453534
C	-3.316685731	0.052868036	-0.10679145	C	-4.130301361	-0.182158629	-1.220490185
C	-2.118911442	0.845465771	0.433722523	C	-2.627574372	-0.080870567	-0.950961461

C	-0.805738145	0.283930869	-0.178292587	C	-1.903952574	0.426581327	-2.230509454
C	-0.614217638	-1.258900302	-0.144522736	C	-2.258964502	-0.2811622	-3.570076386
C	-1.897756084	-1.918133768	-0.67812833	C	-3.791135389	-0.353251956	-3.686566289
C	0.443163057	0.997109388	0.342558152	C	-0.386188014	0.524181651	-2.060104225
C	1.711152138	0.503502489	-0.307546331	C	0.299899656	1.101789835	-3.273811703
C	1.734223487	-0.664956507	-0.955653056	C	-0.324016559	1.132944104	-4.455969802
C	0.547550365	-1.572098719	-1.111713582	C	-1.717940823	0.62906785	-4.693221621
C	2.947401311	1.391837401	-0.174057273	C	1.713539172	1.637469194	-3.062657264
C	3.2265297	1.703644343	1.2966295	C	1.683940831	2.931807614	-2.24720009
C	2.769484213	2.689203035	-0.975723768	C	2.483642634	1.870325172	-4.361972883
O	4.134069709	0.724975321	-0.645869779	O	2.454242058	0.691604848	-2.245101308
O	-1.736241245	-3.345212192	-0.615987672	O	-4.124138317	-1.043493964	-4.902774224
C	-2.159913972	0.925528993	1.95607925	C	-2.086185014	-1.379707814	-0.356931419
C	-0.239764035	-1.80775501	1.241477638	C	-1.620828798	-1.669437182	-3.733422942
H	-2.001992151	-1.612679034	-1.73552216	H	-4.158572804	0.687422033	-3.751015979
H	-0.886365896	0.531033292	-1.252636016	H	-2.279082505	1.457493686	-2.344140231
O	-2.253952371	2.22929573	0.016707225	O	-2.513697349	0.952264421	0.065199094
H	-4.02263664	-1.974152876	-0.358276184	H	-4.110261786	-2.036802422	-2.366512333
H	-3.090285485	-1.736418797	1.118122212	H	-5.533040443	-1.029723583	-2.625369078
H	-3.418854986	0.279226889	-1.178920403	H	-4.627444972	-0.60449142	-0.338884135
H	-4.231767976	0.404020382	0.385437194	H	-4.514588968	0.839070058	-1.351723539
H	0.324675264	2.075152127	0.186366424	H	0.043520672	-0.462663309	-1.84298618
H	0.529371451	0.865720911	1.430247583	H	-0.152117408	1.140002367	-1.182923979
H	2.661256569	-1.011901456	-1.407772355	H	0.176519613	1.558268865	-5.32311862
H	0.184305742	-1.512765722	-2.150953781	H	-1.748564453	0.090151585	-5.649140882
H	0.866563046	-2.612950999	-0.970921117	H	-2.391463383	1.492557611	-4.81995623
H	3.358570584	0.776783221	1.864890247	H	2.707256514	3.275361062	-2.061239587
H	2.401626732	2.269014666	1.737641085	H	1.189042235	2.785343713	-1.28338269
H	4.138593673	2.303662228	1.378105081	H	1.148410173	3.707902167	-2.801577857
H	1.913274132	3.270320598	-0.622420946	H	3.503883327	2.180388495	-4.115989781
H	2.613973733	2.460047359	-2.036525153	H	2.025885888	2.659702832	-4.965660802
H	3.668504236	3.306244675	-0.874354011	H	2.529321403	0.955372949	-4.96284974
H	4.065139557	0.64040234	-1.60607506	H	2.482210304	-0.144258952	-2.730160374
H	-2.516197783	-3.740766125	-1.02483412	H	-5.083991229	-1.008598513	-4.99905292
H	-1.321446687	1.507634239	2.347834283	H	-2.214654095	-2.232264187	-1.025989447
H	-2.142818223	-0.059968489	2.422897728	H	-2.62747672	-1.594463197	0.570797071
H	-3.088653274	1.423785359	2.253488749	H	-1.020361641	-1.298108859	-0.118521275
H	0.665126149	-1.321369286	1.617190557	H	-1.843993839	-2.057781619	-4.730922579
H	-0.033465899	-2.879000825	1.166790739	H	-1.984750396	-2.399390794	-3.007910172
H	-1.028014773	-1.674722567	1.984567984	H	-0.532924808	-1.608618416	-3.636945032
H	-2.265037024	2.243544639	-0.95015562	H	-1.626311112	0.904106774	0.443058068
Compound **19** conformer 5				Compound **19** conformer 6			
C	-3.122209722	-1.465067929	0.110260222	C	-3.1257761	-1.454339443	0.162123532
C	-3.333147832	0.015062187	-0.203377876	C	-3.293482055	0.052029714	-0.018363227
C	-2.175672364	0.893865579	0.289515796	C	-2.077340075	0.846615094	0.461933702

C	-0.829524412	0.323702106	-0.238953828	C	-0.795984888	0.281463738	-0.210844556
C	-0.591017748	-1.203284365	-0.056888449	C	-0.596303434	-1.259023808	-0.150921118
C	-1.839741574	-1.951957367	-0.552719083	C	-1.904759101	-1.945307547	-0.604468875
C	0.383872941	1.122495458	0.239537245	C	0.478261645	1.010886938	0.224342633
C	1.680959294	0.612829962	-0.337745683	C	1.720208778	0.495896069	-0.4627667
C	1.75421297	-0.609418115	-0.87527354	C	1.707872979	-0.685999171	-1.086876171
C	0.601635828	-1.566692354	-0.966225684	C	0.512250277	-1.588498483	-1.170789061
C	2.871398683	1.566432626	-0.275749362	C	2.956515525	1.392875244	-0.402399419
C	2.697715999	2.708674244	-1.27864031	C	4.196414012	0.774638535	-1.034862413
C	4.218962079	0.882913132	-0.504610864	C	3.261166501	1.792274458	1.045482906
O	2.892181995	2.207707264	1.027998017	O	2.708966152	2.595386854	-1.188450349
O	-1.634296118	-3.360312397	-0.353330294	O	-1.80520439	-3.378649917	-0.581294608
C	-2.257427677	1.104139211	1.797977413	C	-2.044215726	0.93424399	1.987075429
C	-0.230249964	-1.607001807	1.381631746	C	-0.148003081	-1.777500604	1.225153268
H	-1.927736068	-1.749262556	-1.636019937	H	-2.051800325	-1.697196317	-1.66616129
H	-0.892368199	0.466243311	-1.333317795	H	-0.943615805	0.510283414	-1.279620577
O	-2.346011884	2.229589972	-0.252506218	O	-2.297732181	2.187236647	-0.053941399
H	-3.968806116	-2.049514864	-0.274068693	H	-4.012566124	-1.974862423	-0.218946752
H	-3.080407542	-1.64040731	1.192461131	H	-3.038856105	-1.716157709	1.22589675
H	-3.412543891	0.135314577	-1.294470324	H	-4.187612986	0.411308367	0.505375276
H	-4.272032528	0.379710202	0.230783359	H	-3.432813317	0.270066364	-1.086397381
H	0.24601485	2.177461669	-0.020998224	H	0.610983145	0.928883963	1.311970791
H	0.450080478	1.10120867	1.335322934	H	0.360889784	2.085353591	0.023677762
H	2.692967407	-0.962488293	-1.296701403	H	2.604317952	-1.045282486	-1.586630104
H	0.262537414	-1.618156105	-2.014071933	H	0.098776301	-1.534466428	-2.191373663
H	0.95217777	-2.577820984	-0.72137246	H	0.832363381	-2.630398226	-1.039527649
H	1.765230913	3.253018356	-1.105376666	H	5.024809724	1.485357949	-0.960022846
H	2.686375888	2.31038328	-2.297273079	H	4.480796516	-0.144940471	-0.516242651
H	3.530978102	3.41384384	-1.18655488	H	4.032615361	0.548508876	-2.092676825
H	4.301581443	0.482482939	-1.519453277	H	3.427414377	0.900258993	1.659455578
H	4.368528003	0.062198633	0.205501435	H	2.434646204	2.359650697	1.485851652
H	5.016872947	1.618753276	-0.364496384	H	4.161457703	2.414546879	1.076884935
H	2.994881507	1.508887011	1.687997989	H	2.054883353	3.131173715	-0.72222692
H	-2.393293879	-3.818348063	-0.735344556	H	-1.801522468	-3.657677458	0.343625249
H	-1.451294881	1.750668976	2.154948789	H	-1.971234576	-0.044599482	2.464464127
H	-2.211351288	0.162101508	2.344781109	H	-1.202605557	1.541692576	2.337090382
H	-3.212007299	1.586307771	2.033744011	H	-2.970516315	1.408118581	2.329160731
H	0.655769942	-1.062720311	1.72111731	H	-0.922624776	-1.699057248	1.991225617
H	0.001625633	-2.67510129	1.414836525	H	0.139386105	-2.831888461	1.149573447
H	-1.034718617	-1.420322487	2.094756043	H	0.731210937	-1.232028896	1.578927414
H	-2.343702485	2.155880836	-1.21663027	H	-1.704637325	2.78912333	0.413513372



The optimized conformers of (1*S*,4*S*,5*S*,10*S*)-**19**

Table S4. Free energy summary of conformer set of compound **19**

	Conformer No.	Energy (a.u.)	Relative Energy (kcal/mol)	Equilibrium Mole Fraction
1*S*, 4*S*, 5*S*, 10*S*	1	-509894.839040418	0.291108009	22.51%
	2	-509894.070797766	1.059350661	6.15%
	3	-509895.130148427	0	36.81%
	4	-509894.323651712	0.806496715	9.43%
	5	-509894.800863102	0.329285325	21.11%
	6	-509893.815545909	1.314602518	4.00%

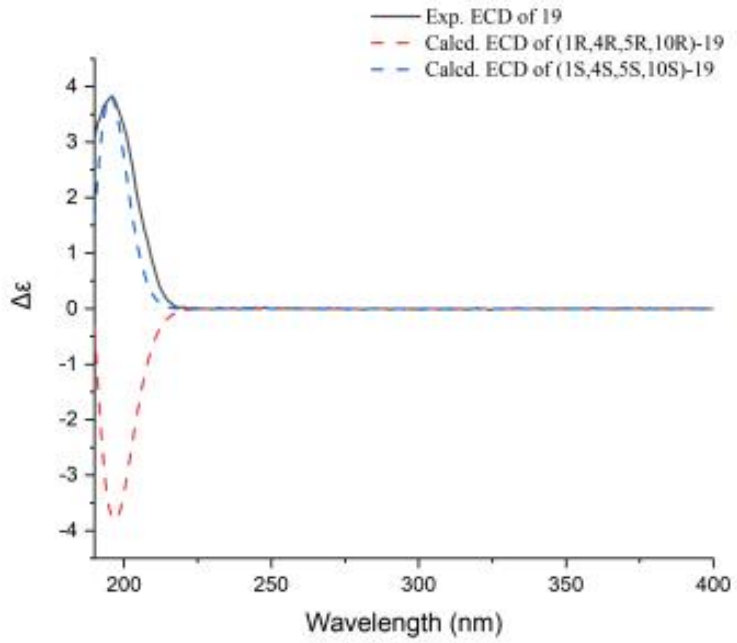
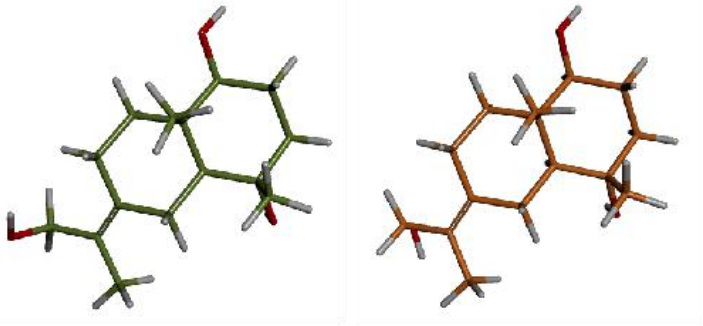


Figure S2. The experimental ECD spectrum of **19** (black), and the calculated ECD spectra of (1*R,* 4*R,* 5*R,* 10*R*)-**19** (dash red) and (1*S,* 4*S,* 5*S,* 10*S*)-**19** (dash blue)

Table S5. Cartesian Coordinates and Equilibrium Populations of Low-energy Conformers of 1*S*,4*S*,5*S*,10*S* in CH_3OH of Compound 20

Compound **20** conformer 1				Compound **20** conformer 2			
C	2.595233165	2.127128598	0.322497666	C	2.532786602	2.108218897	0.113876063
C	3.063416459	0.754404486	-0.156320823	C	2.970583179	0.724352217	-0.363438193
C	2.170217646	-0.392482472	0.337579105	C	2.145970145	-0.415646478	0.251983354
C	0.697040337	-0.064786722	-0.012879456	C	0.640661406	-0.111667004	0.045099803
C	0.173049193	1.330619669	0.438657259	C	0.14808548	1.291732818	0.505127046
C	1.152992291	2.38756572	-0.104175588	C	1.051832353	2.337858475	-0.173500345
C	-0.283984903	-1.193390833	0.361431386	C	-0.285091224	-1.232977798	0.553167999
C	-1.622888679	-0.951614119	-0.287993426	C	-1.690893543	-1.025879445	0.049274533
C	-2.191381606	0.392347478	0.089359671	C	-2.235308163	0.324452827	0.438632088
C	-1.20047946	1.520575088	-0.241587968	C	-1.29144928	1.444578433	-0.032239646
C	-2.179159282	-1.83112307	-1.143176862	C	-2.323563448	-1.94132181	-0.708171275
C	-3.479593772	-1.581633273	-1.854800139	C	-3.7162512	-1.759879278	-1.245939185
C	-1.556279294	-3.175786572	-1.46086833	C	-1.671300512	-3.251932022	-1.111788144
O	0.705416842	3.683768807	0.327284128	O	0.631912763	3.645046281	0.252146126
C	2.424857978	-0.721457474	1.802757567	C	2.554521082	-0.697608578	1.691798522
C	-9.95428E-05	1.493595977	1.961951397	C	0.133123529	1.50597732	2.031575009
H	1.10913658	2.335818865	-1.207599242	H	0.897946476	2.24311889	-1.264212312
H	0.691809074	-0.017034122	-1.117725865	H	0.522704144	-0.098004277	-1.054396425
O	2.554422771	-1.60303054	-0.363309138	O	2.469087351	-1.643445395	-0.449396928
O	-4.542303327	-2.423049787	-1.344199786	O	-3.728159861	-1.514121158	-2.674223716

H	3.23918456	2.90582169	-0.1079329	H	3.119462973	2.878009198	-0.405394008
H	2.685644858	2.213833973	1.412240115	H	2.730424354	2.233917517	1.185383942
H	4.098507856	0.565847012	0.153908716	H	4.033620823	0.557693889	-0.149979777
H	3.047230393	0.740045554	-1.256484502	H	2.848756	0.672951682	-1.455827428
H	0.14975854	-2.145918255	0.053844197	H	0.12173553	-2.194791641	0.237300594
H	-0.411221456	-1.232864712	1.452207034	H	-0.297520788	-1.236570875	1.651926246
H	-2.380303954	0.394324129	1.173433361	H	-2.328052851	0.372139396	1.533957178
H	-3.150273521	0.5980281	-0.391787401	H	-3.231729308	0.509580575	0.031635487
H	-1.624666617	2.48427798	0.062154421	H	-1.693440813	2.41598965	0.277363984
H	-1.056463643	1.553051395	-1.331405871	H	-1.261934553	1.437689614	-1.131628813
H	-3.382035446	-1.862990353	-2.910654828	H	-4.229961164	-0.905279363	-0.804653114
H	-3.78366953	-0.530046039	-1.818128444	H	-4.313955517	-2.658808332	-1.026210011
H	-0.692044842	-3.07068135	-2.1301681	H	-0.767651482	-3.098080951	-1.713187934
H	-2.284992832	-3.818066813	-1.96378774	H	-2.358854438	-3.862882117	-1.706231511
H	-1.21389664	-3.704816518	-0.566474826	H	-1.382048699	-3.850837944	-0.240647026
H	1.308858324	4.337269932	-0.047873422	H	1.189040325	4.289544969	-0.201839101
H	1.782613435	-1.541561636	2.137520591	H	1.944717099	-1.496261204	2.124348873
H	2.24975642	0.138399367	2.4497688	H	2.459548959	0.187314897	2.321448431
H	3.468311068	-1.032136853	1.920993036	H	3.601735351	-1.017461189	1.707725657
H	-0.359933809	0.578246701	2.437770141	H	-0.209622396	0.618971418	2.569824611
H	-0.7297656	2.282666017	2.168174751	H	-0.547659316	2.325785551	2.280359225
H	0.928655907	1.780012016	2.459048945	H	1.114799758	1.772146123	2.428000771
H	2.423034516	-1.448262659	-1.308852309	H	2.230041496	-1.521851719	-1.378547632
H	-4.594710453	-2.253914385	-0.394395323	H	-3.381648623	-2.30176206	-3.112503019



conformer 1 conformer 2

The optimized conformers of (1*S*,4*S*,5*S*,10*S*)-**20**

Table S6. Free energy summary of conformer set of compound 20

	Conformer No.	Energy (a.u.)	Relative Energy (kcal/mol)	Equilibrium Mole Fraction
1*S*, 4*S*, 5*S*, 10*S*	1	-509878.916036390	0.00000000000	69.50%
	2	-509878.422663161	0.49337322952	30.21%

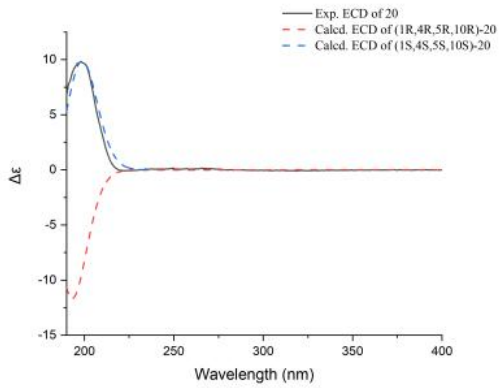


Figure S3. The Experimental ECD Spectrum of 20 (black), and the Calculated ECD Spectra of (1*R*, 4*R*, 5*R*, 10*R*)-20 (dash red) and (1*S*, 4*S*, 5*S*, 10*S*)-20 (dash blue)

Table S7. Antitumor activities of the isolated compounds against MCF-7, BGC823, Hela, A549, HepG2 cell line

Compounds	IC_{50} of MCF-7 (μM)	IC_{50} of BGC823 (μM)	IC_{50} of Hela (μM)	IC_{50} of A549 (μM)	IC_{50} of HepG2 (μM)
1	40.73 ± 0.42	340.53 ± 6.72	283.35 ± 5.72	460.53 ± 10.58	332.76 ± 12.43
2	91.64 ± 3.18	361.26 ± 9.81	301.15 ± 14.93	464.75 ± 13.47	369.49 ± 7.78
3	90.48 ± 2.41	> 500	203.87 ± 16.32	> 500	> 500
4	100.74 ± 9.71	269.76 ± 12.53	398.54 ± 9.47	401.26 ± 16.51	365.68 ± 12.45
5	> 500	> 500	> 500	> 500	> 500
6	147.13 ± 16.26	243.56 ± 19.34	167.57 ± 12.09	387.46 ± 13.64	247.13 ± 17.43
7	101.70 ± 10.01	211.57 ± 16.06	234.64 ± 9.01	306.87 ± 17.24	224.89 ± 21.03
8	229.34 ± 21.96	245.54 ± 20.43	356.87 ± 16.58	324.34 ± 13.48	327.46 ± 9.73
9	249.08 ± 27.08	443.35 ± 23.36	> 500	> 500	389.38 ± 17.74
10	113.59 ± 6.16	387.34 ± 16.53	412.76 ± 21.11	415.78 ± 26.86	315.35 ± 16.34
11	117.03 ± 11.89	315.30 ± 21.89	213.56 ± 10.90	315.53 ± 13.46	317.06 ± 21.69
12	401.01 ± 23.33	> 500	> 500	> 500	> 500
13	160.24 ± 20.04	357.30 ± 26.67	425.67 ± 13.46	409.35 ± 11.36	369.78 ± 22.24
14	249.19 ± 29.26	＞500	＞500	＞500	＞500
15	297.03 ± 12.73	> 500	> 500	> 500	> 500
16	148.09 ± 11.16	245.57 ± 16.24	387.20 ± 16.86	341.35 ± 14.74	457.30 ± 26.47
17	173.83 ± 21.94	357.30 ± 26.67	＞500	＞500	＞500
18	158.03 ± 13.68	335.46 ± 12.35	457.34 ± 8.48	379.36 ± 26.12	414.08 ± 22.45
19	92.01 ± 5.31	289.47 ± 28.44	397.34 ± 24.35	454.35 ± 21.43	453.34 ± 25.76
20	58.77 ± 0.40	321.42 ± 12.57	456.36 ± 22.39	457.00 ± 22.19	482.14 ± 8.24
21	148.63 ± 3.02	387.64 ± 19.69	387.08 ± 25.23	338.58 ± 23.53	455.35 ± 24.34
22	154.81 ± 25.05	＞500	＞500	＞500	335.36 ± 26.38
23	112.91 ± 10.99	456.40 ± 26.10	389.57 ± 23.41	＞500	358.30 ± 27.60
Cisplatin	9.86 ± 0.13	19.32 ± 2.43	6.24 ± 1.54	10.20 ± 0.69	11.34 ± 2.25

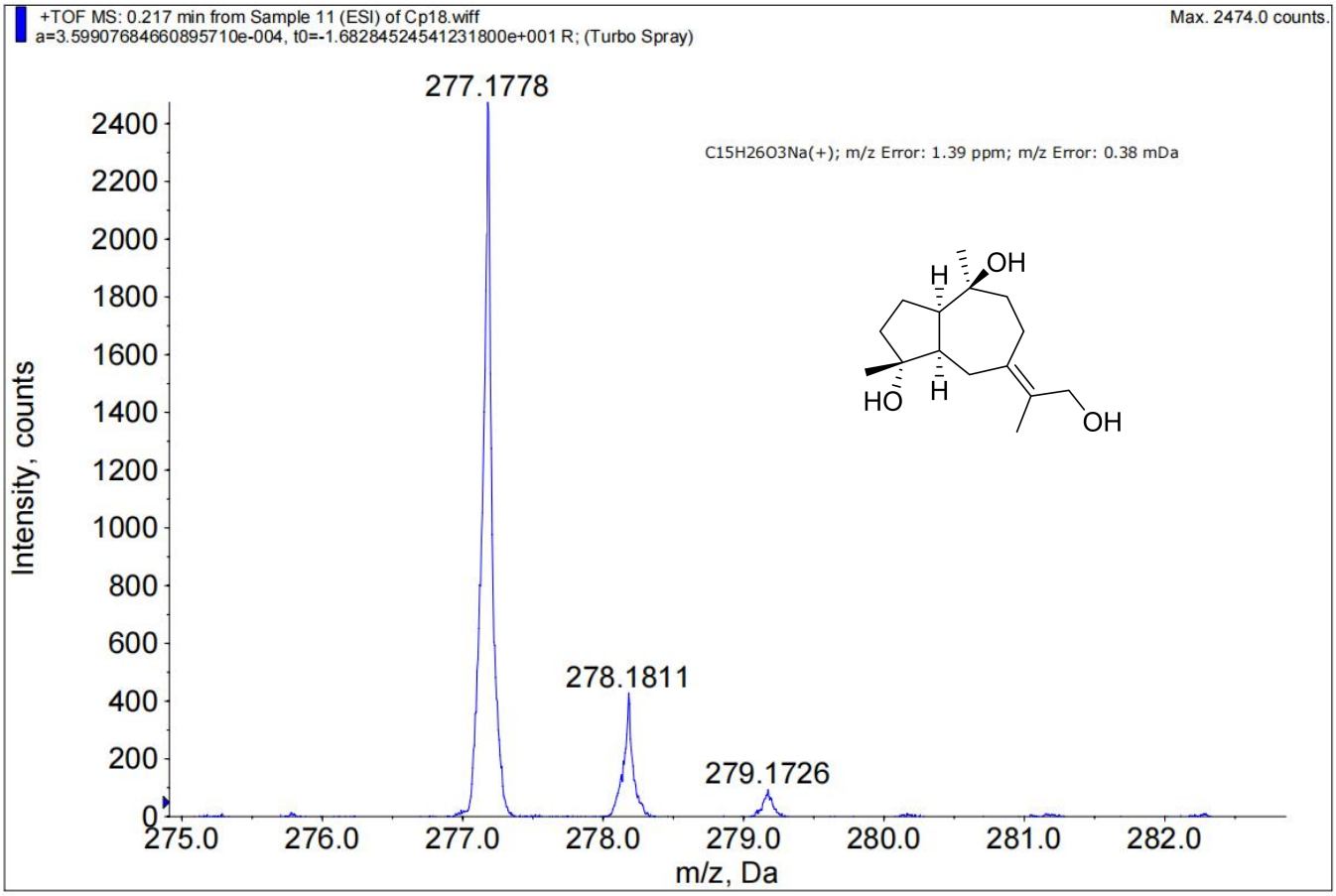


Figure S4. The HR-ESI-MS Spectrum of Compound 1

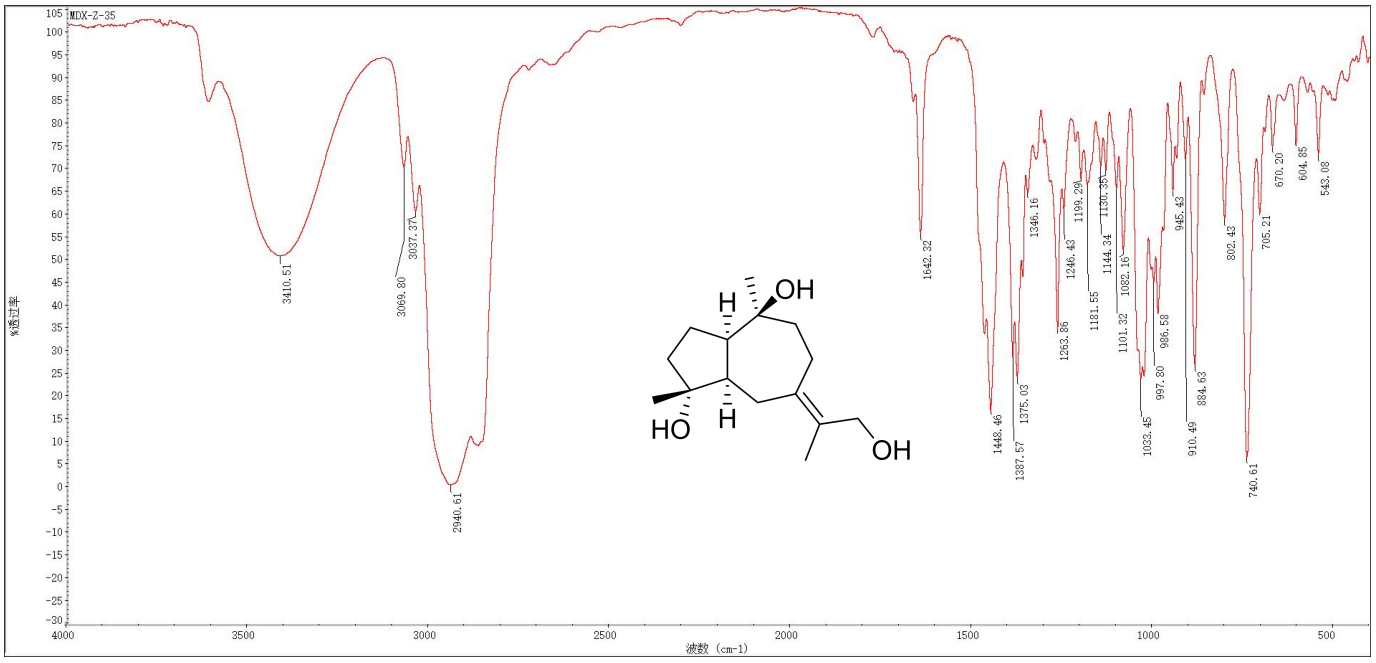


Figure S5. The IR Spectrum of Compound 1

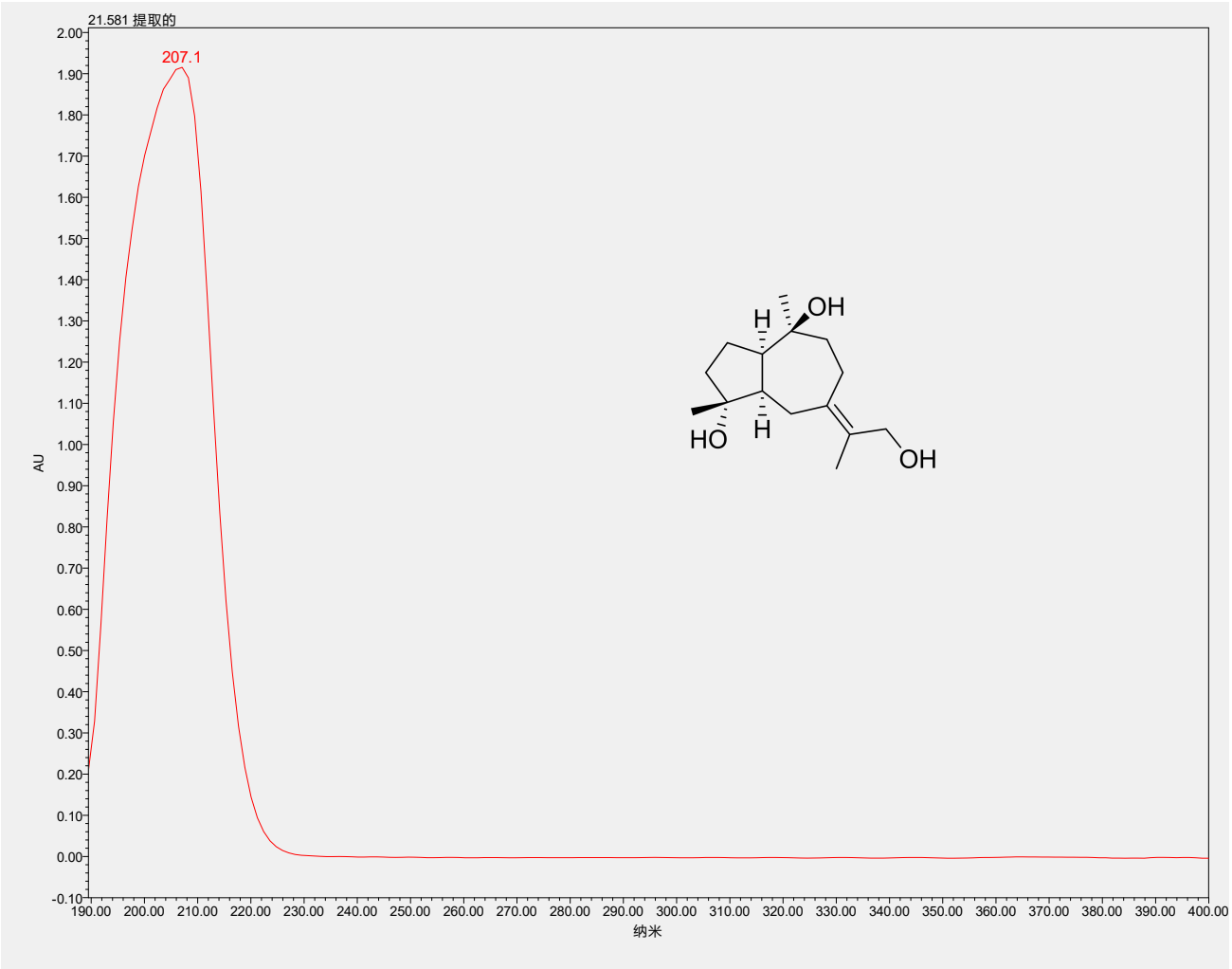


Figure S6. The UV Spectrum of Compound 1

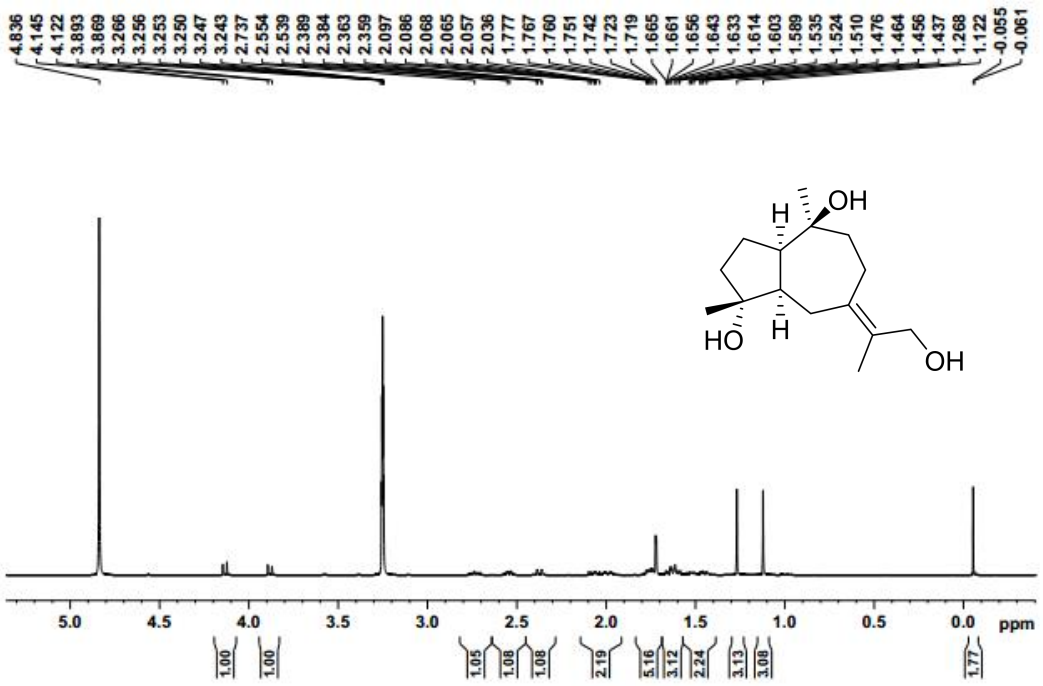


Figure S7. The ^{1}H NMR Spectrum of Compound 1 in CD3OD

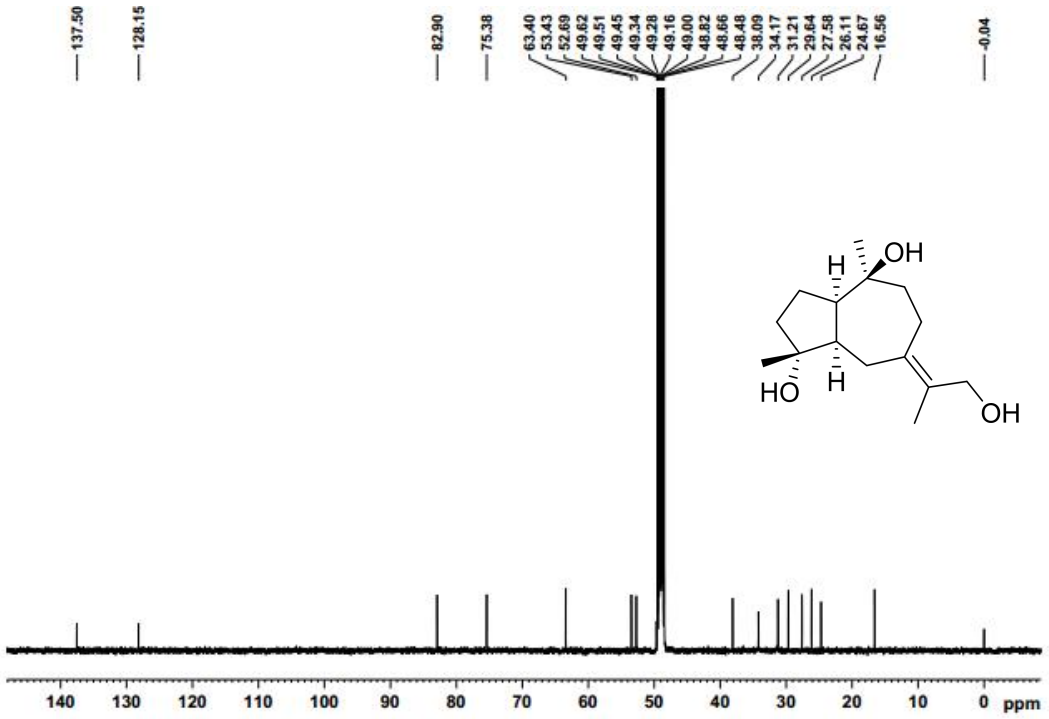


Figure S8. The ^{13}C NMR Spectrum of Compound 1 in CD3OD

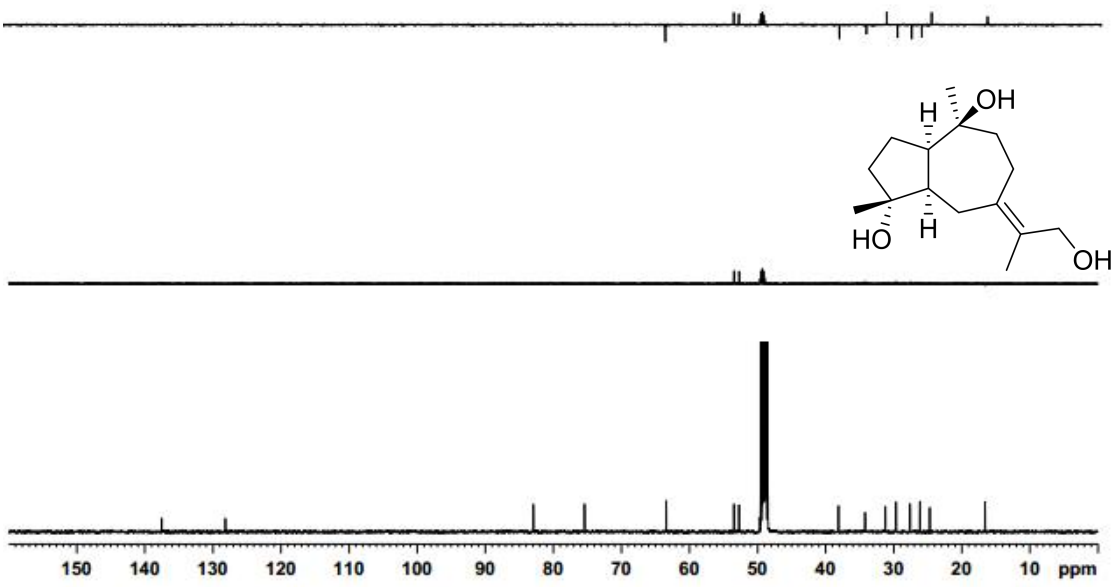


Figure S9. The DEPT Spectrum of Compound 1 in CD3OD

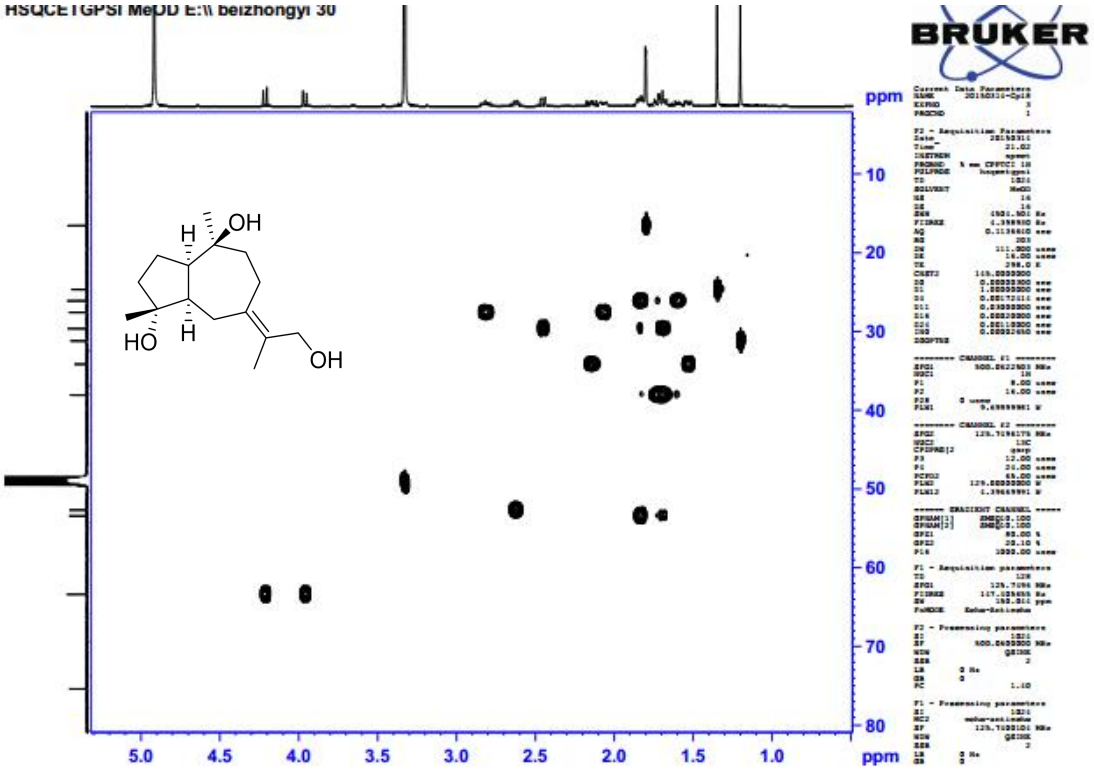


Figure S10. The HSQC Spectrum of Compound 1 in CD3OD

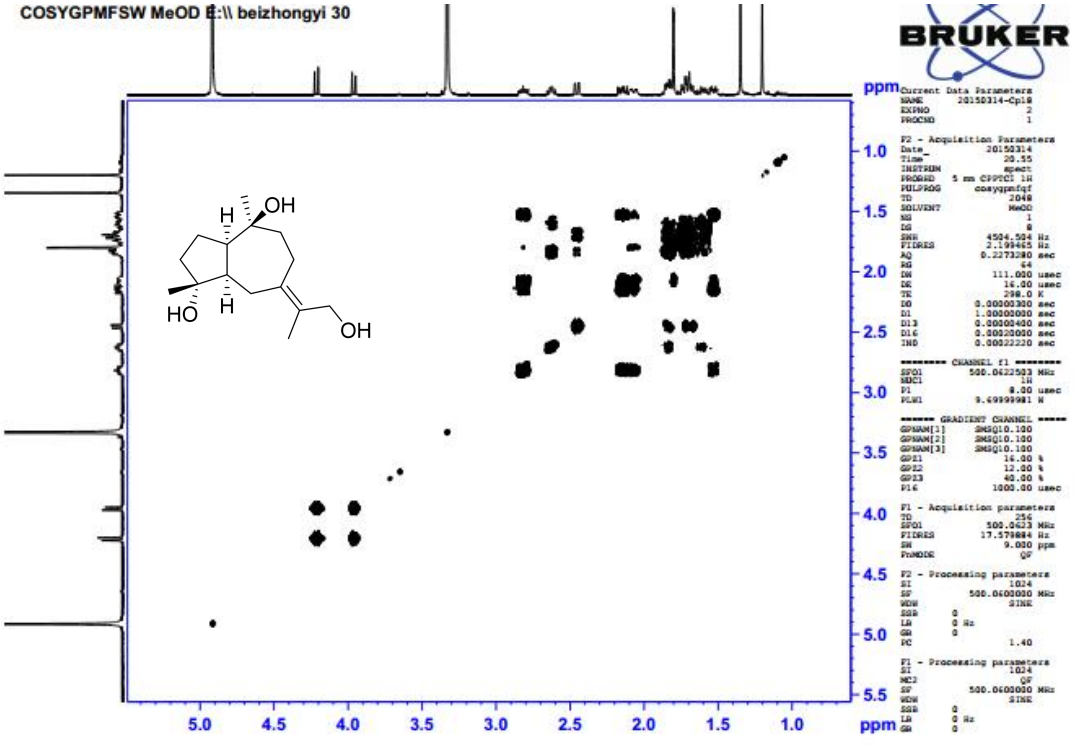


Figure S11. The ^{1}H-^{1}H COSY Spectrum of Compound 1 in CD3OD

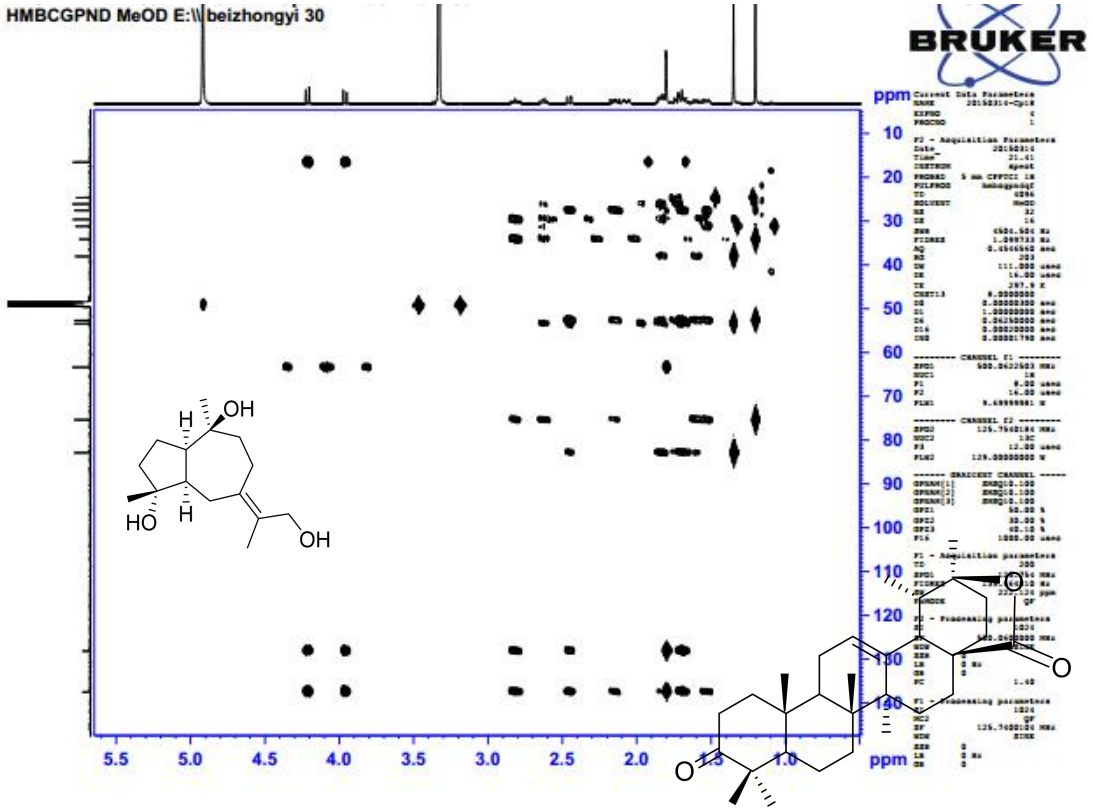


Figure S12. The HMBC Spectrum of Compound 1 in CD3OD

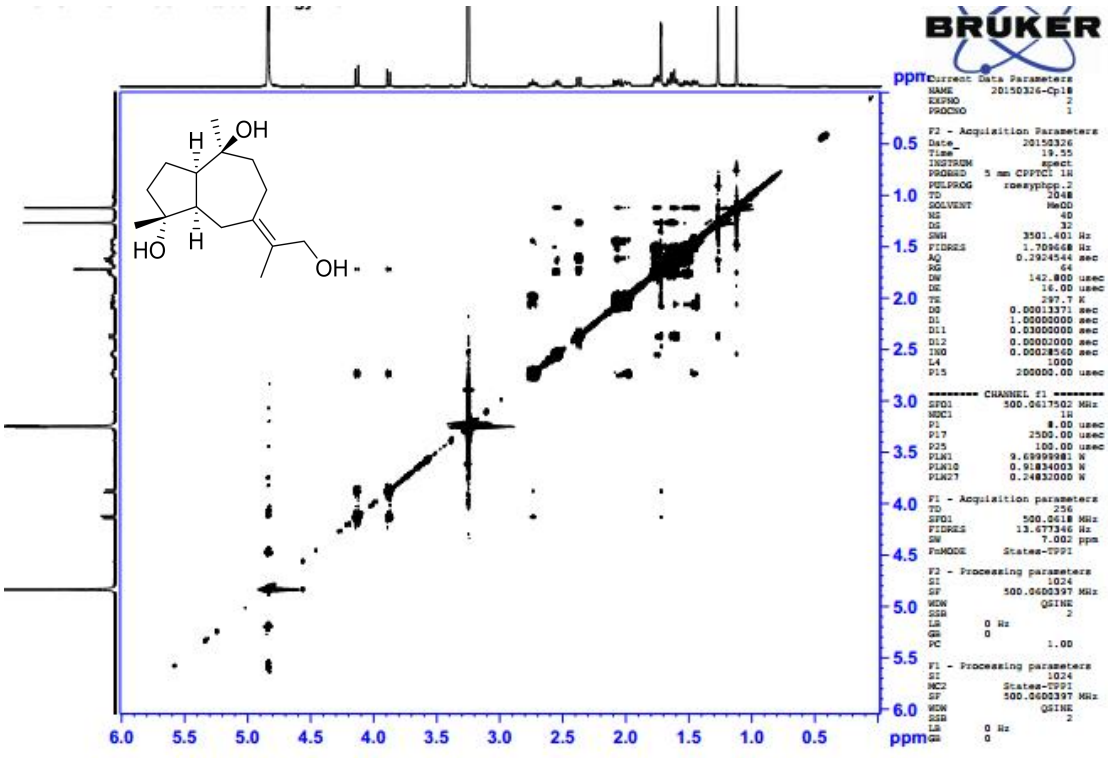


Figure S13. The NOESY Spectrum of Compound 1 in CD3OD

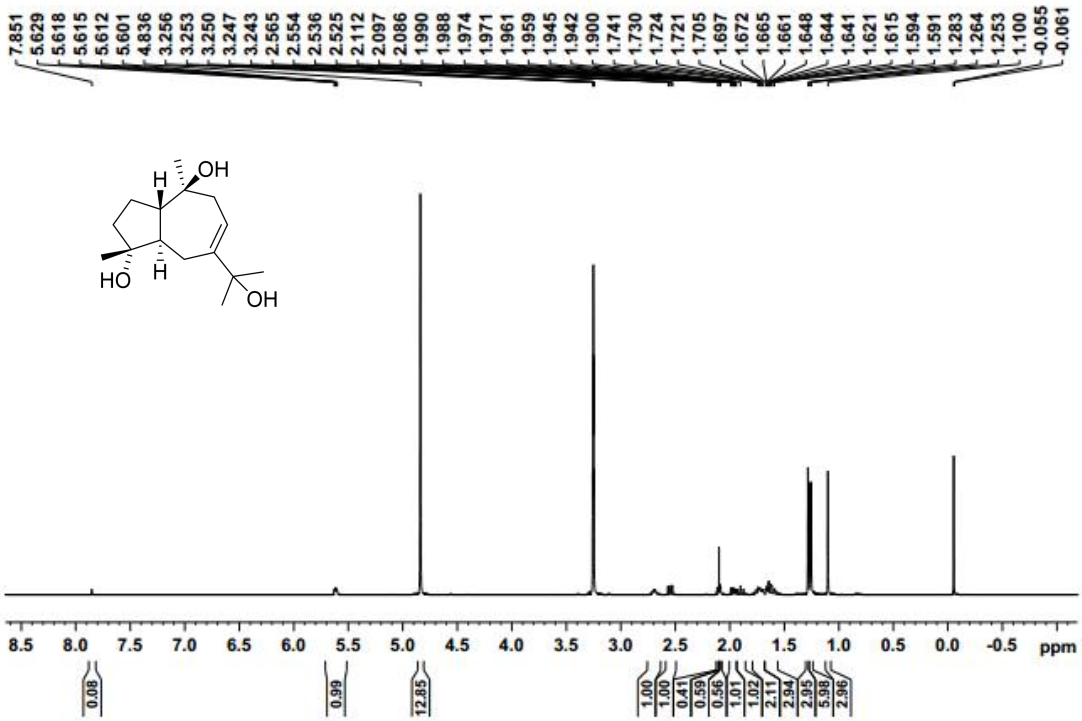


Figure S14. The ^{1}H NMR Spectrum of Compound 2 in CD3OD

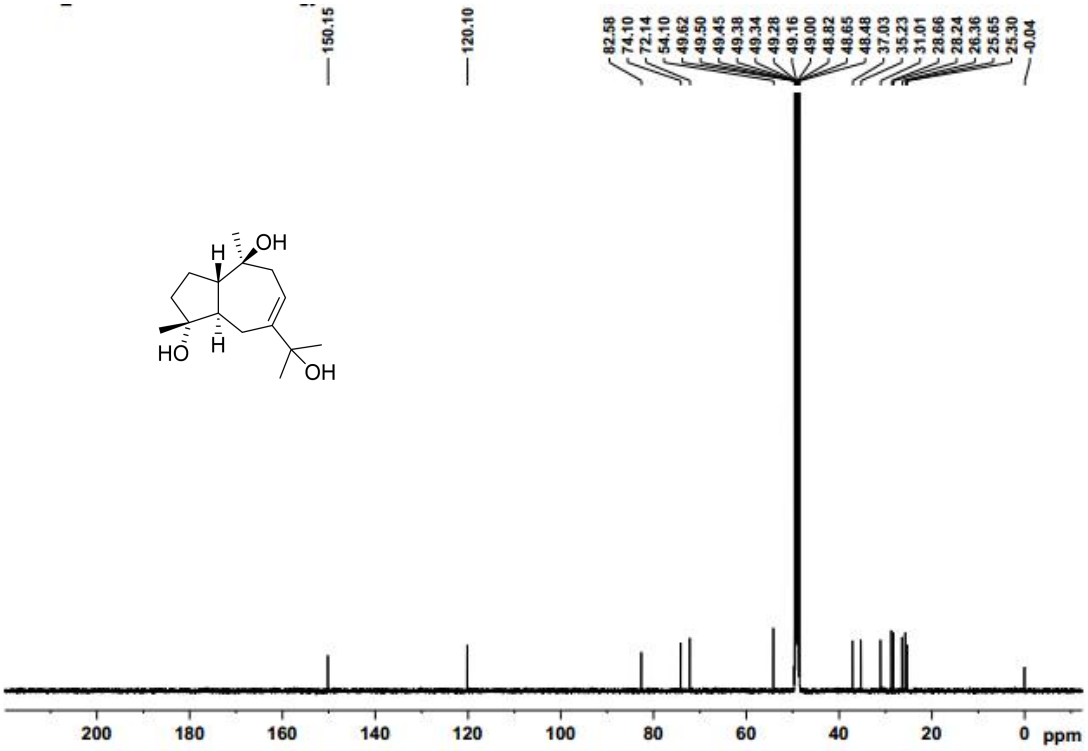


Figure S15. The ^{13}C NMR Spectrum of Compound 2 in CD3OD

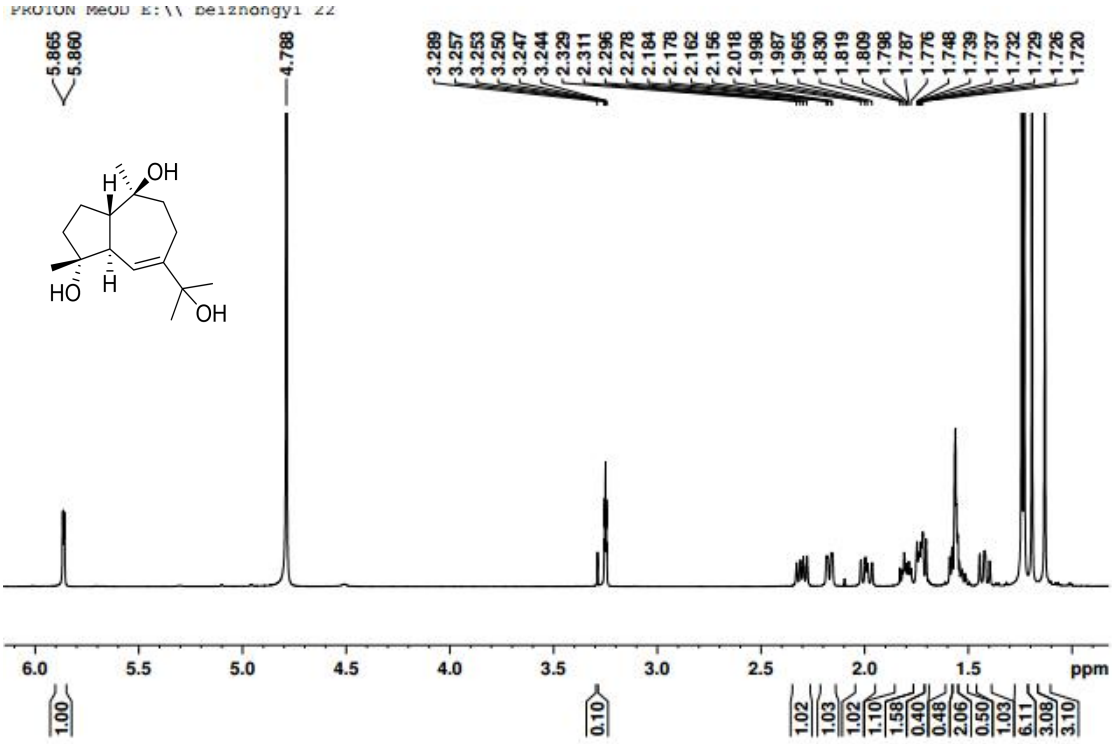


Figure S16. The ^{1}H NMR Spectrum of Compound 3 in CD3OD

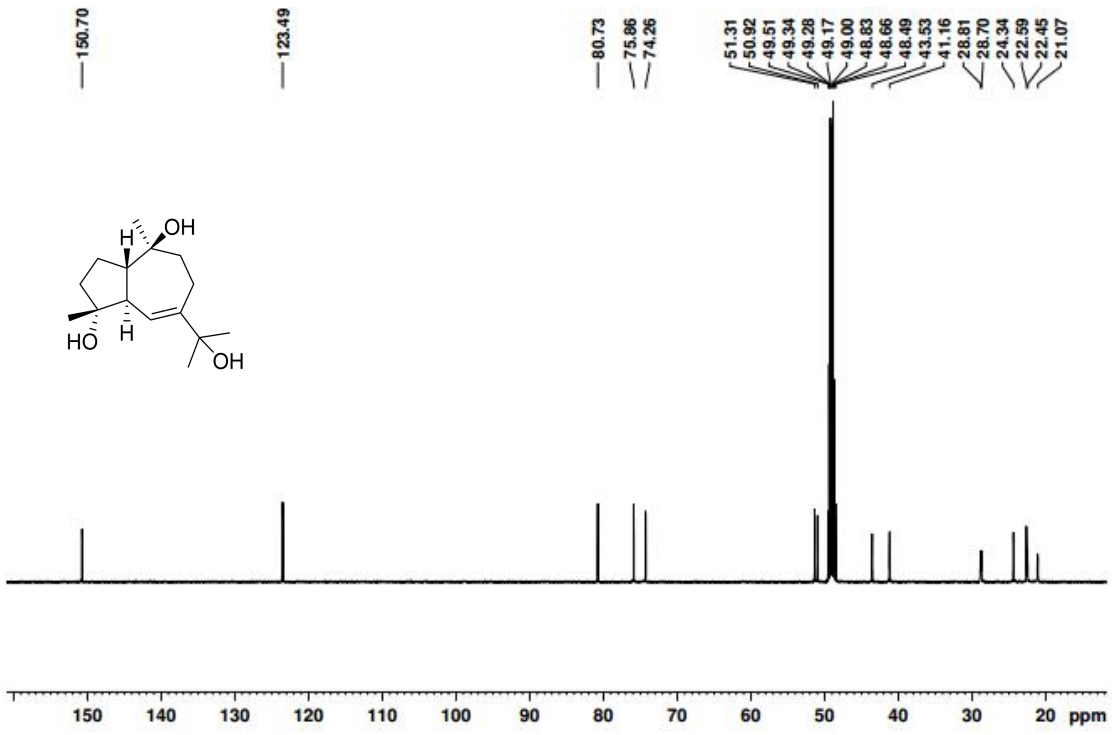


Figure S17. The ^{13}C NMR Spectrum of Compound 3 in CD3OD

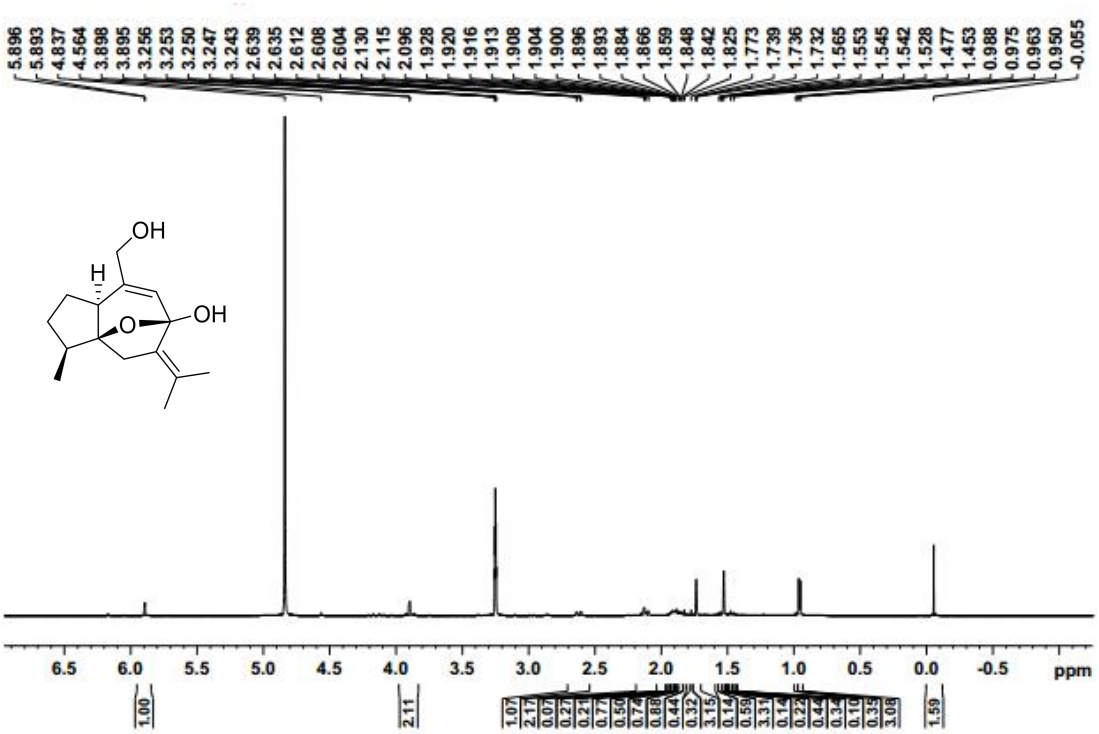


Figure S18. The ^{1}H NMR Spectrum of Compound 4 in CD3OD

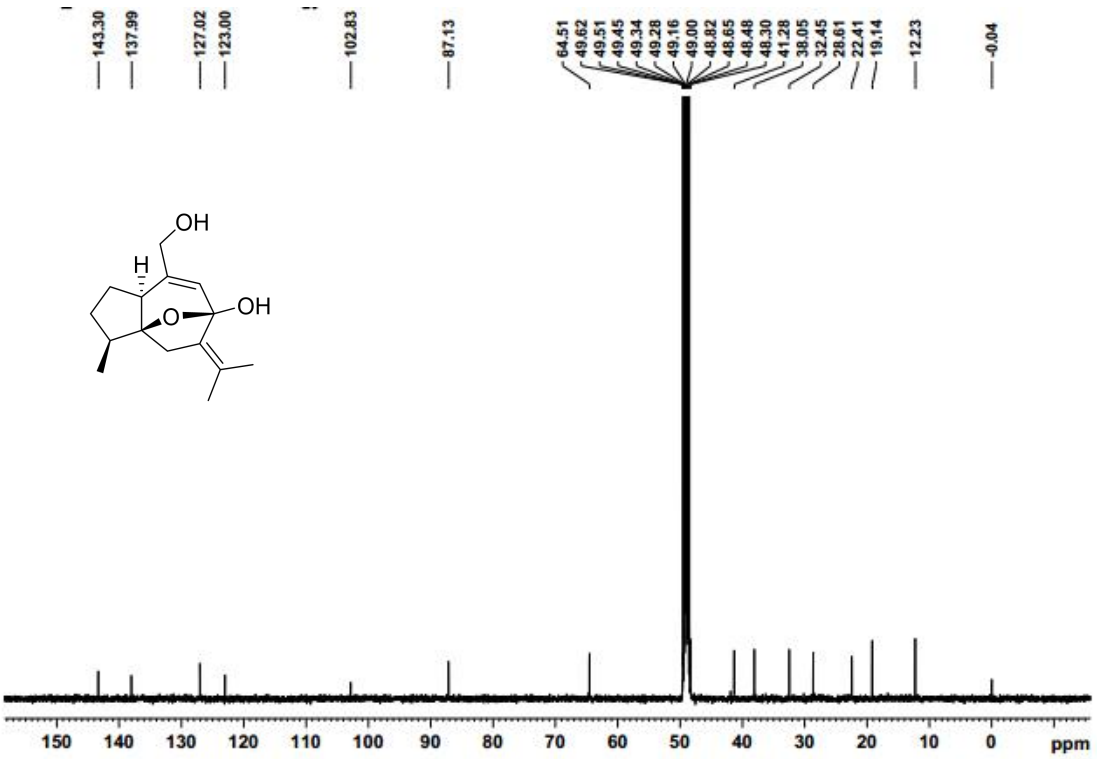


Figure S19. The ^{13}C NMR Spectrum of Compound 4 in CD3OD

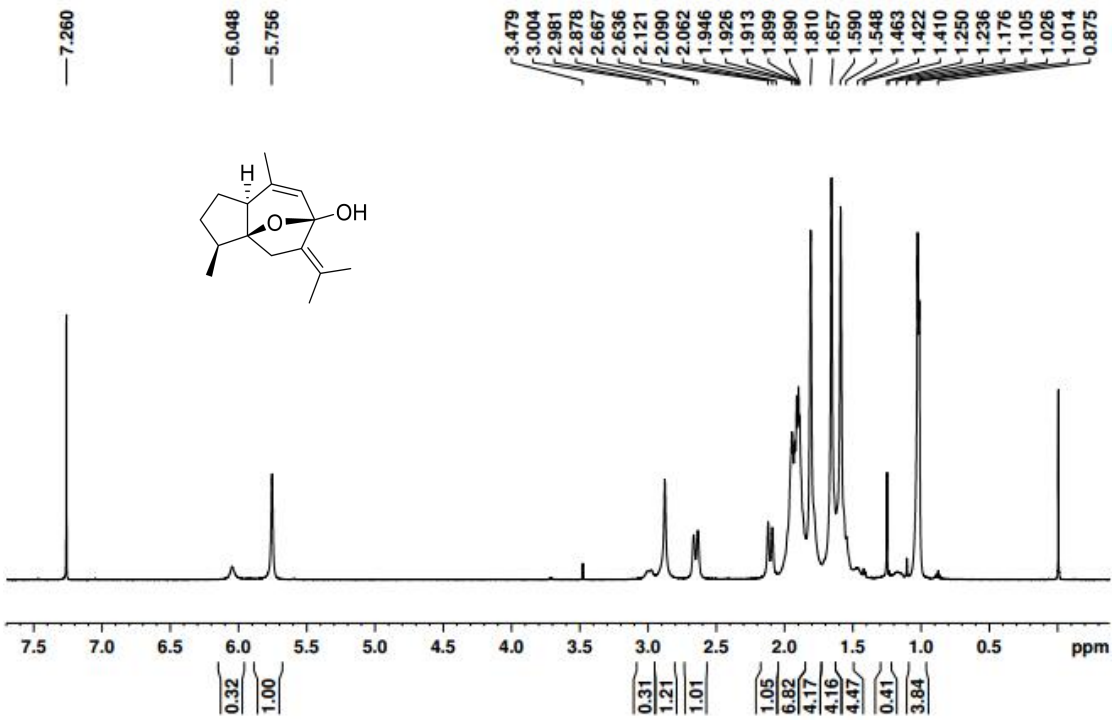


Figure S20. The ^{1}H NMR Spectrum of Compound 5 in CDCCl3

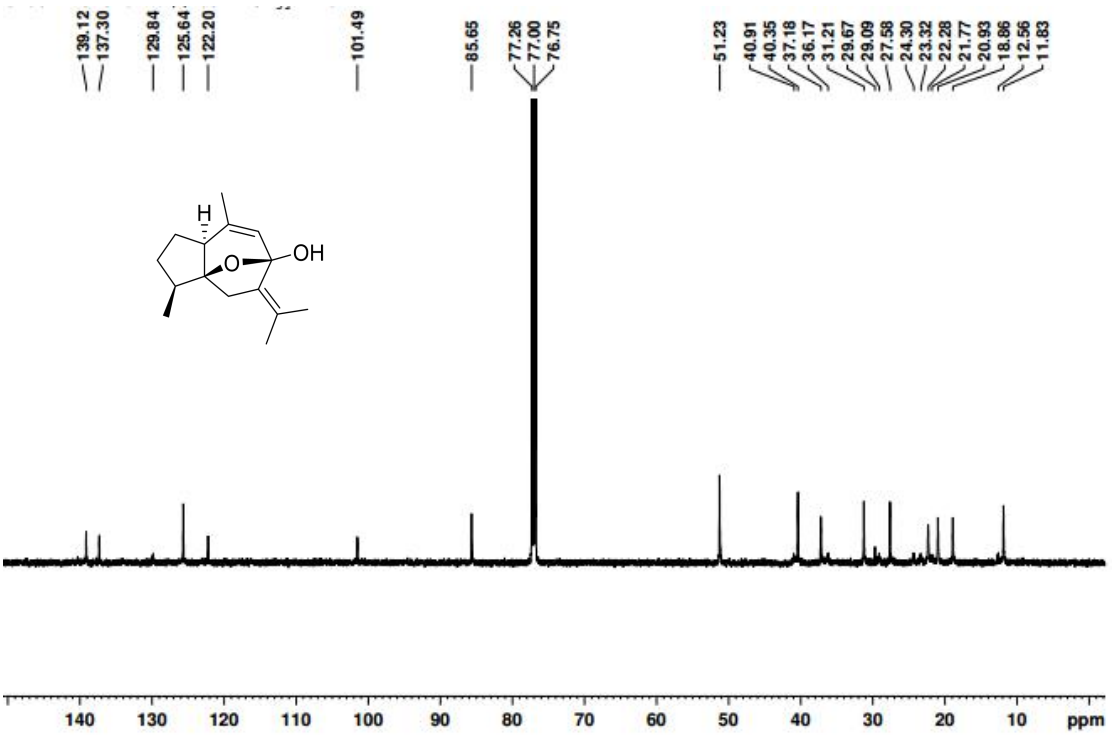


Figure S21. The ^{13}C NMR Spectrum of Compound 5 in CDCCl3

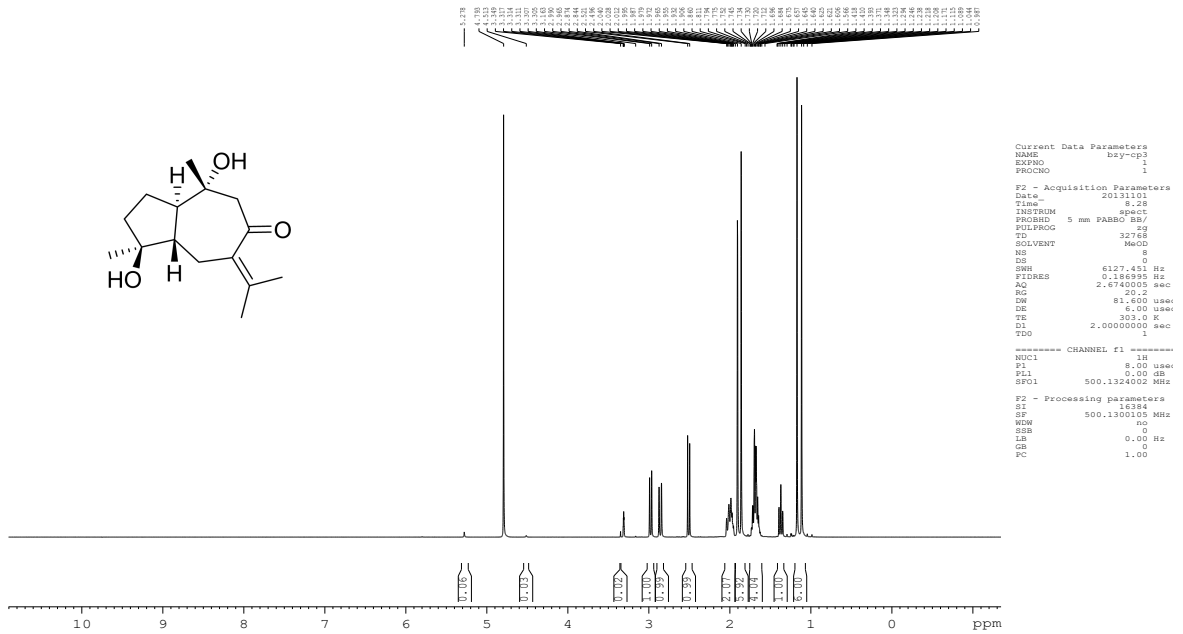


Figure S22. The ^{1}H NMR Spectrum of Compound 6 in CD3OD

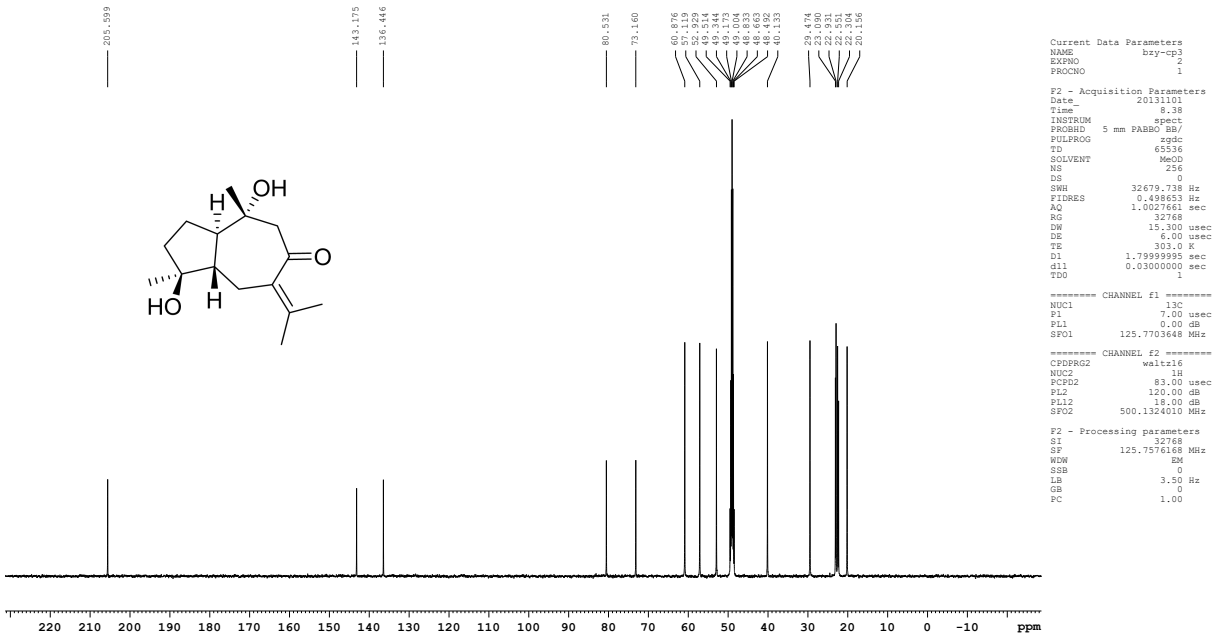


Figure S23. The ^{13}C NMR Spectrum of Compound 6 in CD3OD

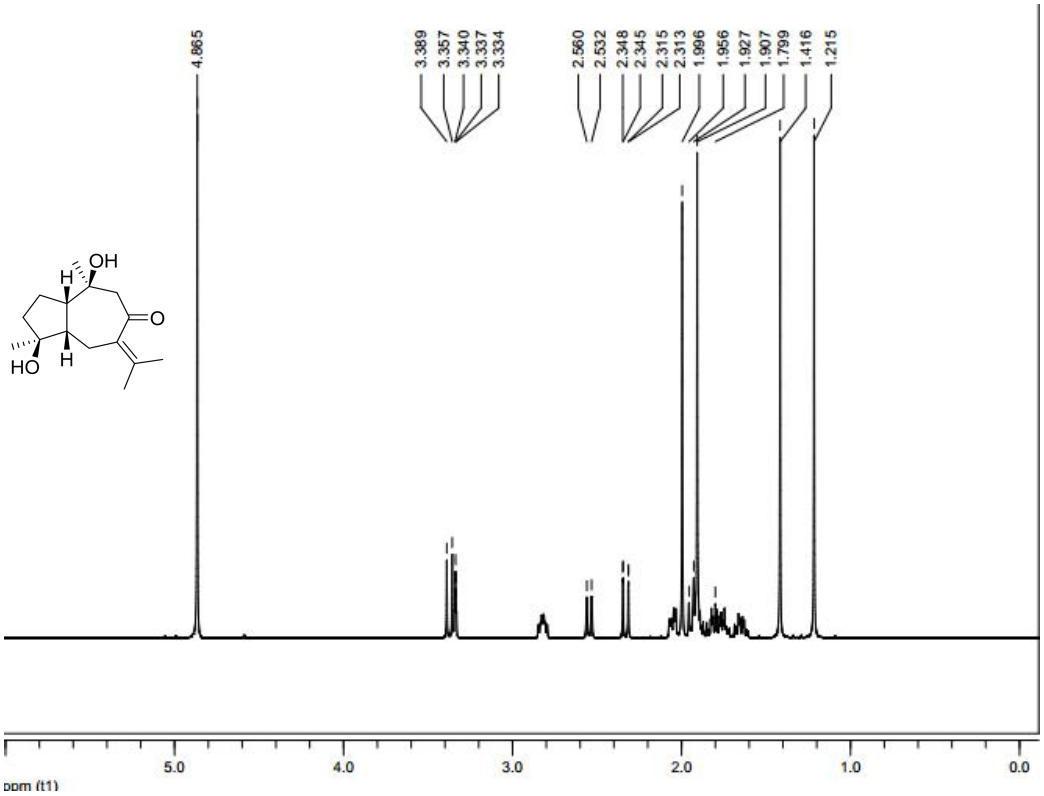


Figure S24. The ^{1}H NMR Spectrum of Compound 7 in CD3OD

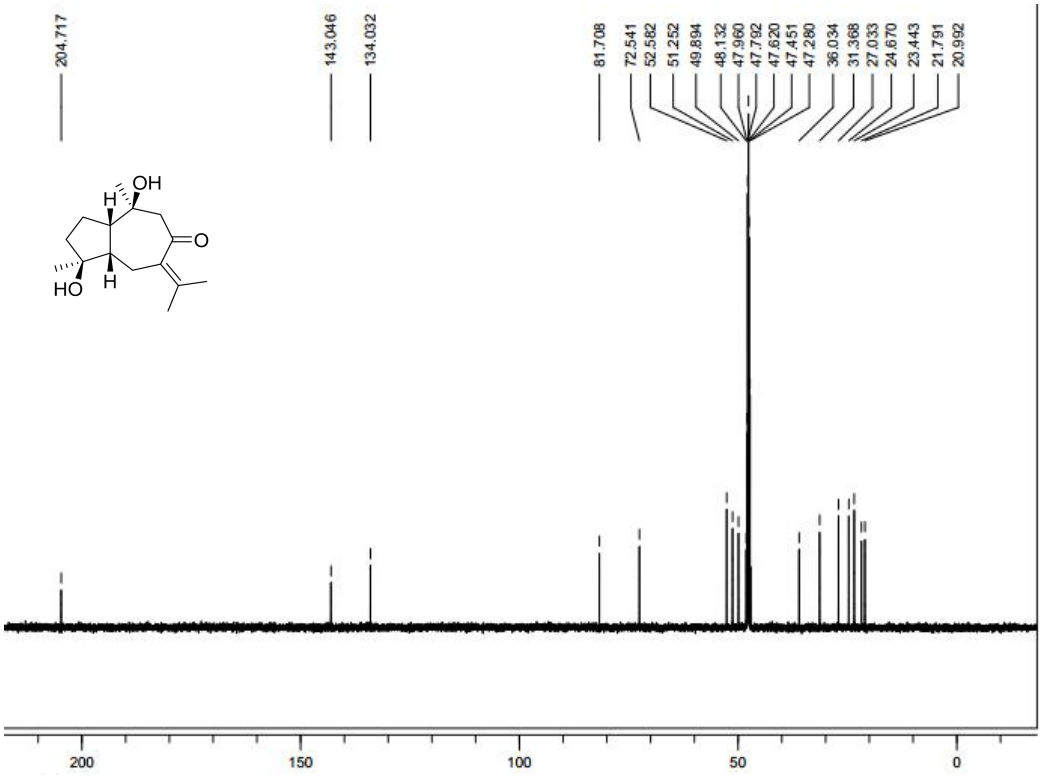


Figure S25. The ^{13}C NMR Spectrum of Compound 7 in CD3OD

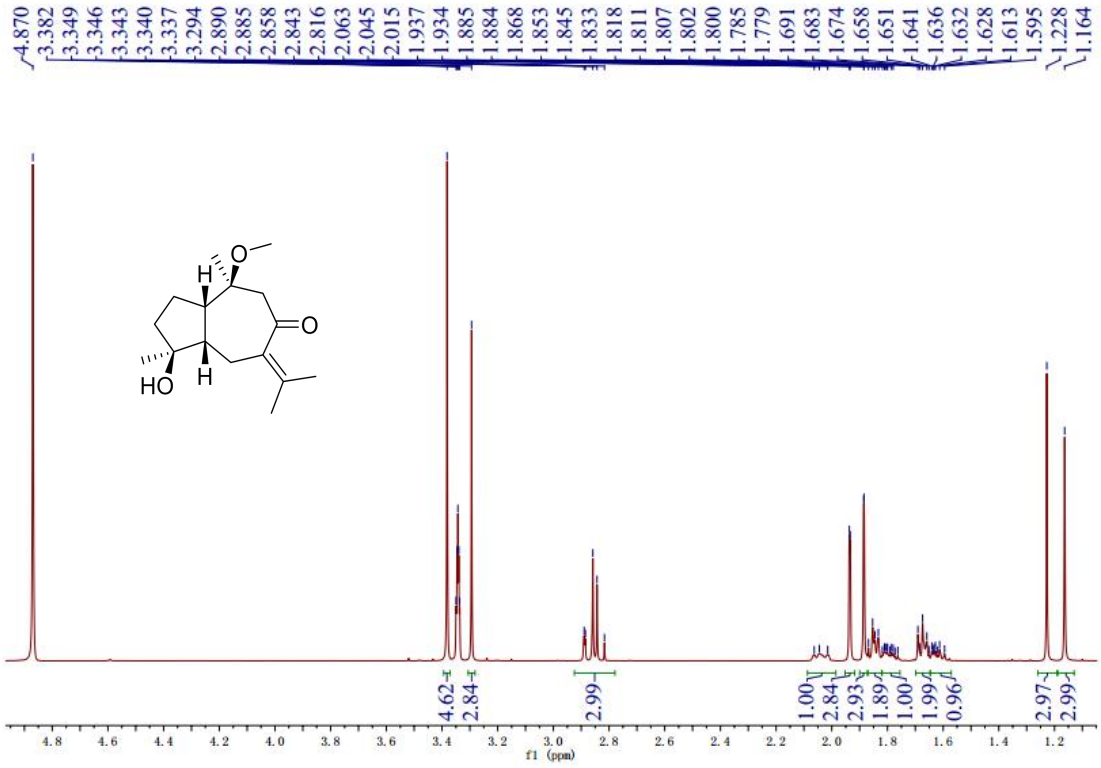


Figure S26. The ^{1}H NMR Spectrum of Compound 8 in CD3OD

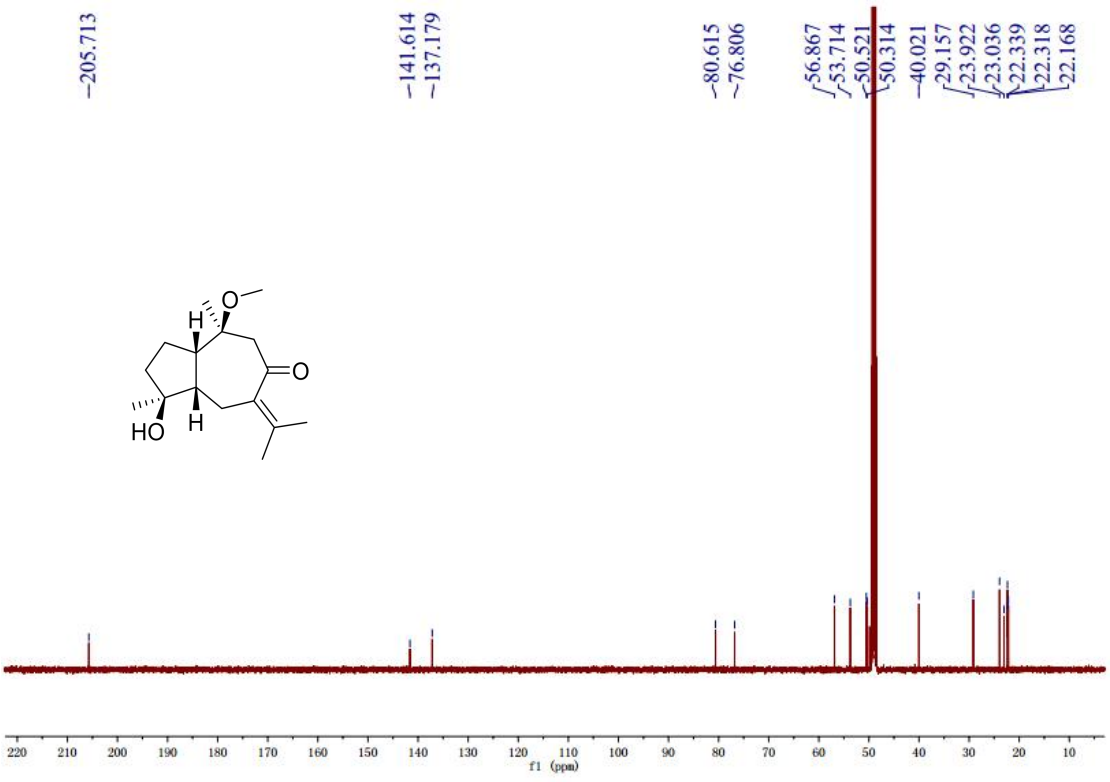


Figure S27. The ^{13}C NMR Spectrum of Compound 8 in CD3OD

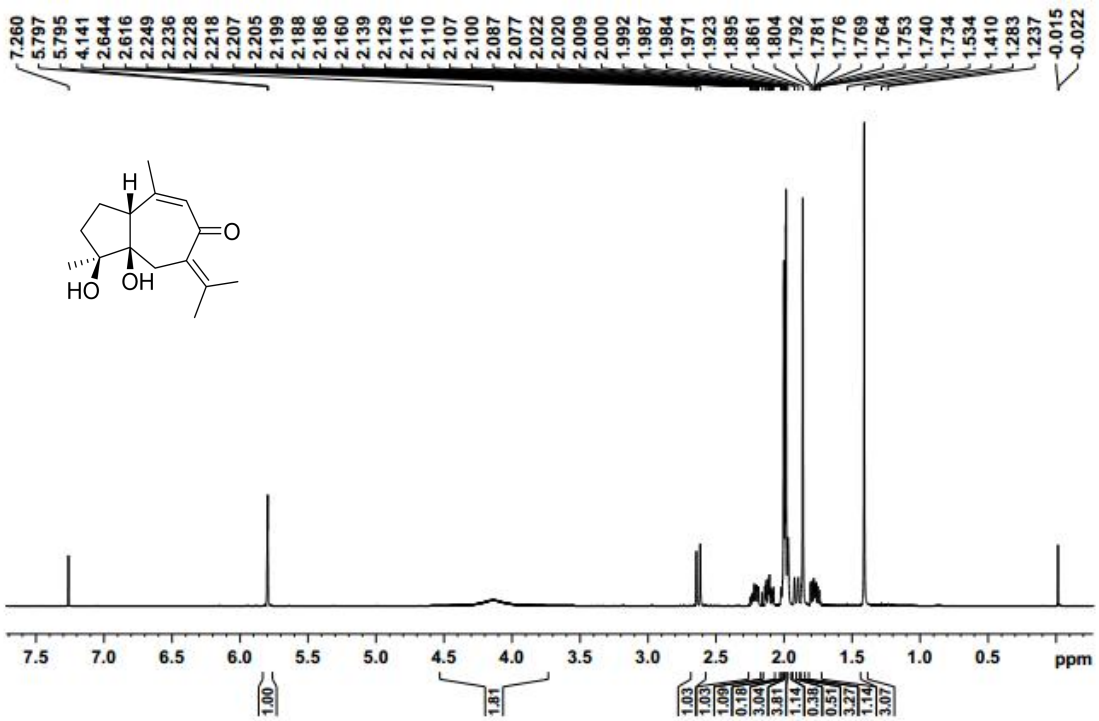


Figure S28. The ^{1}H NMR Spectrum of Compound 9 in CDCl3

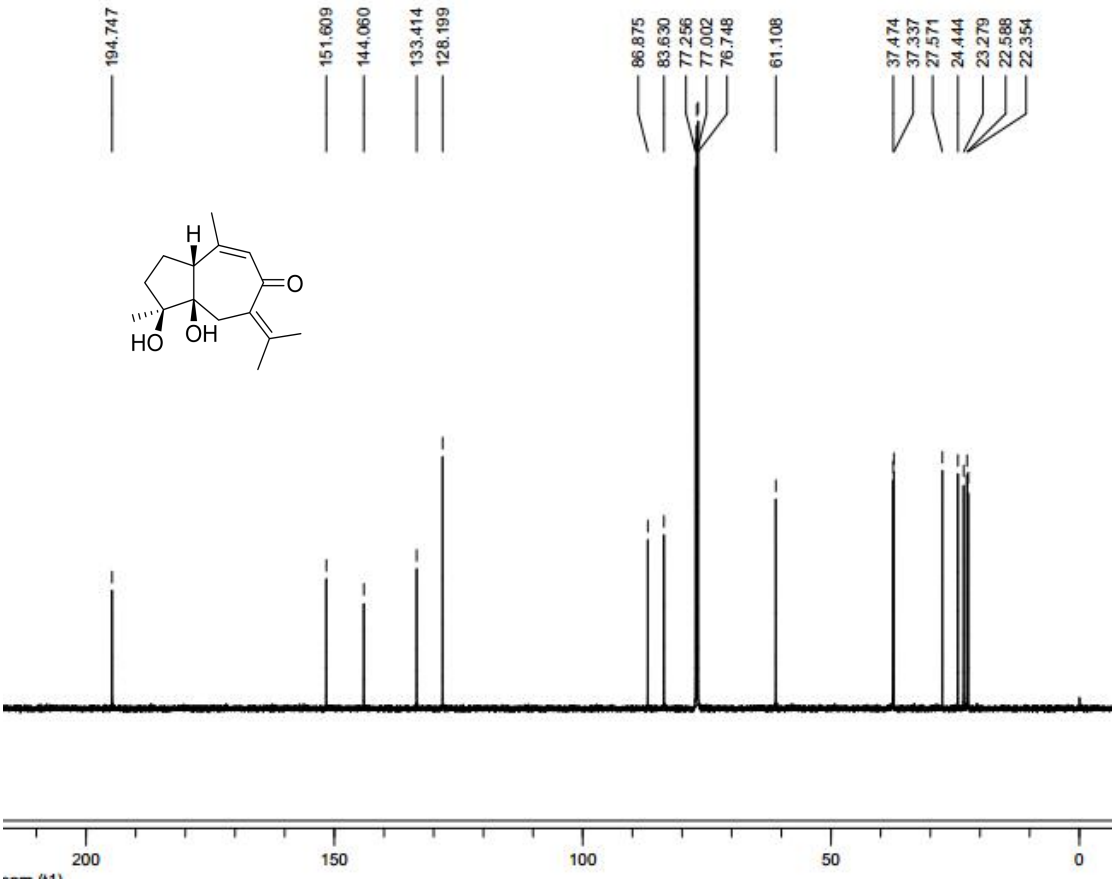


Figure S29. The ^{13}C NMR Spectrum of Compound 9 in CDCl3

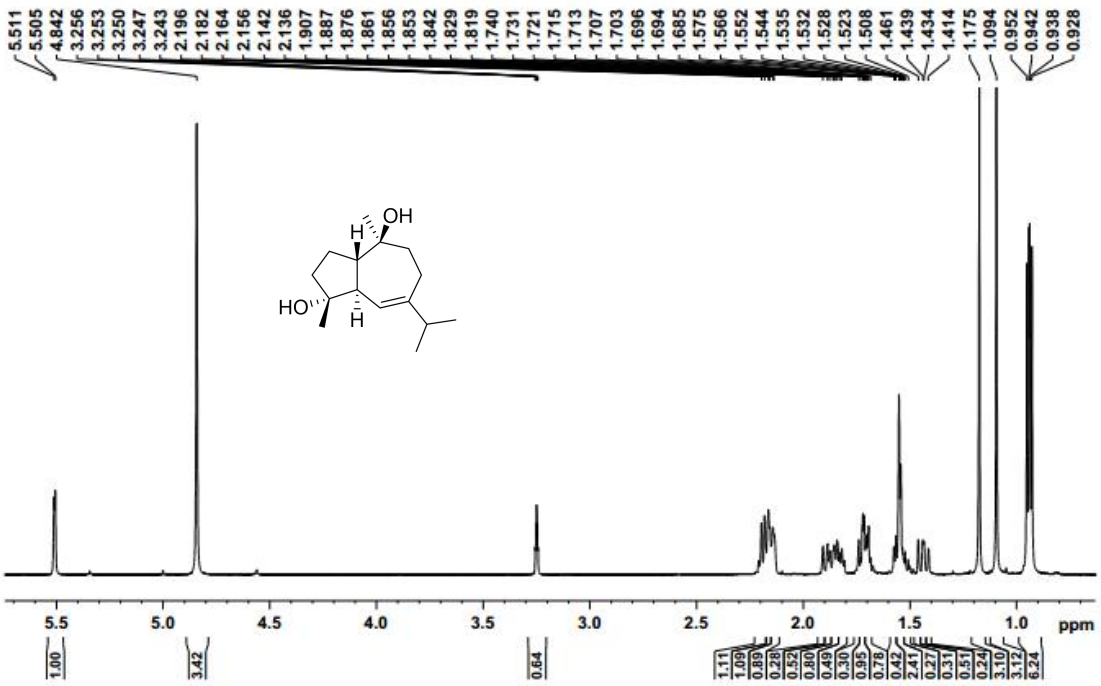


Figure S30. The ^{1}H NMR Spectrum of Compound 10 in CD3OD

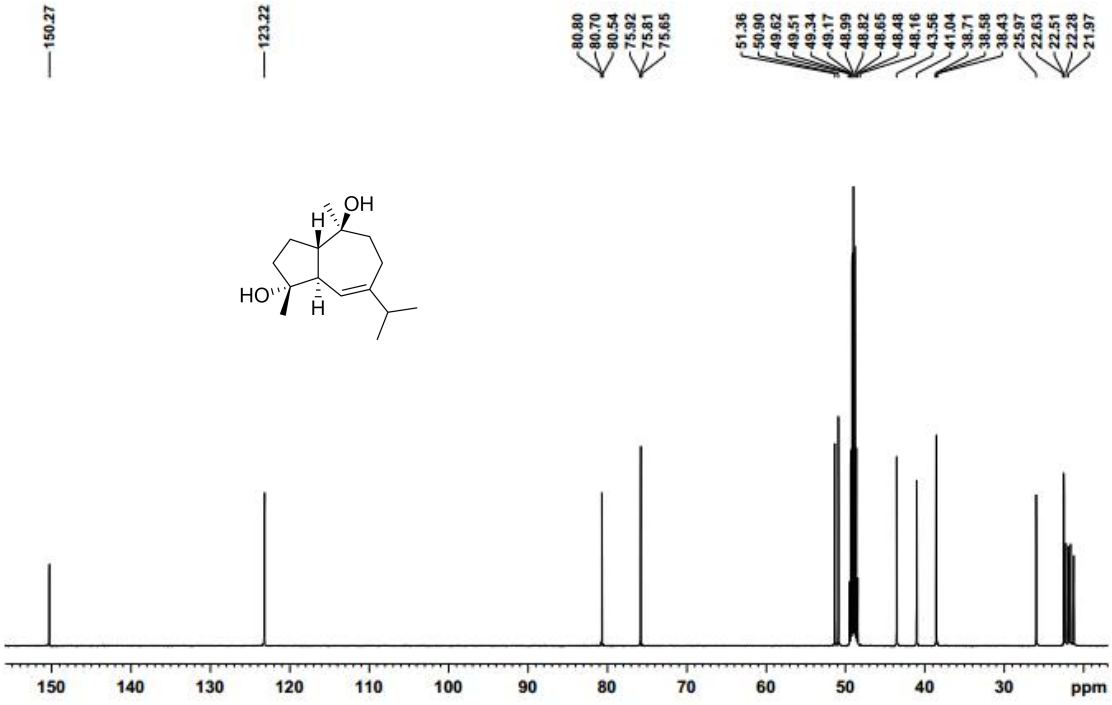


Figure S31. The ^{13}C NMR Spectrum of Compound 10 in CD3OD

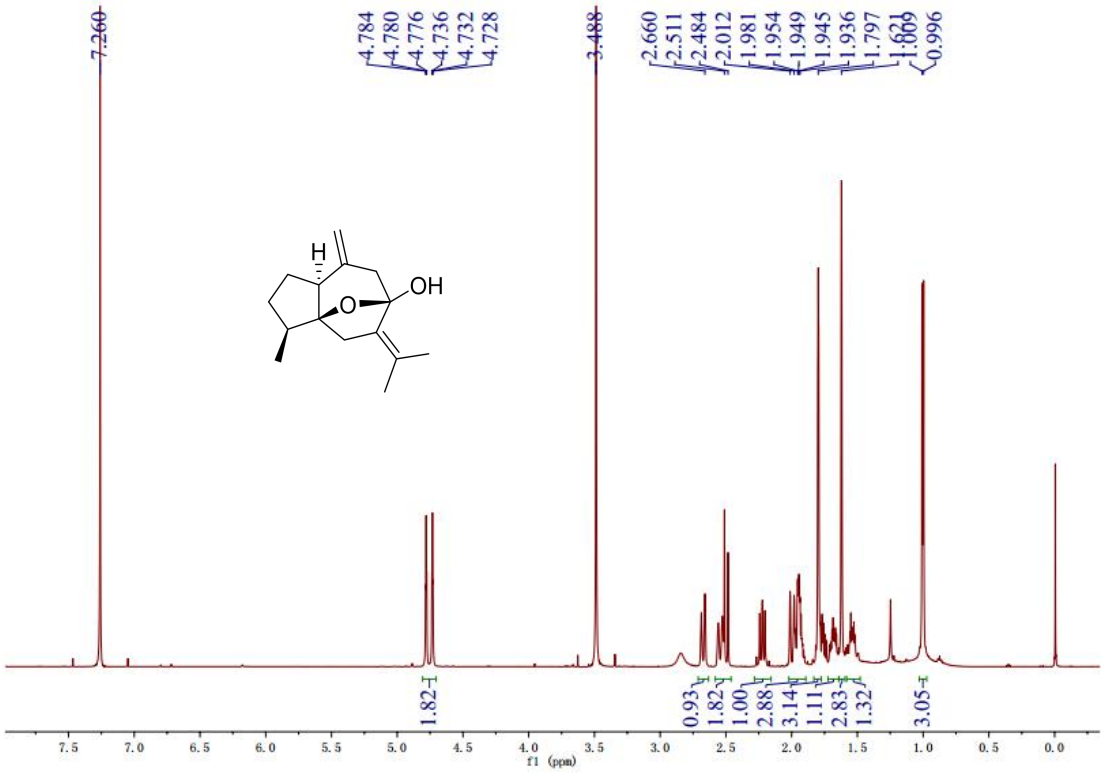


Figure S32. The ^{1}H NMR Spectrum of Compound 11 in CDCl3

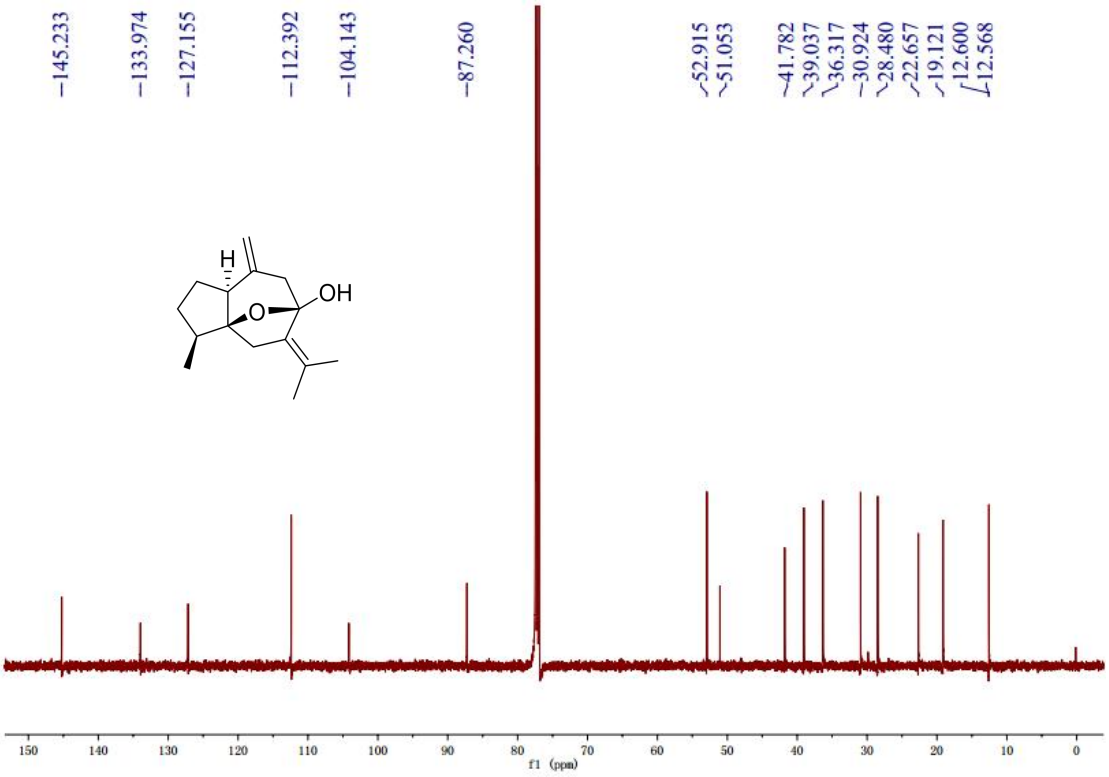


Figure S33. The ^{13}C NMR Spectrum of Compound 11 in CDCl3

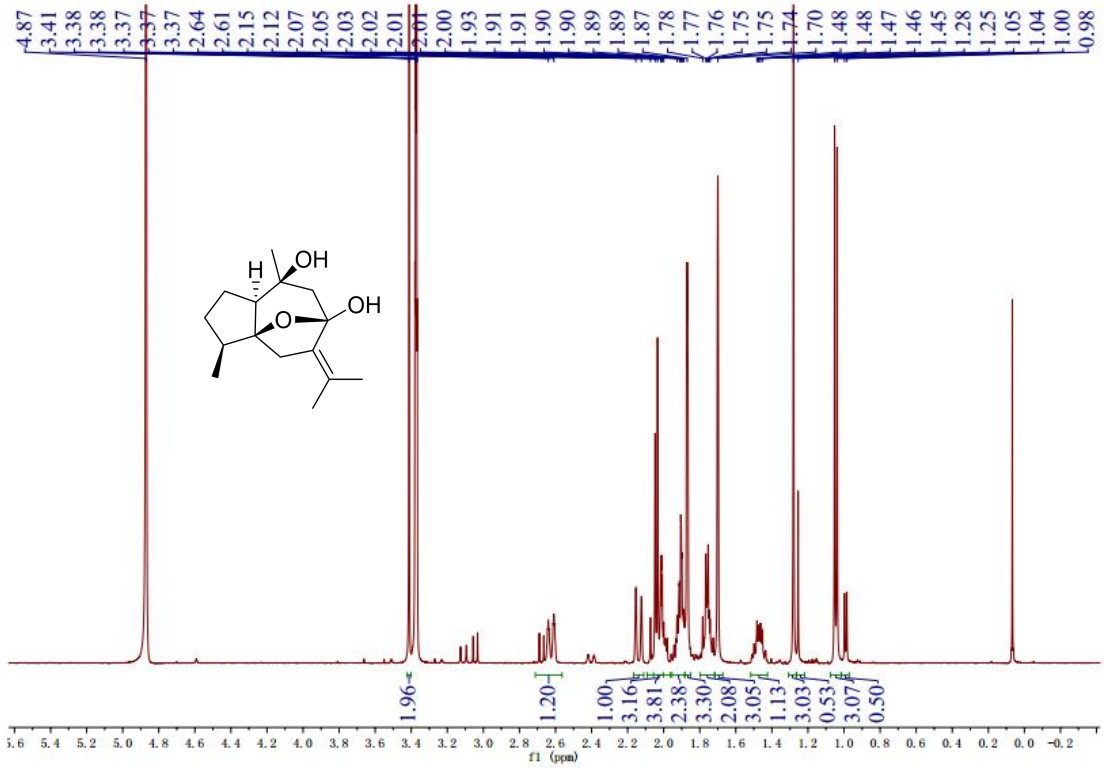


Figure S34. The ^{1}H NMR Spectrum of Compound 12 in CD3OD

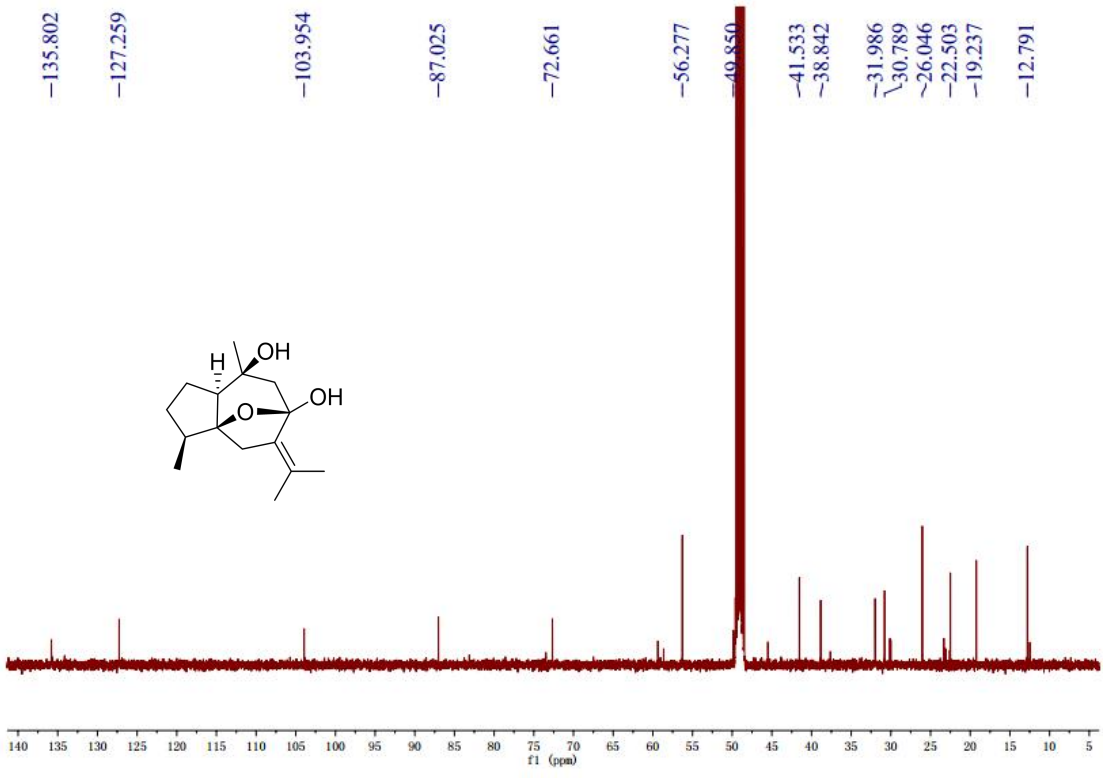


Figure S35. The ^{13}C NMR Spectrum of Compound 12 in CD3OD

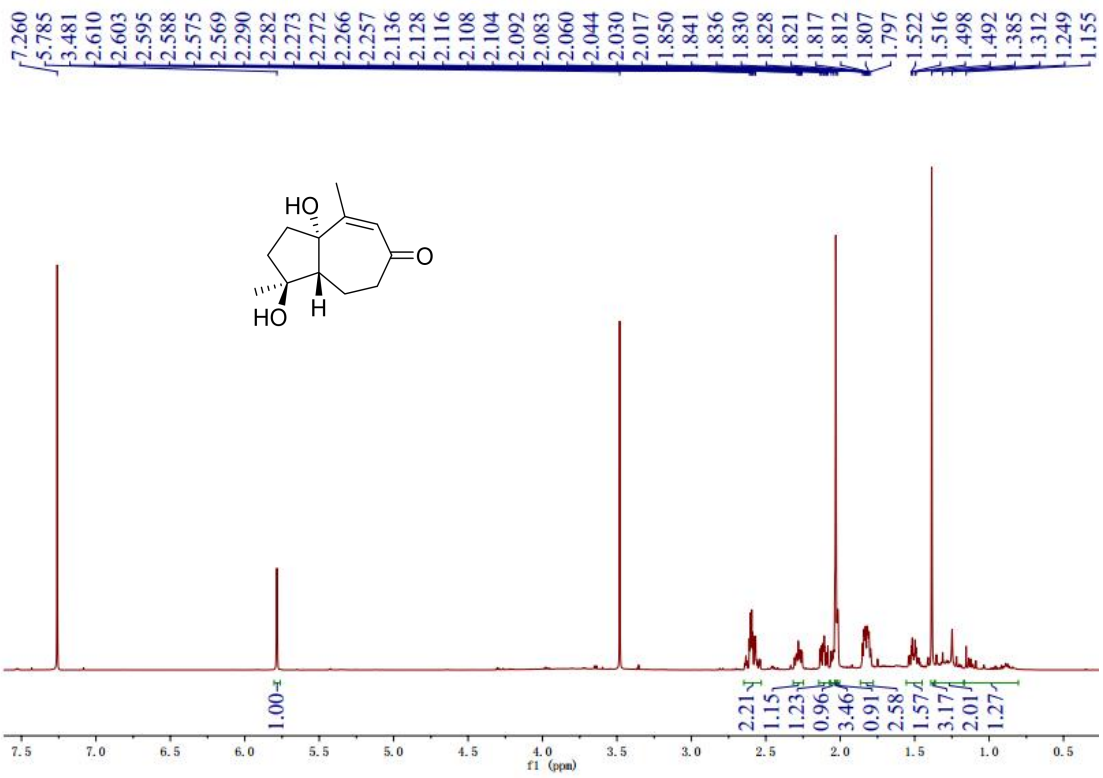


Figure S36. The ^{1}H NMR Spectrum of Compound 13 in CDCl3

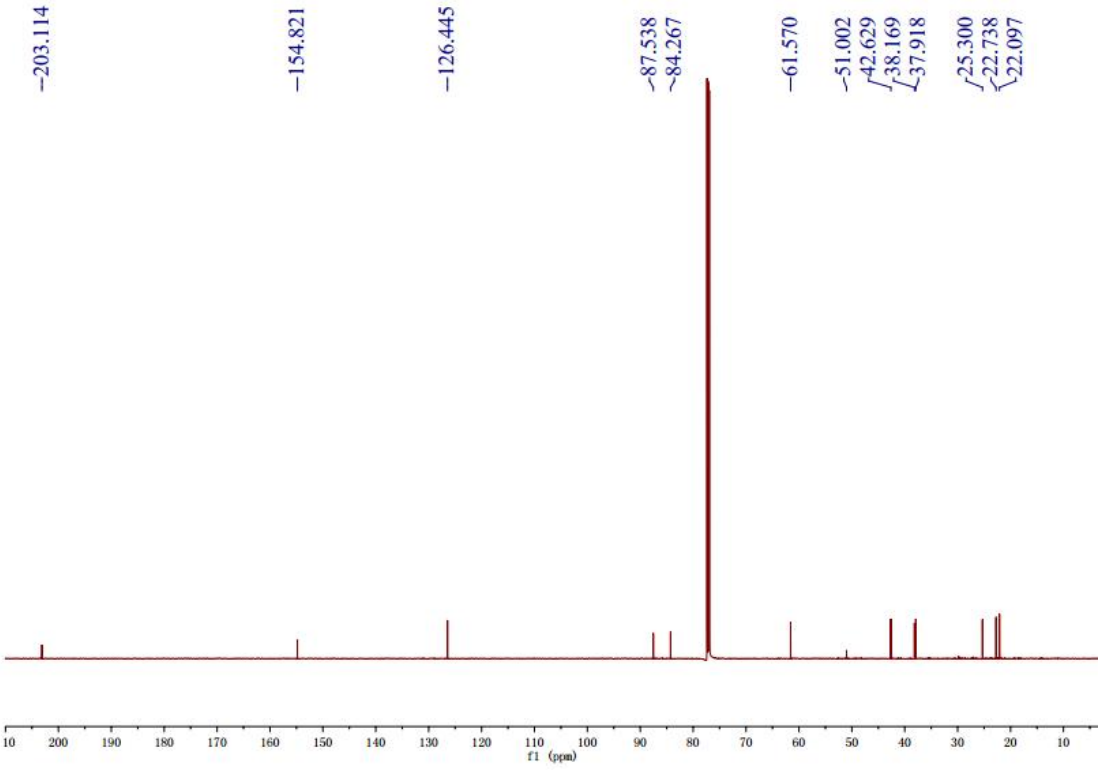


Figure S37. The ^{13}C NMR Spectrum of Compound 13 in CDCl3

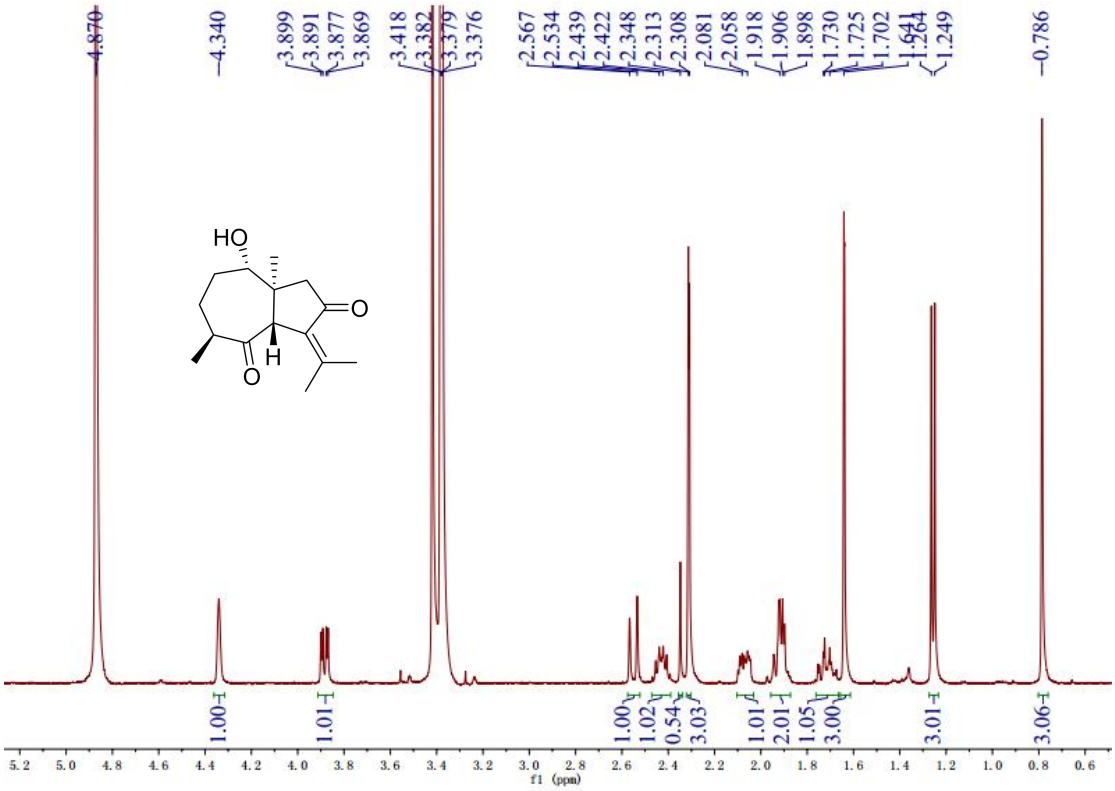


Figure S38. The ^{1}H NMR Spectrum of Compound 14 in CD3OD

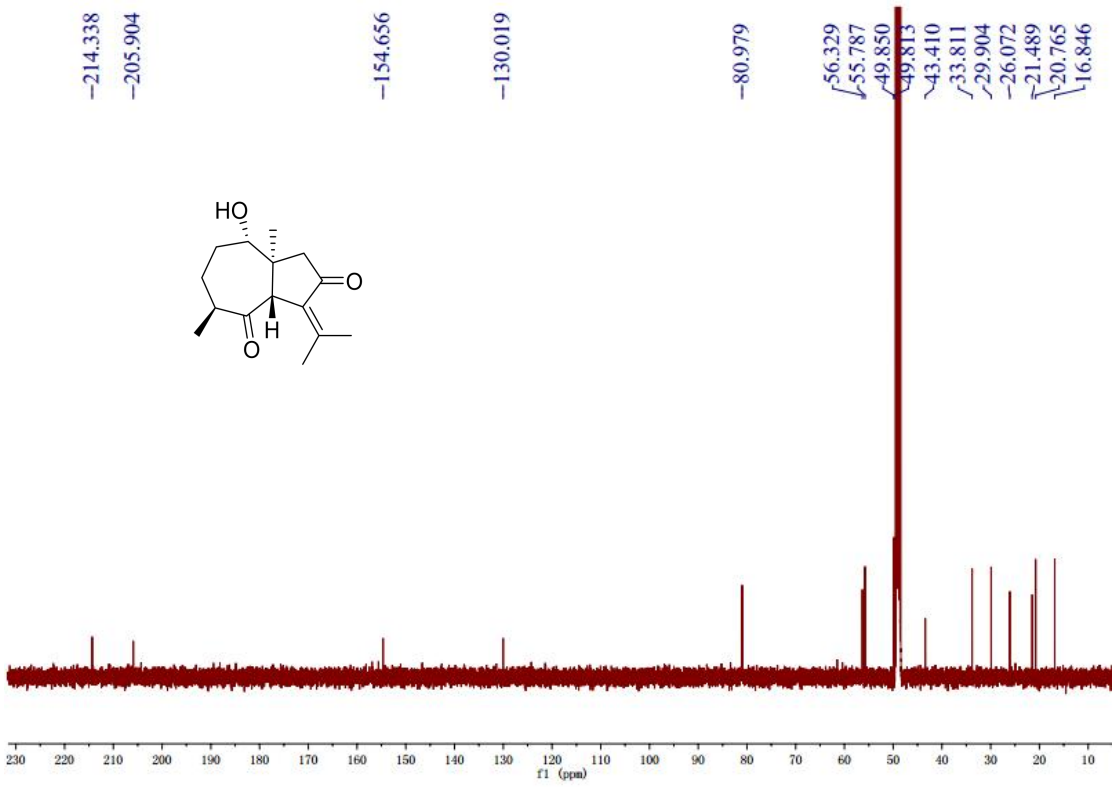


Figure S39. The ^{13}C NMR Spectrum of Compound 14 in CD3OD

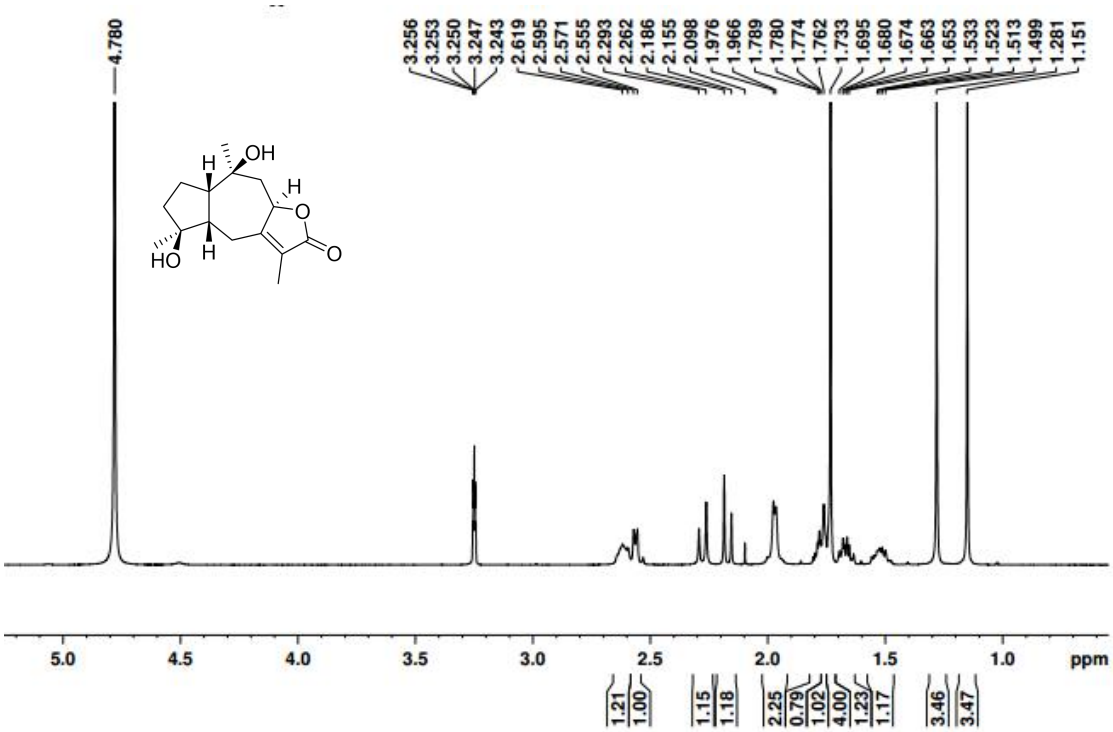


Figure S40. The ^{1}H NMR Spectrum of Compound 15 in CD3OD

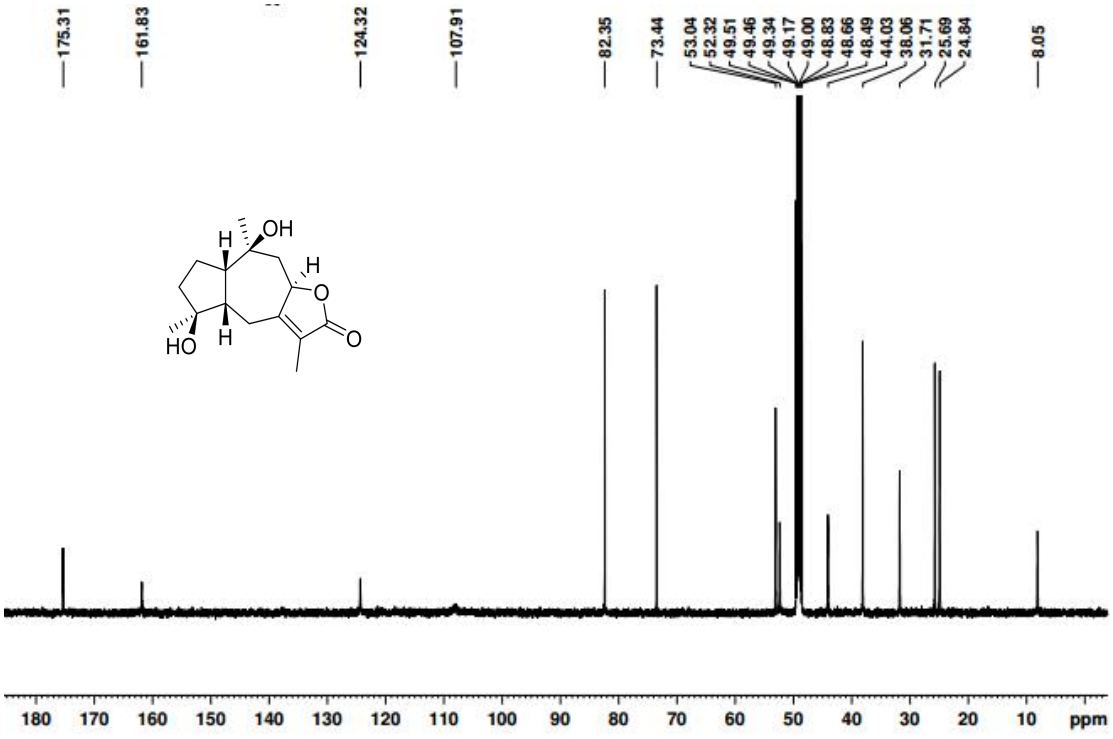


Figure S41. The ^{13}C NMR Spectrum of Compound 15 in CD3OD

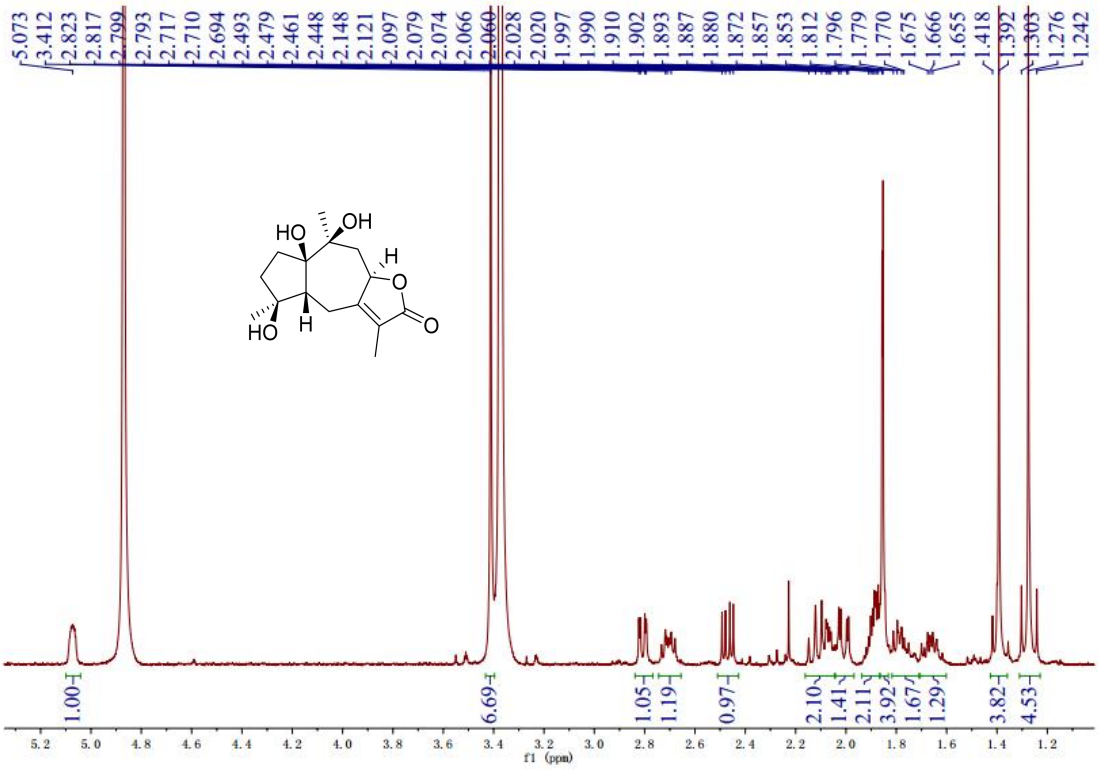


Figure S42. The ^{1}H NMR Spectrum of Compound 16 in CD3OD

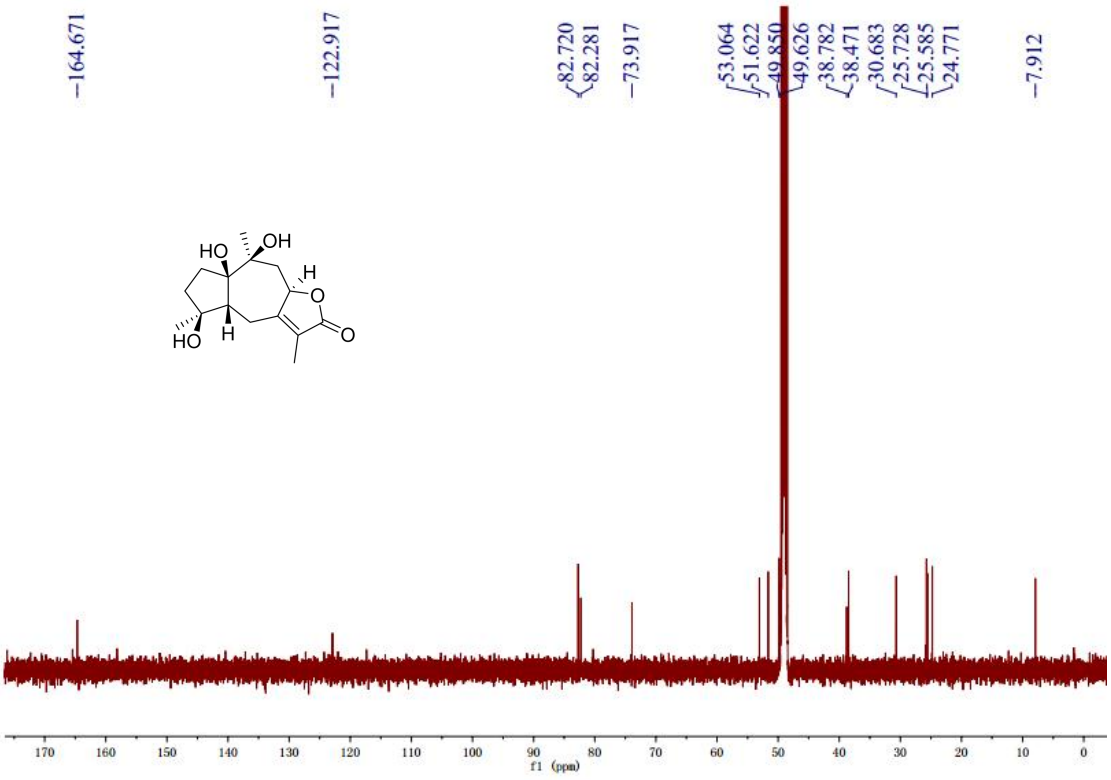


Figure S43. The ^{13}C NMR Spectrum of Compound 16 in CD3OD

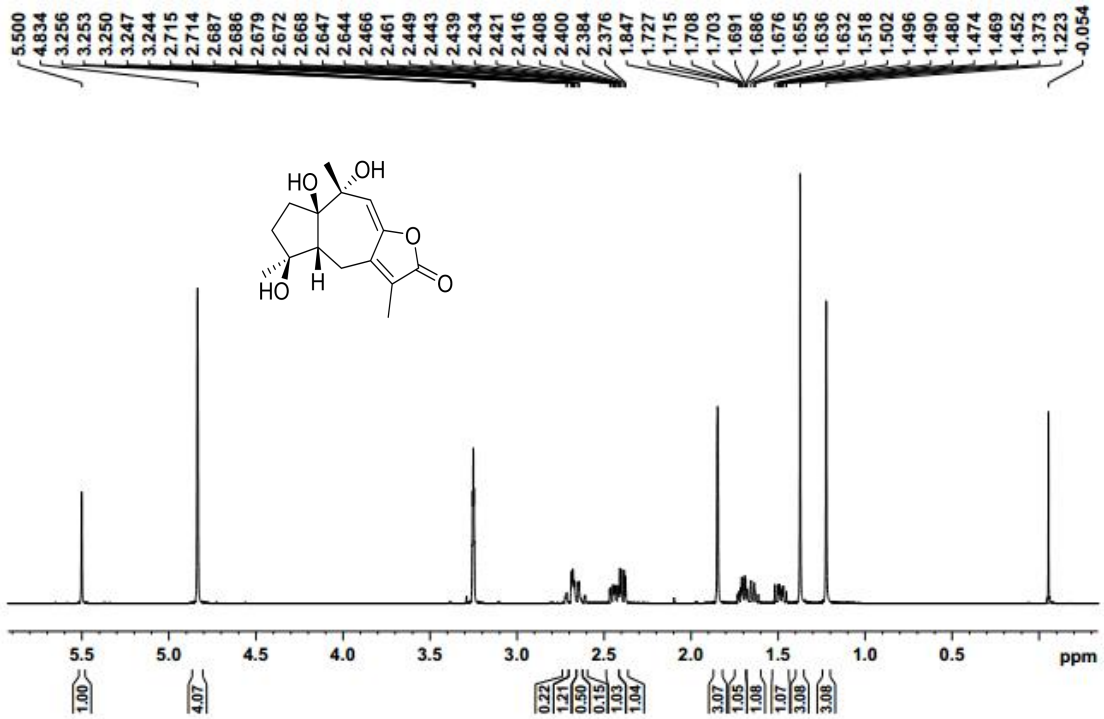


Figure S44. The ^{1}H NMR Spectrum of Compound 17 in CD3OD

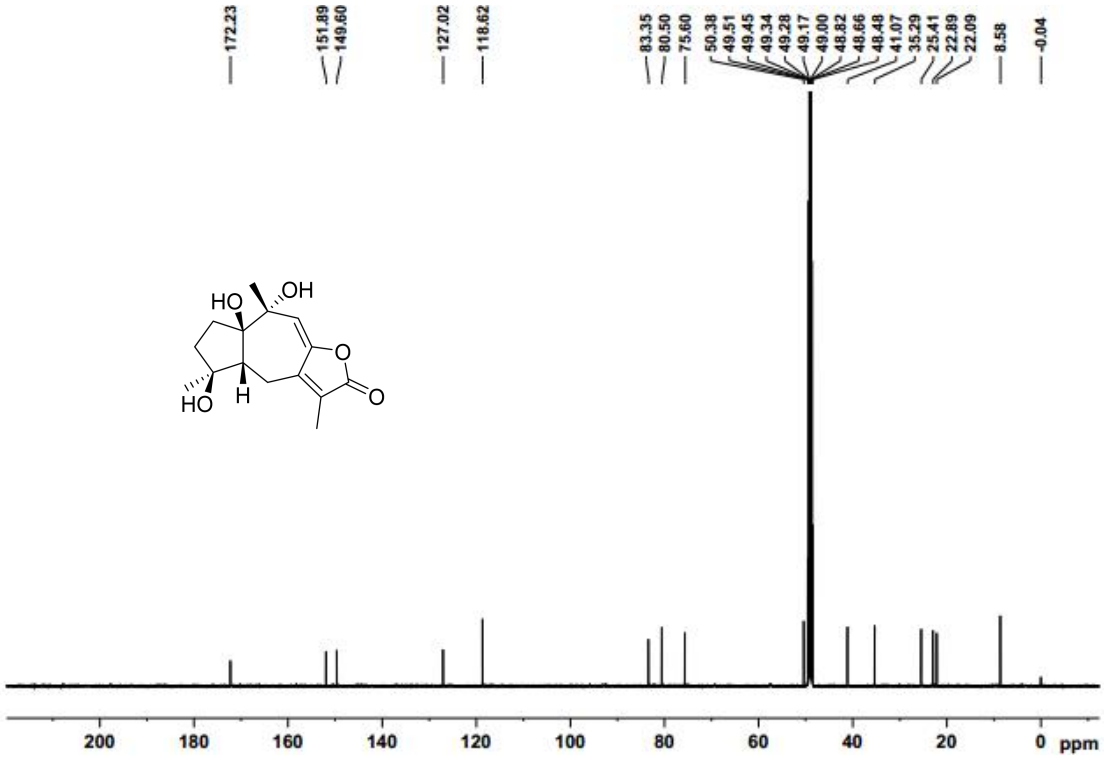


Figure S45. The ^{13}C NMR Spectrum of Compound 17 in CD3OD

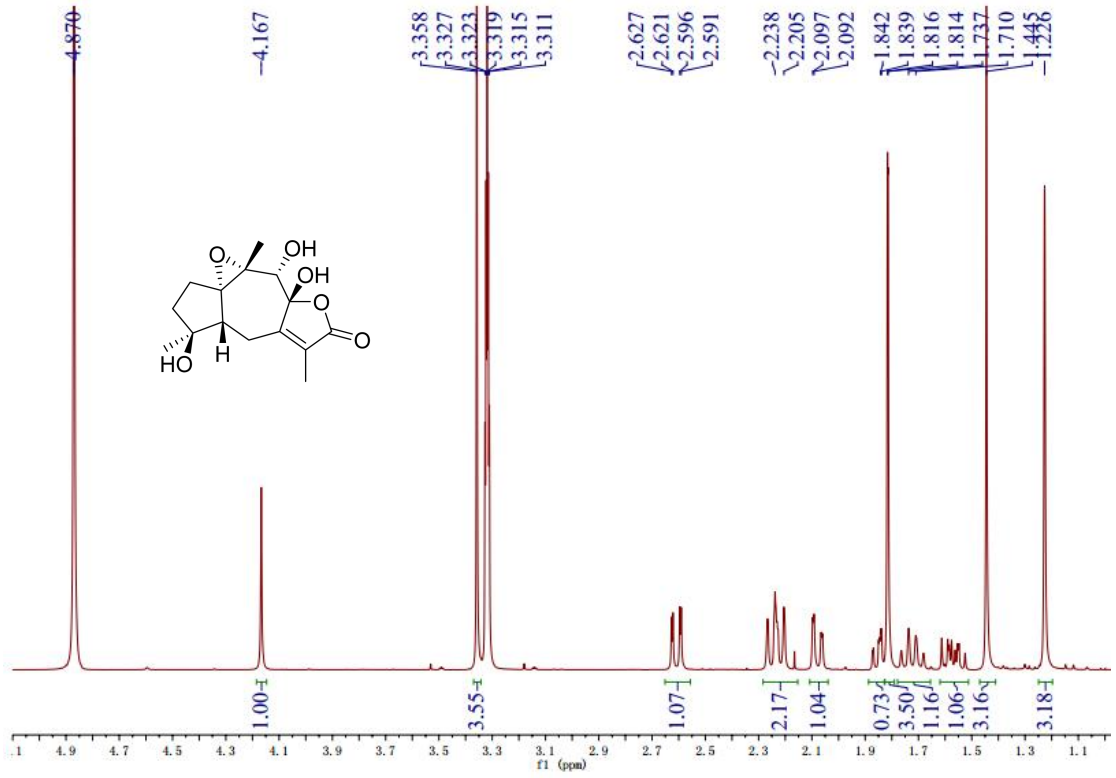


Figure S46. The ^{1}H NMR Spectrum of Compound 18 in CD3OD

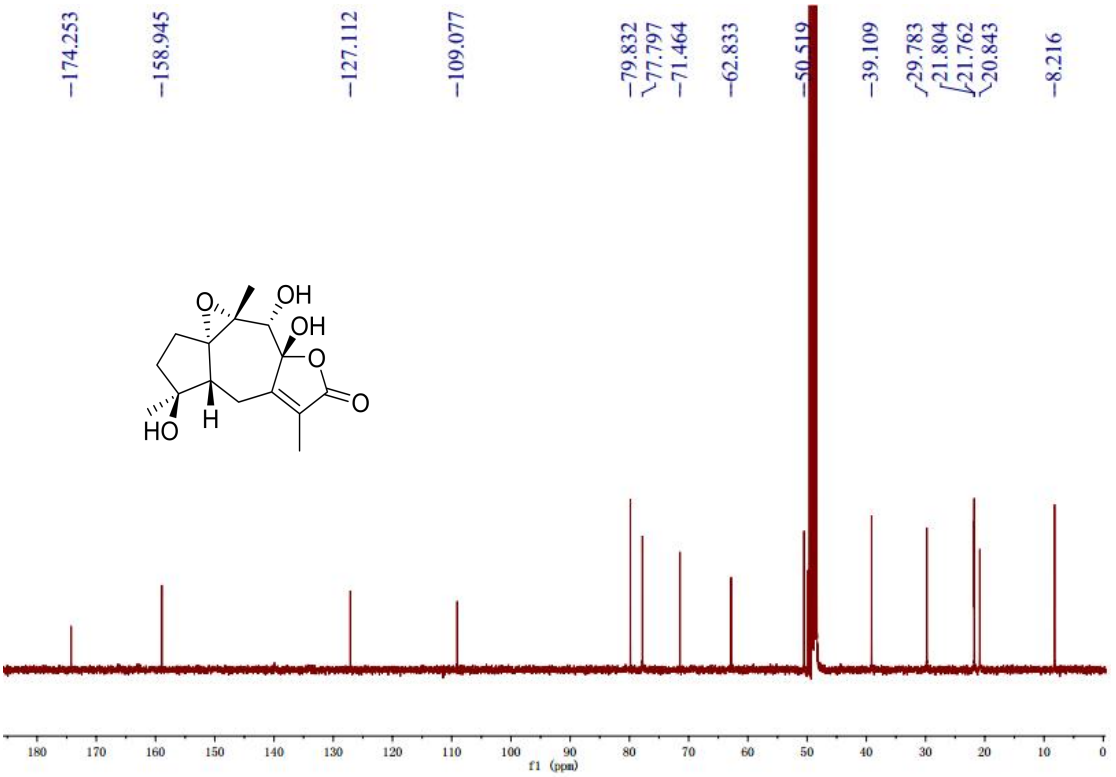


Figure S47. The ^{13}C NMR Spectrum of Compound 18 in CD3OD

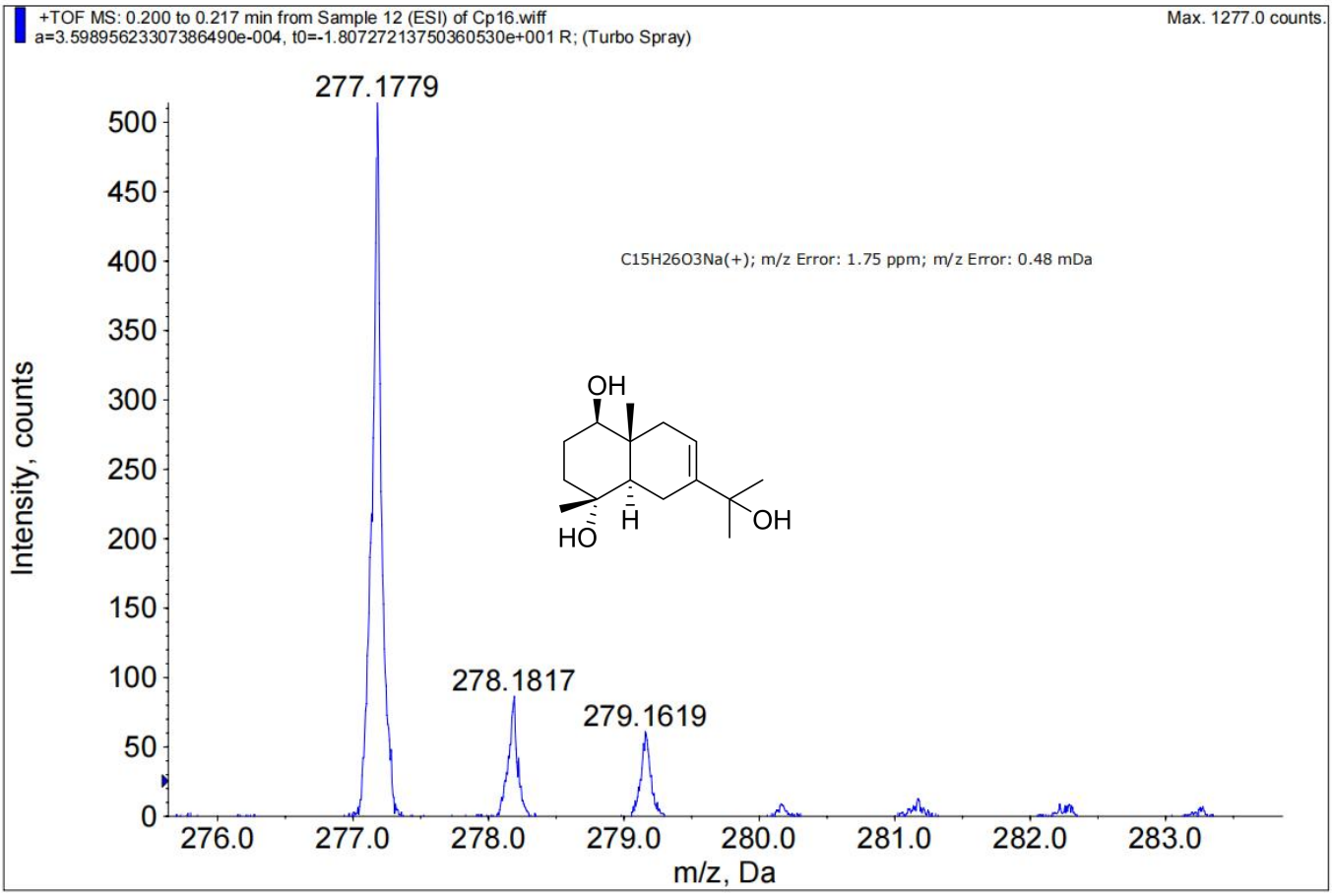


Figure S48. The HR-ESI-MS Spectrum of Compound 19

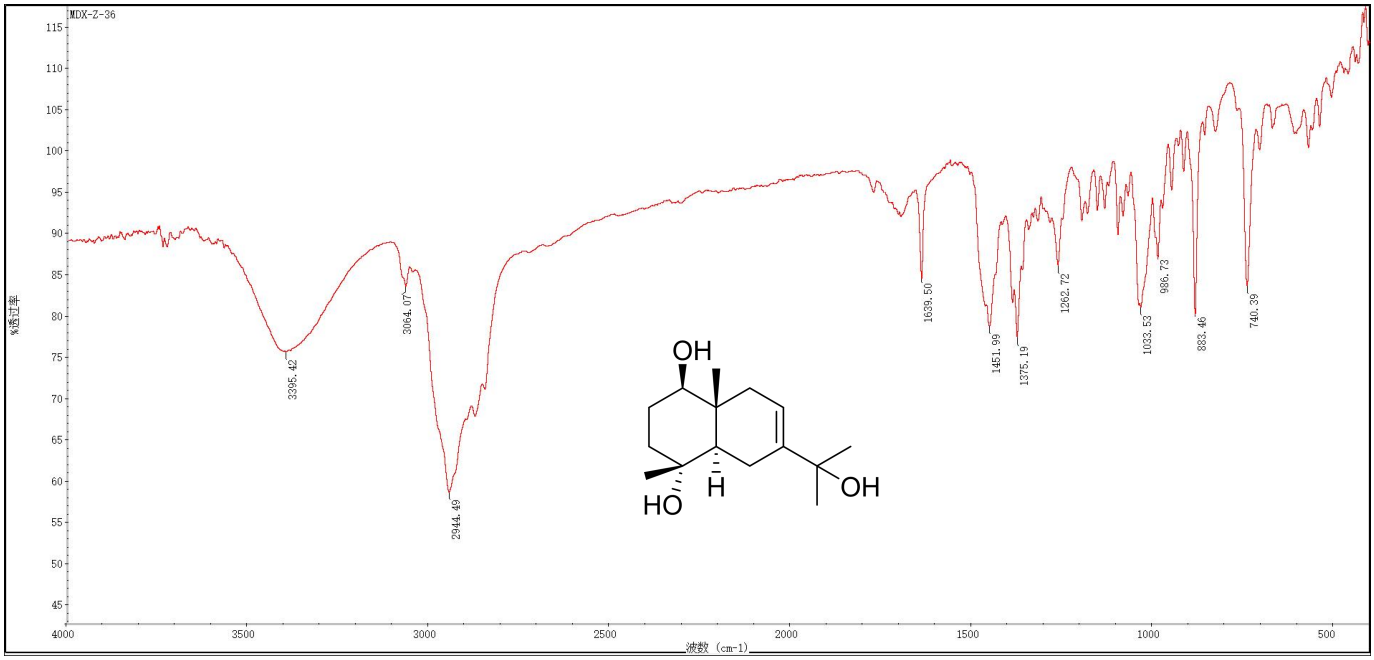


Figure S49. The IR Spectrum of Compound 19

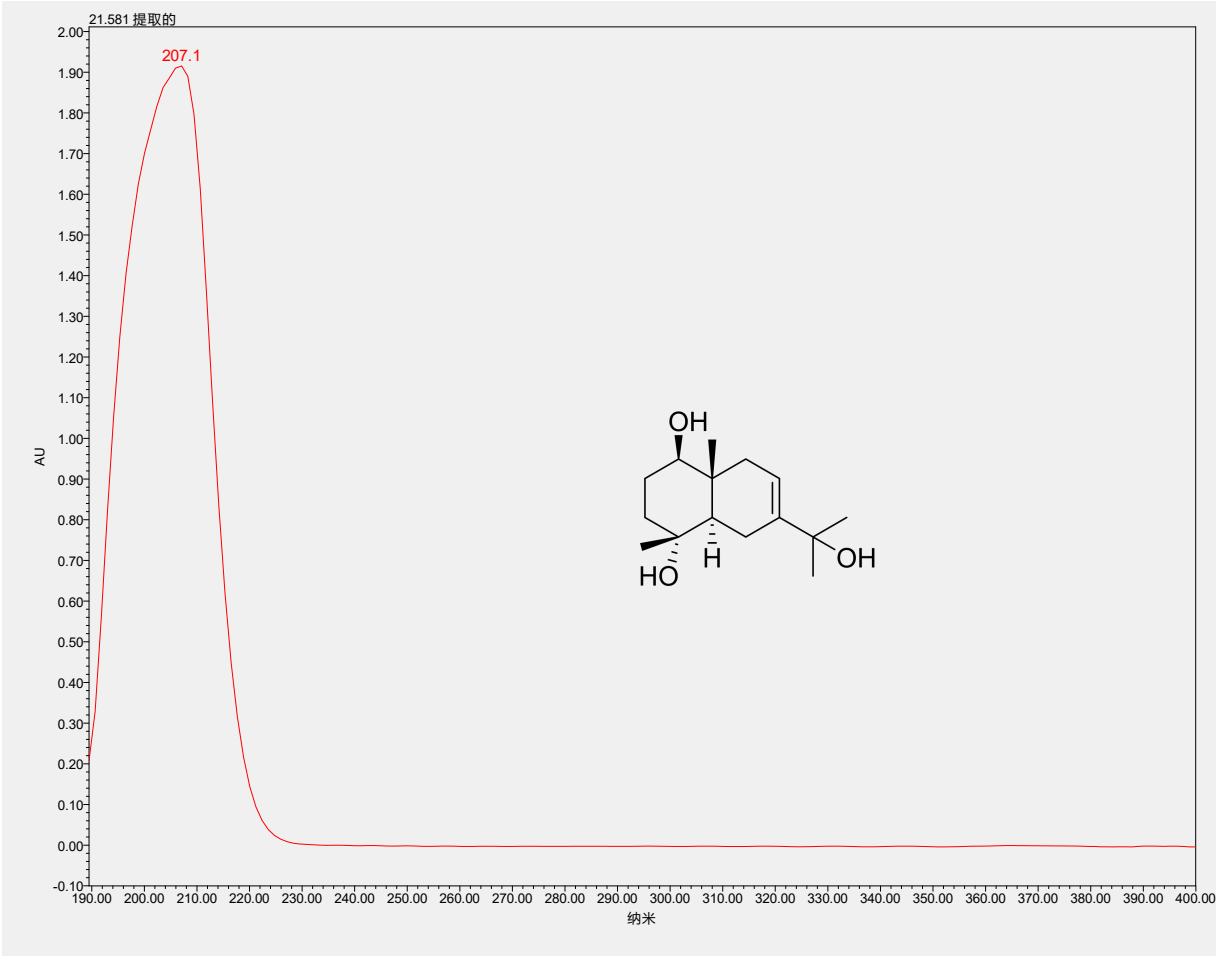


Figure S50. The UV Spectrum of Compound 19

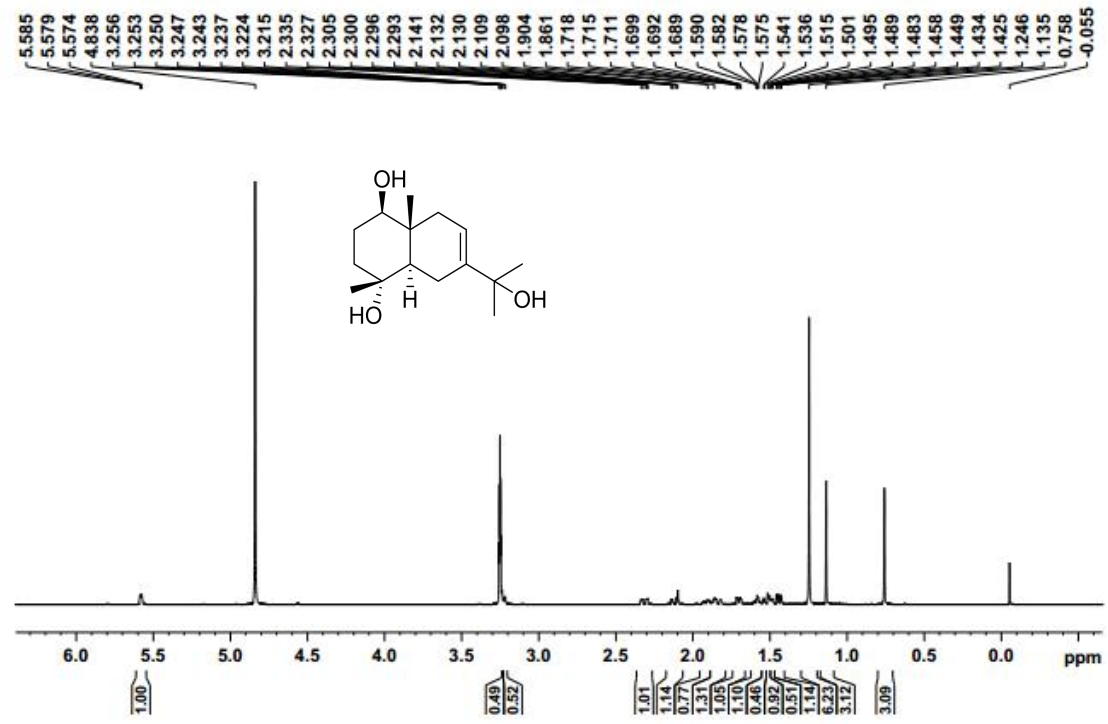


Figure S51. The ^{1}H NMR Spectrum of Compound 19 in CD3OD

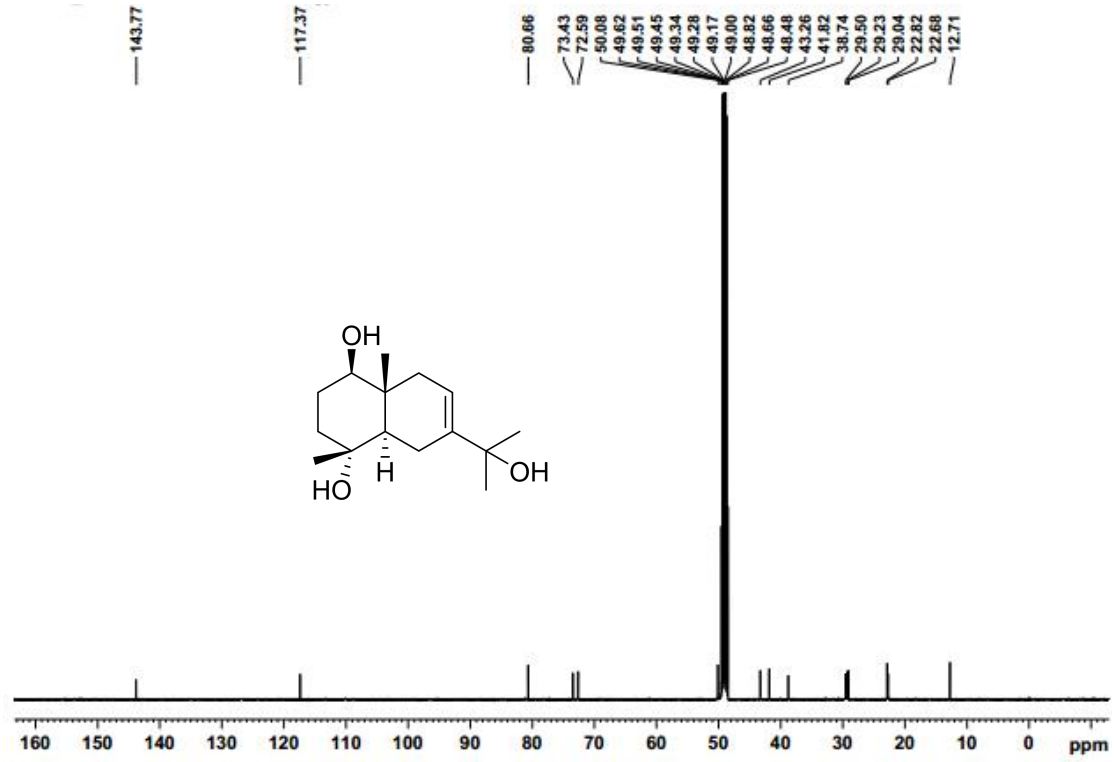


Figure S52. The ^{13}C NMR Spectrum of Compound 19 in CD3OD

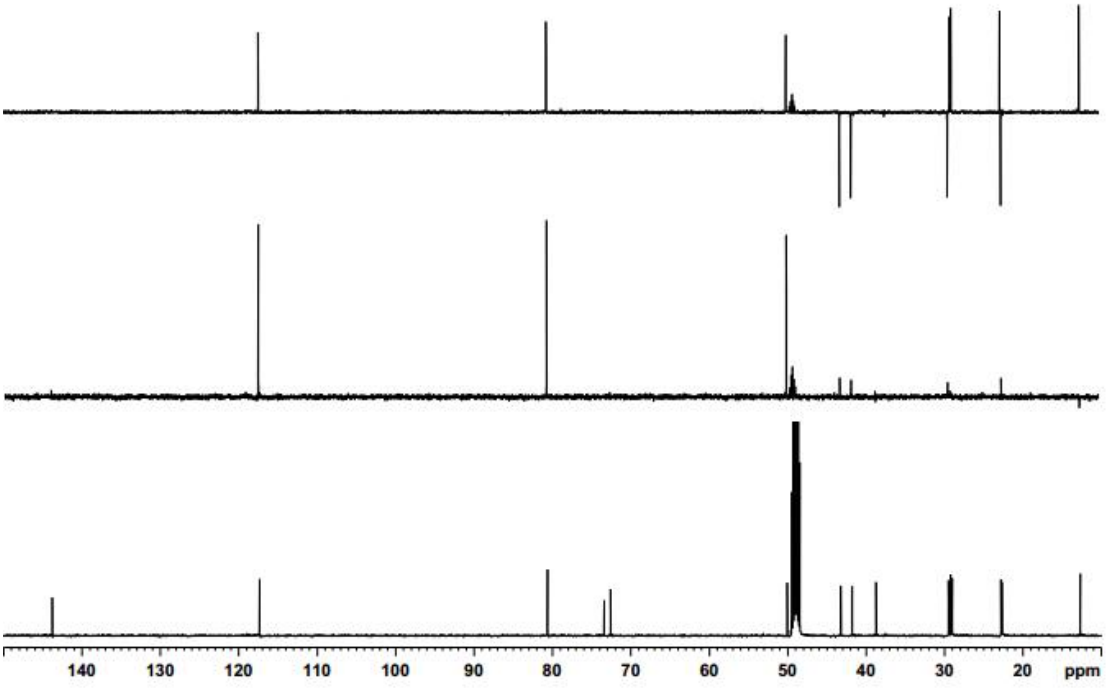


Figure S53. The DEPT Spectrum of Compound 19 in CD3OD

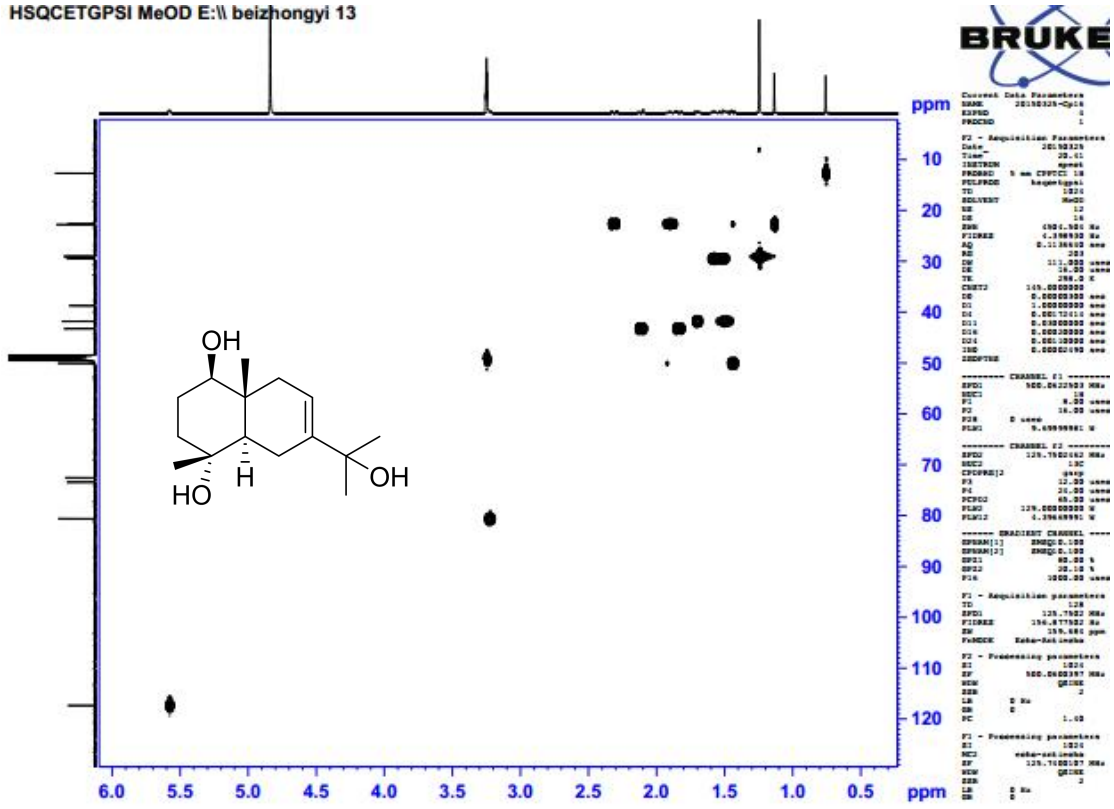


Figure S54. The HSQC Spectrum of Compound 19 in CD3OD

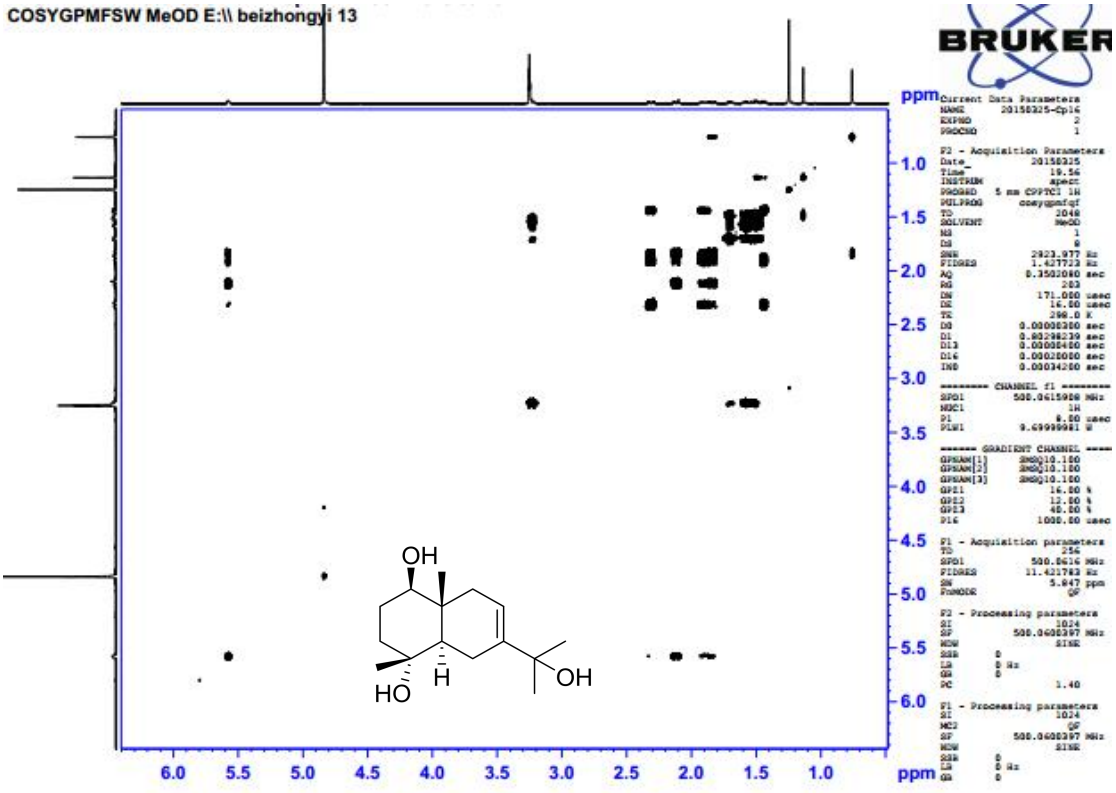


Figure S55. The ^{1}H-^{1}H COSY Spectrum of Compound 19 in CD3OD

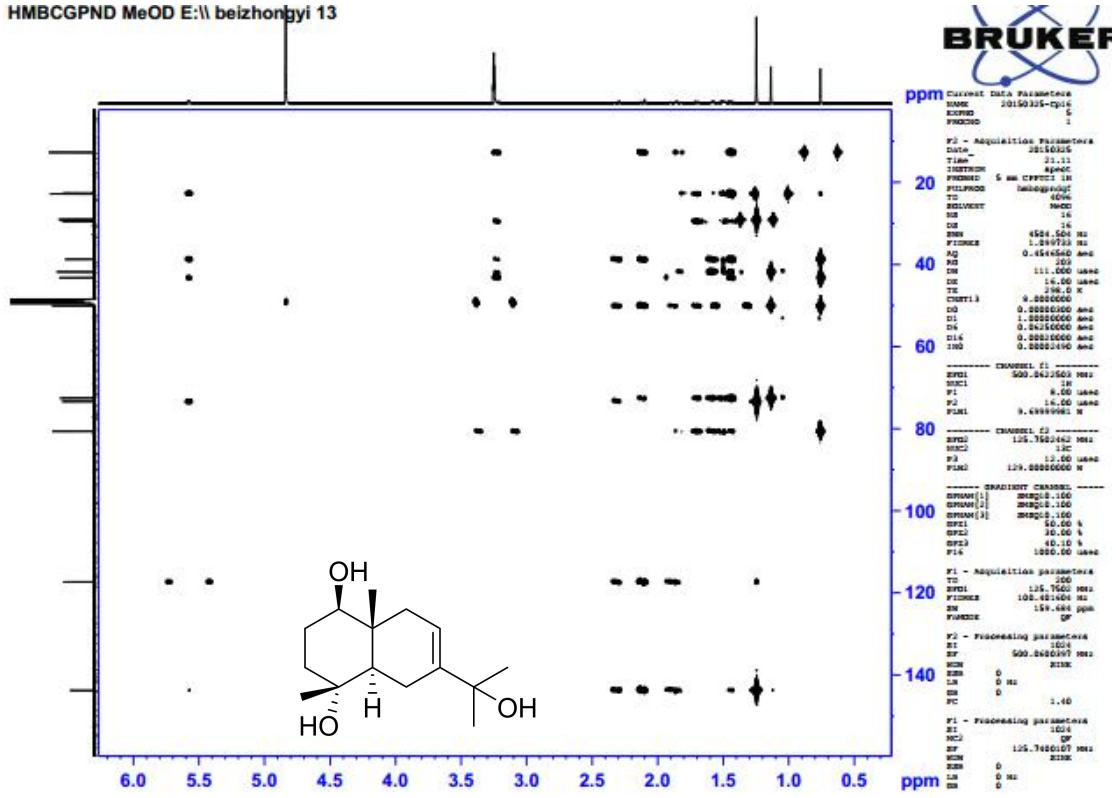


Figure S56. The HMBC Spectrum of Compound 19 in CD3OD

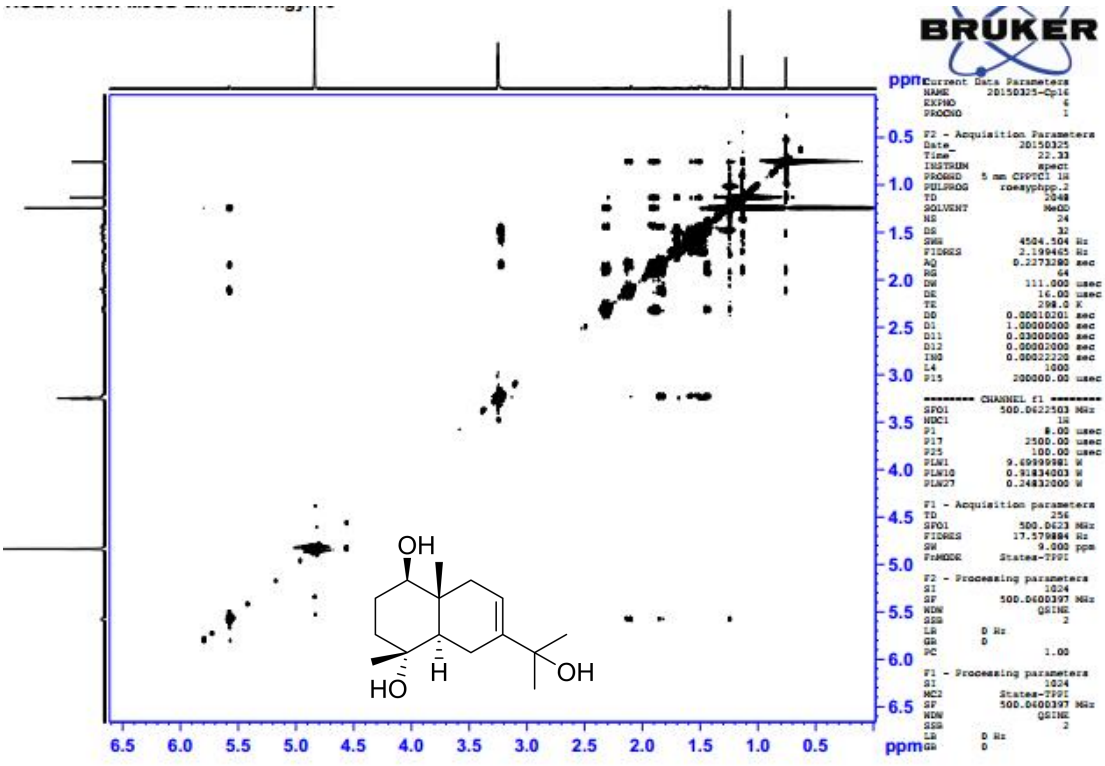


Figure S57. The NOESY Spectrum of Compound 19 in CD3OD

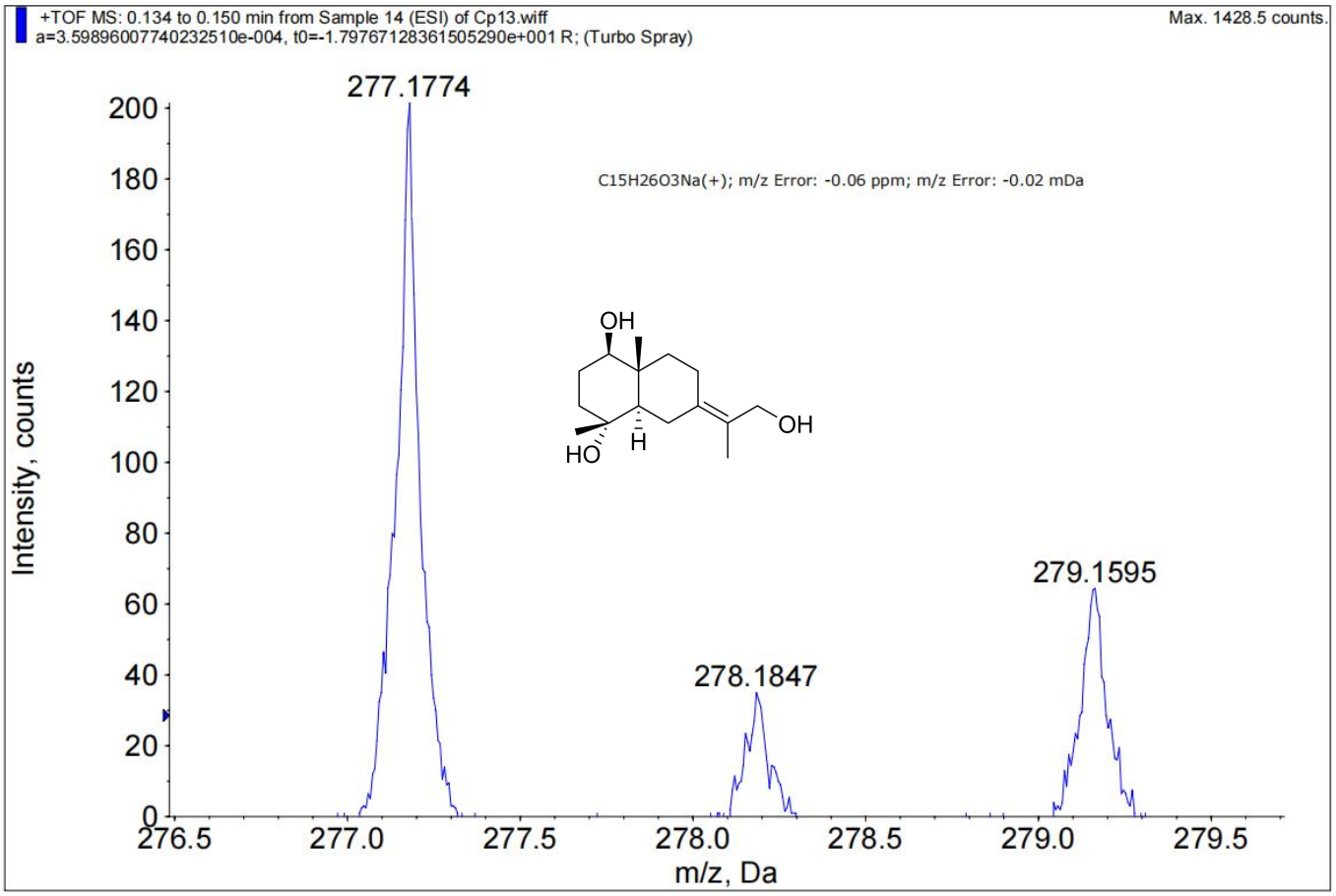


Figure S58. The HR-ESI-MS Spectrum of Compound 20

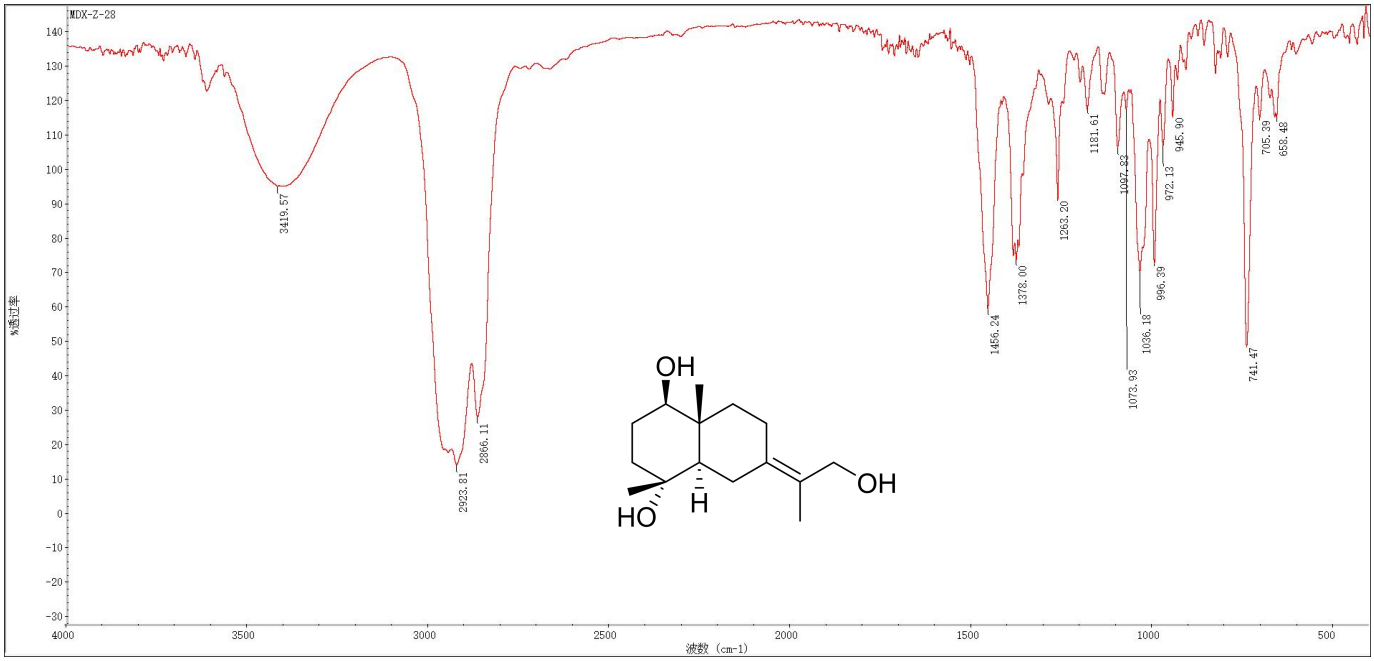


Figure S59. The IR Spectrum of Compound 20

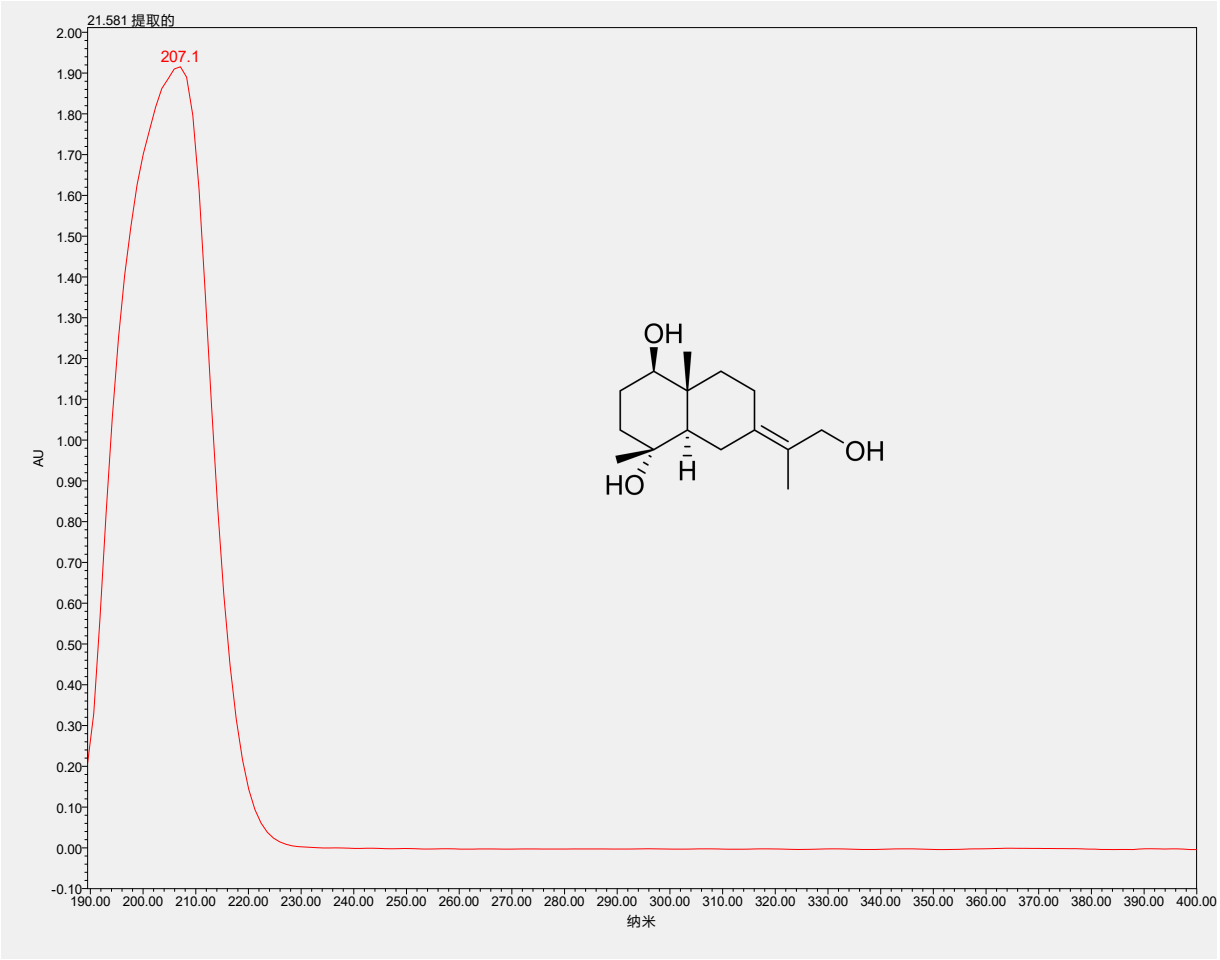


Figure S60. The UV Spectrum of Compound 20

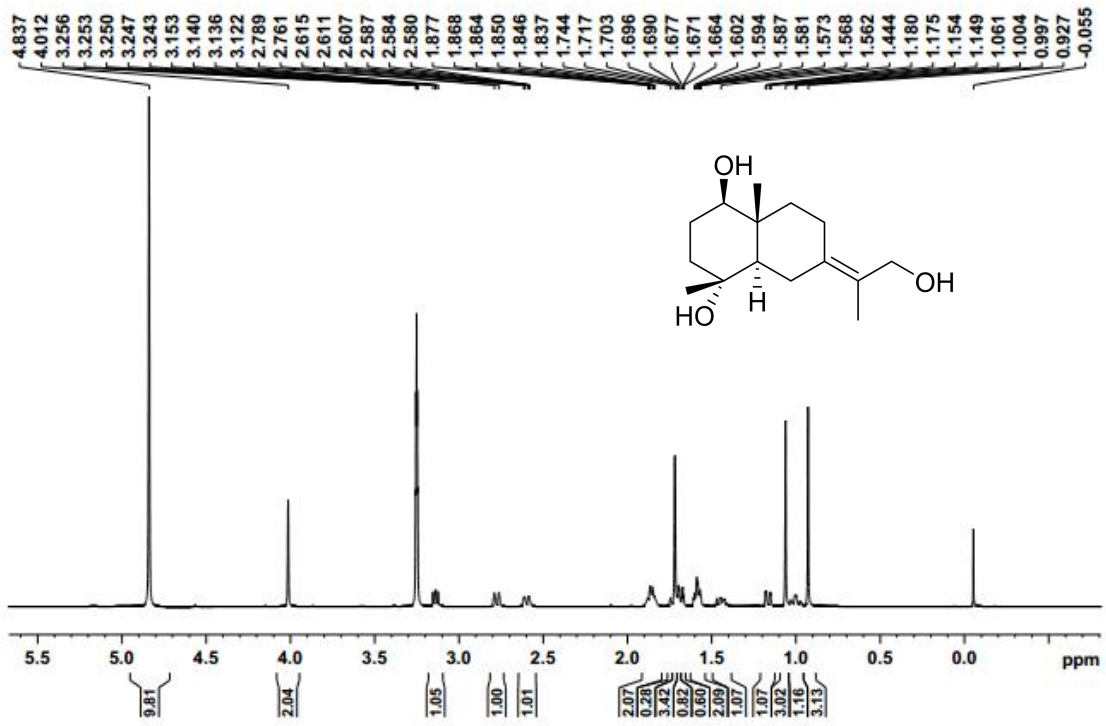


Figure S61. The ^{1}H NMR Spectrum of Compound 20 in CD3OD

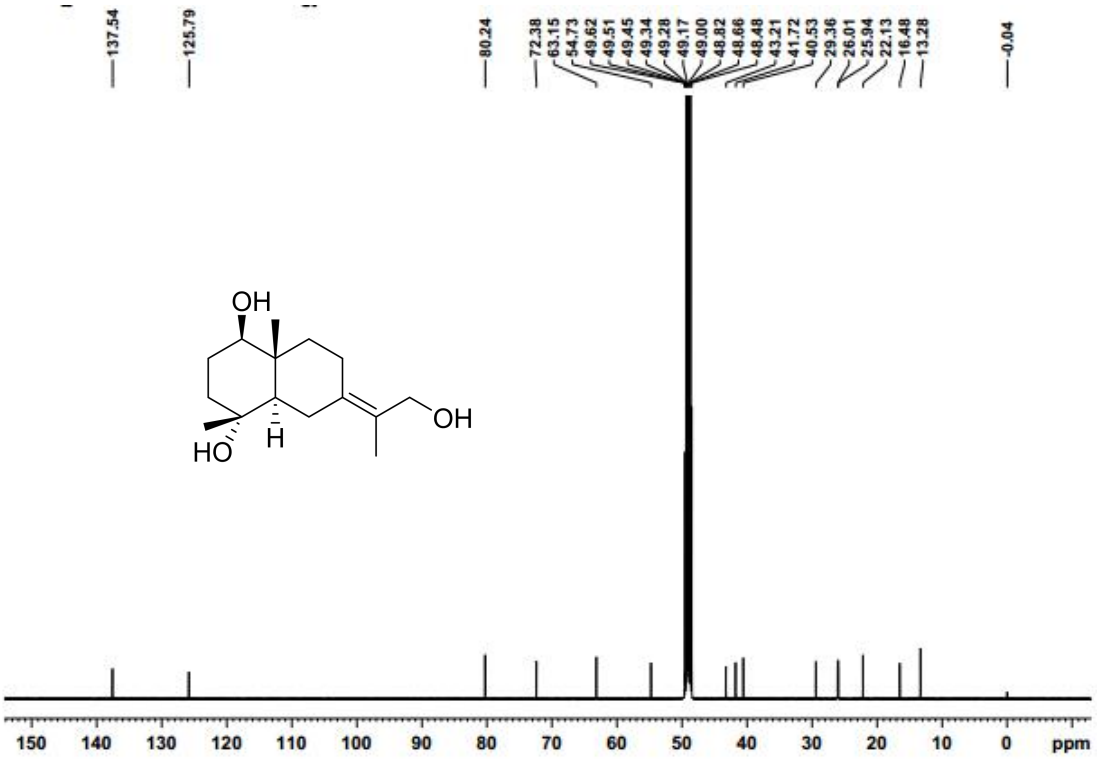


Figure S62. The ^{13}C NMR Spectrum of Compound 20 in CD3OD

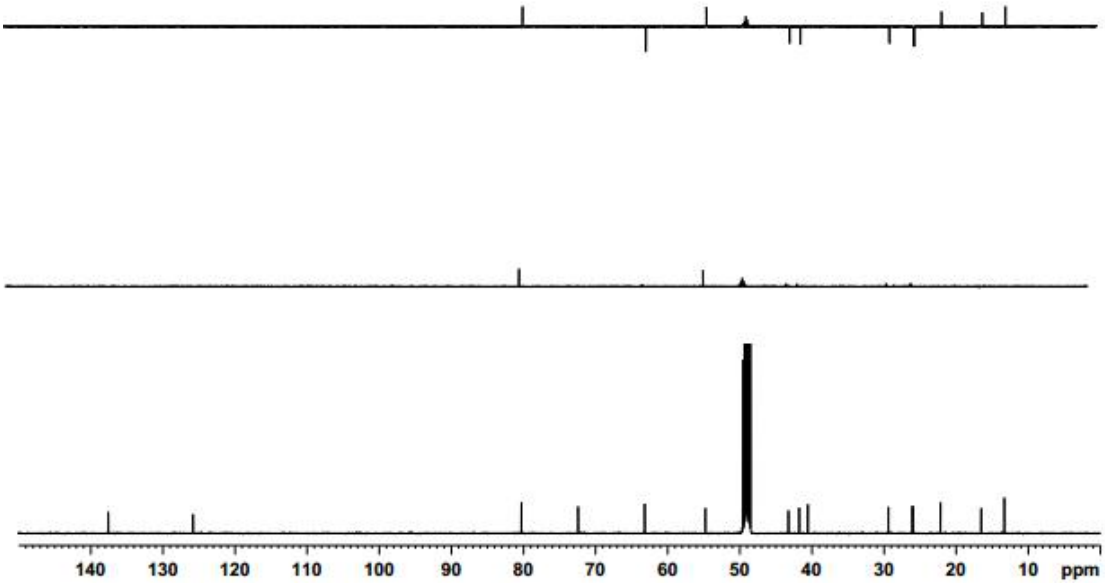


Figure S63. The DEPT Spectrum of Compound 20 in CD3OD

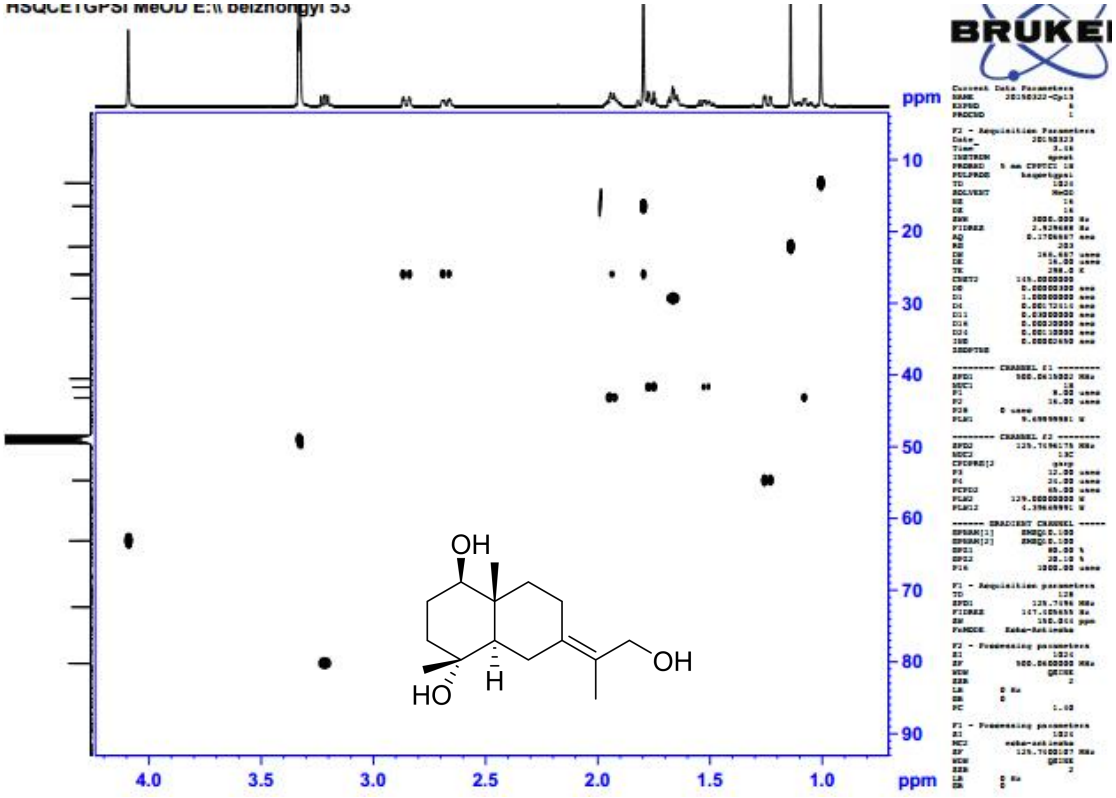


Figure S64. The HSQC Spectrum of Compound 20 in CD3OD

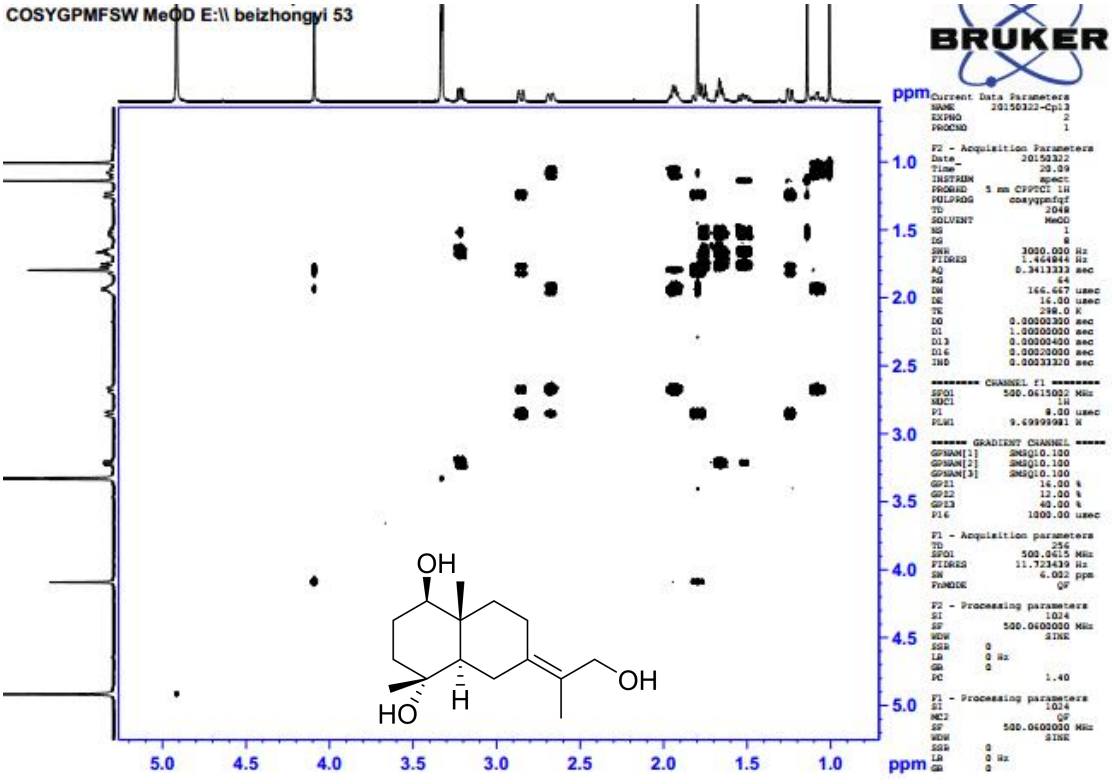


Figure S65. The ^{1}H-^{1}H COSY Spectrum of Compound 20 in CD3OD

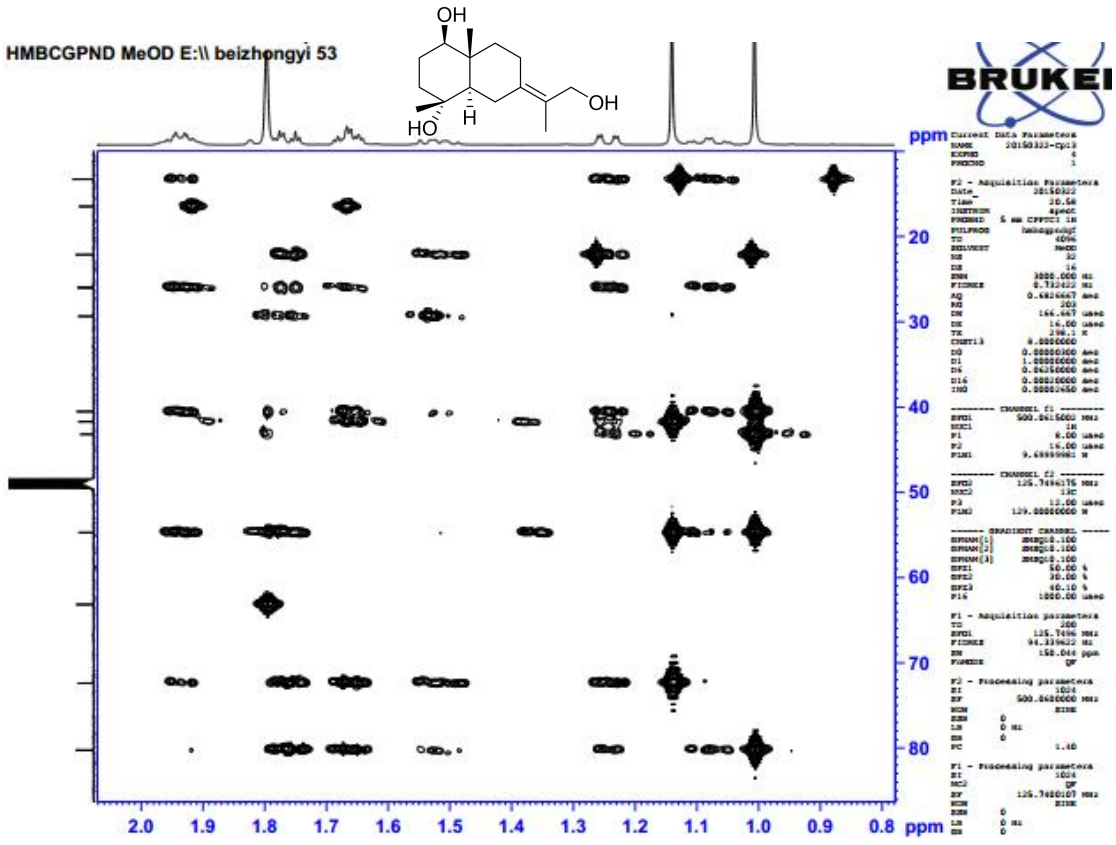


Figure S66. The HMBC Spectrum of Compound 20 in CD3OD

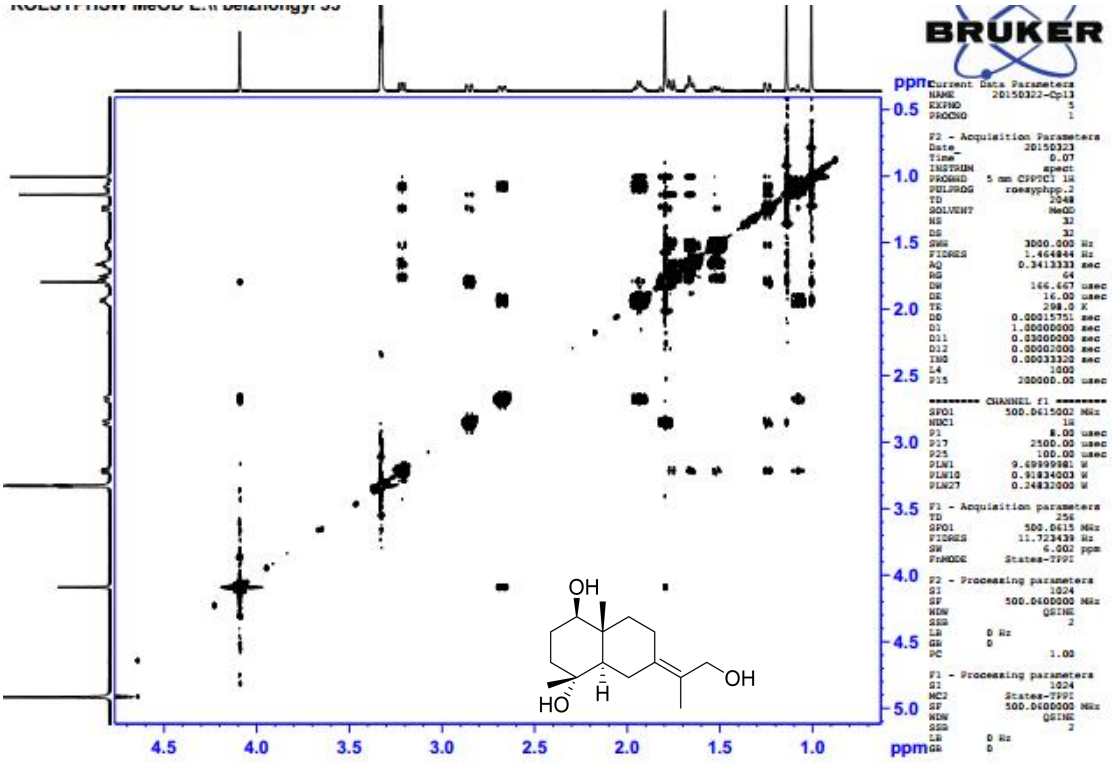


Figure S67. The NOESY Spectrum of Compound 20 in CD3OD

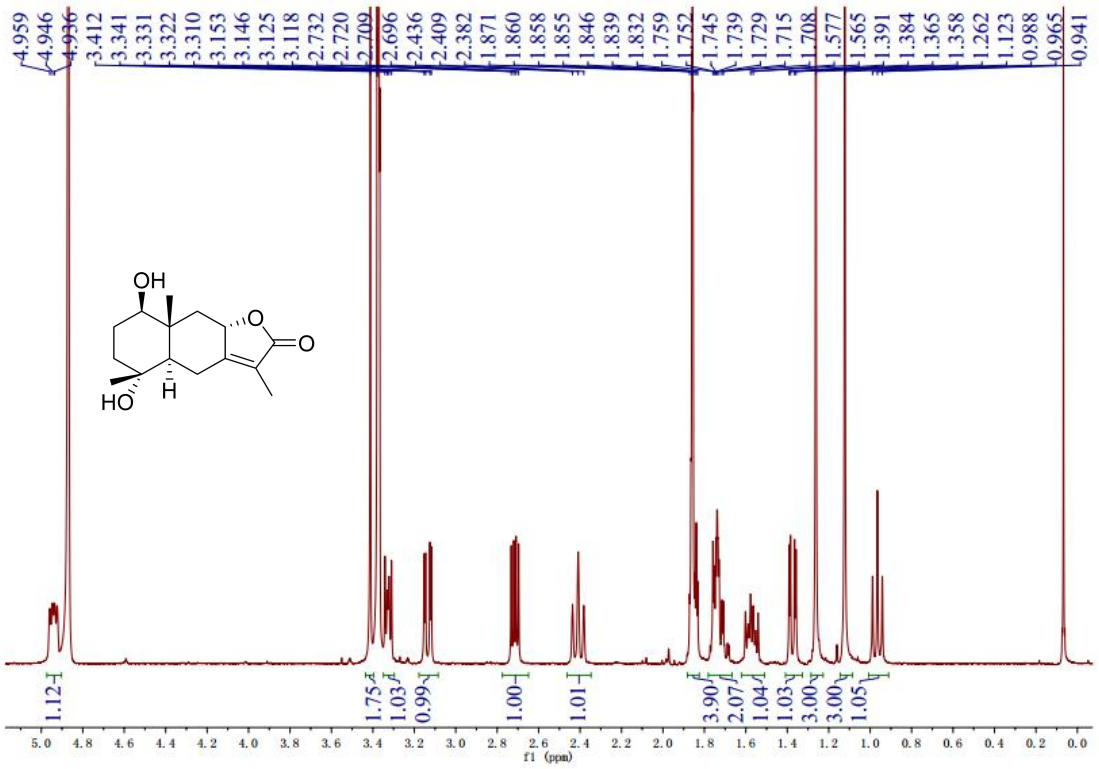


Figure S68. The ^{1}H NMR Spectrum of Compound 21 in CD3OD

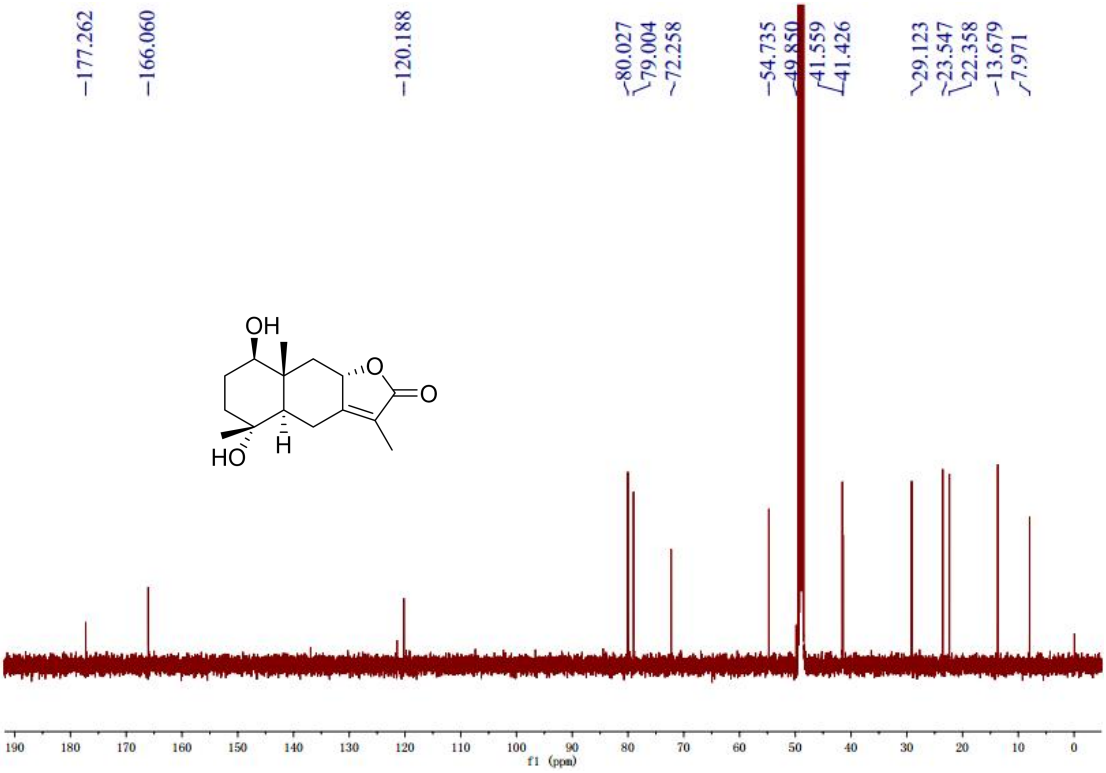


Figure S69. The ^{13}C NMR Spectrum of Compound 21 in CD3OD

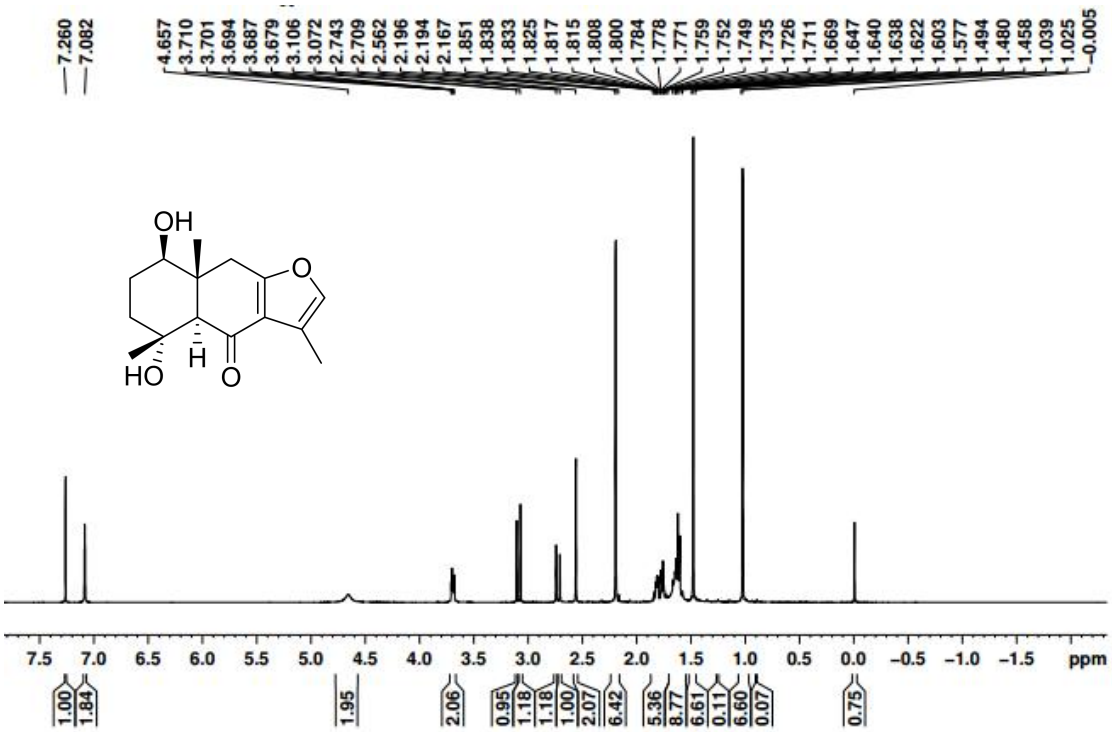


Figure S70. The ^{1}H NMR Spectrum of Compound 22 in CDCl3

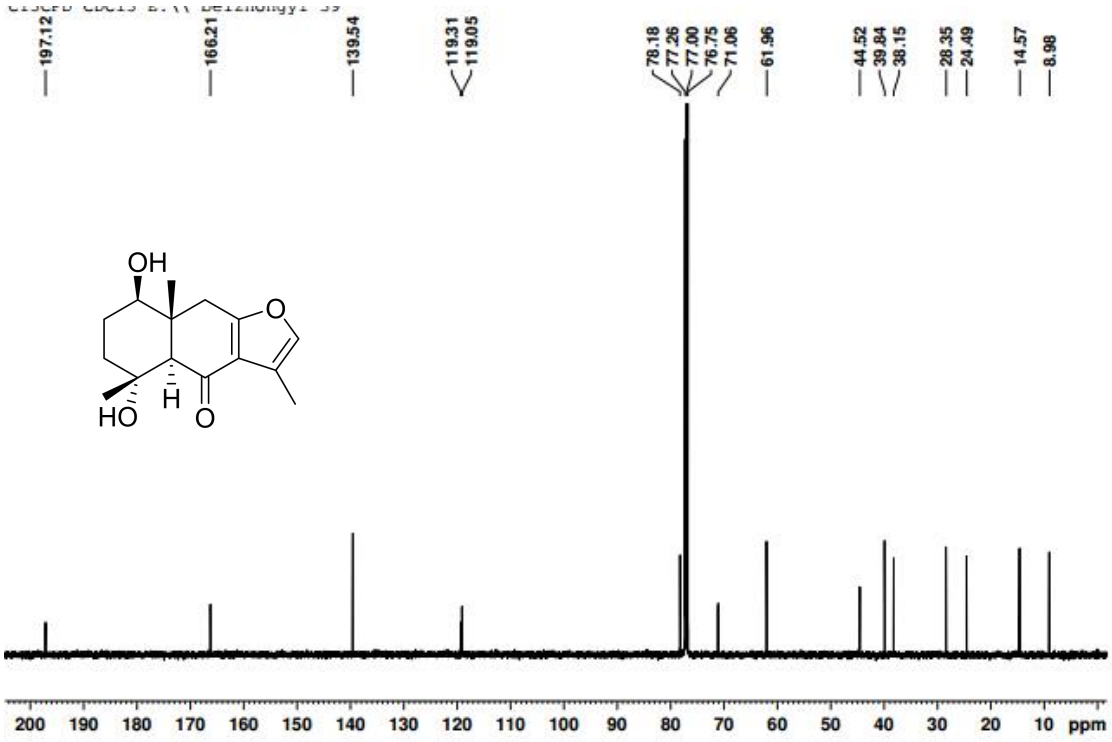


Figure S71. The ^{13}C NMR Spectrum of Compound 22 in CDCl3

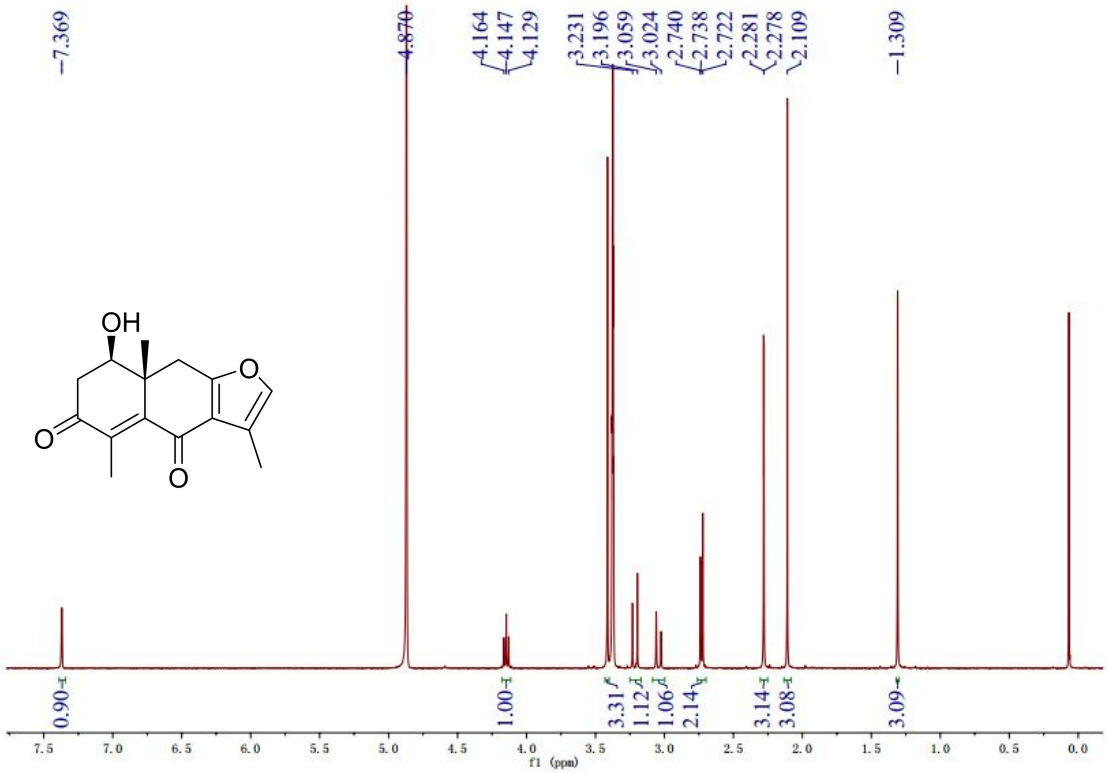


Figure S72. The ^{1}H NMR Spectrum of Compound 23 in CDCl3

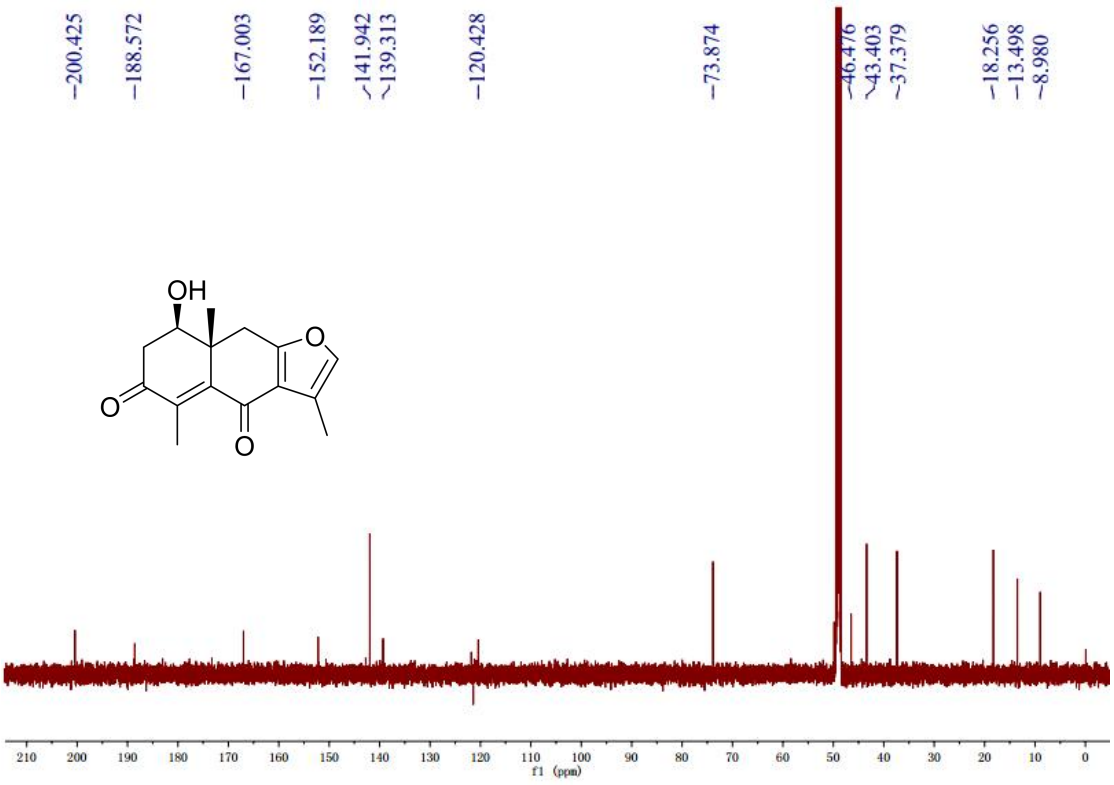


Figure S73. The ^{13}C NMR Spectrum of Compound 23 in CDCl3